ALBERT-LUDWIGS-UNIVERSITÄT FREIBURG IM BREISGAU

Non-Markovian quantum probes for complex systems

Dissertation

zur Erlangung des Doktorgrades der
Fakultät für Mathematik und Physik der
Albert-Ludwigs-Universität
Freiburg im Breisgau

vorgelegt von

Steffen Wißmann

aus Tübingen

betreut von

apl. Prof. Dr. Heinz-Peter Breuer

Juli 2016

Dekan:	Prof. Dr. Dietmar Kröner
Betreuer der Arbeit:	apl. Prof. Dr. Heinz-Peter Breuer
Referent:	apl. Prof. Dr. Heinz-Peter Breuer
Koreferent:	Prof. Dr. Gerhard Stock
Tag der mündlichen Prüfung:	21.10.2016
Prüfer:	apl. Prof. Dr. Heinz-Peter Breuer
	Prof. Dr. Andreas Buchleitner
	Prof. Dr. Hanspeter Helm

Für Else

Zusammenfassung

Die vorliegende Arbeit beschäftigt sich mit verschiedenen aktuellen Fragestellungen aus dem Bereich offener Quantensysteme. Neben der Identifikation von Anfangskorrelationen in der Dynamik offener Systeme, umfasst dies die Charakterisierung von Gedächtniseffekten und deren Auftreten durch korrelierte Umgebungszustände sowie Möglichkeiten ein offenes Quantensystem als Sensor für Eigenschaften seiner Umgebung einzusetzen.

Wie vor geraumer Zeit gezeigt wurde, können Anfangskorrelationen zwischen System und Umgebung zu einem starken Informationsfluss in das offene Quantensystem führen, welcher durch den Spurabstand quantifiziert wird. Die diesem Effekt zugrunde liegende, nicht kontrahierende Systemdynamik kann indessen prinzipiell auch mittels anderer Abstandsmaße auf dem Zustandsraum kenntlich gemacht werden. Eine vegleichende Studie anhand zweier Modellsysteme, die im Zuge dieser Arbeit angefertigt wurde, zeigt jedoch deutlich die bedeutende Rolle des Spurabstandes für die Detektion von Anfangskorrelationen.

Abgesehen hiervon treten solche Informationsflüsse ebenfalls durch starke System-Umgebung-Wechselwirkungen und strukturierte sowie endliche Umgebungen auf, die typischerweise nicht-Markov'schen Dynamiken zugeordnet werden. In dieser Arbeit werden die Eigenschaften der kürzlich eingeführten Charakterisierung nicht-Markov'schen Verhaltens, die dieses einem Informationsaustausch zwischen dem offenen System und seiner Umgebung zuschreibt, und des zugehörigen Maßes resümiert. Insbesondere wird die Funktionsweise und der praktische Nutzen der lokalen Darstellung des Maßes für die Quantifizierung von Gedächtniseffekten anhand eines photonischen Experiments bündig dargelegt.

Durch eine naheliegende Erweiterung dieses auf den Spurabstand aufbauenden Maßes lässt sich zudem eine verallgemeinerte Kennzeichnung von Gedächtniseffekten erzielen, die mit der wohlbekannten Definition für klassische stochastische Prozesse verknüpft ist. Diese Verknüpfung der erweiterten Definition Markov'schen Verhaltens, die gedächtnislose Prozesse mit einer monotonen Zeitentwicklung von Helstrom-Matrizen assoziiert, wird möglich durch seine äquivalente Charakterisierung in Form der Teilbarkeit einer solchen Dynamik bezüglich positiver Abbildungen. Neben derselben Interpretation wie der ursprüngliche Ansatz, genießt das verallgemeinerte Maß ferner ebenso ähnliche mathematische Darstellungen. Es kann gezeigt werden, dass Helstrom-Matrizen, die einen maximalen Informationsrückfluss evozieren, orthogonale Zustände beinhalten und dass für endlich-dimensionale offene Systeme eine lokale und universelle Darstellung des Maßes existiert. Die bestehenden Unterschiede dieses Ansatzes im Vergleich zu anderen wird mittels einiger Beispiele veranschaulicht, anhand derer auch gezeigt werden kann, dass

weder Markov'sche noch, wie kürzlich bewiesen, nicht-Markov'sche Prozesse konvexe Mengen bilden.

Ferner wird die Relevanz spezifischer Anfangskorrelationen in einer zusammengesetzten Umgebung, die einen Informationsrückfluss in vielteiligen offenen Quantensystemen hervorrufen können, beleuchtet. Mittels einer Dekohärenz erzeugenden Dynamik zweier Qubitsysteme, die lokal an ein Multimodenfeld koppeln, das durch zweimodige Gauss-Zustände charakterisiert ist, wird dargelegt, dass solche nicht-lokalen Gedächtniseffekte auch in Abwesenheit von Verschränkung in der Umgebung möglich sind. Wie gezeigt wird, bietet eine für allgemeine Dephasierungsprozesse mit linearer Kopplung und Gauss'schen Umgebungszuständen abgeleitete Bedingung an den Korrelationskoeffizient der in die Wechselwirkung involvierten Umgebungsoperatoren eine Erklärung hierfür. Die Rolle der bosonischen Umgebung für das Auftreten nicht-lokaler Gedächtniseffekte wird schließlich mittels einer effektiven Beschreibung durch endlich-dimensionale Umgebungen in maximal verschränkten Zuständen studiert, die offenlegt, dass mindestens Drei-Niveau-Systeme als Umgebungen gewählt werden müssen.

Motiviert durch die Möglichkeit Parameter zweimodiger Gauss-Zustände mittels nicht-lokaler Gedächtniseffekte zu schätzen, wird im letzten Teil der Arbeit die Fragestellung untersucht, welche Informationen der Umgebung im offenen System zugänglich sind. Zunächst werden hierzu Ansätze betrachtet, die die Korrelationen in Messstatistiken von Observablen des offenen Systems und der Umgebung als Funktion der angewandten Wechselwirkung und der Anfangszustände quantifizieren. Der Versuch eine Relation zwischen der gewonnenen Information und der dadurch hevorgerufenen Störung der Umgebung abzuleiten, ist leider nicht erfolgreich. Wie gezeigt wird, können einige existierende Ansätze nicht auf die beschriebene Situation angewendet werden.

Darüber hinaus werden auch zwei bekannte Sensorstrategien, die die Dynamik des offenen Systems gebrauchen, studiert und erweitert. Für Dephasierungsprozesse offener Systeme, die ähnlich zum quantenmechanischen harmonischen Oszillator sind, kann zum Beispiel gezeigt werden, dass der Erwartungswert gewisser zeitlich gemittelter Observablen gegen den einer Erhaltungsgröße der Umgebung – ob endlich- oder unendlich-dimensional – konvergiert. Die zeitabhängige Messstatistik einer Observable eines offenen Quantensystems mit variabler Energieaufspaltung bietet hingegen die Möglichkeit verschiedene Umgebungseigenschaften bei dissipativen Wechselwirkungen, die jedoch nur virtuelle Übergänge im offenen System hervorrufen, zu erhalten wie anhand der suprafluiden Anregungen im Bose-Hubbard Modell anschaulich dargelegt wird.

Abstract

The purpose of this thesis is to review several recently discussed questions underlying the theory of open quantum systems such as the role of initial system-environment correlations, the essence of memory effects in the quantum regime and their occurrence due to correlated environments as well as the ability to gain information on the environment using the open quantum system.

It is well known that a veritable flow of information to the open quantum system as quantified by the trace distance may be induced by initial correlations between the open system and its environment. But a breakdown of the contractivity of the reduced dynamics may, in principle, be also identified by other distance measures. The prominent role of the trace distance in witnessing initial correlations is eventually confirmed by a comparative study of different quantifiers for two models that is performed in this thesis.

Besides resulting from initial correlations, a flow of information may also be due to strong system-environment couplings and structured or finite reservoirs characterizing non-Markovian processes. The recent characterization of quantum non-Markovianity based on the exchange of information between the open system and its environment is reconsidered in the following, essentially focusing on the local representation of the associated measure. In fact, the functioning of this mathematical representation as well as its use for the experimental determination of the degree of non-Markovianity is convincingly demonstrated by means of an all-optical experiment.

Moreover, by means of a straightforward extension of the trace-distance-based approach to quantum non-Markovianity, it is shown that the so far solely loose connection of quantum and classical non-Markovianity can be made rigorous. Assigning memory effects to the evolution of Helstrom matrices, another characterization of quantum Markovianity in terms of an information flow is obtained which additionally features a clear-cut connection to its classical counterpart due to its equivalence to divisibility of quantum processes with respect to positive maps. In addition, mathematical representations similar to those found for the original trace-distance-based measure are shown to hold true for the associated measure. That is, optimal Helstrom matrices showing a maximal information backflow are proven to consist of orthogonal states and, for finite-dimensional open systems, a local and universal representation of the measure can be established. Several examples are used to illustrate the essential difference between the generalized measure for quantum non-Markovianity and other approaches to quantify memory effects and, moreover, to show that the set of Markovian processes is nonconvex just as that of non-Markovian evolutions, which has been proven recently.

Further, the information flow in multipartite open quantum systems due to correlated local environments, leading to nonlocal memory effects, is studied pertaining to the role of entanglement. Employing the dephasing dynamics of two qubit systems that are coupled locally to multimode fields, being described by two-mode Gaussian states, nonlocal memory effects are shown to occur also in the absence of entanglement. This is explained by a general condition on the correlation coefficient of the environmental coupling operators valid for arbitrary dephasing dynamics with linear interactions and Gaussian environmental states. The significance of the bosonic environment for such a behavior is finally examined by the study of an effective description using finite-dimensional environments in a maximally entangled state. Surprisingly, to obtain such an effective modelling of the coherence factors' evolution, the environments are required to be at least three-dimensional.

Motivated by the opportunity to estimate parameters of the two-mode Gaussian states using nonlocal memory effects, the question about the information on the environment that is accessible by the open quantum system is finally addressed. As a first ansatz to this problem, attempts are studied that quantify how correlated the probability distributions of observables on the open quantum system and the environment – defining a constant of motion or not – are as a function of the initial states and the applied interaction. In order to relate the information gained by such a measurement and the thus-caused disturbance on the environment, several known information-disturbance tradeoffs are studied, but none of these relations can be applied to the given setup as is shown.

Besides this, two general probing schemes are considered that utilize the entire dynamics of the open system. For appropriately adjusted pure dephasing dynamics, open systems that are equivalent to the quantum harmonic oscillator are shown to yield a time-averaged operator mean converging to the expectation value of a constant of motion on the environment which might be of arbitrary dimension. On the contrary, in case of a dissipative coupling inducing only virtual transitions in the open system, environmental properties can be identified from the time-dependent measurement statistics of an observable on an open system with tunable energy splitting as is illustrated for the superfluid excitations in the Bose-Hubbard model.

Contents

Chapter 1

Introduction

In almost any quantum mechanics experiment, it is impossible to perfectly isolate the observed quantum object from its surroundings. As a consequence of the unavoidable interaction with its environment, a quantum object typically exhibits an irreversible dynamics – contrary to the predictions of the standard theory claiming a unitary evolution described by the Schrödinger equation – that is characterized by dissipation of energy, the relaxation to thermal equilibrium or another stationary state, as well as the decay of quantum coherences and correlations (Breuer and Petruccione, 2002). Due to the experimental progress, a profound understanding of these so-called open quantum systems and a reliable description of their dynamics has become more and more important.

Taking the effects of an exchange of energy and information between a quantum system and its environment into account, the theory of open quantum systems (Breuer and Petruccione, 2002) studies and provides methods that target a reliable and efficient description of such an irreversible time evolution. A well-established tool of this theory characterizing the evolution of an open system is given by a quantum master equation which refers to a first-order differential equation for the reduced density operator defining the open system. To derive a master equation for the open system from a microscopic system-environment approach, different methods have been developed within the last decades (see, e.g., Nakajima (1958), Zwanzig (1960), Prigogine (1962), Hashitsumae *et al.* (1977), Shibata *et al.* (1977), Chaturvedi and Shibata (1979), Shibata and Arimitsu (1980)). Among this kind of description for the open system dynamics, a simple and popular ansatz is given by master equations with time-independent generators that lead to dynamical semigroups for the open system's state evolution. To obtain such a dynamics, the generators of these so-called Markovian master equations are forced to have a specific structure which is typically attributed to Lindblad (1976) who derived it at the same time and independently of[1] Gorini *et al.* (1976). Apart from general mathematical and physical principles leading to the Lindblad structure, Markovian master equations can also be deduced from microscopic system-environment approaches to the dynamics if several rather drastic approximations are invoked which explain the basic features required to obtain a semigroup evolution for an open system's dynamics.

[1] As a consequence, the particular structure of a master equation that yields a semigroup dynamics is sometimes also referred to as Lindblad-Gorini-Kossakowski-Sudarshan form in order to acknowledge all researchers that contributed to its discovery.

Due to this fact, it is not surprising that a description by means of a semigroup dynamics fails to give a faithful picture for many open quantum systems (see, e.g., Breuer and Petruccione (2002) for models not obeying such a dynamics). The used approximations which are applied to a differential equation obtained from second-order perturbation theory with respect to the system-environment interaction are, for example, deficient for strong couplings or structured as well as finite environments, low temperatures or nonnegligible initial correlations between the open system and its environment. These properties typically result in environmental correlation times that are not small in comparison with the open system's relaxation times or its intrinsic evolution, finally leading to a breakdown of the usual separation of times scales that is needed for the deployment of the Markov and the rotating wave approximation (Breuer and Petruccione, 2002).

Starting already long ago (see, e.g., Davies (1974), Lindblad (1976, 1979), Accardi *et al.* (1982)), any open system dynamics that may not be faithfully described by a dynamical semigroup has been termed non-Markovian[2], referring to the well-established concept of non-Markovian stochastic processes in classical probability theory which are typically assigned to have memory (see, e.g., Gardiner (2004) and van Kampen (2007)). On the contrary, the semigroup property of a dynamics resulting from a Markovian master equation may clearly be interpreted as characterizing a memoryless dynamical process, whereupon the attribute "memoryless" is additionally supported by the requirements regarding the validity of the previously mentioned approximations needed to derive such a master equation from a microscopic model. However, the connection to the well-known classical concept of Markovian stochastic processes is only loose as the classical definition may not be straightforwardly adapted in quantum theory due to the particular role of measurements in quantum mechanics (cf. Vacchini *et al.* (2011) and Breuer *et al.* (2016)).

Though, for example, Lindblad (1979) and Accardi *et al.* (1982) have tried to define quantum stochastic processes in general, a rigorous and satisfying classification of dynamical processes with and without memory effects – again attributing the terms non-Markovian and Markovian to it – which solely relies on the dynamics of the open quantum system has not been achieved until recently when the topic has again attracted a lot of attention, culminating in a series of proposals for a proper definition of non-Markovianity in the quantum regime. All these approaches are based on appropriate features that characterize memory effects extending the classical notion. However, the question how memory effects manifest themselves in the dynamical behavior of open quantum systems and how they can be uniquely identified has been answered differently. While some proposals invoke analogies to the classical counterpart extending the semigroup property[3] (see, e.g., Rivas *et al.* (2010), Hou *et al.* (2011), Hall *et al.* (2014) and Chruściński and Maniscalco (2014)), several other approaches are based on physically meaningful and intuitive characterizations of the notion of memory effects (see, e.g., Breuer *et al.* (2009),

[2]Previously, the term non-Markovian has also be frequently assigned to dynamics arising from master equations which are not local in time (see, e.g., Zwanzig (1960)) which is, however, not equivalent to a deviation from a semigroup dynamics (cf. Sec. 3.3).

[3]There are yet approaches that stick to the previous classification, defining the border between non-Markovianity and Markovianity by the semigroup property (see, e.g., Wolf *et al.* (2008), Hou *et al.* (2015) and Ali *et al.* (2015)).

Chruściński *et al.* (2011), Luo *et al.* (2012) and Fanchini *et al.* (2014)). Being based on analogies to the classical definition and interpretations of the notion of memory effects, it is not surprising that all these approaches lack a direct connection to the classical definition of a Markov process.

The present thesis reviews the classical notion along with the discussion on the proper definition of quantum non-Markovianity, mainly focusing, however, on the characterization of an exchange of information between the open system and its environment which was proposed by Breuer *et al.* (2009) (see also Breuer *et al.* (2016) and Rivas *et al.* (2014) for reviews on the topic primarily paying attention to this approach and those based on the divisibility of the open system dynamics in terms of completely positive maps). Besides illustrating the representations of the measure quantifying the degree of non-Markovianity in terms of an information flux in an all-optical experiment (cf. Liu *et al.* (2014)), the essence of memory effects and their different sources such as initial correlations in the environment or between the open system and its environment are considered in the first part of the thesis.

Indeed, as has been shown by Laine *et al.* (2012, 2013) (see also Liu *et al.* (2013a) for a photonic realization), initially correlated environments of a multipartite open quantum system can lead to pronounced memory effects albeit the dynamics of the subsystems is Markovian, contrary to the general view as, e.g., detailed by Martinazzo *et al.* (2011) for Brownian motion. Though this peculiar phenomenon has been observed in different open quantum systems, the relevance of the type of correlations for its occurrence has not been studied so far. To address this question, nonlocal memory effects are examined for a dephasing dynamics of a two qubit open quantum system that is linearly coupled to a multimode bosonic environment in a Gaussian state, providing a convenient framework to expose the role of entanglement in the environment along with the primary source of nonlocal memory effects (cf. Wißmann and Breuer (2014)).

Nonfactorizing initial conditions, i.e. if the open system and its environment may not be prepared statistically independent at the initial time, represent another well-known source of memory effects as exposed by Laine *et al.* (2010a) who used this fact to construct a witness for initial system-environment correlations. Apart from the trace distance quantifying the information flow, any other distance measure that is contractive with respect to completely positive and trace preserving maps, subadditive and satisfies the triangle inequality could, in principle, be similarly used to quantify initial correlations from the open system dynamics. To gather insights into the best choice of a distance measure for the purpose of witnessing initial correlations, the comparative study by Dajka *et al.* (2011) is further extended. On the basis of this extension an outstanding capability of the trace distance is demonstrated (cf. Wißmann *et al.* (2013)).

The discussion on non-Markovian open system dynamics is also reviewed in order to address the problem of a "reconciliation" with the classical notion. Of course, a general classification of quantum non-Markovianity allowing for a direct connection to its classical counterpart is particularly interesting if it could additionally be equipped with an intuitive characterization of memory effects. Inspired by the work by Chruściński *et al.* (2011), a generalized criterion which indeed combines a link to the classical notion with an intuitive characterization is introduced

in the first part of the thesis (see also Breuer *et al.* (2016)). As this criterion represents a straightforward extension of the original ansatz quantifying non-Markovian behavior in terms of an information backflow, the associated measure is shown to obey mathematical representations similar to those found for the original trace-distance-based measure (cf. Wißmann *et al.* (2015)). The mathematical structure of the space of thus-assigned Markovian and non-Markovian dynamics is additionally studied by means of examples for two-level systems based on which paradigmatic models are deduced illustrating the essential difference between the different approaches for quantum non-Markovianity.

Besides these fundamental questions concerning the proper definition of quantum memory effects and their primary origin, several recent studies have demonstrated that the non-Markovian dynamics of an open quantum system also reflects characteristic properties of the environment. For example, Haikka *et al.* (2011, 2013, 2012b) has detailed how the effective dimension and the temperature of a Bose-Einstein-condensate significantly influences the non-Markovianity of an immersed impurity atom, and the studies of nonlocal memory effects have shown that nonlocal correlations within composite environments may be associated with the strength of the observed memory effects (see Laine *et al.* (2012, 2013), Liu *et al.* (2013a) and Wißmann and Breuer (2014)). Similarly, the non-Markovianity of polarization states of photon pairs exposes the amount of angular correlations in their environmental states (Smirne *et al.*, 2013a). These examples (see also Apollaro *et al.* (2011), Haikka *et al.* (2012a) and Gessner *et al.* (2014a) for further instances) thus encourage the new perspective that open systems can be exploited as quantum probes for nontrivial features of its environment. On the way towards a general theory of such quantum probes, describing the prospects and limitations of this ansatz, the information on a complex quantum system that can be deduced by means of measurements of a small quantum system as a function of its initial state and the chosen interaction represents a fundamental question. The second part of this thesis is devoted to this topic, studying and explaining different tools that may be used to address this problem on a fundamental level. Apart from approaches quantifying correlations between single measurements of observables on a quantum object and the associated probe, two general strategies are discussed that employ the time evolution of probe observables to gather information on a complex quantum system.

The thesis is organized as follows: To set the stage for the discussion of memory effects in the quantum regime held in the first part, results concerning the quantum state space as well as operations and functionals thereon are recapitulated in *Chapter 2*. In particular, in *Section 2.3* a characterization of the eigenbases of states defining a convex set is proven which deepens the direct connection of the generalized trace-distance-based measure for quantum non-Markovianity to its classical counterpart. In addition to this, the notion of Gaussian states for bosonic systems is introduced in *Section 2.5* and two particular classes of such states are defined which are, later on, employed for the study of nonlocal memory effects.

Chapter 3 provides an introduction to the basic notions used in the theory of open quantum systems such as dynamical maps, the divisibility of a process and master equations where special attention is payed to the exactness of time-

convolutionless master equations of second order for zero-mean Gaussian environmental states and linear couplings. Besides this, the detection of initial system-environment correlations by means of open system dynamics is addressed in *Section 3.5*, focusing on a comparative study that highlights the trace distance's distinguished capability to witness initial correlations.

Starting with a review on classical Markovian processes, different concepts for quantum non-Markovianity are reviewed in *Chapter 3*. After a detailed discussion of the trace-distance-based measure along with an illustration of the functioning and use of its local representation for practical purposes using an all-optical experiment in *Section 4.3*, the generalized criterion of quantum non-Markovianity is introduced and its properties such as its direct connection to the classical definition are exposed in *Section 4.4*. Finally, *Section 4.5* concerns the mathematical structure of the space of Markovian and non-Markovian dynamical processes.

Chapter 5 contains the discussion about the type of environmental correlations that is required to observe nonlocal memory effects. By studying a dephasing dynamics of two qubit systems, it is shown in *Section 5.2* that entanglement is not necessary for nonlocal memory effects which is explained in the subsequent section, i.e. *Section 5.3*, by means of a general dephasing model, leading to a necessary and sufficient condition for the occurrence of such memory effects. The study of nonlocal memory effects is concluded by addressing in *Section 5.4* the question on the significance of an infinite-dimensional environment for perfect nonlocal memory effects.

In the second part, comprising *Chapter 6*, the information content of an open quantum system regarding environmental properties is considered. After an introduction to indirect measurements using tools from the quantum theory of measurements in *Section 6.1*, different quantifiers that can be employed to characterize the performance of an indirect retrieval of information are introduced and possible relations between the gained information and the thus-caused disturbance are studied in *Section 6.2*. Finally, in *Sections 6.3* and *6.4* two strategies are provided that allow to extract information on the environment from the time evolution of the measurement statistics of an observable on an open system for nondissipative and dissipative dynamics.

The results of this thesis are summarized in *Chapter 7* where, additionally, an outlook on further prospects and open questions concerning the addressed topics is given.

Part I

Open quantum systems and non-Markovianity

Chapter 2

States, the state space and operations thereon

In this section, the concept of physical states of a quantum mechanical system are briefly reviewed in order to clarify and fix the notation, and to discuss the structure of this set of states, usually called the state space. Apart from preliminaries concerning quantum states including correlations, endomorphisms and representations of linear operators, the structure of convex subsets of the state space for finite-dimensional Hilbert spaces is examined. Obviously, if such a subset comprises the maximally mixed state, then any orthonormal basis provides an eigenbasis for some state of the subset. It is, however, shown in the present thesis that the converse of this rather trivial statement proves true, too. As a consequence of this result, the coveted connection of quantum and classical non-Markovianity, describing these processes in terms of master equations, can finally be established (see Sec. 4.4.2). Another issue of this section concerns distance measures for states which are relevant for various tasks in quantum physics ranging from the detection of correlations in bipartite systems to ensemble discrimination. For the present work, the trace distance is particularly important due to its remarkable properties and its physical interpretation. Finally, a particular class of states of infinite-dimensional systems, the so-called Gaussian states, is introduced.

2.1 The space of quantum states

The description of a quantum system is based on quantum states which are characterized by density operators ρ encoding the statistics of any type of quantum measurement performed on it. Using an axiomatic approach for the expectation values associated with self-adjoint operators in terms of real functionals (von Neumann, 1932b), it is shown that density operators must be given by bounded linear operators on a Hilbert space $\mathcal{H}$ over the field of complex numbers $\mathbb{C}$ satisfying the additional constraints (Langerholc, 1965) (see also Breuer and Petruccione (2002))

$$\rho = \rho^\dagger \,, \qquad \rho \geq 0 \,, \qquad \mathrm{Tr}\{\rho\} = 1 \,. \tag{2.1}$$

This means that a quantum state is described by a self-adjoint and positive, bounded linear operator with unit trace and, therefore, defines a so-called trace class operator (see also Sec. 2.4.1). While the second requirement, which is the acronym for a state ρ being positive, ensures that positive expectation values are

assigned to events of the theory, the last constraint warrants their probabilistic interpretation. Note that an operator X is said to be positive[1], i.e. $X \geq 0$, if and only if one has $\langle\psi|X|\psi\rangle \geq 0$ for all elements $|\psi\rangle$ of the Hilbert space. Moreover, if X and Y are two Hermitian operators, then one says that $X \geq Y$ if and only if $X - Y \geq 0$.

Quantum states may be equivalently characterized in terms of their eigenstates and eigenvalues. Because self-adjoint operators are in particular normal, that is, an operator that commutes with its Hermitian conjugate, the spectral theorem applies to quantum states (Rudin, 1991). For arbitrary Hilbert spaces a density operator thus admits a spectral decomposition,

$$\rho = \sum_{j=1}^{\dim\mathcal{H}} p_j |\psi_j\rangle\langle\psi_j| \ , \tag{2.2}$$

that is characterized by its eigenvalues p_j and associated eigenstates $|\psi_j\rangle$ which, in addition, constitute an orthonormal basis of the Hilbert space. Positivity of a quantum state is then equivalent to the fact that the eigenvalues are real-valued and nonnegative, i.e. $p_j \geq 0$ for all j. Moreover, according to Lidskii's theorem[2] (see, e.g., Simon (2005)), the last condition of Eq. (2.1) is equivalent to $\sum_j p_j = 1$. For infinite-dimensional systems, the eigenvalues thus define an ℓ^1-convergent series having ℓ^1-norm equal to unity. In the case of a finite-dimensional Hilbert space, the notion of physical states obviously coincides with that of positive matrices whose diagonal elements – and, similarly, its eigenvalues – sum to one. Due to these features of the eigenvalues, they can be interpreted as elements of a probability distribution. It is worth stressing that the requirement on states being self-adjoint is redundant since this already follows from positivity of states as the underlying Hilbert space $\mathcal{H}$ is over the field of complex numbers (Bengtsson and Zyczkowski, 2007).

Throughout the thesis, the set of physical states of a quantum system on the Hilbert space $\mathcal{H}$ is denoted by $\mathcal{S}(\mathcal{H})$, i.e., one has

$$\mathcal{S}(\mathcal{H}) \equiv \{\rho \in \mathcal{B}(\mathcal{H}) \mid \rho \geq 0,\, \mathrm{Tr}(\rho) = 1\} \ , \tag{2.3}$$

where $\mathcal{B}(\mathcal{H})$ indicates the so-called set of bounded linear operators on $\mathcal{H}$ that are characterized by a finite operator norm $\|\cdot\|_\infty$. A fundamental property of the state space is that it defines a convex set. This means, for any pair of states ρ and σ and parameter $\lambda \in [0,1]$, one has

$$\rho_\lambda \equiv (1-\lambda)\sigma + \lambda\rho \in \mathcal{S}(\mathcal{H}) \ . \tag{2.4}$$

Convexity of a set thus signifies that the straight line connecting ρ and σ is entirely contained in $\mathcal{S}(\mathcal{H})$. Clearly, the reverse is not true: there exist states that cannot be written as the convex combination of two unequal states defining the extreme points of the convex set $\mathcal{S}(\mathcal{H})$ (see, e.g., Rockafellar (1972)). These states are consequently termed pure states and it can be shown that they are given by $\rho = |\psi\rangle\langle\psi|$ for

[1] In mathematics, this property is actually referred to as positive semi-definiteness.

[2] The theorem states that the matrix trace of a trace class operator on a separable Hilbert space equals its spectral trace, that is, the sum of its eigenvalues.

$|\psi\rangle \in \mathcal{H}$, representing elements of the projective Hilbert space linked to $\mathcal{H}$. The set of states which can be obtained as convex combination of orthogonal pure states will be studied in the next section.

Note that the notion of orthogonality, which represents a fundamental and important feature of a Hilbert space, is generalized to quantum states in the following way: Two states are called orthogonal, which is henceforth denoted by $\rho \perp \sigma$, if they have orthogonal supports. That is, the complements of the kernels of the linear operators ρ and σ are orthogonal with respect to the inner product of the Hilbert space. As a consequence, such operators have a common spectral decomposition (cf. Eq. (2.2)) with complementary eigenvalues, meaning that the respective sets of eigenvalues regarded as vectors (or series for $\dim\mathcal{H} = \infty$) are orthogonal with respect to the usual scalar product. Because the eigenvalues are positive, one concludes that orthogonal states must have some zero eigenvalues and are thus part of any norm-based boundary of the state space (see below).

It is worth noticing that the seemingly different concept of orthogonality for operators is reconciled with the standard approach by means of the so-called *Hilbert-Schmidt inner product*. The functional $(\rho, \sigma)_{\mathrm{HS}} = \mathrm{Tr}\{\rho^\dagger \sigma\}$ defines an inner product[3] and the previous characterization clearly implies that two states ρ and σ are orthogonal if and only if they satisfy $(\rho, \sigma)_{\mathrm{HS}} = 0$.

2.2 Generalized Bloch representation

A convenient description of the state space for finite-dimensional systems is obtained using representations of the special unitary group. Using the operator basis defined by the representatives of the group's generators, the state space can be characterized as a subset of Euclidean space. This embedding is typically referred to as generalized Bloch representation (Bengtsson and Zyczkowski, 2007) or coherence vector representation (Byrd and Khaneja, 2003), extending the convenient and well-known Bloch representation for two-level systems.

For a quantum system that is described by a Hilbert space $\mathcal{H}$ with dimension N, the generators of the fundamental representation of the (N^2-1)-dimensional special unitary group $\mathrm{SU}(N)$ on $\mathcal{H}$ and the identity operator provide an operator basis for the linear operators on this Hilbert space. Using traceless and Hermitian representatives of the independent generators which satisfy $\mathrm{Tr}\{\sigma_j \sigma_k\} = 2\delta_{jk}$, a Hermitian operator is described as

$$A = \frac{\alpha_0}{N} \mathbb{1}_N + \sum_{j=1}^{N^2-1} \sqrt{\frac{N-1}{2N}} \alpha_j \sigma_j \ , \tag{2.5}$$

where $\alpha_0 = \mathrm{Tr}\{A\}$ as well as $\alpha_j = \mathrm{Tr}\{A\sigma_j\}$ are real-valued constants for all $j \in \{1, \ldots, N^2-1\}$. Apart from being traceless and Hermitian, the $\mathrm{SU}(N)$-

[3] More precisely, it defines a scalar product on the complex vector space of Hilbert-Schmidt operators that are given by the set of operators A for which $\mathrm{Tr}\{A^\dagger A\}$ is finite.

generators σ_j obey

$$\sigma_j\sigma_k = \frac{2}{N}\delta_{jk}\mathbb{1}_N + \sum_{j,k=1}^{N^2-1}(d_{jkl} + if_{jkl})\sigma_l \ , \tag{2.6}$$

where f_{jkl} are the so-called structure constants, defining a completely antisymmetric tensor, and d_{jkl} refers to the symmetric d-tensor (Byrd and Khaneja, 2003). A systematic construction of the generators with respect to an orthonormal basis $\{|j\rangle \,|\, 0 \leq j \leq N-1\}$ of $\mathcal{H}$ is given by

$$\lambda_{j,k} = |j\rangle\langle k| + |k\rangle\langle j| \ , \qquad \tilde{\lambda}_{j,k} = i\{|j\rangle\langle k| - |k\rangle\langle j|\} \ , \tag{2.7}$$

$$\lambda'_l \ = \sqrt{\frac{2}{(l+1)(l+2)}}\left\{(l+1)|l+1\rangle\langle l+1| - \sum_{j=0}^{l}|j\rangle\langle j|\right\} \ , \tag{2.8}$$

where $0 \leq j < k \leq N-1$ and $0 \leq l \leq N-2$ (Hioe and Eberly, 1981). Grouping these N^2-1 operators into a list, the previously used labels σ_j are assigned to the list's elements. In fact, defining for example for two-level systems the operators as $(\sigma_1, \sigma_2, \sigma_3) \equiv (\lambda_{0,1}, \tilde{\lambda}_{0,1}, \lambda'_0)$, this yields the well-known Pauli spin operators. Note that for $N = 3$ one obtains the Gell-Mann matrices known from particle physics (Peskin and Schroeder, 1995).

The operators $\mathbb{1}_N, \sigma_1, \ldots, \sigma_{N^2-1}$ are indeed mutually orthogonal with respect to the Hilbert-Schmidt norm as the generators are traceless (cf. Eq. (2.6)). They thus define an orthogonal operator basis for the vector space of Hermitian operators on $\mathcal{H}$ which is characterized by N^2 free parameters and includes the state space as a subset. As a consequence, the assignment

$$(\alpha_0, \vec{\alpha}) \leftrightarrow A = \frac{\alpha_0}{N}\mathbb{1}_N + \sum_{j=1}^{N^2-1}\sqrt{\frac{N-1}{2N}}\alpha_j\sigma_j \tag{2.9}$$

defines a linear homeomorphism from $\mathbb{R}^{N^2}$ to the set of Hermitian operators on the N-dimensional Hilbert space $\mathcal{H}$. Since any linear operator can be represented as the sum of two Hermitian operators[4], this map extends even to a linear homeomorphism from $\mathbb{C}^{N^2}$ to the bounded linear operators $\mathcal{B}(\mathcal{H})$.

The set of vectors corresponding to the state space is actually contained in a hyperplane of $\mathbb{R}^{N^2}$. According to the normalization of quantum states (cf. Eq. (2.1)), it follows that $\alpha_0 = 1$ for any quantum state so that the assignment reduces to

$$\rho = \frac{1}{N}\mathbb{1}_N + \sum_{j=1}^{N^2-1}\sqrt{\frac{N-1}{2N}}\alpha_j\sigma_j \ . \tag{2.10}$$

The (N^2-1)-dimensional vector $\vec{\alpha} = (\alpha_1, \ldots, \alpha_{N^2-1})^T$ is called the generalized Bloch vector or coherence vector associated with the state ρ (see, e.g., Bengtsson and Zyczkowski (2007), Byrd and Khaneja (2003)). Unfortunately, this representation looks much more innocent than it really is. Clearly, the set of admissible

[4]Given a linear operator X, it may be written as $X = X_+ + iX_-$ where the Hermitian operators $X_+ = (1/2)(X + X^\dagger)$ and $X_- = (-i/2)(X - X^\dagger)$ characterize the Hermitian and anti-Hermitian part of X, respectively.

coherence vectors must be closed and convex as the linear and homeomorphic assignment applies to the closed and convex set $\mathcal{S}(\mathcal{H})$. One furthermore shows that the unit ball with respect to the Euclidean norm in $\mathbb{R}^{N^2-1}$ defines the smallest isotropic superset, whereas the largest isotropic subset is given by a ball that is centered at zero and has radius $R_{\text{in}} = 1/(N-1)$ (Harriman, 1978; Kimura and Kossakowski, 2005). The exact shape of the set of admissible vectors is determined by a lattice of N nested inequalities which are induced by the requirement of positivity of states. Considering the roots of the characteristic polynomial

$$p_\rho(\lambda) = \det(\rho - \lambda \mathbb{1}_N) = (-1)^N \sum_{k=0}^{N} (-1)^k a_k \lambda^{N-k} \ , \tag{2.11}$$

where $a_0 = 1$, it follows from Descartes' rule of signs that the eigenvalues are positive if and only if all coefficients a_k are positive semi-definite (Dickson, 1914; Kimura, 2003). Note that the coefficients for $k > 0$ can be determined using Newton's formula (Lewin, 1994; Byrd and Khaneja, 2003; Kimura, 2003) leading to the recursive relation

$$k \cdot a_k = -\sum_{j=1}^{k} (-1)^j a_{k-j} \mathrm{Tr}\{\rho^j\} \ . \tag{2.12}$$

Employing symmetric parts of traces over the basis elements (Byrd and Khaneja, 2003), the elements $\mathrm{Tr}\{\rho^j\}$ can be expressed in terms of the vectors $\vec{\alpha} \in \mathbb{R}^{N^2-1}$ by means of which the coefficients of the characteristic polynomial may thus be written in terms of the coherence vectors. For the first three coefficients one obtains

$$a_1 = 1 \ , \tag{2.13}$$

$$a_2 = \frac{N-1}{2N} \{1 - \vec{\alpha} \cdot \vec{\alpha}\} \ , \tag{2.14}$$

$$a_3 = \frac{(N-1)(N-2)}{6N^2} \{1 - 3\vec{\alpha} \cdot \vec{\alpha} + 2(\vec{\alpha} \star \vec{\alpha}) \cdot \vec{\alpha}\} \ , \tag{2.15}$$

where the $\star$-product is defined as

$$(\vec{\alpha} \star \vec{\beta})_l = \sqrt{\frac{N(N-1)}{2}} \frac{1}{N-2} d_{jkl} \alpha_j \beta_k \ , \tag{2.16}$$

which hence relies on the algebraic structure of the generators of $\mathrm{SU}(N)$. As the first coefficient is trivially positive, there is only a single constraint given by $a_2 \geq 0$ for two-level systems. One immediately recognizes that this condition implies the well-known Bloch representation for qubit systems, i.e., all vectors in $\mathbb{R}^3$ with norm smaller than or equal to unity warrant positivity of the associated operators. Clearly, for higher-dimensional systems, this condition still constrains the coherence vectors to be contained in the unit ball, providing a first hint on the smallest isotropic superset. The further inequalities $a_j \geq 0$ for $j \geq 3$ impose, however, nontrivial constraints on the vectors breaking the simple symmetry found for two-level systems. Note that pure states are always part of the unit sphere as they are characterized by coherence vectors satisfying $\|\vec{\alpha}\| = 1$ and $\vec{\alpha} \star \vec{\alpha} = \vec{\alpha}$ (Byrd and Khaneja, 2003). However, unless $N = 2$ where the d-tensor vanishes,

the second condition restricts the set of allowable rotations connecting pure states to a proper subset of $\mathrm{SO}(N^2-1)$. Even though it is, for example, only a single further constraint for a three-level system, it is already a tedious task to check whether a vector yields a positive operator or not. Of course, this gets even more challenging for larger Hilbert spaces.

Note that two states are orthogonal if their associated coherence vectors obey $\vec{\alpha}_1 \cdot \vec{\alpha}_2 = \cos(\theta)$ where $\theta = \arccos(-1/\{N-1\})$. For two-dimensional systems, this obviously gives the well-known characterization of orthogonal states in terms of pairs of antipodal Bloch vectors on the unit sphere.

2.3 Boundaries and convex subsets

In the following, the study of the structure of the set of physical states is continued, focusing on its boundaries and convex subsets. In fact, besides the definition and characterization of boundaries and the corresponding interiors which will be needed later on, features of convex subsets of the state space regarding the decomposition of elements into pure states are considered.

According to the standard procedure, a boundary of the state space $\partial_{\|\cdot\|}\mathcal{S}(\mathcal{H})$ with respect to some norm $\|\cdot\|$ is defined as

$$\partial_{\|\cdot\|}\mathcal{S}(\mathcal{H}) = \{\rho \in \mathcal{S}(\mathcal{H}) \mid \forall \epsilon > 0 : \hat{B}_\epsilon^{(p)}(\rho) \cap \mathcal{S}(\mathcal{H})^c \neq \emptyset\} \ , \tag{2.17}$$

where $\mathcal{S}(\mathcal{H})^c \equiv \mathcal{E}_1(\mathcal{H}) \setminus \mathcal{S}(\mathcal{H})$ denotes the relative complement of $\mathcal{S}(\mathcal{H})$ with respect to the set of Hermitian operators with unit trace $\mathcal{E}_1(\mathcal{H}) = \{A \in \mathcal{B}(\mathcal{H}) \mid A = A^\dagger, \mathrm{Tr}\{A\} = 1\}$. Moreover, $\hat{B}_\epsilon(\rho) = \{\sigma \in \mathcal{S}(\mathcal{H}) \mid \|\rho - \sigma\| \leq \epsilon\}$ describes the closed ball relative to the considered norm which is centered at ρ. Note that it is irrelevant which norm is chosen as long as the Hilbert space is not infinite-dimensional since all norms on finite-dimensional vector spaces are equivalent (Rudin, 1991). As clarified in Sec. 2.2, the set of Hermitian matrices indeed represents a finite-dimensional vector space over the reals, so this result indeed applies here. It is worth noticing that one has $\partial_{\|\cdot\|}\mathcal{S}(\mathcal{H}) \subset \mathcal{S}(\mathcal{H})$ by definition.

To determine the boundary explicitly, one must, of course, first fix a norm. A convenient choice is given by the Schatten p-norm[5] (Schatten and von Neumann, 1946),

$$\|A\|_p = \left(\sum_{j=1}^{\dim\mathcal{H}} s_j(A)^p\right)^{1/p} = \left(\mathrm{Tr}\{|A|^p\}\right)^{1/p}, \quad p \in [1,\infty] \ , \tag{2.18}$$

where $s_j(A)$ denote the eigenvalues of the positive operator $|A| = \sqrt{A^\dagger A}$ associated with A which are also referred to as singular values. For a normal operator A admitting a spectral decomposition with eigenvalues a_j and eigenstates $|\psi_j\rangle$ (cf. Eq. (2.2)), the modulus of such an operator is simply given by

[5] Note that the Schatten p-norm for $p = \infty$ is determined by $\|A\|_\infty = \sup_j s_j(A)$. It equals the operator norm which is typically defined as the supremum of $\|A|\psi\rangle\|_\mathcal{H}$ over the set of unit vectors $|\psi\rangle$.

$|A| = \sum_{j=1}^{n} |a_j||\psi_j\rangle\langle\psi_j|$. Note that the second equality sign in Eq. (2.18) is a simple consequence of the functional calculus. Due to positivity of states, the third condition on states, i.e. $\mathrm{Tr}\{\rho\} = 1$ (cf. Eq. (2.1)), can thus be written in terms of the Schatten 1-norm, the so-called *trace norm* (see Sec. 2.4.1), as $\|\rho\|_1 = 1$ showing that these norms represent a natural choice. Hence, the state space defines a particular subset of the trace class operators being characterized by finite trace norms.

To get a better understanding of the associated boundary, it is advantageous to determine a characterization of its elements in terms of their spectral properties. For finite-dimensional systems, it can be shown that the boundary is determined by $\partial_{\|\cdot\|_p}\mathcal{S}(\mathcal{H}) = \{\rho \in \mathcal{S}(\mathcal{H}) \mid 0 \in \mathrm{spec}(\rho)\}$ for any $p \in [1, \infty)$ where $\mathrm{spec}(\rho)$ refers to the spectrum of the state (Wißmann, 2012). The boundary comprises, thus, exactly those states that have zero eigenvalues corresponding to a rank deficiency of the boundary's elements (Bengtsson and Zyczkowski, 2007). Due to this, orthogonal states are located on the boundary and, moreover, pure states completely determine the boundary of a two-level system which agrees with the basic intuition gathered from the Bloch representation (see Sec. 2.2). This characterization is, however, only true for finite systems. Quite remarkably, all states are part of the boundary for infinite-dimensional Hilbert spaces implying that the interior is empty, i.e. $\mathring{\mathcal{S}}(\mathcal{H}) = \emptyset$ (Wißmann, 2012).

The convex structure of the state space itself gives yet rise to a boundary $\partial\mathcal{S}(\mathcal{H})$. In convex analysis one defines a boundary of a convex set, which is referred to as the relative boundary, as follows (Rockafellar, 1972): A state $\rho \in \mathcal{S}(\mathcal{H})$ is on the boundary of the convex set $\mathcal{S}(\mathcal{H})$ if and only if there exists a state $\sigma \in \mathcal{S}(\mathcal{H})$ such that for any real number $\lambda > 1$ the operator $\rho_\lambda = (1-\lambda)\sigma + \lambda\rho$ (cf. Eq. (2.4)) is not contained in $\mathcal{S}(\mathcal{H})$. That is, the set of states defining the boundary of the state space $\partial\mathcal{S}(\mathcal{H})$ is given by

$$\partial\mathcal{S}(\mathcal{H}) = \{\rho \in \mathcal{S}(\mathcal{H}) \mid \exists\, \sigma \in \mathcal{S}(\mathcal{H}), \text{ s.t. } \rho_\lambda \notin \mathcal{S}(\mathcal{H}) \text{ for any } \lambda > 1\}\ . \tag{2.19}$$

Having in mind the precise meaning of convexity, an inner point has thus the property that any line terminating in this point can be extended. However, the extension of the convex combination ρ_λ to values $\lambda > 1$ fails for points on the boundary (cf. Fig. 2.1). This illustration also applies to the boundaries based on norms since the relative boundary is in fact equivalent to those boundaries, regardless of the dimension of the underlying Hilbert space (Wißmann *et al.*, 2012; Wißmann, 2012).

After this introduction of boundaries of the state space along with the spectral properties of the states representing the boundary, one now considers the eigenbases of states defining a convex subset of the state space which will be relevant for a link of quantum non-Markovianity to its classical counterpart as will be shown in Sec. 4.4.2. In fact, to render such a link rigorous, the question is important whether or not the eigenbases corresponding to the states found in the images of dynamical maps (see Sec. 3.2), which define convex subsets of the state space, actually provide all possible orthonormal bases of the Hilbert space.

As a result of this thesis, it is shown in the following that any orthonormal basis of a finite-dimensional Hilbert space indeed defines the eigenbasis of some state of a convex subset of the state space if and only if the maximally mixed state

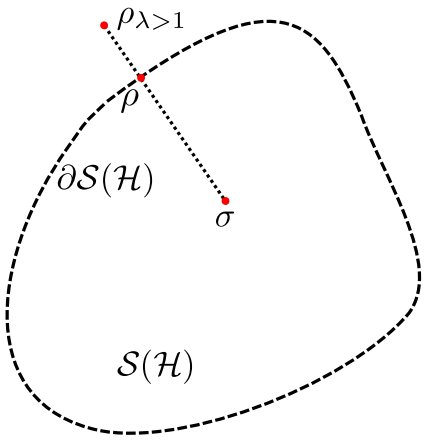

Figure 2.1 – Illustration of the definition of the boundary $\partial\mathcal{S}(\mathcal{H})$. While the state ρ is on the boundary and, therefore, rank deficient, the state σ defines an inner point.

is contained in it, too. Clearly, if the subset includes the maximally mixed state, the statement trivially follows from the fact that any orthonormal basis $\{|\psi_j\rangle\}$ defines a resolution of identity[6], i.e. one has $\sum_j |\psi_j\rangle\langle\psi_j| = \mathbb{1}_{\mathcal{H}}$. To prove the converse implication, one uses the Hahn-Banach separation theorem for normed vector spaces (Rudin, 1991). Note that the state space is embedded in the set of finite Hermitian matrices which represents a normed vector space. In fact, it defines even a Hilbert space with respect to the Hilbert-Schmidt scalar product so that Riesz' representation theorem applies (see, e.g., Rudin (1991)). That is, any continuous linear functional on the set of Hermitian matrices can be represented by a Hermitian operator.

Lemma 2.1. *Let* $\dim\mathcal{H} = N < \infty$ *and denote by* $\mathcal{C} \subset \mathcal{S}(\mathcal{H})$ *a nonempty and convex subset of the state space. Then, any orthonormal basis* $\{|\psi_j\rangle\}$ *of* $\mathcal{H}$ *defines the eigenbasis of some quantum state* $\rho \in \mathcal{C}$ *if and only if* $\frac{1}{N}\mathbb{1}_N \in \mathcal{C}$.

Proof. The 'if' statement is obviously true since any orthonormal basis defines a resolution of identity as mentioned before.

To show the reverse, suppose that $\frac{1}{N}\mathbb{1}_N \notin \mathcal{C}$. According to the Hahn-Banach separation theorem, there exists a continuous real-valued linear functional φ_Y separating the two disjoint nonempty and convex sets $\mathcal{C}$ and $\{\frac{1}{N}\mathbb{1}_N\}$. That is, one has

$$\varphi_Y(\tfrac{1}{N}\mathbb{1}_N) < \gamma \leq \varphi_Y(\rho) \tag{2.20}$$

for some $\gamma \in \mathbb{R}$ and all $\rho \in \mathcal{C}$. Due to the Riesz representation theorem (see, e.g., Rudin (1991)), the functional can be written as $\varphi_Y(X) = \mathrm{Tr}\{XY\}$ for some Hermitian operator Y. Moreover, one may assume that the operator Y is traceless as replacing Y by $Y' \equiv Y - \mathrm{Tr}\{Y\}\mathbb{1}_N$ only leads to a constant shift – given by $\mathrm{Tr}\{Y\}$ – of the functional φ_Y for all states.

[6]This fact is, of course, also true for infinite-dimensional Hilbert space. However, neither the identity operator nor any nonzero scalar multiple of it are trace class operators in this case.

It then follows that the set $\mathcal{X}_Y \equiv \{X \in \mathcal{B}(\mathcal{H}) | X = X^\dagger, \mathrm{Tr}\{X\} = 1, \varphi_Y(X) = 0\}$, describing a hyperplane, contains the maximally mixed state and separates it from the convex set $\mathcal{C}$. Now, let the spectral decomposition of Y be given by

$$Y = \sum_{j=0}^{N-1} \lambda_j |\lambda_j\rangle\langle\lambda_j| \ , \tag{2.21}$$

where the eigenvalues satisfy $\sum_j \lambda_j = 0$ as Y is traceless. To prove the claim, one shows that there exists an orthonormal basis $\{|\psi_k\rangle\}$ of the Hilbert space $\mathcal{H}$ where each of its elements is part of $\mathcal{X}_Y$. Clearly, for any unitary operator U on $\mathcal{H}$ the vectors $|\psi_k\rangle \equiv U|\,\lambda_k\rangle = \sum_{j=0}^{N-1} u_{jk}|\lambda_j\rangle$ where $u_{jk} = \langle\lambda_j|U|\lambda_k\rangle$ define an orthonormal basis. Moreover, one finds

$$\mathrm{Tr}\{Y|\psi_k\rangle\langle\psi_k|\} = \langle\psi_k|Y|\psi_k\rangle = \sum_{j=0}^{N-1} |u_{jk}|^2 \lambda_j \ , \tag{2.22}$$

which vanishes if one has $|u_{jk}| = c$ for all $0 \leq j, k \leq N-1$. This condition is, for example, satisfied by the Vandermonde matrix, introduced by Sylvester (1867) and known from discrete Fourier transforms, whose coefficients obey $u_{jk} = (1/\sqrt{N})\omega_N^{j\cdot k}$ where $\omega_N = \exp[-2\pi i/N]$ and, therefore, $c = 1/\sqrt{N}$. The associated operator

$$U = \tfrac{1}{\sqrt{N}} \sum_{j,k=0}^{N-1} \omega_N^{j\cdot k} |j\rangle\langle k| \tag{2.23}$$

is indeed unitary as one readily obtains $(1/N)\sum_{j=0}^{N-1} \exp[-2\pi i m \cdot j/N] = \delta_{k,l}$ for all $m \in \mathbb{Z}$ using the finite geometric series $\sum_{j=0}^{N-1} q^j = (1-q^N)/(1-q)$ for $q \neq 1$.

Thus, the set $\{|\psi_k\rangle\}$ defines an orthonormal basis satisfying $|\psi_k\rangle\langle\psi_k| \in \mathcal{X}_Y$ for all k. By linearity of the functional φ_Y, all states with spectral decomposition given by $\sum_k p_k |\psi_k\rangle\langle\psi_k|$ are contained in $\mathcal{X}_Y$, too, implying that there does not exist a quantum state $\rho \in \mathcal{C}$ with eigenbasis given by $\{|\psi_k\rangle\}$. □

Clearly, the Vandermonde operator remains unitary if one multiplies each column or row by a phase factor $\exp[i\phi_k]$ where $\phi_k \in [0, 2\pi)$ for all $0 \leq k \leq N-1$ which, of course, does not change the modulus of the entries. Hence, the proof reveals also that an infinite set of orthonormal bases is actually contained in the hyperplane $\mathcal{X}_Y$ defined by the real-valued functional associated with the Hermitian matrix Y.

This result can be easily illustrated with the help of the two-dimensional case. Employing the Bloch representation (see Sec. 2.2 for details), convex subsets of the state space are mapped to convex subsets of the unit ball in $\mathbb{R}^3$. If the maximally mixed state, which is represented by the origin, is not contained in a convex set $\mathcal{C}$, there then exist two-dimensional planes that do not touch $\mathcal{C}$ but intersect the maximally mixed state and, thus, comprise opposite lying points of the boundary (cf. Fig. 2.2). However, states corresponding to opposing points on the boundary define pure and orthogonal states which hence define an orthonormal basis of $\mathbb{C}^2$. It also follows from this illustration that an infinite set of orthonormal bases is encountered within a single plane. The intersection of the plane with the boundary of the state space defines a circle on the unit sphere which thus contains infinitely

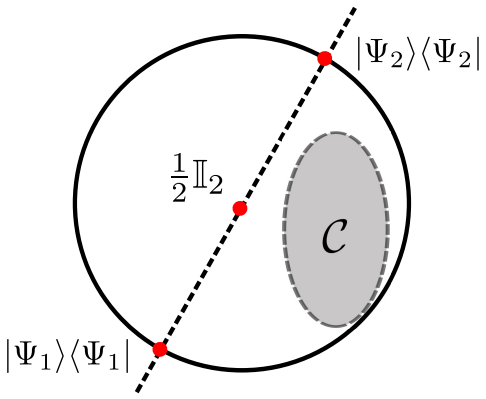

Figure 2.2 – Two-dimensional cut of a hyperplane in the Bloch representation of a two-level system separating the two disjoint nonempty and convex sets $\{\frac{1}{2}\mathbb{1}_2\}$ and $\mathcal{C}$. As the plane contains the maximally mixed state its intersection with the state space, that is, the unit ball comprises an infinite set of pure and orthogonal states on the unit sphere defining orthonormal bases of $\mathbb{C}^2$ (cf. Fig. 3 in Wißmann *et al.* (2015)).

many pairs of opposing points, that is, orthogonal states. Note that lemma 2.1 has no counterpart in infinite dimensions since the identity as well as all of its non-zero multiples are not trace class, making the statement ill-defined in this case.

2.4 Operations and functionals on the state space

Operations on the state space including endomorphisms of and functionals on the state space are important for several tasks in quantum physics. While the former are used to describe the effect of quantum measurements, the latter play a role in ensemble discrimination, parameter estimation and the detection and classification of correlations. In fact, correlations in composite systems feature a link between these two seemingly different classes of maps on the state space. To be appropriate, such maps must, of course, have certain properties which will be deduced in the following. In addition to the introduction of basic concepts in quantum physics such as entanglement and completely positive and trace preserving maps, four distinguished distance measures on the state space are stated along with their properties which will be used later on to detect initial correlations in composite quantum systems (see Sec. 3.5.2) and to quantify non-Markovian behavior in open quantum systems (see Sec. 4.3). Finally, a particular quantifier for the entanglement in a bipartite state, the so-called concurrence, will be introduced in Sec. 2.4.3 and discussed for special states which will be needed later on for a thorough analysis of the study concerning initial correlations and nonlocal memory effects (see Ch. 5).

Clearly, a map that transforms states to states[7] must leave the trace invariant and has to assign positive operators to positive operators in accordance with the

[7]The input and output spaces do not necessarily be the same. That is, the state spaces may be associated with Hilbert spaces having different dimensions.

conditions on states (see Eq. (2.1)). This amounts to require that a map Λ satisfies $\mathrm{Tr}\{\Lambda(X)\} = \mathrm{Tr}\{X\}$ for any linear operator X with finite trace, and $\Lambda(Y) \geq 0$ for any positive operator $Y \geq 0$ which one abbreviates by calling Λ trace preserving and positive, respectively. However, these conditions do not suffice, in general, due to correlations in bipartite quantum systems (Horodecki *et al.*, 1996). Before turning to this issue, one observes that physical requirements additionally force the map to be affine[8]. That is, for any collection of states ρ_j and nonnegative real numbers $p_j \geq 0$ satisfying $\sum_j p_j = 1$, the map obeys

$$\Lambda\Big(\sum_j p_j \rho_j\Big) = \sum_j p_j \Lambda(\rho_j) \ . \tag{2.24}$$

The map's image thus inherits the convex structure of the state space. This condition can even be motivated in the broader context of positive maps that do not necessarily preserve the trace but satisfy $0 \leq \mathrm{Tr}\{\Lambda(\rho)\} \leq 1$ for any state. In this case, the coefficients $p(\Lambda) \equiv \mathrm{Tr}\{\Lambda(\rho)\}$ can still be interpreted as the probability describing the likelihood that the map Λ was applied to the state ρ. Clearly, the operator $p(\Lambda)^{-1}\Lambda(\rho)$ is positive and has unit trace.

Moreover, if the initial state is interpreted as an ensemble $\rho = \sum_j p_j \rho_j$ of states ρ_j that are prepared with probabilities p_j, it is natural to expect this to be true also for the state $p(\Lambda)^{-1}\Lambda(\rho)$. That is, the final state should be a mixture of the single output states $\mathrm{Tr}\{\Lambda(\rho_j)\}^{-1}\Lambda(\rho_j)$ and their associated probabilities $p(j|\Lambda)$ which implies the following relation

$$p(\Lambda)^{-1}\Lambda(\rho) = \sum_j p(j|\Lambda)\mathrm{Tr}\{\Lambda(\rho_j)\}^{-1}\Lambda(\rho_j) \ . \tag{2.25}$$

The conditional probability $p(j|\Lambda)$ represents the probability that the state ρ_j has been prepared given that the map Λ was applied to the quantum system. According to Bayes' rule, it can be rewritten as

$$p(j|\Lambda) = p(\Lambda|j)\frac{p_j}{p(\Lambda)} = \mathrm{Tr}\{\Lambda(\rho_j)\}\frac{p_j}{\mathrm{Tr}\{\Lambda(\rho)\}} \ , \tag{2.26}$$

so that Eq. (2.25) eventually reduces to relation (2.24). It is worth stressing that any affine map has a unique linear extension to the underlying linear vector space (Hayashi, 2006) which is given by the set of bounded linear operators $\mathcal{B}(\mathcal{H})$ in this case. Henceforth, affine maps on the state space are identified with their linear extensions and, therefore, referred to as being linear. As a consequence of the linearity, an appropriate map on the state space must indeed be positive and trace preserving.

However, taking a closer look, one recognizes that positivity does actually not suffice as dilations of such maps to bipartite Hilbert spaces occur in quantum physics. More specifically, one may face the situation where a positive map Λ acts nontrivially only on one part of a composite Hilbert space $\mathcal{H}_{AB} \equiv \mathcal{H}_A \otimes \mathcal{H}_B$ whereas the second factor of the tensor product remains unchanged. Due to the particular type of correlations in quantum theory, this dilation of a positive map to a bipartite

[8]The term *convex linear* is frequently used for this property in the literature, too (see, e.g., Nielsen and Chuang (2000), Breuer and Petruccione (2002)).

system fails to be positive. To introduce this peculiar fact in more detail, one first recalls that states of a bipartite system $\mathcal{H}_{AB}$ which can be approximated in trace norm (cf. Eq. (2.18) for $p = 1$) by states of the form

$$\rho_{AB} = \sum_j p_j \rho_{A,j} \otimes \rho_{B,j} \ , \tag{2.27}$$

where $\rho_{A,j}$ and $\rho_{B,j}$ refer to states of the subsystems corresponding to the Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively, and one has $p_j \geq 0$ satisfying $\sum_j p_j = 1$ as before, are conventionally said to be separable[9]. Being separable is the complement of being entangled, so entangled states cannot be approximated by such states, extending the well-known concept of entanglement for pure states to the full state space. Clearly, one recovers the characterization in terms of the number of nonzero Schmidt coefficients α_j for pure states described by

$$|\psi\rangle_{AB} = \sum_j \alpha_j |\chi_j\rangle_A \otimes |\phi_j\rangle_B \tag{2.28}$$

for some orthonormal bases $\{|\chi_j\rangle_A\}$ and $\{|\phi_j\rangle_B\}$, that is, a state $|\psi\rangle_{AB}$ is said to be entangled if and only if there are more than two nonzero Schmidt coefficients. Note that one speaks of a maximally entangled state if the coefficients obey $\alpha_j = 1/\sqrt{\min_{K=A,B} N_K}$ for all j where $N_K \equiv \dim \mathcal{H}_K$.

As shown by Horodecki *et al.* (1996), the operator $(\Lambda \otimes I_B)(\rho_{AB})$, where I_B denotes the identity map on $\mathcal{H}_B$, may be nonpositive if ρ_{AB} defines an entangled state, even though the linear map Λ is positive. Here, the operator $\Lambda \otimes I_B$ is defined as the linear tensor extension of the map $(\Lambda \otimes I_B)(X \otimes Y) = \Lambda(X) \otimes Y$ for bounded linear operators X and Y on the Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively. Complete positivity of a map warrants, however, that this straightforward dilation of a positive linear map to arbitrary Hilbert spaces is indeed positive again.

Definition 2.1. *A linear map Λ is said to be completely positive if and only if the dilated map*

$$\Lambda_n^\star \equiv \Lambda \otimes I_n : \mathcal{B}(\mathcal{H}_A) \otimes \mathcal{M}_n(\mathbb{C}) \to \mathcal{B}(\mathcal{H}_A) \otimes \mathcal{M}_n(\mathbb{C}) \tag{2.29}$$

is positive for all $n \in \mathbb{N}$ where $\mathcal{M}_n(\mathbb{C})$ refers to the set of complex-valued $n \times n$-matrices. In particular, Λ is called n-positive if $\Lambda_n^\star$ is positive

It thus follows that $(\Lambda \otimes I_B)(\rho_{AB}) \geq 0$ for any Hilbert space $\mathcal{H}_B$ and state ρ_{AB} of the joint system if the linear map Λ is completely positive. Hence, completely positive linear maps are insensitive to the particular structure of correlations in quantum systems. Note that the action of $\Lambda_n^\star$ can also be written as

$$\Lambda_n^\star\big((X_{jk})\big) = \big(\Lambda(X_{jk})\big) \tag{2.30}$$

for $(X_{jk}) \in \mathcal{M}_n(\mathcal{B}(\mathcal{H}_A))$ if one identifies $\mathcal{B}(\mathcal{H}_A) \otimes \mathcal{M}_n(\mathbb{C})$ with the C^*-algebra $\mathcal{M}_n(\mathcal{B}(\mathcal{H}_A))$ of $n \times n$-matrices with entries in $\mathcal{B}(\mathcal{H}_A)$. This characterization of the dilation has the advantage that it also applies to nonlinear maps (Ando and Choi, 1986).

[9] The presented definition of separable states is due to Werner (1989) who called them classically correlated states because of their similarity to classical probability measures.

It is also worth noticing that the concept of n-positivity is evidently hierarchical, that is, n-positivity of Λ implies that the map is also k-positive for all $1 \leq k \leq n$ (Choi, 1972; Blackadar, 2006) where 1-positivity is obviously equivalent to the map being positive. However, the converse is not true in general (Choi, 1972; Stinespring, 1955; Arveson, 1969). This relation is summarized as

$$\mathcal{P}_1(\mathcal{B}(\mathcal{H}_A)) \supsetneq \mathcal{P}_2(\mathcal{B}(\mathcal{H}_A)) \supsetneq \cdots \supsetneq \mathcal{P}_\infty(\mathcal{B}(\mathcal{H}_A)) \ , \tag{2.31}$$

where $\mathcal{P}_n(\mathcal{B}(\mathcal{H}_A))$ denotes the set of n-positive linear endomorphisms of $\mathcal{B}(\mathcal{H})$. For an N_A-dimensional quantum system, it has been shown that complete positivity is equivalent to N_A-positivity and, therefore, $\mathcal{P}_{N_A}(\mathcal{B}(\mathcal{H}_A)) = \mathcal{P}_k(\mathcal{B}(\mathcal{H}_A))$ for all $k \geq N_A$ (Choi, 1975).

An alternative characterization of completely positive maps is given by the so-called Kraus representation (Kraus, 1983). It was shown by Choi (1975) that a linear map $\Lambda : \mathcal{B}(\mathcal{H}_A) \to \mathcal{B}(\mathcal{H}_A)$ is completely positive if and only if there exist operators Ω_j on the Hilbert space $\mathcal{H}_A$ such that Λ can be written as

$$\Lambda(X) = \sum_j \Omega_j X \Omega_j^\dagger \tag{2.32}$$

for any $X \in \mathcal{B}(\mathcal{H}_A)$. Because the map is similarly described by any set of Kraus operators $\{\tilde{\Omega}_j\}$ satisfying $\tilde{\Omega}_j = \sum_k U_{jk}\Omega_k$ for some unitary $U = (U_{jk})$, it follows that at most N_A^2 Kraus operators are required to represent any such map on an N_A-dimensional Hilbert space (Breuer and Petruccione, 2002). Employing the cyclicity of the trace, one easily shows that the map is trace preserving if and only if the Kraus operators obey $\sum_j \Omega_j^\dagger \Omega_j = \mathbb{1}_{\mathcal{H}_A}$. Completely positive linear maps that do not increase the trace are nevertheless important in quantum theory (see, e.g., Nielsen and Chuang (2000)). In fact, quantum measurements are described by so-called quantum operations which refer to sets $\{\Lambda_k\}_{k\in\mathcal{M}}$ of completely positive and linear maps whose Kraus operators satisfy $\sum_{j,k} \Omega_{k,j}^\dagger \Omega_{k,j} = \mathbb{1}_{\mathcal{H}_A}$ that one assigns to the possible outcomes $\mathcal{M} \subset \mathbb{R}$ of a measurement. The effects $E_k \equiv \sum_j \Omega_{k,j}^\dagger \Omega_{k,j}$ thus define a resolution of identity (cf. Sec. 2.3) which is typically not be projective. While the map Λ_k specifies the state change caused by a measurement with outcome k, the associated effect E_k determines the probability for the occurrence of this outcome in a state ρ according to $\mathrm{Tr}\{E_k\rho\}$. Note that the map $k \mapsto E_k$ defines a positive operator-valued measure which is abbreviated as POVM (Nielsen and Chuang, 2000). It is furthermore worth stressing that the probabilities are unaffected by unitary transformations of the Kraus operators, at variance with the quantum operations itself which are determined by the details of the measurement setup.

Summarizing the previous discussion, completely positive (**CP**) and trace preserving (**T**) linear maps, which are henceforth abbreviated as **CPT**-maps, represent the class of maps transforming states to states that are consistent with quantum theory. In particular, the structure of correlations in quantum physics led to some of these significant constraints. To detect and quantify entanglement, functionals on the state space are typically used in quantum theory[10]. Given a distance

[10] Of course, a positive but not 2-positive map already provides the basis for an entanglement witness (Peres, 1996; Horodecki *et al.*, 1996) just as the violation of Bell's inequalities (Bell, 1987). However, they typically fail to detect all entangled states as they define solely witnesses (Gisin, 1996).

measure $\mathcal{D} : \mathcal{S}(\mathcal{H}_{AB}) \times \mathcal{S}(\mathcal{H}_{AB}) \to \mathbb{R}$, the deduced quantity

$$\mathcal{E}_{\mathcal{D}}(\rho) \equiv \inf_{\sigma \in \tilde{\mathcal{S}}(\mathcal{H}_{AB})} \mathcal{D}(\rho, \sigma) \ , \tag{2.33}$$

where $\tilde{\mathcal{S}}(\mathcal{H}_{AB})$ denotes the set of separable states (cf. Eq. (2.27)), provides, for example, a means to quantify the amount of entanglement contained in an arbitrary state. Such quantifiers are referred to as geometric measures of entanglement. To obtain proper entanglement measures which are also called entanglement monotone, it suffices, for example, to require that used distance measure defines a metric and that it is unitarily invariant and contractive under CPT-maps[11]. That is, it must obey

$$\mathcal{D}(U\rho_1 U^\dagger, U\rho_2 U^\dagger) = \mathcal{D}(\rho_1, \rho_2) \ , \tag{2.34}$$

$$\mathcal{D}(\Lambda(\rho_1), \Lambda(\rho_2)) \leq \mathcal{D}(\rho_1, \rho_2) \tag{2.35}$$

for any pair of states, unitary operator U and CPT-map Λ where a distance measure $\mathcal{D} : \mathcal{S}(\mathcal{H}) \times \mathcal{S}(\mathcal{H}) \to \mathbb{R}_+$ clearly defines a metric if and only if it satisfies

$$\mathcal{D}(\rho_1, \rho_2) = \mathcal{D}(\rho_2, \rho_1) \ , \tag{2.36}$$

$$\mathcal{D}(\rho_1, \rho_2) = 0 \Leftrightarrow \rho_1 = \rho_2 \ , \tag{2.37}$$

$$\mathcal{D}(\rho_1, \rho_2) \leq \mathcal{D}(\rho_1, \rho_3) + \mathcal{D}(\rho_2, \rho_3) \tag{2.38}$$

for any states ρ_1, ρ_2 and ρ_3. Note that positivity of the range of $\mathcal{D}$ directly follows from these three properties.

Another particular property of a distance measure is given by the so-called subadditivity, i.e.

$$\mathcal{D}(\rho_1 \otimes \sigma_1, \rho_2 \otimes \sigma_2) \leq \mathcal{D}(\rho_1, \rho_2) + \mathcal{D}(\sigma_1, \sigma_2) \ . \tag{2.39}$$

Distance measures having all these four features define witnesses for arbitrary initial correlations between open quantum system and their environments as will be shown in Sec. 3.5. In the following, several frequently used distance measures are introduced along with a thorough discussion about their properties and interpretations. Apart from their use for geometric measures of entanglement (cf. Eq. (2.33)), they are frequently employed, for example, in quantum information and estimation theory as well as in the study of dynamics of open quantum systems. To give an overview and motivate the distance measures properly, these quantifiers are introduced by means of their classical counterparts, defined on the space of classical probability distributions.

2.4.1 The trace distance

Foremost, the trace distance defines a particular distance measure on the state space that does not only satisfy all of the previously mentioned properties but admits a significant physical interpretation, too. Due to these features, one may

[11] See the work by Vedral *et al.* (1997) and Vedral and Plenio (1998) for a detailed list of requirements on entanglement monotones.

use it to quantify non-Markovian behavior of open quantum systems as will be shown in Sec. 4.3. Note that additional properties and most of the proofs of the stated properties can be found in the works by Nielsen and Chuang (2000), Fuchs and van de Graaf (1999) and Hayashi (2006).

The *trace distance* is proportional to the metric induced by the trace norm (cf. Sec. 2.3), i.e., it is defined as

$$\mathcal{D}_T(\rho_1, \rho_2) = \tfrac{1}{2}\|\rho_1 - \rho_2\|_1 \ . \tag{2.40}$$

In addition to the metric property, the trace distance also inherits unitary invariance from the Schatten 1-norm (2.18). Its range is the unit interval $[0, 1]$ where the upper bound is attained for orthogonal states, i.e.

$$\mathcal{D}_T(\rho_1, \rho_2) = 1 \qquad \Leftrightarrow \qquad \rho_1 \perp \rho_2 \ , \tag{2.41}$$

and the lower bound is obviously realized if the states are equal due to the metric property. Furthermore, the trace distance is contractive under CPT-maps, in contrast to the Hilbert-Schmidt norm (Ozawa, 2000) for example, and even the larger class of positive trace preserving linear maps actually define contractions for this distance measure (Ruskai, 1994). That is, one has

$$\mathcal{D}_T(\Upsilon(\rho_1), \Upsilon(\rho_2)) \leq \mathcal{D}_T(\rho_1, \rho_2) \tag{2.42}$$

for any positive, trace preserving linear map Υ which are consistently called PT-maps. Note that the trace distance obeys the characterizations

$$\mathcal{D}_T(\rho_1, \rho_2) = \max_{0 \leq E \leq \mathbb{1}} \mathrm{Tr}\{E(\rho_1 - \rho_2)\} \ , \tag{2.43}$$

where the maximizing positive operator is given by the projection $\Pi_{\{\rho_1 - \rho_2 \geq 0\}}$ onto the subspace spanned by the eigenvectors that correspond to positive eigenvalues of the Hermitian operator $\rho_1 - \rho_2$.

The trace distance can be seen as the generalization of the *Kolmogorov distance*[12] which represents a frequently used tool for classical probability distributions. For $P_1 = \{p_{1,j}\}_{j \in I}$ and $P_2 = \{p_{2,j}\}_{j \in I}$ over an index set $I \subset \mathbb{N}$ satisfying $p_{k,j} \geq 0$ and $\sum_{j \in I} p_{k,j} = 1$, the Kolmogorov distance is given by (see, e.g., Nielsen and Chuang (2000))

$$d_K(P_1, P_2) = \tfrac{1}{2}\|P_1 - P_2\|_{\ell^1} = \tfrac{1}{2} \sum_{j \in I} |p_{1,j} - p_{2,j}| \ , \tag{2.44}$$

which obviously defines a metric on the set of probability distributions. Clearly, Eq. (2.44) represents the special instance obtained for Dirac measures of the general measure theoretic formulation of the Kolmogorov distance. As the Kolmogorov distance can also be characterized as $d_K(P_1, P_2) = \max_{S \subset I} |\sum_{j \in S}(p_{1,j} - p_{2,j})|$ where S refers to any subset of the index set I, it thus quantifies the maximal difference between the probabilities P_1 and P_2 that may be observed for an event. In the following, it is shown that its quantum generalization obeys a similar interpretation with respect to the discrimination of states.

[12] In the literature, one also encounters the name *(total) variational distance* for this quantity (see, e.g., Hayashi (2006)).

Ensemble discrimination Based on the representation (2.43), it can be shown that the trace distance defines a measure for the distinguishability of two states relying on an operational meaning that is similar to the findings for the Kolmogorov distance.

Consider a so-called one-shot, two-state discrimination problem where a sender (Alice) and a receiver (Bob) have the tasks to prepare and to discriminate two states by a single measurement, respectively (Hayashi, 2006). Alice prepares one out of two quantum states $\rho_{1,2}$ with corresponding probability $p_{1,2} \neq 1$ and sends it to Bob who performs a single generalized measurement (see above) in order to infer which one of the two states he had received. As Bob has only a single try, it might happen that it is impossible to distinguish the pair of states with certainty. To guess best the state from a measurement with possible outcomes $\Omega \subset \mathbb{R}$, Bob defines two sets of possible results, R and $\Omega \backslash R$, and assigns the state to be ρ_1 if the measurement outcome is in R and ρ_2 if a value in $\Omega \backslash R$ occurs. This strategy effectively results in a two-valued POVM $\{E_R, \mathbb{1} - E_R\}$ where E_R refers to the collection of effects corresponding to outcomes in R. The probability for correct state discrimination according to this strategy is then given by

$$\begin{aligned} P_{\text{success}} &= p_1 \text{Tr}\{E_R \rho_1\} + p_2 \text{Tr}\{(\mathbb{1} - E_R)\rho_2\} \\ &= p_2 + \text{Tr}\{\Delta E_R\} \ , \end{aligned} \tag{2.45}$$

where the operator Δ is defined as $\Delta \equiv p_1\rho_1 - p_2\rho_2$. Clearly, the probability is maximized by the projection $\Pi_{\{\Delta \geq 0\}}$ onto the positive part this operator. Employing that $\text{Tr}\{|X|\} = \text{Tr}\{X(\Pi_{\{X \geq 0\}} - \Pi_{\{X<0\}})\}$ and $\mathbb{1}_{\mathcal{H}} = \Pi_{\{X \geq 0\}} + \Pi_{\{X<0\}}$ holds for any Hermitian operator X, one shows that the maximal success probability for correct discrimination is given by (Hayashi, 2006)

$$P_{\text{success}}^{\max} = \max_{0 \leq E_R \leq \mathbb{1}} P_{\text{success}} = \frac{1}{2}\left(1 + \|\Delta\|_1\right) \ . \tag{2.46}$$

For an unbiased a prior distribution, i.e. $p_1 = p_2 = 1/2$, this eventually reduces to

$$\tilde{P}_{\text{success}}^{\max} = \frac{1}{2}(1 + \mathcal{D}_T(\rho_1, \rho_2)) \ , \tag{2.47}$$

so the trace distance defines the bias in favor for correct state identification establishing its interpretation as a measure for the distinguishability of two states (Holevo, 1982; Hayashi, 2006; Helstrom, 1976). Note that the optimal measurement strategy is given by a two-valued observable with eigenspaces $\{\rho_1 - \rho_2 \geq 0\}$ and $\{\rho_1 - \rho_2 < 0\}$, which clearly depends on the pair of states.

2.4.2 Classical and quantum f-divergences

Another relevant class of distance measures that are inspired by classical quantities, serving for the important task of comparison of probability measures, is provided by generalizations of the so-called *f-divergences* which were introduced by Csiszár, Marimoto, Ali and Silvey (see the work by Österreicher and Vajda (2003) and references therein). In the following, particular f-divergences and their quantum mechanical counterparts, the quantum Hellinger distance, the Bures metric and

the quantum Jensen-Shannon divergence are considered.

Following Österreicher and Vajda (2003), one defines the intervals $\mathbb{R}_+ = [0, \infty)$ and $\mathbb{R}_0 = \mathbb{R}_+ \backslash \{0\}$ and denotes by $\mathcal{F}$ the set of convex functions $f : \mathbb{R}_+ \to \mathbb{R} \cup \infty$ which are finite on $\mathbb{R}_O$ and continuous on $\mathbb{R}_+$. Note that the function f^* defined by $f^*(x) = x \cdot f(1/x)$ for $x \in \mathbb{R}_0$ is convex and continuous for any $f \in \mathcal{F}$, too, and one obtains $x \cdot f^*(y/x) = y \cdot f(x/y)$ for all $x, y \in \mathbb{R}_+$ and $f \in \mathcal{F}$ by setting $0 \cdot f(v/0)$ equal to zero if $v = 0$ and $0 \cdot f(v/0) = v \cdot f^*(0)$ for $v > 0$.

Definition 2.2. *Let $P_k = \{p_{k,j}\}_{j \in I}$ for $k = 1, 2$ denote two discrete*[13] *probability distributions over the same index set $I \subset \mathbb{N}$. For $f \in \mathcal{F}$ the functional*

$$d_f(P_1, P_2) = \sum_{j \in I} p_{1,j} f\left(\frac{p_{2,j}}{p_{1,j}}\right) \tag{2.48}$$

is called the f-divergence[14]*.*

The well-known *relative entropy* (Kullback and Leibler, 1951) defines, for example, the f-divergence associated with the convex function $f(x) = x \cdot \ln x$ which is typically denoted as $H(P_1 \parallel P_2)$ (see, e.g., Nielsen and Chuang (2000)). Clearly, an f-divergence typically fails to be symmetric and, therefore, to define a metric. However, if the convex function is strictly convex at 1 and satisfies $f(1) = 0$ as well as $f^*(x) = f(x)$ for all $x \in \mathbb{R} \cup \infty$, the associated f-divergence is symmetric as well as positive semidefinite and nondegenerate as proven by Österreicher and Vajda (2003). It is yet more complicate to warrant that the triangle inequality holds. For the class of convex functions

$$f_\beta(x) = \begin{cases} \frac{1}{1-\frac{1}{\beta}} \left[(1 + x^\beta)^{\frac{1}{\beta}} - 2^{\frac{1}{\beta}-1}(1+x) \right] & \text{if } \beta \in \mathbb{R}_0 \backslash \{1\} \ , \\ (1+x)\ln 2 + x \ln x - (1+x)\ln(1+x) & \text{if } \beta = 1 \end{cases} \tag{2.49}$$

on $\mathbb{R}_+$, it is indeed satisfied by the quantities (Österreicher and Vajda, 2003)

$$\tilde{d}_{f_\beta}(P_1, P_2) = d_{f_\beta}(P_1, P_2)^{\min(\beta, \frac{1}{2})} \ . \tag{2.50}$$

As the functions f_β also obey the other conditions mentioned before, these functionals thus represent metrics. The distance measures corresponding to the parameters $\beta = 1/2$ and $\beta = 1$ are of particular interest as they provide the basis for important quantifiers on the state space. More precisely, the functionals

$$d_H(P_1, P_2) \equiv \sqrt{\tfrac{1}{2} d_{f_{1/2}}(P_1, P_2)} \ , \tag{2.51}$$

$$d_J^*(P_1, P_2) \equiv \tfrac{1}{2} d_{f_1}(P_1, P_2) \tag{2.52}$$

are called the *Hellinger distance* (Hellinger, 1909) and the *Jensen-Shannon divergence* (Wong and You, 1985; Lin and Wong, 1990), respectively, where

$$d_{f_{1/2}}(P_1, P_2) = \sum_{j \in I} \left(\sqrt{p_{1,j}} - \sqrt{p_{2,j}} \right)^2 \ , \tag{2.53}$$

$$d_{f_1}(P_1, P_2) = H\big(P_1 \parallel \tfrac{1}{2}(P_1 + P_2)\big) + H\big(P_2 \parallel \tfrac{1}{2}(P_1 + P_2)\big) \ . \tag{2.54}$$

[13] One may similarly define f-divergences in the general framework of probability measures on some measure space (Endres and Schindelin, 2003).

[14] Note that the name *f-relative entropy* is also used in the literature (see, e.g., Hayashi (2006)).

Both quantities are obviously symmetric supporting the common attribution that the Jensen-Shannon divergence defines the symmetric version of the relative entropy. While d_H defines a metric[15], the Jensen-Shannon divergence is the square of a metric on the space of probability distributions according to the previous result (see also Endres and Schindelin (2003)). Note that the f_β-divergence in the limit $\beta \to \infty$ is half of the Kolmogorov distance (2.44) as one easily verifies that $\lim_{\beta\to\infty} f_\beta(x) = \frac{1}{2}|1-x|$. In the following, the quantum counterparts of the Hellinger distance and the Jensen-Shannon divergence are introduced.

The Hellinger distance Besides the relative entropy, the Hellinger distance represents a fundamental distance between two probability distributions that allows to express the Fisher information (Hayashi, 2006), well-known from parameter estimation (Helstrom, 1976). To generalize it to the quantum regime, one first observes that the Hellinger distance may be rewritten in terms of the ℓ^2-norm, i.e.,

$$d_H(P_1, P_2) = \sqrt{\tfrac{1}{2}}\|\sqrt{P_1} - \sqrt{P_2}\|_{\ell^2} \ . \tag{2.55}$$

Replacing this norm by the Hilbert-Schmidt norm $\|\cdot\|_2$ (see Eq. (2.18)), when passing from classical probability distributions to quantum states, one obtains the distance measure

$$\mathcal{D}_H(\rho_1, \rho_2) \equiv \sqrt{\tfrac{1}{2}}\,\|\sqrt{\rho_1} - \sqrt{\rho_2}\|_2 = \sqrt{\tfrac{1}{2}\mathrm{Tr}\{(\sqrt{\rho_1} - \sqrt{\rho_2})^2\}}\ , \tag{2.56}$$

which will be called *quantum Hellinger distance*[16]. Using the cyclic property of the trace and the normalization of quantum states, one may rewrite Eq. (2.56) as

$$\mathcal{D}_H(\rho_1, \rho_2) = \sqrt{1 - A(\rho_1, \rho_2)}\ , \tag{2.57}$$

where $A(\rho_1, \rho_2) \equiv \mathrm{Tr}\{\sqrt{\rho_1}\sqrt{\rho_2}\}$ is referred to as the *affinity* (Luo and Zhang, 2004) which obviously coincides with the classical fidelity, defined as $f(P_1, P_2) = \sum_{j\in I}(p_{1,j}p_{2,j})^{1/2}$ (Nielsen and Chuang, 2000), for commuting operators. The quantum Hellinger distance is clearly symmetric and, in addition, nondegenerate (2.37). Its range is given by the unit interval where the upper limit is attained if and only if the states are orthogonal. Moreover, by means of a theorem by Schoenberg (1938), one may prove the triangle inequality (see, e.g., Mendonça *et al.* (2008)) showing that the quantum Hellinger distance indeed defines a metric on the state space.

Apart from defining a metric, this distance measure is also shown to be invariant under unitary transformations, subadditive and contractive under CPT-maps (cf. Eqs. (2.34), (2.39) and (2.35), respectively) (Luo and Zhang, 2004) as required in the beginning of this section. Clearly, unitary invariance is simply inherited from the Schatten p-norms, and the subadditivity follows from the fact that the affinity is multiplicative (Luo and Zhang, 2004), i.e.,

$$A(\rho_1 \otimes \sigma_1, \rho_2 \otimes \sigma_2) = A(\rho_1, \rho_2)A(\sigma_1, \sigma_2)\ . \tag{2.58}$$

[15]The fact that the Hellinger distance satisfies the triangle inequality can also be shown by means of an elementary proof (see, e.g., Hayashi (2006)).

[16]Note that Luo and Zhang (2004) defined the quantum Hellinger distance as twice the given distance measure.

In fact, similarly to the proof given for the Bures metric in (Wißmann *et al.*, 2013), the subadditivity is obtained by considering the real-valued function $Q : [0,1] \times [0,1] \to \mathbb{R}$ defined by

$$Q(x,y) = \sqrt{1-\sqrt{x}} + \sqrt{1-\sqrt{y}} - \sqrt{1-\sqrt{xy}}\,, \tag{2.59}$$

which is readily shown to be nonnegative. As the affinity satisfies $0 \leq A(\rho_1,\rho_2) \leq 1$ for any two states, the function $Q\big(A(\rho_1,\rho_2), A(\sigma_1,\sigma_2)\big)$ is thus nonnegative for any four quantum states which may be rewritten as

$$\sqrt{1-\sqrt{A(\rho_1,\rho_2)A(\sigma_1,\sigma_2)}} \leq \sqrt{1-\sqrt{A(\rho_1,\rho_2)}} + \sqrt{1-\sqrt{A(\sigma_1,\sigma_2)}}\,. \tag{2.60}$$

It is easily seen that this inequality is equivalent to the subadditivity of the quantum Hellinger distance (2.39) employing its definition (2.57) and the multiplicativity of the affinity.

Finally, it is worth remarking that the quantum Hellinger distance is bounded from below by its classical counterpart just as the trace distance (cf. Sec. 2.4.1). That is, one finds $\mathcal{D}_H(\rho_1,\rho_2) \geq d_H(P_1,P_2)$ for any probability distribution $P_k = \{\mathrm{Tr}\{E_j\rho_k\}\}$ associated with the measurement of a POVM $\{E_j\}$ in the state ρ_k.

The Bures metric There exists yet another possibility to generalize the classical Hellinger distance to the quantum realm. According to Hayashi (2006), a quantum version is provided by

$$\mathcal{D}_B(\rho_1,\rho_2) \equiv \min_{U\,\text{unitary}} \sqrt{\tfrac{1}{2}\mathrm{Tr}\big\{(\sqrt{\rho_1}-\sqrt{\rho_2}U)(\sqrt{\rho_1}-\sqrt{\rho_2}U)^\dagger\big\}}\,, \tag{2.61}$$

defining a symmetric functional on the state space, too. By means of the characterization $\mathrm{Tr}\{|X|\} = \max_U \mathrm{Tr}\{UX\}$, this quantity is rewritten as

$$\mathcal{D}_B(\rho_1,\rho_2) = \sqrt{1-\mathrm{Tr}\{|\sqrt{\rho_1}\sqrt{\rho_2}|\}} = \sqrt{1-\sqrt{F(\rho_1,\rho_2)}}\,, \tag{2.62}$$

which is the well-known *Bures metric*[17] (Bures, 1969; Bengtsson and Zyczkowski, 2007). The *fidelity*[18] $F(\rho_1,\rho_2) = \big(\mathrm{Tr}\{\sqrt{\sqrt{\rho_2}\rho_1\sqrt{\rho_2}}\}\big)^2$, which was introduced by Uhlmann (1976) in order to generalize the Berry phase (Berry, 1984; Simon, 1983) to mixed states as it extends the notion of a transition probability, is obviously very similar to the affinity. In fact, these two quantities equal the classical fidelity for commuting states, they are multiplicative (cf. Eq. (2.58)) and range from 0 to 1 where the lower and upper bounds are attained if and only if $\rho_1 \perp \rho_2$ or $\rho_1 = \rho_2$ holds, respectively (Nielsen and Chuang, 2000; Luo and Zhang, 2004).

Hence, the very same proof as for the quantum Hellinger distance applies to the Bures metric proving that it is subadditive (2.39), too, as shown in (Wißmann

[17] Note that the frequently present factor $\sqrt{2}$ in the definition of the Bures metric (2.62) is omitted in order to restrict its range to the unit interval. It appears that this quantity is referred to as the *sine distance* in the literature (see, e.g., Mendonça *et al.* (2008)).

[18] Unfortunately, the square root of $F(\rho_1,\rho_2)$ is also termed "fidelity" in the literature (see, e.g., Nielsen and Chuang (2000)).

et al., 2013). And similarly, one has $0 \leq \mathcal{D}_B(\rho_1, \rho_2) \leq 1$ where $\mathcal{D}_B(\rho_1, \rho_2) = 1$ holds if and only if the states are orthogonal. Note that the Bures metric dominates the quantum Hellinger distance, that is, one has $\mathcal{D}_H(\rho_1, \rho_2) \leq \mathcal{D}_B(\rho_1, \rho_2)$ where equality holds for any pair of commuting quantum states. Finally, as the name already suggests, the Bures metric $\mathcal{D}_B$ defines indeed a metric on the state space (see Gilchrist *et al.* (2005) and Mendonça *et al.* (2008) for a proof) as well as a contraction with respect to CPT-maps (Nielsen and Chuang, 2000).

The Bures metric is particularly interesting because it is contractive under CPT-maps and, in addition, Riemannian. That is, its infinitesimal form represents a Riemannian metric (Bengtsson and Zyczkowski, 2007) which actually is the quantum Fisher information (see (Hübner, 1992, 1993) and (Braunstein and Caves, 1994)). The quantum Fisher information is well-known from quantum parameter estimation (Helstrom, 1976; Holevo, 1982) as its inverse defines a sharp lower bound for the variance of an unbiased estimator for parameters characterizing quantum states. The (infinitesimal) Bures metric is thus part of the quantum version of a *Cramér-Rao inequality* (Braunstein and Caves, 1994).

The Jensen-Shannon divergence To define a quantum version of the classical Jensen-Shannon divergence, one first observes that the classical distance measure d_J^* (cf. Eq. (2.52)) may be rewritten, as for the Hellinger distance before. In fact, one finds

$$d_J^*(P_1, P_2) = H\big(\tfrac{1}{2}(P_1 + P_2)\big) - \tfrac{1}{2}\sum_{j=1}^{2} H(P_j) \ , \tag{2.63}$$

where the Shannon entropy[19] for a discrete probability distribution $P_k = \{p_{k,j}\}_{j\in I}$ reads

$$H(P_k) = -\sum_{j\in I} p_{k,j} \ln p_{k,j} \ , \tag{2.64}$$

so that the range of the Jensen-Shannon divergence is found to be $0 \leq d_J^*(P_1, P_2) \leq \ln 2$ (Majtey *et al.*, 2005). Based on the representation (2.63), one may also generalize this distance measure to multiple probability distributions over the same index set with weights π_k. The so-called *general Jensen-Shannon divergence* (Lin, 1991)

$$d_{J,\mathrm{gen}}^*(\{P_k\}, \{\pi_k\}) \equiv H\Big(\sum_k \pi_k P_k\Big) - \sum_k \pi_k H(P_k) \tag{2.65}$$

has a wide range of applications including biological tasks and graph theory theory (see Briet and Harremoës (2009) and references therein). Obviously, the initially considered quantity d_J^* is recovered when comparing only two probability distributions with unbiased weights which provides both the lower and upper bounds to Bayes' probability of error (Lin, 1991) and can be related to the mutual information (Grosse *et al.*, 2002).

[19] Note that this quantity is also frequently defined with respect to other logarithms, mainly to base 2 (see, e.g., Helstrom (1976) and Holevo (1982)).

The quantum counterpart of this distance measure is then obtained by replacing the Shannon entropy with the *von-Neumann entropy* $S(\rho) \equiv -\mathrm{Tr}\{\rho \ln \rho\}$ (see, e.g., Nielsen and Chuang (2000)). The *quantum Jensen-Shannon divergence* is thus given by

$$\mathcal{D}_J^*(\rho_1, \rho_2) \equiv S\Big(\tfrac{1}{2}(\rho_1 + \rho_2)\Big) - \frac{1}{2}\sum_{i=1}^{2} S(\rho_i) \ , \tag{2.66}$$

which is symmetric, bounded and well-defined employing the convention $0 \cdot \ln 0 = 0$. In fact, it obeys $0 \leq \mathcal{D}_J^*(\rho_1, \rho_2) \leq \ln 2$ for any pair of quantum states, where the extremal values are again obtained for identical and orthogonal states as before (Majtey *et al.*, 2005). Just as its classical version, the quantum Jensen-Shannon divergence clearly represents a smoothed and symmetric version of the quantum counterpart of the relative entropy. Moreover, it is evident that it represents a special instance (choosing $\pi_j = 1/2$ for $j = 1, 2$) of the quantum counterpart of Eq. (2.65)

$$\mathcal{D}_{J,\mathrm{gen}}^*(\{\rho_k\}, \{\pi_k\}) \equiv S\Big(\sum_k \pi_k \rho_k\Big) - \sum_k \pi_k S(\rho_k) \ , \tag{2.67}$$

which is known as the *Holevo χ quantity*, used in quantum information theory to quantify the maximally retrievable amount of classical information encoded by the quantum states $\{\rho_k\}$ with the a priori probability distribution $\{\pi_k\}$ (Holevo, 1973, 1977).

To define a metric, it remains to verify that the triangle inequality holds for the quantum Jensen-Shannon divergence. Unfortunately, the validity of this property has not yet been proven in general. It could, however, be shown that the square root of $\mathcal{D}_J^*$ satisfies the triangle inequality for two-level systems (Briet and Harremoës, 2009) and, in addition, if restricted to pure states of arbitrary Hilbert spaces (Lamberti *et al.*, 2008). Note that Lamberti *et al.* (2008) obtained, in addition, numerical evidence that the triangle inequality is indeed true on the full set of quantum states for any Hilbert space.

It is worth stressing that the quantum Jensen-Shannon divergence and, thus, its square root is contractive under CPT-maps and invariant under unitary transformations (cf. Eqs. (2.35) and (2.34), respectively), but satisfies solely the restricted additivity (Majtey *et al.*, 2005)

$$\mathcal{D}_J^*(\rho_1 \otimes \sigma, \rho_2 \otimes \sigma) = \mathcal{D}_J^*(\rho_1, \rho_2) \ , \tag{2.68}$$

at variance with the distance measures introduced before. Henceforth, the quantity

$$\mathcal{D}_J(\rho_1, \rho_2) \equiv \sqrt{\mathcal{D}_J^*(\rho_1, \rho_2)} \ , \tag{2.69}$$

will be referred to as the *quantum Jensen-Shannon divergence* which thus defines a contractive, with respect to CPT-maps, and unitarily invariant metric for two-level systems satisfying[20] $0 \leq \mathcal{D}_J(\rho_1, \rho_2) \leq \sqrt{\ln 2}$. For convenience, the addendum *quantum* for the quantum counterparts of the various distance measures presented in this section will be omitted in the sequel if no confusion can arise.

[20] Note that it was erroneously claimed in Wißmann *et al.* (2013) that $\mathcal{D}_J$ is upper bounded by unity which does, however, not change the results presented therein (cf. Sec. 3.5). Clearly, replacing the natural logarithm by that to the base 2, one indeed obtains the bounds $0 \leq \mathcal{D}_J \leq 1$.

2.4.3 Entanglement of formation

Besides geometric measures of entanglement as defined in Eq. (2.33), there exist, of course, other measures for entanglement in bipartite systems such as the negativity or those based on entropic quantifiers measuring how entangled a given bipartite quantum state ρ_{AB} is by means of the distribution of the eigenvalues of its associated reduced states ρ_A or ρ_B. Clearly, a maximally entangled state (cf. Eq. (2.28)) yields maximally mixed reduced states whereas one obtains pure states if a pure bipartite state is separable which thus may, for example, be distinguished using the von-Neumann entropy introduced in the preceding section. The so-called entanglement of formation indeed quantifies entanglement of arbitrary bipartite quantum states in this way, generalizing the entanglement entropy quantifying pure state entanglement. A related quantifier is given by the so-called concurrence which is easily evaluated for two-qubit systems and will therefore be used to examine the detection of initial correlations in open quantum system and the effect of nonlocal memory effects later on in Sec. 3.5.2 and Ch. 5, respectively.

As argued before, the entanglement in pure bipartite states $\rho_{AB} \in \mathcal{S}(\mathcal{H}_A \otimes \mathcal{H}_B)$ may be quantified by $S_{\log_2}(\mathrm{Tr}_B\{\rho_{AB}\})$, where the von Neumann entropy is to the base 2, which one calls entanglement entropy (Nielsen and Chuang, 2000). This quantifier is then extended to arbitrary quantum states by means of a convex roof construction. That is, the *entanglement of formation* is defined according to (Bennett *et al.*, 1996)

$$E_F(\rho_{AB}) = \min_{\{(p_j,\rho_{AB,j})\}} \sum_j p_j S_{\log_2}(\mathrm{Tr}_B\{\rho_{AB,j}\}) \ , \tag{2.70}$$

where the minimum[21] is thus taken over all ensembles[22] of pure states representing the state ρ_{AB}, i.e. $\rho_{AB} = \sum_j p_j \rho_{AB,j}$. By construction, the entanglement of formation reduces to the entanglement entropy and it describes the least expected entanglement of any ensemble of pure states providing a decomposition of the state. In this sense, it basically specifies the amount of entanglement that needs to be shared in advance in order to create the state by means of local operations. Note that the entanglement of formation is invariant under local unitary operations and nonincreasing under local operations and classical communication (Bennett *et al.*, 1996).

Despite of its attractive interpretation, the entanglement of formation is typically hard to determine as the convex roof construction defines a high dimensional optimization problem. Surprisingly, there exists an analytic expression for a bipartite system consisting of two-level systems. In fact, Wootters (1998) has shown that the entanglement of formation for states $\rho_{AB} \in \mathcal{S}(\mathbb{C}^2 \otimes \mathbb{C}^2)$ reads (see also Hill and Wootters (1997))

$$E_F(\rho_{AB}) = h(\tfrac{1}{2}(1 + \sqrt{1 - C_2(\rho_{AB})^2}) \ , \tag{2.71}$$

[21] Note that the minimum must, in fact, be replaced by the infimum as it may not be attained in general.

[22] The quantity is unchanged if the minimization is extended to any ensemble of states representing ρ_{AB} as the minimal value is always attained for pure states $\rho_{AB,j}$ (Hayashi, 2006).

where the binary entropy h is given by $h(x) = -x\log_2 x - (1-x)\log_2(1-x)$ and C_2 refers to the previously mentioned concurrence which is defined as

$$C_2(\rho) = \max\{0, \lambda_1 - \sum_{j=2}^{4}\lambda_j\} \ . \tag{2.72}$$

Here, the nonnegative real numbers λ_j refer to the eigenvalues of the operator[23] $(\sqrt{\rho}\tilde{\rho}\sqrt{\rho})^{1/2}$ in decreasing order, i.e. $\lambda_1 \geq \cdots \geq \lambda_4$, where $\tilde{\rho} \equiv \sigma_2 \otimes \sigma_2 \rho^* \sigma_2 \otimes \sigma_2$ defines the so-called spin flipped state. The operator σ_2 refers to the usual Pauli spin operator[24] (cf. Sec. 2.2) and the complex conjugate ρ^* is defined with respect to the standard computational basis for qubit systems $\{|j,k\rangle = |j\rangle\otimes|k\rangle \,|\, j,k = 0,1\}$ where $\{|j\rangle\}$ denotes the eigenbasis of σ_3, i.e. one has $\sigma_3|j\rangle = (-1)^{j+1}|j\rangle$. Note that the spin flipped state is similarly obtained by complex conjugation with respect to the so-called "magic basis" (2.78)–(2.81) (Wootters, 1998).

It is readily shown that the concurrence takes values in the unit interval, where product states have zero concurrence and it attains its maximal value if a state is maximally entangled. Because the entanglement of formation as a function of the concurrence is strictly monotonic on the interval $[0,1]$, the concurrence defines a measure of entanglement in its own right[25] (Coffman *et al.*, 2000). For a pure two-qubit state $\rho = |\psi\rangle\langle\psi|$ so that one has $\tilde{\rho} = |\tilde{\psi}\rangle\langle\tilde{\psi}|$ with $|\tilde{\psi}\rangle = \sigma_2 \otimes \sigma_2 \sum_{j,k}\langle\psi|j,k\rangle\,|j,k\rangle$, the concurrence simply reads

$$C_2(|\psi\rangle\langle\psi|) = |\langle\psi|\tilde{\psi}\rangle| \ , \tag{2.74}$$

as the only possibly nonzero eigenvalue of the operator $(\sqrt{\rho}\tilde{\rho}\sqrt{\rho})^{1/2} = |\langle\psi|\tilde{\psi}\rangle|\,|\psi\rangle\langle\psi|$ is given by $|\langle\psi|\tilde{\psi}\rangle|$. This can, of course, be rewritten as

$$C_2(|\psi\rangle) = \sqrt{2(1 - \mathrm{Tr}\{\rho_A^2\})} \ , \tag{2.75}$$

where $\rho_A \equiv \mathrm{Tr}_B\{|\psi\rangle\langle\psi|\}$ denotes the reduced, single qubit state associated with $|\psi\rangle \in \mathbb{C}^2 \otimes \mathbb{C}^2$. This characterization defines the starting point for a generalization of the concurrence to pure states of arbitrary systems (Rungta *et al.*, 2001; Albeverio and Fei, 2001) which may, in turn, be extended to any state by a convex roof construction just as the entanglement of formation (2.70) (Chen *et al.*, 2005). Hence, for a bipartite state $\rho_{AB} \in \mathcal{S}(\mathcal{H}_A \otimes \mathcal{H}_B)$ of a $N_A \times N_B$-dimensional system the concurrence is defined by

$$C_{\mathrm{gen}}(\rho_{AB}) = \min_{\{p_j, |\psi_j\rangle_{AB}\}} \sum_j p_j C_{\mathrm{gen}}(|\psi_j\rangle_{AB}) \ , \tag{2.76}$$

[23] One may also show that they define the square roots of the eigenvalues of the non-Hermitian operator $\rho\tilde{\rho}$ (Hayashi, 2006).

[24] Employing the representatives $\lambda_{j,k}$, $\tilde{\lambda}_{j,k}$ and λ'_l of the SU(2)-generators (cf. Eq. (2.6)) along with the assignment $(\sigma_1, \sigma_2, \sigma_3) \equiv (\lambda_{0,1}, \tilde{\lambda}_{0,1}, \lambda'_0)$, one obtains the common representation

$$\sigma_1 = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right) \ , \quad \sigma_2 = \left(\begin{smallmatrix} 0 & -i \\ i & 0 \end{smallmatrix}\right) \ , \quad \sigma_3 = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right) \ , \tag{2.73}$$

of the Pauli spin operators if the basis $\{|j\rangle \,|\, 0 \leq j \leq 1\}$, used to construct the generators, is associated with the canonical basis of $\mathbb{R}^2$.

[25] Note that the square of the concurrence characterizes obviously entanglement, too. In the literature, the square of C_2 is referred to as the tangle (see, e.g., Adesso (2006)).

where any ensemble $\{p_j, |\psi_j\rangle_{AB}\}$ again provides a decomposition of the bipartite state ρ_{AB}, i.e. $\rho_{AB} = \sum_j p_j |\psi_j\rangle_{AB}\langle\psi_j|$. Moreover, one has

$$C_{\text{gen}}(|\psi\rangle_{AB}) \equiv \sqrt{2(1 - \text{Tr}\{\rho_A^2\})} \ , \tag{2.77}$$

for any pure states $|\psi\rangle_{AB} \in \mathcal{H}_A \otimes \mathcal{H}_B$ with $\rho_A = \text{Tr}_B\{|\psi\rangle_{AB}\langle\psi|\}$ in analogy to Eq. (2.75). Obviously, the concurrence vanishes for pure product states $|\psi\rangle_{AB} = |\psi\rangle_A \otimes |\psi'\rangle_B$, whereas a maximally entangled state yields $C_{\text{gen}} = \sqrt{2(1 - 1/N_A)}$ as one has $\rho_A = \frac{1}{N_A}\mathbb{1}_{N_A}$ in this case. However, as for the entanglement of formation, the convex roof makes it difficult to determine the concurrence explicitly, in general.

A special class of states for which the concurrence has an explicit and remarkably simple form, is given by Bell diagonal states. They are defined as $\rho_{\text{Bell}} = \sum_{j=0}^{3} p_j |\Psi_j\rangle\langle\Psi_j|$ where $\{p_j\}$ refers to a probability distribution and the pure states $|\Psi_j\rangle$ are defined as

$$|\Psi_0\rangle = \frac{1}{\sqrt{2}}(|1,1\rangle + |0,0\rangle) \ , \tag{2.78}$$

$$|\Psi_1\rangle = \frac{i}{\sqrt{2}}(|0,1\rangle + |1,0\rangle) = i\sigma_1 \otimes \mathbb{1}_2 |\Psi_0\rangle \ , \tag{2.79}$$

$$|\Psi_2\rangle = \frac{i}{\sqrt{2}}(|0,1\rangle - |1,0\rangle) = \sigma_2 \otimes \mathbb{1}_2 |\Psi_0\rangle \ , \tag{2.80}$$

$$|\Psi_3\rangle = \frac{1}{\sqrt{2}}(|1,1\rangle - |0,0\rangle) = \sigma_3 \otimes \mathbb{1}_2 |\Psi_0\rangle \ , \tag{2.81}$$

thus denoting the Bell states with particular phases which is known as the "magic basis" (Bennett *et al.*, 1996). Employing that $\rho_{\text{Bell}}^* = \rho_{\text{Bell}}$ as well as $\sigma_2 \otimes \sigma_2 \rho_{\text{Bell}} \sigma_2 \otimes \sigma_2 = \rho_{\text{Bell}}$ holds for any probability distribution $\{p_j\}$ (Hayashi, 2006), one shows that the concurrence is given by (Bennett *et al.*, 1996; Hill and Wootters, 1997)

$$C_2(\rho_{\text{Bell}}) = \max\{0, 2 \max_j p_j - 1\} \ . \tag{2.82}$$

In addition, one may show that the concurrence is determined by the coherence factor for any Bell state $\rho_{\Psi_j} = |\Psi_j\rangle\langle\Psi_j|$ subject to decoherence. In fact, focusing on ρ_{Ψ_1} without loss of generality, one recognizes that the time-evolved state

$$\rho_{\Psi_1}(t) = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & \kappa(t) & 0 \\ 0 & \kappa(t)^* & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \ , \tag{2.83}$$

can be rewritten as $\rho_{\Psi_1}(t) = U_t \otimes \mathbb{1}_2 \rho_{\text{Bell}} U_t^\dagger \otimes \mathbb{1}_2$ where the probability distribution characterizing the Bell state is given by $p_{0,3} = 0$ and $p_j = \frac{1}{2}(1 - (-1)^j |\kappa(t)|)$ for $j = 1, 2$. Moreover, the unitary obeys $U_t = e^{i\varphi(t)}|1\rangle\langle 1| + |0\rangle\langle 0|$ with an phase factor $\varphi(t) = \arg(\kappa(t))$. Since one has $\sigma_2 U_t^* = e^{-i\varphi(t)} U_t \sigma_2$, the relation

$$\sqrt{\sqrt{\rho_1(t)}\tilde{\rho}_{\Psi_1}(t)\sqrt{\rho_1(t)}} = \sqrt{U_t \otimes \mathbb{1}_2 \rho_{\text{Bell}}^2 U_t^\dagger \otimes \mathbb{1}_2} \tag{2.84}$$

is readily proven so that Eq. (2.82) applies which finally leads to

$$C_2(\rho_{\Psi_1}(t)) = 2 \cdot \frac{1}{2}(1 + |\kappa(t)|) - 1 = |\kappa(t)| \ , \tag{2.85}$$

as the coherence factor satisfies $0 \leq |\kappa(t)| \leq 1$ for all times t. Note that Chruściński and Kossakowski (2010) have shown that the concurrence of any so-called X state

$$\rho_X(t) = \begin{pmatrix} \rho_{11}(t) & 0 & 0 & \rho_{14}(t) \\ 0 & \rho_{22}(t) & \rho_{23}(t) & 0 \\ 0 & \rho_{32}(t) & \rho_{33}(t) & 0 \\ \rho_{41}(t) & 0 & 0 & \rho_{44}(t) \end{pmatrix} \tag{2.86}$$

is determined by

$$C_2(\rho_X(t)) = 2 \cdot \max\{c_1, c_2, 0\} \,, \tag{2.87}$$

where the parameters c_j are defined as $c_1 = |\rho_{23}(t)| - \sqrt{\rho_{11}(t)\rho_{44}(t)}$ and $c_2 = |\rho_{14}(t)| - \sqrt{\rho_{22}(t)\rho_{33}(t)}$. One immediately recognizes that this reduces to Eq. (2.85) for $\rho_X(t) = \rho_{\Psi_1}(t)$. Due to this result, the nonlocal memory effects of a two-qubit open quantum system presented in Ch. 4 can be associated with the revivals of entanglement.

2.5 Gaussian states in bosonic systems

In quantum physics, the complexity of tasks such as the previously touched characterization and quantification of correlations scales, in general, polynomially or even exponentially with the dimension of the underlying Hilbert space. It thus seems unlikely that one is able to deal effectively with continuous variable systems describing ubiquitous quantized physical systems like opto- or nanomechanical oscillators for example. Quite remarkably, there exists, however, a distinguished class of states in infinite-dimensional systems that refutes this conjecture: Gaussian states allow for a feasible characterization and quantification of entanglement in terms of the covariance matrix of the canonical operators. From a theoretical and practical point of view, they are also interesting as Gaussian states approximate the peculiar state containing infinite entanglement that was considered by Einstein *et al.* (1935) in order to demonstrate the incompleteness of quantum theory. Because their production and manipulation is also routinely and reliably done in the lab nowadays, these states are of great practical relevance for implementations of quantum information tasks and quantum communication protocols (Weedbrook *et al.*, 2012).

2.5.1 Continuous variable systems

The Hilbert space of a bosonic many-particle system, describing indistinguishable particles on a Hilbert space $\mathcal{H}$, is given by the infinite-dimensional Fock space

$$\mathcal{F}_+(\mathcal{H}) = \overline{\bigoplus_{n=0}^{\infty} S_+\Big(\bigotimes_{k=0}^{n} \mathcal{H}\Big)} \,, \tag{2.88}$$

which is the closure of the infinite direct sum of the symmetrized n-fold tensor power of the single-particle mode space $\mathcal{H}$ of the system. The Fock space is thus

stacked according to the particle number. In the one-dimensional case, that is, $\mathcal{H} = \mathbb{C}$ for example, it is represented by the set of Lebesgue square-integrable functions over the reals, i.e. $\mathcal{F}_+(\mathbb{C}) = \mathbb{L}_2(\mathbb{R})$ (Fannes, 2015). The natural isomorphism[26] $U : \mathcal{F}_+(\mathcal{H}_1 \oplus \mathcal{H}_2) \to \mathcal{F}_+(\mathcal{H}_1) \otimes \mathcal{F}_+(\mathcal{H}_2)$ then allows to construct the Fock space corresponding to any single-particle Hilbert space by means of the single mode factors $\mathcal{F}_+(\mathbb{C})$. In particular, one obtains $\mathcal{F}_+(\mathbb{C}^n) = \bigotimes_{k=1}^n \mathbb{L}_2(\mathbb{R})$ which in turn can be identified with $\mathbb{L}_2(\mathbb{R}^n)$ according to Fubini's theorem (Elstrodt, 2009).

A Hilbert space basis for the single mode Fock space $\mathbb{L}_2(\mathbb{R})$ is given by the so-called number basis $\{|m\rangle\}_{m\in\mathbb{N}_0}$, where $\mathbb{N}_0 \equiv \mathbb{N}\cup\{0\}$, defining eigenstates of the number operator $\hat{b}^\dagger\hat{b}$. Here, $\hat{b}$ and $\hat{b}^\dagger$ refer to the Fock annihilation and creation operators for $\mathcal{F}_+(\mathbb{C})$, respectively, which thus satisfy $[\hat{b}, \hat{b}^\dagger] = 1$ and $[\hat{b}, \hat{b}] = [\hat{b}^\dagger, \hat{b}^\dagger] = 0$. Defining $|0\rangle$ to be the so-called vacuum state which is annihilated by $\hat{b}$, i.e. it satisfies $\hat{b}\,|0\rangle = 0$, one determines the other elements of the number basis using the relations $\hat{b}^\dagger|m\rangle = \sqrt{m+1}|m+1\rangle$ and $\hat{b}\,|m\rangle = \sqrt{m}|m-1\rangle$ for all $m \in \mathbb{N}_0$. With respect to the position representation, these operators satisfy

$$\langle x|\hat{b}|\psi\rangle = \frac{1}{\sqrt{2}}\{x\psi(x) + i\frac{\mathrm{d}}{\mathrm{d}x}\psi(x)\} \ , \tag{2.89}$$

$$\langle x|\hat{b}^\dagger|\psi\rangle = \frac{1}{\sqrt{2}}\{x\psi(x) - i\frac{\mathrm{d}}{\mathrm{d}x}\psi(x)\} \tag{2.90}$$

for $|\psi\rangle \in \mathbb{L}_2(\mathbb{R})$ where $\psi(x) \equiv \langle x|\psi\rangle$ and the vacuum state is given by $\psi_0(x) = (1/\pi^{1/4})\exp[-(1/2)x^2]$ (Schrödinger, 1926; von Neumann, 1931; Fannes, 2015).

An n-mode bosonic system $\mathcal{F}_+(\mathbb{C}^n)$ is accordingly spanned by the sets of number bases $\{|m\rangle_k\}_{m\in\mathbb{N}_0}$ corresponding to each mode of the modes k, i.e. the so-called Fock basis is given by $\{\bigotimes_{k=1}^n |m\rangle_k \,|\, m \in \mathbb{N}_0\}$. Note that the creation and annihilation operators of the different modes commute, that is, they satisfy the fundamental commutation relations

$$[\hat{b}_j, \hat{b}_k^\dagger] = \delta_{jk} \ , \qquad [\hat{b}_j, \hat{b}_k] = [\hat{b}_j^\dagger, \hat{b}_k^\dagger] = 0 \ , \tag{2.91}$$

which in terms of the dimensionless canonical position and momentum operators[27]

$$\hat{q}_j \equiv \frac{1}{\sqrt{2}}(\hat{b}_j + \hat{b}_j^\dagger) \ , \qquad \hat{p}_j \equiv \frac{-i}{\sqrt{2}}(\hat{b}_j - \hat{b}_j^\dagger) \tag{2.92}$$

are given by $[\hat{q}_j, \hat{p}_k] = i\delta_{jk}$ and $[\hat{q}_j, \hat{q}_k] = [\hat{p}_j, \hat{p}_k] = 0$. Grouping the position and momentum operators into a $2n$-component operator-valued vector

$$\hat{X} = (\hat{q}_1, \hat{p}_1, \ldots, \hat{q}_n, \hat{p}_n)^T \ , \tag{2.93}$$

these relations may be compactly written as

$$[\hat{X}_j, \hat{X}_k] = i(\Omega_n)_{jk} \ , \tag{2.94}$$

[26] Note that for one-dimensional fermionic systems, which are described by the antisymmetrized Fock spaces $\mathcal{F}_-(\mathbb{C}) = \mathbb{C}^2$, the natural isomorphism U between $\mathcal{F}_-(\mathbb{C}^n)$ and $\mathbb{C}^{2n}$ is called the Jordan-Wigner transform, connecting fermionic mode operators and the Pauli spin operators known from the study of spin chains (Sachdev, 2011).

[27] It is worth emphasizing that in quantum optics one typically uses a different convention regarding the prefactor of $\hat{q}_j$ and $\hat{p}_j$. The quantum optical convention corresponds to a prefactor $1/2$, thus defining the quadrature components of $\hat{b}_j$.

where the matrix Ω_n obeys

$$\Omega_n = \bigoplus_{k=1}^{n} \omega \qquad \text{with} \qquad \omega = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} . \tag{2.95}$$

This skew-symmetric and invertible matrix is also well-known in classical Hamilton mechanics as it induces an alternating[28] and nondegenerate bilinear form on $\mathbb{R}^{2n}$ that allows to write the Poisson bracket on classical phase space in a compact way (Arnold, 1997; Dragt, 2005). In addition, the $2n \times 2n$-matrices that are characterized by the relation

$$S\Omega_n S^T = \Omega_n \tag{2.96}$$

represent canonical transformations of the classical variables leaving Hamilton's equation of motion invariant. The so-called symplectic matrices define a group (in fact even a Lie group, see Appendix A) which actually is the defining representation of the real symplectic group $\mathrm{Sp}(2n, \mathbb{R})$ (Simon *et al.*, 1994).

Elements of $\mathrm{Sp}(2n, \mathbb{R})$ are, however, not only relevant in classical physics but also in quantum theory. A linear transformations $\hat{X}' = S\hat{X}$ of the canonical operators specified by a $2n \times 2n$-matrix S is said to be canonical if $\hat{X}'$ obeys the same commutation relations as $\hat{X}$. It is easily shown that this yields Eq. (2.96), implying that canonical linear transformations are in one-to-one correspondence with the real symplectic group. On account of the Stone-von Neumann theorem (Stone, 1930, 1932; von Neumann, 1932a, 1931), it follows that these transformations of the canonical operators are unitarily implementable. For each $S \in \mathrm{Sp}(2n, \mathbb{R})$ there thus exists a unitary operator U_S acting on $\mathbb{L}_2(\mathbb{R}^{2n})$ such that

$$\hat{X}'_j = \sum_k S_{jk} \hat{X}_k = U_S^\dagger \hat{X}_j U_S \ , \tag{2.97}$$

where the phase of the unitaries U_S, which is initially free, can be narrowed down to a sign ambiguity. The general composition law, which follows from the irreducibility of $\hat{X}'$, thus reads[29]

$$U_S U_{S'} = \pm U_{SS'} \ . \tag{2.98}$$

This unitary representation is eventually generated by the set of Hermitian operators that are quadratic in the canonical operators (Arvind *et al.*, 1995; Ma and Rhodes, 1990). Note that the Hermitian operators that are quadratic at maximum, i.e., (Ferraro *et al.*, 2005)

$$H = \sum_k^n \alpha_k \hat{b}^\dagger + \sum_{l>k=1}^{n} \beta_{kl} \hat{b}_k^\dagger \hat{b}_l + \sum_{k,l=1}^{n} \gamma_{kl} \hat{b}_k^\dagger \hat{b}_l^\dagger + \text{h.c.} \ , \tag{2.99}$$

with complex-valued constants α_k, β_{kl} and γ_{kl}, generate the unitary representation of the affine symplectic group $\mathrm{ISp}(2n, \mathbb{R})$, describing transformations $\hat{X} \to S\hat{X} + \vec{d}$.

[28] A bilinear form $b : V \times V \to \mathbb{F}$ on a vector space V over the field $\mathbb{F}$ is said to be alternating if it obeys $b(v, v) = 0$ for all $v \in V$. It is moreover called nondegenerate if $b(v, w) = 0$ for all $w \in V$ implies $v = 0$.

[29] The two-valued unitary representation actually defines a faithful unitary representation of the metaplectic group $\mathrm{Mp}(2n)$ which is a two-fold covering of $\mathrm{Sp}(2n, \mathbb{R})$ (Arvind *et al.*, 1995).

One easily recognizes that the second term leaves the total number of quanta unchanged, which is referred to as passive device, whereas the first and third term change the amount of quanta, thus being called an active apparatus. Examples for these kinds of devices are provided by beam splitters and (non)degenerate amplifiers in quantum optics (Ferraro *et al.*, 2005).

Another important issue concerning the symplectic group is the diagonalization of real symmetric and not indefinite matrices. Clearly, any real symmetric matrix is diagonalizable by an element of the orthogonal group according to the spectral theorem. If a $2n \times 2n$-matrix is either positive or negative definite, it can, however, also be diagonalized using symplectic matrices. The so-called symplectic diagonalization follows from Williamson's theorem (Williamson, 1936; Arnold, 1997) which states that there exists a symplectic matrix $S \in \mathrm{Sp}(2n, \mathbb{R})$ for any real symmetric, positive-definite (negative-definite) $2n \times 2n$-matrix $V > 0$ ($V < 0$) such that

$$SVS^T = D_V = \mathrm{diag}(\kappa_1, \kappa_1, \ldots, \kappa_n, \kappa_n) \; . \tag{2.100}$$

The parameters κ_j, being called symplectic eigenvalues, are strictly positive (negative) and characterize the spectrum of the matrix $\Omega_n V$ completely according to $\mathrm{spec}(\Omega_n V) = \{\pm i\kappa_j | j = 1, \ldots, n\}$ (Olivares, 2012; Arvind *et al.*, 1995). Note that the symplectic matrix S and the Williamson normal form of V, that is, D_V are solely unique up to a permutation of the symplectic eigenvalues (Ferraro *et al.*, 2005).

2.5.2 Mathematical description of Gaussian states

Having introduced the formalism used to describe continuous variable systems in quantum physics, one now focuses on the previously mentioned Gaussian states for such systems. In complete analogy to Gaussian distributions in classical probability theory (van Kampen, 2007), these states are fully characterized by the first two moments of an operator, implying that the associated characteristic function is Gaussian. In fact, a state of a continuous variable system $\rho \in \mathcal{S}(\mathbb{L}_2(\mathbb{R}^n))$ is said to be an n-mode Gaussian state if and only if for all $\vec{x}, \vec{y} \in \mathbb{R}^n$ the observable

$$\hat{Y} = \sum_{j=1}^{n} (x_j \hat{p}_j - y_j \hat{q}_j) \tag{2.101}$$

has a normal distribution on the real line in the state ρ (Parthasarathy, 2010). Equivalently, the characteristic function $\chi_\rho^t(\vec{x} + i\vec{y}) \equiv \langle \exp[-it\hat{Y}] \rangle_\rho$ of $\hat{Y}$ in the state ρ obeys (Olivares, 2012; Weedbrook *et al.*, 2012; Parthasarathy, 2010)

$$\chi_\rho^t(\vec{z}) = \exp\left[-it\vec{v}^T \Omega_n \langle \hat{X} \rangle_\rho - \frac{t^2}{2} \vec{v}^T \Omega_n \boldsymbol{\sigma}_{\hat{X},\rho} \Omega_n^T \vec{v} \right] \; , \tag{2.102}$$

where $\vec{v} = (x_1, y_1, \ldots, x_n, y_n)^T$ and $\langle \cdot \rangle_\rho = \mathrm{Tr}\{\rho \cdot\}$ denotes the quantum mechanical expectation values. Clearly, the exponential of $\hat{Y}$ is related to the famous Weyl or (n-mode) displacement operator $D(\vec{z})$ for $\vec{z} \in \mathbb{C}^n$ (Parthasarathy, 2010; Scully, 1997) according to

$$\exp[-it\hat{Y}] = D\Big(\frac{t}{\sqrt{2}}\vec{z}\Big) = \exp\left[\frac{t}{\sqrt{2}} \sum_{j=1}^{n} (z_j \hat{b}_j^\dagger - z_j^* \hat{b}_j) \right] \; . \tag{2.103}$$

The moments of the canonical operators can be determined by the derivatives of χ_ρ^t with respect to the variables x_j and y_j at the origin just as in the classical case. Note that the characteristic function is well-defined for any operator and any state, even if the moments actually do not exist. One shows that the $2n$-dimensional real vector $\langle \hat{X} \rangle_\rho$ is composed of the mean position $\langle \hat{p}_j \rangle_\rho$ and momenta $\langle \hat{q}_j \rangle_\rho$, as its notation already suggests, whereas the $2n \times 2n$-matrix $\boldsymbol{\sigma}_{\hat{X},\rho}$ denotes the covariance matrix of the operator $\hat{X} = (\hat{q}_1, \hat{p}_1, \ldots, \hat{q}_n, \hat{p}_n)^T$ whose components are specified by

$$\left(\boldsymbol{\sigma}_{\hat{X},\rho}\right)_{jk} = \tfrac{1}{2}\langle\{\hat{X}_j, \hat{X}_k\}\rangle_\rho - \langle \hat{X}_j \rangle_\rho \langle \hat{X}_k \rangle_\rho \ . \tag{2.104}$$

While the diagonal elements yield the variances $\langle\langle \hat{X}_j \rangle\rangle_\rho \equiv \langle \hat{X}_j^2 \rangle_\rho - \langle \hat{X}_j \rangle_\rho^2$ of the canonical operators, the off-diagonal terms characterize the correlation coefficient of these operators, i.e.,

$$K_{\hat{X}_j,\hat{X}_k}(\rho) \equiv \frac{\frac{1}{2}\langle\{\hat{X}_j, \hat{X}_k\}\rangle_\rho - \langle \hat{X}_j \rangle_\rho \langle \hat{X}_k \rangle_\rho}{\sqrt{\langle\langle \hat{X}_j \rangle\rangle_\rho \langle\langle \hat{X}_k \rangle\rangle_\rho}} = \frac{\left(\boldsymbol{\sigma}_{\hat{X},\rho}\right)_{jk}}{\sqrt{\left(\boldsymbol{\sigma}_{\hat{X},\rho}\right)_{jj}\left(\boldsymbol{\sigma}_{\hat{X},\rho}\right)_{kk}}} \ . \tag{2.105}$$

Note that the correlation coefficient ranges from -1 to $+1$ and the covariance matrix is positive apart from being real and symmetric, as is known from classical probability distributions over a classical phase space (Simon *et al.*, 1994).

Positivity of quantum states and the noncommutative structure of quantum mechanics in opposition to classical physics sets, however, some further restrictions on the covariance matrix. Indeed, the canonical commutation relations impose the constraint

$$\boldsymbol{\sigma}_{\hat{X},\rho} + \frac{i}{2}\Omega_n \geq 0 \tag{2.106}$$

on the covariance matrix of the canonical operators of any, generally non-Gaussian, continuous variable state ρ (Simon *et al.*, 1994). This inequality follows from the fundamental Schrödinger uncertainty relation (Schrödinger, 1930; Griffiths, 2004) and Williamson's theorem (cf. Eq. (2.100)) as is demonstrated in Appendix B.

Summarizing, a state $\rho \in \mathcal{S}(\mathbb{L}_2(\mathbb{R}^n))$ is Gaussian with mean momenta and position given by the elements of $\langle \hat{X} \rangle_\rho$ and a covariance matrix $\boldsymbol{\sigma}_{\hat{X},\rho}$ if its characteristic function obeys (2.102). However, does really any tuples of elements in $\mathbb{R}^{2n}$ and real symmetric and positive $2n \times 2n$-matrices that satisfy relation (2.106) correspond to a Gaussian state? The answer is "yes" which can be shown using the theory of positive definite kernels and quantum Bochner's theorem.

Theorem 2.1. *(Parthasarathy, 2010) Given $\vec{r} \in \mathbb{R}^{2n}$ and let $V \in \mathcal{M}_{2n}(\mathbb{R})$ be a real symmetric and positive-definite $2n \times 2n$-matrix. The function*

$$g_t(\vec{x} + i\vec{y}) = \exp\left[-it\vec{v}^T\Omega_n\vec{r} - \tfrac{t^2}{2}\vec{v}^T\Omega_n V \Omega_n^T \vec{v}\right] \tag{2.107}$$

with $\vec{v} = (x_1, y_1, \ldots, x_n, y_n)^T$ defines the characteristic function of an n-mode Gaussian state with mean position and momenta given by $\langle \hat{X} \rangle_\rho = \vec{r}$ and covariance matrix $\boldsymbol{\sigma}_{\hat{X},\rho} = V$ if and only if the matrix V satisfies

$$V + \frac{i}{2}\Omega_n \geq 0 \ . \tag{2.108}$$

In particular, there are no constraints imposed on the mean position and momenta for Gaussian states. They can even be removed without changing the covariance matrix because the characteristic function transforms under a Weyl transform, leading to a state $\rho' \equiv D(\vec{\alpha})\rho D(\vec{\alpha})^\dagger$, according to

$$\chi^t_{\rho'}(\vec{z}) = \chi^t_\rho(\vec{z}) \exp\Big[2i\frac{t}{\sqrt{2}}\sum_k \mathrm{Im}(\alpha_k^* z_k)\Big] \ . \tag{2.109}$$

Obviously, such a transformation does not alter the terms that are quadratic in $\vec{z}$ which correspond to the covariance matrix. Due to this. choosing $\vec{\alpha} \in \mathbb{C}^n$ such that $\mathrm{Re}(\alpha_j) = -\frac{1}{\sqrt{2}}\langle\hat{q}_j\rangle_\rho$ and $\mathrm{Im}(\alpha_j) = -\frac{1}{\sqrt{2}}\langle\hat{p}_j\rangle_\rho$, the transformed Gaussian state ρ' has zero means while its covariance matrix equals that of ρ, i.e., one has $\langle\hat{X}\rangle_{\rho'} = 0$ and $\boldsymbol{\sigma}_{\hat{X},\rho'} = \boldsymbol{\sigma}_{\hat{X},\rho}$. One may thus always assume that a Gaussian state has zero means when studying solely properties of the covariance matrix.

It is also worth noticing that the famous Wigner function (Wigner, 1932; Glauber, 1963; Cahill and Glauber, 1969)

$$W_{\rho,n}(\vec{v}) \equiv \frac{1}{(2\pi)^n}\int_{\mathbb{R}^n} \mathrm{d}^n\vec{u}\ e^{-i\vec{y}^T\vec{u}}\langle\vec{x}+\tfrac{1}{2}\vec{u}|\rho|\vec{x}-\tfrac{1}{2}\vec{u}\rangle \qquad (\hbar = 1) \tag{2.110}$$

is related[30] to the characteristic function (2.102) for $t = 1$. More precisely, the quasi-probability distribution $W_{\rho,n}$ and the characteristic function are connected by means of a Fourier transformation, i.e.,

$$W_{\rho,n}(\vec{v}) = \frac{1}{(2\pi^2)^n}\int_{\mathbb{R}^{2n}} \mathrm{d}^{2n}\vec{w}\ \ e^{i\vec{v}^T\vec{w}}\,\chi^{t=1}_\rho(\Omega_n\vec{w}) \ , \tag{2.111}$$

$$\chi^{t=1}_\rho(\Omega_n\vec{w}) = \int_{\mathbb{R}^{2n}} \mathrm{d}^{2n}\vec{v}\ e^{-i\vec{w}^T\vec{v}}\,W_{\rho,n}(\vec{v}) \ , \tag{2.112}$$

where $\Omega_n\vec{w}$ is associated with $\vec{z} \in \mathbb{C}^n$ according to $z_j = (\Omega_n\vec{w})_{2j-1} + i(\Omega_n\vec{w})_{2j}$. For $\vec{w} = (x_1, y_1, \ldots, x_n, y_n)^T$ one thus finds $z_j = y_j - ix_j$. As a Fourier transformation maps Gaussian distributions onto Gaussian distributions (see Eq. (C.41)), one may similarly characterize Gaussian states by Gaussian Wigner functions (Weedbrook *et al.*, 2012). In fact, performing the Fourier transform explicitly, Eq. (2.102) is shown to be equivalent to

$$W_{\rho,n}(\vec{w}) = \frac{1}{\pi^n\sqrt{\det(\boldsymbol{\sigma}_{\hat{X},\rho})}}\ \exp\Big[-\tfrac{1}{2}(\vec{w}-\langle\hat{X}\rangle_\rho)^T\boldsymbol{\sigma}^{-1}_{\hat{X},\rho}(\vec{w}-\langle\hat{X}\rangle_\rho)\Big] \ . \tag{2.113}$$

Note that the ordering of the canonical operators in the operator-valued vector $\hat{X}$ is crucial for the exact form of the relation (2.106). Another convenient choice is given by $\hat{X}' = (\hat{p}_1, \ldots, \hat{p}_n, \hat{q}_1, \ldots, \hat{q}_n)^T$ which then corresponds to the inequality (Ferraro *et al.*, 2005)

$$\boldsymbol{S} \pm \frac{i}{2}\beta_n \geq 0 \ , \qquad \text{where} \qquad \beta_n \equiv \begin{pmatrix} 0 & \mathbb{1}_n \\ -\mathbb{1}_n & 0 \end{pmatrix} \ , \tag{2.114}$$

[30] The characteristic function can similarly be related to the Husimi Q-function (Husimi, 1940) and the P-representation (Glauber, 1963; Sudarshan, 1963) which thus provide further descriptions of Gaussian states.

as one easily deduces from the original form (2.106) using the orthogonal transformation induced by the permutation matrix P mapping $\hat{X}$ onto $\hat{X}'$. The characteristic function transforms accordingly to

$$\chi_\rho^t(\vec{z}) = \exp\left[-it(\boldsymbol{l}^T\vec{x} - \boldsymbol{m}^T\vec{y}) - \frac{t^2}{2}(-\vec{x}^T, \vec{y}^T)\boldsymbol{\sigma}_{\hat{X}',\rho}\begin{pmatrix}-\vec{x}\\ \vec{y}\end{pmatrix}\right] , \tag{2.115}$$

where one has $\boldsymbol{l}_j = \langle\hat{p}_j\rangle_\rho$ and $\boldsymbol{m}_j = \langle\hat{q}_j\rangle_\rho$.

2.5.3 Correlations in two-mode Gaussian states

As outlined in the introduction to this section, Gaussian states allow for a feasible quantification of correlations. For two-mode Gaussian states for instance, entanglement is characterized by a relation for the state's covariance matrix that is similar to Eq. (2.106). The covariance matrix determines also the quantum discord for this kind of continuous variable systems as shown by Giorda and Paris (2010) and by (Adesso and Datta, 2010). This fact should actually not surprise since Gaussian states are completely characterized by the first two moments, but the first moments can be removed by local operations (cf. Eq. (2.109)) which thus cannot be relevant for correlations.

In the following, the Peres-Horodecki criterion at the level of second moments is introduced verifying entanglement in two-mode Gaussian states. First, recall that the Peres-Horodecki criterion employs the fact that positive but not completely positive maps might yield nonpositive states if applied to entangled states. Of course, at first glance, this doesn't seem to be advantageous compared to direct attempts finding convex combinations that decompose a given state, characterizing separability (see Eqs. (2.27)). Fortunately, a single positive map suffices in some cases to reveal entanglement unambiguously. In fact, it can be shown that positivity of the partial transpose $\rho_{AB}^{T_K}$, which refers to the state obtained due to matrix transposition with respect to one subsystem only ($K = A$ or B), provides a necessary[31] and sufficient condition for ρ_{AB} being separable for finite systems of dimension 2×2 and 2×3 (Horodecki *et al.*, 1996) as well as Gaussian states[32] (Simon, 2000). The positivity under partial transpose (PPT) which is also known as *Peres-Horodecki-criterion* represents one of the most powerful tools in the context of quantum entanglement known so far.

The validity of the PPT criterion for two-mode Gaussian states relies basically on the necessary and sufficient condition (2.106) on the covariance matrix of

[31] Clearly, the partial transpose of separable states of any kind of system is always positive (Peres, 1996). Positivity under partial transposition is, however, not sufficient in general. Entangled states with positive partial transpose are known as bound entangled states (Horodecki, 1997). For finite systems of dimension 2×2 and 2×3 it turns out to be sufficient, too, since any positive map on $\mathbb{C}^2$ can be decomposed as $\Lambda_1 + \Lambda_2 T$ where Λ_1 and Λ_2 refer to completely positive maps, whereas T denotes the transpose (Strømer, 1963; Horodecki *et al.*, 1996).

[32] The PPT criterion defines a necessary and sufficient condition for all $(1 + N)$-mode Gaussian states under $1 \times N$ bipartitions (Werner and Wolf, 2001) as well as $M \times N$ Gaussian states which are invariant under local mode permutations in the M-mode an N-mode partitions (Serafini *et al.*, 2005; Adesso, 2006). Other necessary and sufficient conditions for bipartite entanglement were, e.g., derived by Giedke *et al.* (2001, 2003b).

quantum states. As Simon (2000) observed, the operation of transposition translates to a mirror reflection[33] in the phase space, described by a sign change of the momentum variables, so that the partial transposition (say, of the first subsystem) transforms the canonical operators $\hat{X} = (\hat{q}_1, \hat{p}_1, \hat{q}_2, \hat{p}_2)^T$ of a two-mode system according to $\hat{X} \to \hat{X}^{(1)} = \Delta_1 \hat{X}$ where

$$\Delta_1 \equiv \mathrm{diag}(1, -1) \oplus \mathbb{1}_2 \ . \tag{2.116}$$

The covariance matrix of a generic two-mode state ρ thus changes to $\boldsymbol{\sigma}_{\hat{X}^{(1)},\rho} = \Delta_1 \boldsymbol{\sigma}_{\hat{X},\rho} \Delta_1$ which must satisfy inequality (2.106), too, if the partial transpose of the state is supposed to be positive. Hence, the Peres-Horodecki criterion at the level of second moments reads

$$\Delta_1 \boldsymbol{\sigma}_{\hat{X},\rho} \Delta_1 + \frac{i}{2} \Omega_n \geq 0 \ , \tag{2.117}$$

which is satisfied by definition by any separable two-mode state. However, for Gaussian states, Simon (2000) has proven that separability of a state also follows from this inequality.

A convenient and manifestly $\mathrm{Sp}(2, \mathbb{R}) \oplus \mathrm{Sp}(2, \mathbb{R})$ invariant form of this constraint, which was actually used to prove that inequality (2.117) is indeed sufficient for a state to be separable and allows for a direct characterization of many states, is obtained using the four quantities

$$I_1 = \det(A) \ , \quad I_2 = \det(B) \ , \quad I_3 = \det(C) \ , \quad I_4 = \det(\boldsymbol{\sigma}_{\hat{X},\rho}) \ , \tag{2.118}$$

associated with the covariance matrix

$$\boldsymbol{\sigma}_{\hat{X},\rho} = \begin{pmatrix} A & C \\ C^T & B \end{pmatrix} \ . \tag{2.119}$$

Clearly, these four quantities are invariant under any transformation induced by $S_{\mathrm{loc}} = \left(\begin{smallmatrix} S_1 & 0 \\ 0 & S_2 \end{smallmatrix} \right) \in \mathrm{Sp}(2, \mathbb{R}) \oplus \mathrm{Sp}(2, \mathbb{R})$. In terms of these invariants the PPT criterion (2.117) can be written as

$$I_1 + I_2 - 2I_3 \leq 4I_4 + \frac{1}{4} \ , \tag{2.120}$$

which, in fact, directly follows from the representation of the necessary and sufficient constraint on covariance matrices (2.106) (Simon, 2000)

$$I_1 + I_2 + 2I_3 \leq 4I_4 + \frac{1}{4} \ , \tag{2.121}$$

as all but I_3 are also invariant under the partial mirror reflection, changing I_3 to $-I_3$. As a consequence of this characterization, it is immediately clear that Gaussian states with $I_3 \geq 0$ are separable (Simon, 2000). Moreover, two-mode Gaussian states having zero discord[34] obey $I_3 = 0$ as zero discord is equivalent to

[33] This is explained by the fact that the transpose of a Hermitian operator is equivalent to its complex conjugate which corresponds to a time reversal transformation.

[34] Even though a bipartite state is not entangled, there can sill be quantumness in the correlations which is quantified by the so-called quantum discord (Ollivier and Zurek, 2001; Henderson and Vedral, 2001). Zero discord states, containing solely classical correlations, are characterized by separable states of the form $\rho_{AB} = \sum_j p_j |\chi_j\rangle_A \langle\chi_j| \otimes \rho_{B,j}$ where $\{|\chi_j\rangle_A\}$ defines an orthonormal basis of $\mathcal{H}_A$.

$C = 0$. Thus, all but completely uncorrelated Gaussian states have nonclassical correlations (Giorda and Paris, 2010; Adesso and Datta, 2010).

Common tools to quantify entanglement are given by the so-called negativity and logarithmic negativity (Vidal and Werner, 2002) which measure the degree to which the partially transposed state fails to be positive. For two-mode Gaussian states the logarithmic negativity is for example defined as

$$E(\boldsymbol{\sigma}_{\hat{X},\rho}) = \max\{0, -\ln(2\kappa_-^{(1)})\} \ , \tag{2.122}$$

representing a monotonically decreasing function of the symplectic eigenvalues of the partially mirrored covariance matrix $\boldsymbol{\sigma}_{\hat{X}^{(1)},\rho}$. Note that one obtains for the symplectic eigenvalues of a two-mode state in terms of the symplectic invariants I_j (Serafini *et al.*, 2004)

$$\kappa_\pm = \left[\frac{1}{2}\Big\{I_1 + I_2 + 2I_3 \pm \sqrt{(I_1 + I_2 + 2I_3)^2 - 4I_4}\Big\}\right]^{1/2} \ . \tag{2.123}$$

Besides the logarithmic negativity, one can also use the entanglement of formation (2.70) for symmetric Gaussian states as is shown by Giedke *et al.* (2003b).

It is worth noticing that the standard or normal form of covariance matrices associated with two-mode states is given by (Botero and Reznik, 2003; Giedke *et al.*, 2003a,b)

$$\boldsymbol{\sigma}_{\hat{X},\rho} = \begin{pmatrix} a & 0 & c_1 & 0 \\ 0 & a & 0 & c_2 \\ c_1 & 0 & b & 0 \\ 0 & c_2 & 0 & b \end{pmatrix} \ , \tag{2.124}$$

where the diagonalization of the blocks A, B and C is achieved by local symplectic transformations (Botero and Reznik, 2003; Giedke *et al.*, 2003a). Clearly, a pure[35] two-mode Gaussian state requires $a = b$ since the von Neumann entropies of the two subsystems, which are determined by $S_V(\rho_{1,2}) = f(\sqrt{I_{1,2}})$ where $f(x) = (x + \frac{1}{2})\ln(x + \frac{1}{2}) - (x - \frac{1}{2})\ln(x - \frac{1}{2})$, must be equal (Olivares, 2012).

2.5.4 Two classes of Gaussian states

The basic definition of Gaussian states for bosonic systems is now illustrated by means of two important classes of these states which are obtained from thermal states using symplectic transformations. Later on, these two classes will be used to characterize the type of correlations needed to obtain nonlocal memory effects (see Sec. 5.2).

It is easily proven that an n-mode thermal state

$$\begin{aligned} \rho_{\rm th}^{(n)} &= \bigotimes_{j=1}^{n} \frac{e^{-\hbar\omega_j/(k_BT)\hat{b}_j^\dagger\hat{b}_j}}{\mathrm{Tr}\left\{e^{-\hbar\omega_j/(k_BT)\hat{b}_j^\dagger\hat{b}_j}\right\}} \\ &= \bigotimes_{j=1}^{n} \frac{1}{N_j+1}\sum_{m=0}^{\infty}\left(\frac{N_j}{N_j+1}\right)^m |m\rangle_j\langle m| \end{aligned} \tag{2.125}$$

[35]The purity, i.e., $P(\rho) = \mathrm{Tr}\{\rho^2\}$ is given by $P(\rho) = [2^{2n}\det(\boldsymbol{\sigma}_{\hat{X},\rho})]^{-1/2}$ for Gaussian states (Olivares, 2012). Hence, a two-mode Gaussian state is pure if and only if one has $I_4 = (1/16)$.

at temperature T with frequencies $\{\omega_j \,|\, j = 1, \ldots, n\}$ defines a zero-mean Gaussian state with diagonal covariance matrix $\boldsymbol{\sigma}_{\hat{X},\rho_{\mathrm{th}}^{(n)}}$. More precisely, one finds for the associated covariance matrix

$$\boldsymbol{\sigma}_{\hat{X},\rho_{\mathrm{th}}^{(n)}} = \mathrm{diag}(\kappa_1, \kappa_1, \ldots, \kappa_n, \kappa_n) \;, \tag{2.126}$$

where $\kappa_j = N_j + 1/2$ and $N_j \equiv \langle \hat{b}_j^\dagger \hat{b}_j \rangle_\rho = \left\{\exp[\hbar\omega_j/(k_B T)] - 1\right\}^{-1}$ defines the average number of photons in the jth mode (Olivares, 2012; Ferraro *et al.*, 2005) whose associated number basis is denoted by $\{|m\rangle_j\}$. Obviously, the coefficients κ_j satisfy $\kappa_j \geq 1/2$ where equality holds if and only if the vacuum state is chosen, corresponding to $N_j = 0$ for all modes. Hence, thermal states are Gaussian with covariance matrices that are already in the Williamson normal form (2.100). Williamson's theorem thus shows that any n-mode Gaussian state ρ can be obtained from a thermal state $\rho_{\mathrm{th}}^{(n)}$ by means of a unitary transformation U_S corresponding to a symplectic matrix $S \in \mathrm{Sp}(2n, \mathbb{R})$ which are generated by Hamilton operators that are linear and quadratic in the creation and annihilation operators (see Eq. (2.99)). That is, one has

$$\rho = U_S \rho_{\mathrm{th}}^{(n)} U_S^\dagger \tag{2.127}$$

for any n-mode Gaussian state whose symplectic eigenvalues are determined by $\kappa_j = N_j + 1/2$ for some coefficients $N_j \in \mathbb{R}$.

In the following, the so-called *squeezed thermal* and *mixed thermal states*, defining two particular classes of two-mode Gaussian states, are introduced and discussed.

Squeezed thermal states By means of the unitary operator

$$U_{\mathrm{STS}}^{(2)}(\zeta) = \exp[\zeta \hat{b}_1^\dagger \hat{b}_2^\dagger - \zeta^* \hat{b}_1 \hat{b}_2] \;, \tag{2.128}$$

one obtains so-called squeezed thermal states when applied to $\rho_{\mathrm{th}}^{(n)}$ (Kim *et al.*, 1989; Olivares, 2012). Here, $\zeta = r \exp[i\phi]$ is called the squeezing parameter where $r \in \mathbb{R}_+$ and $\phi \in [-\pi, \pi)$ are denoted squeezing factor and angle, respectively. Values about $r = 2$ can, for example, be realized with a Josephson parametric amplifier (Zhong *et al.*, 2013). Note that this unitary corresponds to the symplectic matrix

$$S_{\mathrm{STS}}^{(2)}(\zeta) = \begin{pmatrix} \cosh(r)\mathbb{1}_2 & R_{r,\phi} \\ R_{r,\phi} & \cosh(r)\mathbb{1}_2 \end{pmatrix} \tag{2.129}$$

with $R_{r,\phi} = \sinh(r) \left(\begin{smallmatrix} \cos(\phi) & \sin(\phi) \\ \sin(\phi) & -\cos(\phi) \end{smallmatrix}\right)$ and, therefore, the covariance matrix of a two-mode thermal state with mean photon number N_j is shown to transform to (see, e.g., Marian *et al.* (2003))

$$\boldsymbol{\sigma}_{\hat{X},r,\phi,N_j}^{\mathrm{STS}} = \begin{pmatrix} a\mathbb{1}_2 & C \\ C & b\mathbb{1}_2 \end{pmatrix} \;, \tag{2.130}$$

where $C = c \begin{pmatrix} \cos(\phi) & \sin(\phi) \\ \sin(\phi) & -\cos(\phi) \end{pmatrix}$ and one has

$$a = \frac{1}{2}\cosh(2r) + N_1 \cosh^2(r) + N_2 \sinh^2(r) \ , \tag{2.131}$$

$$b = \frac{1}{2}\cosh(2r) + N_2 \cosh^2(r) + N_1 \sinh^2(r) \ , \tag{2.132}$$

$$c = \frac{1}{2}(1 + N_1 + N_2)\sinh(2r) \ . \tag{2.133}$$

Obviously, for a real-valued squeezing parameter ζ corresponding to $\phi = 0, -\pi$, the block matrix C is diagonal and, thus, the covariance matrix is in standard form (2.124). For convenience, one describes this case by setting $\phi = 0$ and assuming that the squeezing factor can also be negative, i.e. one has $r \in \mathbb{R}$.

It is worth mentioning that the squeezing operator $U^{(2)}_{\mathrm{STS}}(r, \phi)$ describes an active device meaning that it adds energy to the thermal states. The difference in the mean occupation number $\hat{b}_1^\dagger \hat{b}_1 - \hat{b}_2^\dagger \hat{b}_2$ is, however, conserved implying that the squeezing operator shifts excitations between the two modes (Olivares, 2012). Moreover, employing the PPT criterion (2.117), one deduces that a two-mode squeezed thermal state is separable if and only if the squeezing factor satisfies the following inequality (Marian *et al.*, 2003)

$$\cosh^2(r) \leq \cosh^2(r_{\mathrm{ent}}) \equiv \frac{(N_1 + 1)(N_2 + 1)}{N_1 + N_2 + 1} \ . \tag{2.134}$$

Hence, for a sufficiently strong squeezing with respect to fixed mean occupation numbers N_1 and N_2, specifying the threshold r_{ent}, positivity under partial transposition is violated so that $\boldsymbol{\sigma}^{\mathrm{STS}}_{\hat{X},r,\phi,N_j}$ describes an entangled two-mode Gaussian state.

A special squeezed thermal state for a real-valued squeezing parameter is given by the two-mode squeezed vacuum. As one has $N_1 = N_2 = 0$, it is clearly symmetric, i.e., one has $a = b$ (cf. Eqs. (2.131) and (2.132)) and, in addition, it shows perfect correlations in the photon numbers for which reason it is also referred to as twin-beam state (Ferraro *et al.*, 2005). The covariance matrix is thus given by

$$\boldsymbol{\sigma}^{\mathrm{EPR}}_{\hat{X},r} \equiv \boldsymbol{\sigma}^{\mathrm{STS}}_{\hat{X},r,\phi=(0,\pi),N_j=0} = \frac{1}{2}\begin{pmatrix} \cosh(2r)\mathbb{1}_2 & \sinh(2r)\sigma_3 \\ \sinh(2r)\sigma_3 & \cosh(2r)\mathbb{1}_2 \end{pmatrix} \ , \tag{2.135}$$

where $r \in \mathbb{R}$ and σ_3 denotes the usual Pauli spin operator. By comparison with Eq. (2.134), one recognizes immediately that this Gaussian state is entangled if and only if $r \neq 0$. This is also readily understood by looking at the state's representation in the Fock basis (Giedke *et al.*, 2003b)

$$|\psi_u\rangle \equiv U^{(2)}_{\mathrm{STS}}(\zeta)|0\rangle \otimes |0\rangle = \sqrt{1 - u^2} \sum_{n=0}^{\infty} u^n |n\rangle \otimes |n\rangle \ , \tag{2.136}$$

where $u = \tanh(r)$ (see Appendix C). In the limit $|r| \to \infty$, this state represents the analog of the maximally entangled Bell states (2.78)–(2.81) for continuous variable systems and may therefore be seen as the physical realization of the model used by Einstein, Podolski and Rosen in their famous Gedankenexperiment (Einstein *et al.*, 1935). Due to this, the two-mode squeezed vacuum is also called EPR

state (Weedbrook *et al.*, 2012). The strong correlations or anti-correlations in the particle positions are clearly seen by looking at the position representation

$$\psi_u(x,y) = \frac{1}{\sqrt{\pi}} \exp\left[-\frac{1}{4}\frac{1-u}{1+u}(x+y)^2 - \frac{1}{4}\frac{1+u}{1-u}(x-y)^2\right] . \tag{2.137}$$

For $r \to +\infty$, the exponent is dominated by the second term yielding a wave function with strongly correlated particle positions, whereas the opposite limit ($r \to -\infty$) leads to a wave function describing strong anti-correlations of the positions of the particles. Hence, $\psi_u(q_1, q_2)$ approximates a delta function $\delta(q_1 \mp q_2)$ for $r \to \pm\infty$. This implies in particular that this state approaches an eigenstate of the operator

$$\hat{A}_{\mp} = \hat{q}_1 \mp \hat{q}_2 \tag{2.138}$$

in the appropriate limit which accordingly leads to a vanishing variance, i.e., it leads to $\langle\langle \hat{A}_{\mp}\rangle\rangle_{|\psi_u\rangle} \to 0$ for $r \to \pm\infty$.

The basic intuition gathered from Eq. (2.136) concerning the dependence of the strength of bipartite correlations on the squeezing factor is supported by the concurrence (2.77) which is fount to be given by

$$C_{\text{gen}}(|\psi_u\rangle) = \sqrt{2(1 - \sqrt{1 - K_{\hat{q}_1,\hat{q}_2}(|\psi_u\rangle)^2})} \tag{2.139}$$

for the EPR state where the correlation coefficient (2.105) obeys

$$K_{\hat{q}_1,\hat{q}_2}(|\psi_u\rangle) = \frac{c_+}{\sqrt{ab}} = \tanh(2r) . \tag{2.140}$$

Hence, the squeezing factor indeed determines the amount of entanglement. Note that any pure two-mode Gaussian state can be transformed into a two-mode squeezed vacuum by virtue of local symplectic operations which means that the EPR states' orbit under local symplectic groups contains all pure two-mode Gaussian states. Note that this result generalizes also to arbitrary pure $2n$-mode Gaussian states (Botero and Reznik, 2003; Giedke *et al.*, 2003a). As the purity of $|\psi_u\rangle$, determining $C_{\text{gen}}(|\psi_u\rangle)$, is given by the local symplectic invariant I_1 defined in Eq. (2.118) (see Appendix B), one directly concludes that the generalized concurrence for any pure two-mode Gaussian state is given by Eq. (2.139).

Finally, it is worth noticing that two-mode squeezing can be realized by means of single-mode squeezing and the action of beamsplitters. More precisely, the two-mode squeezing operator (2.128) can be represented as

$$U^{(2)}_{\text{STS}}(\zeta) = U^{(2)}_{\text{MTS}}(\frac{\pi}{4}e^{i\theta})\, U^{(1)}_{\text{STS},1}(\zeta e^{i\theta}) \otimes U^{(1)}_{\text{STS},2}(-\zeta e^{-i\theta})\, U^{(2)}_{\text{MTS}}(\frac{\pi}{4}e^{i\theta})^{\dagger} , \tag{2.141}$$

where

$$U^{(2)}_{\text{MTS}}(\chi) = \exp[\chi \hat{b}_1^{\dagger}\hat{b}_2 - \chi^* \hat{b}_1 \hat{b}_2^{\dagger}] \tag{2.142}$$

describes the action of a beam splitter on two modes of the electromagnetic field and $U^{(1)}_{\text{STS},j}(\zeta e^{i\theta}) = \exp[\frac{1}{2}(\zeta(\hat{b}_j^{\dagger})^2 - \zeta^*(\hat{b}_j)^2)]$ defines the single mode squeezing operator (Ferraro *et al.*, 2005).

Mixed thermal states If the mixing unitary $U^{(2)}_{\mathrm{MTS}}(\chi)$ is not accompanied by the single-mode squeezing, then one obtains mixed thermal states, defining the second important class of zero-mean two-mode Gaussian states. The symplectic matrix corresponding to the linear mixing of modes reads

$$S^{(2)}_{\mathrm{MTS}}(\chi) = \begin{pmatrix} \cos(\tau)\mathbb{1}_2 & \tilde{R}_{\tau,\theta} \\ \tilde{R}^T_{\tau,\theta} & \cos(\tau)\mathbb{1}_2 \end{pmatrix} , \tag{2.143}$$

where $\chi = \tau \exp[i\theta]$ with $\theta \in [0, 2\pi)$ and $\tau \in \mathbb{R}_+$, as well as

$$\tilde{R}_{\tau,\theta} = \sin(\tau) \begin{pmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{pmatrix} . \tag{2.144}$$

One readily shows that this operation does not entangle a thermal state and that the total number of quanta in the two modes is unchanged, implying that the two-mode vacuum is invariant under this transformation. If it represents the action of a beam splitter, then the coupling χ is proportional to the interaction length and the linear susceptibility of the linear optical medium. Moreover, the quantity $\cos^2(\tau)$ is typically referred to as the transmissivity of the beam splitter (Ferraro *et al.*, 2005).

For a real-valued parameter χ, the covariance matrix of a two-mode thermal state $\rho^{(2)}_{\mathrm{th}}$ with mean occupation numbers N_1 and N_2 is then transformed to

$$\boldsymbol{\sigma}^{\mathrm{MTS}}_{\hat{X},\tau,N_j} = \begin{pmatrix} (\cos^2(\tau)N_1 + \sin^2(\tau)N_2 + \frac{1}{2})\,\mathbb{1}_2 & \sin(\tau)\cos(\tau)(N_2 - N_1)\,\mathbb{1}_2 \\ \sin(\tau)\cos(\tau)(N_2 - N_1)\,\mathbb{1}_2 & (\cos^2(\tau)N_2 + \sin^2(\tau)N_1 + \frac{1}{2})\,\mathbb{1}_2 \end{pmatrix},$$

defining a covariance matrix that is in standard form for any possible values of τ and the mean occupation numbers. Moreover, for non-vacuum states these states are obviously mixed as a direct calculation of the purity shows.

A representation that is similar to the EPR state's covariance matrix is obtained by assuming a perfect beam splitter, characterized by $\cos^2(\tau) = 1/2$, and mean occupation numbers $N_1 = 0$ as well as $N_2 = \cosh(2r) - 1$ with $r \in \mathbb{R}$. For this configuration, the previous covariance matrix reads

$$\boldsymbol{\sigma}^{\mathrm{MTS}}_{\hat{X},r} = \frac{1}{2} \begin{pmatrix} \cosh(2r)\mathbb{1}_2 & \{\cosh(2r) - 1\}\mathbb{1}_2 \\ \{\cosh(2r) - 1\}\mathbb{1}_2 & \cosh(2r)\mathbb{1}_2 \end{pmatrix} , \tag{2.145}$$

which is symmetric and describes a separable two-mode Gaussian state since the 2×2-matrix in the upper right corner is obviously positive definite for any nonzero value of r (cf. Eq. (2.120)). Hence, these states indeed represent separable but correlated two-mode Gaussian states. Comparing the covariance matrices of the mixed thermal state (2.145) to those of the EPR state (2.135), it is clear that the relative sign of the cross-covariances $\langle \hat{q}_1 \hat{q}_2 \rangle_\rho$ and $\langle \hat{p}_1 \hat{p}_2 \rangle_\rho$ discriminates these two types of symmetric Gaussian states along with the type of correlations described by them.

To complete the analysis of this particular kind of mixed thermal state, one considers its position representation which is obtained by means of the Weyl transform representing the inverse of the Wigner transform (see Appendix D). In fact,

one finds for the density matrix $\rho_{\boldsymbol{\sigma}^{\mathrm{MTS}}_{\hat{X},r}}(\vec{x},\vec{y}) \equiv \langle\vec{x}|\rho_{\boldsymbol{\sigma}^{\mathrm{MTS}}_{\hat{X},r}}|\vec{y}\rangle$ with $\vec{x},\vec{y}\in\mathbb{R}^2$

$$\begin{aligned}\rho_{\boldsymbol{\sigma}^{\mathrm{MTS}}_{\hat{X},r}}(\vec{x},\vec{y}) =& \frac{1}{\pi}\sqrt{\frac{1}{2\cosh(2r)-1}}\,\exp\Big[-\frac{1}{4}(\vec{x}-\vec{y})^T B(\vec{x}-\vec{y})\Big] \\ & \cdot\exp\Big[-\frac{1}{4}(\vec{x}+\vec{y})^T B^{-1}(\vec{x}+\vec{y})\Big]\,, \end{aligned} \tag{2.146}$$

where

$$B = \begin{pmatrix}\cosh(2r) & \cosh(2r)-1\\ \cosh(2r)-1 & \cosh(2r)\end{pmatrix}\,. \tag{2.147}$$

The inverse is approximately given by $B^{-1}\approx\frac{1}{2}\left(\begin{smallmatrix}1 & -1\\ -1 & 1\end{smallmatrix}\right)$ for $r\gg 1$ so that the diagonal elements of the density matrix obey

$$\rho_{\boldsymbol{\sigma}^{\mathrm{MTS}}_{\hat{X},r}}(\vec{x},\vec{x}) \approx \frac{1}{\pi}\sqrt{\frac{1}{2\cosh(2r)-1}}\,\exp\left[-\frac{1}{2}(x_1-x_2)^2\right]\,, \tag{2.148}$$

representing a Gaussian distribution with constant variance with respect to difference in the particle positions. Hence, these states have a nonzero second moment of the operator $\hat{A}_- = \hat{q}_1-\hat{q}_2$ (cf. Eq. (2.138)) which converges to unity for $r\gg 1$ as one easily shows. This fact is in contrast to the behavior for the EPR state (2.137) where the diagonal elements in the position representation are increasingly correlated in the particle positions with corresponding variance $\exp[-2r]$ for positive squeezing parameters, thus approaching a delta function.

Chapter 3

Open quantum systems

Having introduced the state space along with some results concerning its structure, the current chapter is dedicated to open systems and their dynamics providing the framework for the description of almost every quantum physical system of practical relevance. Indeed, the interaction of a quantum system with an environment is ubiquitous in any realistic physical system necessitating a proper and efficient description of the arising, irreversible dynamics of the quantum system. The theory of open quantum system offers numerous methods such as projection operator techniques (Nakajima, 1958; Zwanzig, 1960; Prigogine, 1962; Hashitsumae *et al.*, 1977; Shibata *et al.*, 1977; Chaturvedi and Shibata, 1979; Shibata and Arimitsu, 1980), influence functional and path integral techniques (Grabert *et al.*, 1988) achieving this task. In addition, it provides advanced methods such as quantum Monte Carlo methods and stochastic wave function techniques (Breuer *et al.*, 1999; Piilo *et al.*, 2008) to simulate the Feynman-Vernon path integral and to determine the solution of master equations, respectively. By means of the mentioned techniques, an effective description of actual systems present in various experiments is in fact possible. In the following the fundamental concepts used in the theory of open quantum systems, such as dynamical maps and quantum master equations, are reviewed and the exactness of the second order time-convolutionless projection operator technique is discussed. Finally, the implication of nonfactorizing initial conditions for the open system dynamics and their possible detection by means of distance measures are studied. As a result of this thesis employing two exactly solvable models, the trace distance is shown to represent a much more sensitive means to witness initial correlations in comparison to the other measures introduced in Sec. 2.4.2.

3.1 Microscopic approach to open systems

The concept of open quantum systems applies to the setup of joint, interacting physical systems where only a description for a part of the total system is requested. The *open system* S is comprised of the relevant degrees of freedom which are in contact with its environment E referring to the remaining degrees of freedom of the total system. When performing the splitting of the total system's Hilbert space $\mathcal{H}_{SE}$ into the two subsystems $\mathcal{H}_S$ and $\mathcal{H}_E$ associated with the open system

and the environment, respectively, it is typically assumed that the environment is sufficiently large so that the total system is closed. That is, the time evolution of any of its states $\rho \in \mathcal{S}(\mathcal{H}_{SE})$ is presumably governed by the *Liouville-von Neumann equation* (in the Schrödinger picture) (Breuer and Petruccione, 2002)

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{SE}(t) = -i[H(t), \rho_{SE}(t)] \equiv \mathcal{L}(t)\rho_{SE}(t) \ , \tag{3.1}$$

where Planck's constant $\hbar$ is again set to unity, and $H(t)$ refers to the possibly time-dependent Hamiltonian of the total system. In fact, one may actually assume that the Hamiltonian is time-independent if the system is sufficiently large. A convenient approach in the theory of open quantum systems i to split the Hamiltonian into two parts

$$H(t) = H_0(t) + H_I(t) \ , \tag{3.2}$$

separating the free evolution of the open system and its environment, which is represented by $H_0(t) = H_S(t) \otimes \mathbb{1}_E + \mathbb{1}_S \otimes H_E(t)$, from the interaction between them which is described by $H_I(t)$. Employing the notation of the Liouville-von Neumann equation (3.1) in terms of the Liouvillian superoperator $\mathcal{L}(t)$, the formal solution of Eq. (3.1) for a state $\rho_{SE}(t_0)$ at some initial time t_0 is given by

$$\rho_{SE}(t) = \mathcal{G}(t, t_0)\rho_{SE}(t_0) \ , \tag{3.3}$$

where the propagator $\mathcal{G}$ obeys

$$\mathcal{G}(t, t_0) = \mathrm{T}_{\leftarrow} \exp\left[\int_{t_0}^{t} \mathrm{d}s \, \mathcal{L}(s)\right] \ . \tag{3.4}$$

It obviously satisfies $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{G}(t, t_0) = \mathcal{L}(t)\mathcal{G}(t, t_0)$ with initial condition $\mathcal{G}(t_0, t_0) = I$, where I denotes the identity on the level of superoperators. Note that $\mathrm{T}_{\leftarrow}$ refers to the chronological time-ordering meaning that the superoperators are ordered with decreasing time arguments from left to right. Correspondingly, $\mathrm{T}_{\rightarrow}$ describes the anti-chronological time-ordering of operators.

The actual state of the open system at time t is finally determined by averaging over the environmental degrees of freedom which is described by the partial trace over the Hilbert space $\mathcal{H}_E$ of the time-evolved total state $\rho_{SE}(t)$, i.e.,

$$\rho_S(t) = \mathrm{Tr}_E\{\mathcal{G}(t, t_0)\rho_{SE}(t_0)\} \ . \tag{3.5}$$

One may equivalently write this as

$$\rho_S(t) = \mathrm{Tr}_E\{U(t, t_0)\rho_{SE}(t_0)U^{\dagger}(t, t_0)\} \ , \tag{3.6}$$

where the unitary operator $U(t, t_0)$ defines the solution of the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t}U(t, t_0) = -iH(t)U(t, t_0) \tag{3.7}$$

for the initial condition $U(t_0, t_0) = \mathbb{1}_{SE}$. For time-independent Hamiltonians Eq. (3.7) gives rise to the one-parameter family of operators $U(t, t_0) = \exp[-i(t - t_0)H]$.

Despite the clear and elegant formulation of the dynamics of an open quantum system, the determination of the propagator still represents the challenging major difficulty. Even in the simple case of time-independent Hamiltonians, the open system's dynamics is not easily solved in general. An objective of the theory of open quantum systems is exactly to tackle this issue by providing an analytically or numerically feasible formulation of the dynamical evolution of the open system (Breuer and Petruccione, 2002). Most of the strategies developed within this endeavor are defined in the interaction picture removing the free evolution of the open system and the environment. The Liouville-von Neumann equation in this picture reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{SE}(t) = -i[\tilde{H}_I(t), \rho_{SE}(t)] \equiv \tilde{\mathcal{L}}(t)\rho_{SE}(t) \ , \tag{3.8}$$

where $\tilde{H}_I(t)$ refers to the interaction picture representation of the Hamiltonian $H_I(t)$ which is given by

$$\tilde{H}_I(t) = U_0^\dagger(t, t_0) H_I(t) U_0(t, t_0) \ , \tag{3.9}$$

Here, $U_0(t, t_0)$ solves the differential equation (3.7) for $H_0(t)$ generating the free evolution. Based on these preliminaries, some of the concepts and descriptions used in the theory of open quantum systems are introduced in the subsequent section.

3.2 Quantum dynamical maps

Before turning to the efficient description for the reduced dynamics provided by the time-convolutionless projection operator technique, the fundamental mathematical properties of the dynamical evolution defined by Eq. (3.6) are considered. Clearly, if one assigns a reduced state $\rho_S(t_0)$ to the "initial" total system state $\rho_{SE}(t_0)$, Eq. (3.6) defines a closed equation for the time evolution of the reduced state. Assuming that such an assignment can be established for any reduced state, this results in a map which completely characterizes the dynamical evolution of the open system. Indeed, upon introducing the so-called *assignment map* $\mathcal{A} : \mathcal{S}(\mathcal{H}_\mathcal{S}) \to \mathcal{S}(\mathcal{H}_{SE})$, which assigns a unique total system state to any given state of the open system, the so-called quantum dynamical map $\Phi_{t,t_0} : \mathcal{S}(\mathcal{H}_\mathcal{S}) \to \mathcal{S}(\mathcal{H}_\mathcal{S})$ is defined by

$$\Phi_{t,t_0}(\cdot) = \mathrm{Tr}_E\{U(t, t_0)\mathcal{A}(\cdot)U^\dagger(t, t_0)\} \ , \tag{3.10}$$

so that one has $\rho_S(t) = \Phi_{t,t_0}\big(\rho_S(t_0)\big)$. Clearly, Φ_{t_0,t_0} represents the identity operator for t_0. Since it determines the open system state $\rho_S(t)$ at time t according to the action of the dynamics for any initial state $\rho_S(t_0)$, it is actually referred to as the quantum dynamical map corresponding to time t with initial time t_0. Obviously, this map combines the three parts in which the microscopic treatment (3.6) for the reduced dynamics can be split up: the assignment of a state of the total system, a subsequent unitary evolution and, finally, the partial trace over the environment.

To define a proper map on the state space, the dynamical maps for any initial time must be trace preserving and completely positive as discussed in Sec. 2.4. It follows from the structure of a dynamical map that these constraints boil down to the very same requirements on the assignment map. Moreover, to ensure that Φ_{t_0,t_0} is the identity operator, it must additionally be consistent, i.e., it has to satisfy

$$\rho_S(t_0) = \mathrm{Tr}_E\{\mathcal{A}(\rho_S(t_0))\} \; . \tag{3.11}$$

Clearly, factorizing initial conditions corresponding to $\mathcal{A}(\rho_S) = \rho_S \otimes \rho_E$ for a fixed environmental state ρ_E are one possibility for an assignment map which obeys these constraints. In addition to the mentioned necessary properties of an assignment map, this particular approach is also linear and, thus, leads to a linear dynamical map. As shown by Pechukas (1994) and Jordan *et al.* (2004), any assignment map $\mathcal{A}$ that is not only positive and consistent but also convex linear (cf. Eq. (2.24)) on $\mathcal{S}(\mathcal{H}_\mathcal{S})$ corresponds already to factorizing initial conditions (see also Lindblad (1996)). That is, there is no other type of assignment map than $\mathcal{A}(\rho_S) = \rho_S \otimes \rho_E$ obeying all these constraints.

The rather drastic assumption of factorizing initial conditions is consequently the only possibility to obtain a *linear* dynamical map defined on the *entire* state space unless, e.g., either the trivial action for $t = 0$ or linearity of the map is abandoned (Pechukas, 1994, 1995; Alicki, 1995). This means that there exist assignment maps that are not consistent or linear which still lead to a description of the open system dynamics in terms of completely positive and trace preserving maps. One may just as well restrict the domain of the maps, which is equivalent to abandon positivity of the assignment map, in order to obtain a CPT-dynamics[1] in the presence of initial correlations in the total state (Masillo *et al.*, 2011; Rodríguez-Rosario *et al.*, 2010, 2008). Table 3.1 summarizes the properties of assignment maps in the presence of different kinds of initial correlations in the total state. Due to the structure of the state space and the reduced dynamics, it is, however, rather natural to require consistency and linearity for any dynamical map so that factorizing initial conditions indeed represent the most reasonable ansatz[2].

Now, assuming a factorizing assignment map associated with a fixed initial environmental state $\rho_E(t_0)$, the dynamical map (3.10) reads

$$\Phi_{t,t_0}(\rho_S(t_0)) = \mathrm{Tr}_E\{U(t,t_0)\rho_S(t_0) \otimes \rho_E(t_0)U^\dagger(t,t_0)\} \; , \tag{3.12}$$

which obviously defines a linear map on the state space $\mathcal{S}(\mathcal{H}_S)$ at any time t (see Fig. 3.1 for an illustration of the definition of Φ). The lack of correlations in

[1] The fundamental requirement of complete positivity may be questioned since one may raise the objections that there is either no entangled ancillary system, as it is part of the environment, or the simple dilation of the dynamical process to the compound system of the open system and ancilla provides an incorrect description of the dynamics of the joint system which may thus cause unphysical results if complete positivity is not given (Dominy and Lidar, 2016).

[2] A more general approach achieving this type of subdynamics is based on restricting not only the set of admissible open system states but also the applied unitary evolutions which might result in (physically valid but) non-CP evolutions (Dominy *et al.*, 2016; Dominy and Lidar, 2016). The constraints imposed on the unitaries ensure that two different total states with the same reduced state evolve in the same way which may fail in general (see, e.g., Štelmachovič and Bužek (2001, 2003)). The case of a factorizing assignment map is recovered within this ansatz if no constraints on the set of unitaries are imposed.

type of correlations	assignment map		
	consistent	linear	positive
none	✓	✓	✓
classical	–	✓	✓
quantum	✓	✓	–

Table 3.1 – Properties of assignment maps for different types of system-environment correlations in the associated total states (cf. Tab. 1 in Rodríguez-Rosario *et al.* (2010)). Note that classical and quantum correlations are defined with respect to quantum discord (Ollivier and Zurek, 2001; Henderson and Vedral, 2001). Classically correlated states, having zero discord, are represented as $\rho_{AB} = \sum_j p_j |\chi_j\rangle_A\langle\chi_j| \otimes \rho_{B,j}$ for some orthonormal basis $\{|\chi_j\rangle_A\}$ of $\mathcal{H}_A$, whereas states having nonzero discord are said to have quantum correlations which is not necessarily given by entanglement.

the initial total system state can, for example, be realized by measuring the open system at the initial time t_0. Of course, one can also imagine that the open system is first brought into contact with the environment at time t_0, ensuing that the two subsystems are statistically independent before. Note that one typically obtains different dynamical maps by changing the environmental state whereas the total system still evolves due to the same unitary dynamics.

It is directly proven that the above dynamical map preserves the trace and Hermiticity, and is completely positive, i.e. one has

$$\mathrm{Tr}_S\{\Phi_{t,t_0}(X)\} = \mathrm{Tr}_S\{X\} \ , \tag{3.13}$$

$$\Phi_{t,t_0}(X)^\dagger = \Phi_{t,t_0}(X^\dagger) \ , \quad \forall \ X \in \mathcal{B}(\mathcal{H}_S) \tag{3.14}$$

and

$$(\Phi_{t,t_0})^\star_n(Y) \geq 0 \ , \quad \forall \ 0 \leq Y \in \mathcal{B}(\mathcal{H}_S) \otimes \mathcal{M}_n(\mathbb{C}) \ , \tag{3.15}$$

for any $n \in \mathbb{N}$ (cf. definition 2.1), respectively. The latter property can, for example, be confirmed by a direct calculation of the Kraus representation (2.32). Upon inserting the spectral decomposition of the environmental state $\rho_E = \sum_j \lambda_j |j\rangle\langle j|$ in Eq. (3.12) and performing the partial trace, one obtains

$$\Phi_{t,t_0}\big(\rho_S(t_0)\big) = \sum_{j,k} \Omega_{j,k} \rho_S(t_0) \Omega_{j,k}^\dagger \ , \tag{3.16}$$

$$\begin{array}{ccc} \rho_{SE}(t_0) = \rho_S(t_0) \otimes \rho_E(t_0) & \xrightarrow{U(t,t_0)} & \rho_{SE}(t) = U(t,t_0)\rho_S(t_0) \otimes \rho_E(t_0) U^\dagger(t,t_0) \\ \mathrm{Tr}_E \big\downarrow \ \big\uparrow \mathcal{A} & & \mathrm{Tr}_E \big\downarrow \\ \rho_S(t_0) & \xrightarrow{\Phi_{t,t_0}} & \rho_S(t) = \mathrm{Tr}_E\{U(t,t_0)\rho_S(t_0) \otimes \rho_E(t_0) U^\dagger(t,t_0)\} \end{array}$$

Figure 3.1 – Commutative diagram that uniquely defines the linear CPT-map (3.12) associated with a factorizing assignment map.

where the Kraus operators obey $\Omega_{j,k} = \sqrt{\lambda_k}\langle j|U(t,t_0)|k\rangle$. In summary, any reduced dynamics based on a microscopic approach, associated with a unitary dynamics of the joint system of the open system and the environment, as well as factorizing initial conditions is described by a linear CPT-map.

It is worth noticing that Stinespring's dilation theorem (Stinespring, 1955) provides somewhat of the reverse statement. In fact, it states that any linear CPT-map between states of any Hilbert spaces is precisely of the kind of Eq. (3.12). That is, given a linear CPT-map Λ on $\mathcal{S}(\mathcal{H}_S)$, there exists an auxiliary system $\mathcal{H}_A$ and a unitary operator U on $\mathcal{H}_S \otimes \mathcal{H}_A$ such that the CPT-map may be written as

$$\Lambda(\rho_S) = \mathrm{Tr}_A(U\rho_S \otimes \rho_A U^\dagger) \tag{3.17}$$

for all $\rho_S \in \mathcal{S}(\mathcal{H}_S)$, where ρ_A refers to some state on $\mathcal{H}_A$. The auxiliary system's Hilbert space can be chosen such that $\dim\mathcal{H}_A \leq (\dim\mathcal{H}_S)^2$. Note that the representation is only unique up to unitary equivalence and can also be extended to output Hilbert spaces that are different from $\mathcal{H}_S$ (Hayashi, 2006). However, it is an open problem whether the Stinespring dilation of a quantum dynamical process given by the one-parameter family of dynamical maps associated with the initial time t_0, i.e.,

$$\Phi = \{\Phi_{t,t_0} \mid t \geq t_0,\, \Phi_{t_0,t_0} = I_S\}\ , \tag{3.18}$$

results in a one-parameter group of unitary operators $\{U(t,t_0) \mid t \geq t_0,\ U(t_0,t_0) = \mathbb{1}_{SA}\}$ describing an ordinary unitary evolution of the open system and some fixed, auxiliary system.

Clearly, the one-parameter family of dynamical maps (3.18) provides full information about the time evolution of any state of the open system as it determines the reduced state at any time for any initial state. It is generally assumed that any quantum dynamical process of an open quantum system may be described by such a family of maps. Properties of the open system dynamics such as quantum non-Markovianity (see Ch. 4) then correspond to particular features of the one-parameter family of maps. Henceforth, one sticks to the convention that a dynamical map defines a linear CPT-map if not stated differently.

3.3 General master equation

The formal description of the dynamical evolution of the open quantum system in terms of dynamical maps is obviously of no help if the exact dynamics must be determined. To this end, one still needs to determine a solution to the Liouville-von Neumann equation (3.1). This task may, for example, be accomplished using several theoretical and numerical approaches that are formally exact but allow for feasible approximations of the exact dynamics. In fact, the projection operator techniques (Nakajima, 1958; Zwanzig, 1960) provides a famous example of such an approach leading to an exact description for the dynamical evolution of the open quantum system in terms of a so-called quantum master equation (see Sec. 3.3.1). Before turning to the details of this method, the commonly used characterization based on time-local quantum master equations is introduced along with a discussion on general features of this representation arising from the fundamental

properties of dynamical maps.

Similar to the Liouville-von Neumann equation, a quantum master equation describes the dynamics of an open quantum system by a first-order differential equation. That is, one has

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_S(t) = \mathcal{K}_t\rho_S(t) \;, \tag{3.19}$$

where the generator $\mathcal{K}_t$ must obviously preserve Hermiticity and the trace to generate a physical evolution which is equivalent to the relations

$$\{\mathcal{K}_t X\}^\dagger = \mathcal{K}_t X \qquad \text{and} \qquad \mathrm{Tr}_S\{\mathcal{K}_t X\} = 0 \;, \tag{3.20}$$

that must be satisfied for all t and any Hermitian operators X on $\mathcal{H}_S$. One may show that these two constraints imply that the generator has the general form (Gorini *et al.*, 1976; Breuer, 2012a)

$$\begin{aligned}\mathcal{K}_t\rho_S(t) = &- i[H'_S(t), \rho_S(t)] \\ &+ \sum_j \gamma_j(t)\Big[A_j(t)\rho_S(t)A_j^\dagger(t) - \tfrac{1}{2}\{A_j^\dagger(t)A_j(t), \rho_S(t)\}\Big] \;,\end{aligned} \tag{3.21}$$

where $A_j(t)$ denote arbitrary bounded linear operators on $\mathcal{H}_S$ which are called generalized Lindblad operators describing the various decay channels of the system with associated decay rates given by $\gamma_j(t)$. Note that the Hermitian operator $H'_S(t)$ does typically not coincide with the free Hamiltonian of a microscopic approach (3.2). In fact, it may contain additional terms due to the interaction of the open system with its environment. Looking at the structure of the generator, it is clear that a time-local master equation extends the description provided by a Liouville-von Neumann equation: while the first term of $\mathcal{K}_t$ is an ordinary Liouville-von Neumann contribution, which thus represents the reversible, Hamiltonian evolution of the open system – even though with respect to the altered Hamiltonian $H'_S(t)$ –, the second term induces irreversible effects like dissipation. The latter term is accordingly referred to as the dissipator (see, e.g., Ingarden and Kossakowski (1975)).

It is clear that the dynamics generated by such a differential equation must be completely positive, too. Unfortunately, this property is not guaranteed by the very structure of the generator, so further constraints must be imposed. A sufficient condition is given by positivity of the decay rates, that is, if $\gamma_j(t) \geq 0$ for all j and $t \geq t_0$, the generated dynamical map is indeed completely positive (see theorem 3.2). However, the most general constraints on the components of the generator (3.21) leading to a completely positive and trace preserving dynamics are not known yet.

A particular generator of CPT-dynamics is provided by choosing positive and time-independent rates as well as Lindblad operators which thus leads to a generator

$$\mathcal{K}_L\rho_S(t) = -i[H'_S, \rho_S(t)] + \sum_j \gamma_j\Big[A_j\rho_S(t)A_j^\dagger - \tfrac{1}{2}\{A_j^\dagger A_j, \rho_S(t)\}\Big] \;, \tag{3.22}$$

representing the famous *Lindblad form* (Gorini *et al.*, 1976; Lindblad, 1976). This kind of generator deserves special attention as the induced dynamics has the particular feature of being described by a one-parameter semigroup[3] of dynamical maps. This means that the concatenation of two maps for times t and s gives the dynamical map at the later time $t+s$, i.e., one has

$$\Phi_{t+s,t_0} = \Phi_{t,t_0} \circ \Phi_{s,t_0} \tag{3.23}$$

for any $t, s \geq t_0$. The exact form of the solution for the initial time $t_0 = 0$, which is given by

$$\Phi_{t,0} = \exp\left[\mathcal{K}_L t\right] \ , \tag{3.24}$$

already suggests, for example, that the semigroup property holds.

Due to the universal action of the dynamical maps on the states' evolution, one may consider such dynamical processes as being memoryless. Indeed, the map's effect on a state is independent of the point in time when it is applied which directly reflects the neglect of any kind of memory effects. Dynamical evolutions which are governed by a completely positive semigroup are thus called Markovian in the style of the notion for stochastic processes (see Sec. 4.1). Note that the processes obtained from generators $\mathcal{K}_t$ with time-dependent but positive rates are usually referred to as a time-dependent Markovian process which can be motivated by the fact that the associated generators are still in Lindblad form (3.22) at any instance of time t.

It is rather obvious that there are dynamical processes which do not satisfy the drastic property required for a one-parameter semigroup. Conversely, one might ask whether all such particular dynamical processes are generated by time-local master equations in Lindblad form. The answer is "yes": first, under very general mathematical conditions [4], one shows that any semigroup has an infinitesimal generator and, thus, any element of the semigroup is given by the exponential of the generator as, e.g., in Eq. (3.24). Secondly, the popular Gorini-Kossakowski-Sudarshan-Lindblad theorem (Gorini *et al.*, 1976; Lindblad, 1976) establishes the one-to-one connection between the Lindblad form (3.22) of the generator and the existence of semigroups of completely positive and trace preserving maps (see theorem 3.2). Thus, time-local master equations with a generator in Lindblad form provide the prototype of an admissible dynamics explaining their intensive use for phenomenological approaches to open system dynamics.

However, employing several rather drastic assumptions assisting the memoryless character, it is also possible to obtain such a master equation from a microscopic approach for the total system (Breuer and Petruccione, 2002): assuming that the coupling between system and environment is weak, one expands the Liouville-von Neumann equation in the interaction picture (3.8) up to second order in the interaction strength and applies the Born approximation, which supposes the state of the composite system factorizes, yielding a second-order differential equation for the open system density operator. Before using the rotating wave approximation,

[3] The term *semi* indicates that the family of dynamical maps typically defines not a group as the parameter t is restricted to values larger than t_0.

[4] The semigroup must be continuous with respect to some topology. For example, one can require $\lim_{t\to 0}\|\Phi_{t,0}A - A\|_\infty = 0$ for every $A \in \mathcal{B}(\mathcal{H}_S)$, where $\|\cdot\|_\infty$ denotes the operator norm (see, e.g., Rudin (1991)).

which erases the rapidly oscillating terms in the differential equation, the so-called Markov approximation is invoked which presupposes a separation of the intrinsic time scales of the system and environment. That is, the system's relaxation time τ_S must be much larger than the correlation time of the environment τ_E, i.e., one must have $\tau_E \ll \tau_S$ which means that the degrees of freedom of the open system are slow compared to those of the environment. Similarly, the rotating wave approximation is reliable if the time scale of the intrinsic evolution of the open system τ_I is much smaller than the system's relaxation.

These approximations clearly support the attribution of a lack of memory effects for a semigroup evolution, which is considered to define the prototype of a memoryless, that is, Markovian dynamics. Although there are many examples of physical interest for which these assumptions result in very good approximations of the exact dynamics, its validity is not ensured in general. Strong system-environment couplings or an environment at low temperatures typically lead to drastic deviations from the semigroup dynamics (Breuer and Petruccione, 2002). It is widely believed that such a "non-Markovian" dynamics can only be properly described by a master equation which is non-local in time due to the fundamental understanding that only a non-trivial memory kernel accounts for memory effects as the term already suggests. However, one readily proves the existence of a time-local master equation for the evolution of an open system, even in the presence of memory effects: Assuming a sufficiently smooth time dependence of the one-parameter family of CPT-maps Φ describing the open system's evolution, one obtains a time-local master equation upon differentiating $\rho_S(t) = \Phi_{t,t_0}(\rho_S(t_0))$ with respect to the parameter t if the dynamical evolution is invertible. More precisely, one finds

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_S(t) = \dot{\Phi}_{t,t_0} \circ \Phi_{t,t_0}^{-1}(\rho_S(t)) \ . \tag{3.25}$$

where Φ_{t,t_0}^{-1} denotes the inverse of the dynamical map Φ_{t,t_0} within the algebra of superoperators acting on bounded linear operators on $\mathcal{H}_S$. Note that the existence of the left-inverse, requiring injectivity of the maps Φ_{t,t_0}, would actually be sufficient to establish such a time-local master equation.

Unfortunately, the dynamics is not invertible for all times in general as, e.g., the damped Jaynes-Cummings model on resonance (Breuer and Petruccione, 2002; Laine *et al.*, 2010b; Breuer *et al.*, 2016) or instances of quantum semi-Markov processes show (Vacchini *et al.*, 2011). Nevertheless, one can show (Štelmachovič and Bužek, 2001, 2003) that the inverse and, therefore, the generator $\mathcal{K}_t = \dot{\Phi}_{t,t_0}\Phi_{t,t_0}^{-1}$ exists apart from isolated singularities if the time dependence is analytic. In the intermediate time intervals, the reduced dynamics can thus be described by a time-local master equation (see, e.g., Laine *et al.* (2010b)). It is worth stressing that the inverse Φ_{t,t_0}^{-1} is not required to be completely positive and it indeed satisfies neither this property nor positivity in general. Note that the exact features of the inverse map influence the dynamical process' property of being divisible (see Sec. 3.4) which will be important in the discussion on a proper definition of quantum non-Markovianity later on.

3.3.1 The TCL projection operator method

As shown in the preceding section, a time-local master equations may indeed be used to describe dynamical systems even in the presence of strong memory effects. A systematic and efficient approach to obtain the time-local master equation associated with a certain microscopic model is given by the time-convolutionless projection operator technique (Prigogine, 1962; Nakajima, 1958; Zwanzig, 1960). This technique relies on the idea that the ignorance of the environmental degrees of freedom, which is implemented by taking the partial trace, can be regarded as the formal action of a projection superoperator $\mathcal{P}$ on the total state space which singles out the *relevant part* of the information on the open system. A convenient choice of this superoperator is given by

$$\mathcal{P}\rho_{SE} = \mathrm{Tr}_E\{\rho_{SE}\} \otimes \rho_E \ , \tag{3.26}$$

where ρ_E refers to some fixed state of the environment. Clearly, $\mathcal{P}\rho_{SE}$ contains all the relevant information allowing to reconstruct the reduced state ρ_S of the open quantum system. The remaining degrees of freedom, defining the irrelevant part, are accordingly determined by the superoperator $\mathcal{Q} \equiv I_{SE} - \mathcal{P}$ where I_{SE} refers to the identity map on the joint state space $\mathcal{H}_S \otimes \mathcal{H}_E$. The basic properties of these superoperators are summarized by the relations

$$\mathcal{P}^2 = \mathcal{P} \ , \qquad \mathcal{Q}^2 = \mathcal{Q} \qquad \mathcal{P}\mathcal{Q} = \mathcal{Q}\mathcal{P} = 0 \ , \tag{3.27}$$

where, in addition, $\mathcal{P} + \mathcal{Q} = I_{SE}$ obviously holds.

To obtain a closed and exact equation for the reduced density operator $\rho_S(t) = \mathrm{Tr}_E\{\rho_{SE}(t)\}$, one applies the projection superoperators $\mathcal{P}$ and $\mathcal{Q}$ to the Liouville-von Neumann equation (3.1) and, finally, separates the emerging coupled partial differential equations for the relevant and irrelevant part. Following Breuer and Petruccione (2002), one introduces a dimensionless expansion parameter α in the total time-independent Hamiltonian (3.2), i.e. $H = H_0 + \alpha H_I$, so that one obtains the equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\tilde{\rho}_{SE}(t) = \alpha\mathcal{P}\tilde{\mathcal{L}}(t)\mathcal{P}\tilde{\rho}_{SE}(t) + \alpha\mathcal{P}\tilde{\mathcal{L}}(t)\mathcal{Q}\tilde{\rho}_{SE}(t) \ , \tag{3.28}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{Q}\tilde{\rho}_{SE}(t) = \alpha\mathcal{Q}\tilde{\mathcal{L}}(t)\mathcal{P}\tilde{\rho}_{SE}(t) + \alpha\mathcal{Q}\tilde{\mathcal{L}}(t)\mathcal{Q}\tilde{\rho}_{SE}(t) \ , \tag{3.29}$$

when working in the interaction picture (cf. Eq. (3.8)). The formal solution of the equation of motion for the irrelevant part (3.29) for a given initial state $\tilde{\rho}_{SE}(t_0)$ reads

$$\mathcal{Q}\rho_{SE}(t) = \tilde{\mathcal{G}}_{\mathcal{Q}}(t,t_0)\mathcal{Q}\tilde{\rho}_{SE}(t_0) + \alpha\int_{t_0}^{t}\mathrm{d}s\ \tilde{\mathcal{G}}_{\mathcal{Q}}(t,s)\mathcal{Q}\tilde{\mathcal{L}}(s)\mathcal{P}\tilde{\rho}_{SE}(s) \ , \tag{3.30}$$

where

$$\tilde{\mathcal{G}}_{\mathcal{Q}}(t,s) = \mathrm{T}_{\leftarrow}\exp\left[\alpha\int_{s}^{t}\mathrm{d}s'\mathcal{Q}\tilde{\mathcal{L}}(s')\right] \tag{3.31}$$

defines the propagator of the irrelevant part in the interaction picture. Upon inserting the formal solution (3.30) into the equation for the relevant part (3.28),

one arrives at the so-called *Nakajima-Zwanzig equation*

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\tilde{\rho}_{SE}(t) = \alpha\mathcal{P}\tilde{\mathcal{L}}(t)\tilde{\mathcal{G}}_{\mathcal{Q}}(t,t_0)\mathcal{Q}\tilde{\rho}_{SE}(t_0) + \alpha\mathcal{P}\tilde{\mathcal{L}}(t)\mathcal{P}\tilde{\rho}_{SE}(t) + \alpha^2\int_{t_0}^{t}\mathrm{d}s\mathcal{P}\tilde{\mathcal{L}}(t)\tilde{\mathcal{G}}_{\mathcal{Q}}(t,s)\mathcal{Q}\tilde{\mathcal{L}}(s)\mathcal{P}\tilde{\rho}_{SE}(s)\ . \tag{3.32}$$

Obviously, Eq. (3.32) represents a closed and exact equation for the relevant part which, however, is nonlocal and therefore difficult to treat. This practical disadvantage is, of course, not cured when a perturbative expansion of the memory kernel $\mathcal{P}\tilde{\mathcal{L}}(t)\tilde{\mathcal{G}}_{\mathcal{Q}}(t,s)\mathcal{Q}\tilde{\mathcal{L}}(s)\mathcal{P}$ in the parameter α is employed even though this approach already simplifies the derivation and the solution of the equations of motion. Note that the Nakajima-Zwanzig equation is typically said to account for non-Markovian time evolutions due to the time convolution contained in it.

To remove the nonlocality, resulting in a time-local master equation, one uses the method known as time-convolutionless projection operator technique (Shibata *et al.*, 1977; Chaturvedi and Shibata, 1979; Shibata and Arimitsu, 1980). Following Breuer and Petruccione (2002), one eliminates the convolution by virtue of the backward propagator

$$\tilde{\mathcal{G}}^{\dagger}(t,s) = \mathrm{T}_{\rightarrow}\exp\left[-\alpha\int_{s}^{t}\mathrm{d}s'\,\tilde{\mathcal{L}}(s')\right]\ , \tag{3.33}$$

allowing to express the density matrix at time s by $\tilde{\rho}_{SE}(s) = \tilde{\mathcal{G}}^{\dagger}(t)(t,s)(\mathcal{P}+\mathcal{Q})\tilde{\rho}_{SE}(t)$. The irrelevant part's solution (3.30) may then be written as

$$\mathcal{Q}\tilde{\rho}_{SE}(t) = \tilde{\mathcal{G}}_{\mathcal{Q}}(t,t_0)\mathcal{Q}\tilde{\rho}_{SE}(t_0) + \alpha\int_{t_0}^{t}\mathrm{d}s\ \tilde{\mathcal{G}}_{\mathcal{Q}}(t,s)\mathcal{Q}\tilde{\mathcal{L}}(s)\mathcal{P}\tilde{\mathcal{G}}^{\dagger}(t,s)(\mathcal{P}+\mathcal{Q})\tilde{\rho}_{SE}(t)\ , \tag{3.34}$$

which is equivalent to

$$[I_{SE}-\Sigma(t,t_0)]\mathcal{Q}\tilde{\rho}_{SE}(t) = \tilde{\mathcal{G}}_{\mathcal{Q}}(t,t_0)\mathcal{Q}\tilde{\rho}_{SE}(t_0) + \Sigma(t,t_0)\mathcal{P}\tilde{\rho}_{SE}(t)\ , \tag{3.35}$$

using the superoperator

$$\Sigma(t,t_0) \equiv \alpha\int_{t_0}^{t}\mathrm{d}s\ \tilde{\mathcal{G}}_{\mathcal{Q}}(t,s)\mathcal{Q}\tilde{\mathcal{L}}(s)\mathcal{P}\tilde{\mathcal{G}}^{\dagger}(t,s)\ , \tag{3.36}$$

which obviously satisfies $\Sigma(t_0,t_0) = 0$ and $\Sigma(t,t_0)|_{\alpha=0} = 0$. Due to this, $I_{SE} - \Sigma(t,t_0)$ is invertible for sufficiently small couplings α and in any case for a small difference $t-t_0$. Assuming that one of these conditions is met, the irrelevant part $\mathcal{Q}\tilde{\rho}_{SE}(t)$ can thus be expressed as a function of the relevant part at time t and the initial condition $\mathcal{Q}\tilde{\rho}_{SE}(t_0)$. By virtue of this representation of $\mathcal{Q}\tilde{\rho}_{SE}(t)$ and the idempotence of the projection superoperators, one finally deduces the following exact time-convolutionless master equation for the relevant part from Eq. (3.28):

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\tilde{\rho}_{SE}(t) = \mathcal{K}(t,t_0)\mathcal{P}\tilde{\rho}_{SE}(t) + \mathcal{I}(t,t_0)\mathcal{Q}\tilde{\rho}_{SE}(t_0)\ . \tag{3.37}$$

Here, the time-local generator, which is known as *TCL generator*, is given by

$$\mathcal{K}(t,t_0) = \alpha\mathcal{P}\tilde{\mathcal{L}}(t)[I_{SE}-\Sigma(t,t_0)]^{-1}\mathcal{P}\ , \tag{3.38}$$

and the so-called inhomogeneity obeys

$$\mathcal{I}(t,t_0) = \alpha\mathcal{P}\tilde{\mathcal{L}}(t)[I_{SE} - \Sigma(t,t_0)]^{-1}\tilde{\mathcal{G}}_Q(t,t_0)\mathcal{Q} \ . \tag{3.39}$$

Note that the second term of Eq. (3.37) vanishes for factorizing initial conditions because $\mathcal{Q}\tilde{\rho}_S(t_0) \otimes \tilde{\rho}_E(t_0) = 0$. However, the treatment is not limited to this particular situation.

The TCL generator as well as the inhomogeneity are still complicated objects but, fortunately, they provide the starting point for a systematic perturbative expansion which is formally exact. As both superoperators rely on the existence of the inverse of $I_{SE} - \Sigma(t,t_0)$, one may assume that it indeed exists and may be written as a geometric series

$$[I_{SE} - \Sigma(t,t_0)]^{-1} = \sum_{n=0}^{\infty} [\Sigma(t,t_0)]^n \ . \tag{3.40}$$

Upon expanding the forward and backward propagators $\tilde{\mathcal{G}}_{\mathcal{Q}}$ and $\tilde{\mathcal{G}}^{\dagger}$ in powers of the coupling strength α, the superoperator $\Sigma(t,t_0)$ admits a decomposition into a power series

$$\Sigma(t,t_0) = \sum_{k=1}^{\infty} \alpha^k \Sigma_k(t,t_0) \ , \tag{3.41}$$

which finally allows to write the TCL generator as

$$\mathcal{K}(t,t_0) = \sum_{n=1}^{\infty} \alpha^n \mathcal{K}_n(t,t_0) \ . \tag{3.42}$$

A similar treatment naturally applies to the inhomogeneity, too. The first to third order contributions to the generator $\mathcal{K}(t,t_0)$ are shown to be given by

$$\mathcal{K}_1(t,t_0) = \mathcal{P}\tilde{\mathcal{L}}(t)\mathcal{P} \ , \tag{3.43}$$

$$\mathcal{K}_2(t,t_0) = \mathcal{P}\tilde{\mathcal{L}}(t)\Sigma_1(t,t_0)\mathcal{P} \ , \tag{3.44}$$

$$\mathcal{K}_3(t,t_0) = \mathcal{P}\tilde{\mathcal{L}}(t)\left\{[\Sigma_1(t,t_0)]^2 + \Sigma_2(t,t_0)\right\}\mathcal{P} \ , \tag{3.45}$$

where one has

$$\Sigma_1(t,t_0) = \int_{t_0}^{t} \mathrm{d}s \ \mathcal{Q}\tilde{\mathcal{L}}(s)\mathcal{P} \ , \tag{3.46}$$

$$\Sigma_2(t,t_0) = \int_{t_0}^{t} \mathrm{d}s \int_{t_0}^{s} \mathrm{d}s' \ \left\{\mathcal{Q}\tilde{\mathcal{L}}(s)\mathcal{Q}\tilde{\mathcal{L}}(s')\mathcal{P} - \mathcal{Q}\tilde{\mathcal{L}}(s')\mathcal{P}\tilde{\mathcal{L}}(s)\right\} \ . \tag{3.47}$$

It is worth noticing that several contributions such as $[\Sigma_1(t,t_0)]^2$ are eliminated due to the orthogonality of the projection superoperators $\mathcal{P}$ and $\mathcal{Q}$ (cf. Eq. (3.27)). A further drastic simplification of the contributions $\mathcal{K}_n(t,t_0)$ is achieved for particular choices of the interaction Hamiltonian $\tilde{H}_I(t)$ and the reference state associated with $\mathcal{P}$ (cf. Eq. (3.26)). More precisely, choosing ρ_E such that the odd moments of the interaction Hamiltonian $\tilde{H}_I(t)$ vanish, i.e.

$$\mathrm{Tr}_E\{\tilde{H}_I(t_1)\tilde{H}_I(t_2)\cdots\tilde{H}_I(t_{2n+1})\rho_E\} = 0 \tag{3.48}$$

for $n \in \mathbb{N}_0$, the Liouvillian satisfies the relation

$$\mathcal{P}\tilde{\mathcal{L}}(t_1)\tilde{\mathcal{L}}(t_2)\cdots\tilde{\mathcal{L}}(t_{2n+1})\mathcal{P} = 0 \ . \tag{3.49}$$

This implies that the first and third order contributions (cf. Eqs. (3.43) and (3.45)) to the TCL generator vanish, whereas $\mathcal{K}_2(t,t_0)$ (cf. Eq. (3.44)) is simply given by

$$\mathcal{K}_2(t,t_0) = \int_{t_0}^{t} \mathrm{d}s \ \mathcal{P}\tilde{\mathcal{L}}(t)\tilde{\mathcal{L}}(s)\mathcal{P} \ . \tag{3.50}$$

Note that one speaks of a *TCL n master equation* if solely contributions up to nth order in α of the TCL generator are taken into account. The second-order time-convolutionless master equation is the most prominent and frequently used representative of this stack of approximations which thus reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\tilde{\rho}_S(t) = -\alpha^2 \int_{t_0}^{t} \mathrm{d}s \ \mathrm{Tr}_E\{[\tilde{H}_I(t),[\tilde{H}_I(s),\tilde{\rho}_S(t)\otimes\rho_E]]\} \tag{3.51}$$

in case of factorizing initial conditions and a reference state ρ_E that implies condition (3.49).

3.3.2 Exactness of TCL 2

The perturbative expansion of the TCL master equation defines a convenient way to describe the open system dynamics, but it cannot be hoped to yield the exact dynamics. However, there are instances where these approximate master equations are exact (Ban *et al.*, 2010; Doll *et al.*, 2008). In fact, the second-order time-convolutionless master equation for an open quantum system that is linearly coupled to a thermal bath, described by a collection of bosonic modes in a Gaussian state with zero-means, represents such a specific physical model where TCL 2 determines the exact solution. This kind of systems are frequently considered in physics due to their relevance for modelling decoherence in which case the dynamics is even exactly solvable (Breuer and Petruccione, 2002). In summary, the total Hamiltonian corresponding to these models obeys

$$H = H_S \otimes \mathbb{1}_E + \mathbb{1}_S \otimes H_E + \hat{S} \otimes \sum_k \left(g_k \hat{b}_k^\dagger + g_k^* \hat{b}_k\right) \ , \tag{3.52}$$

where $\hat{S}$ refers to a Hermitian operator on $\mathcal{H}_S$ and the free Hamiltonian of the bath is assumed to be given by $H_E = \sum_k \omega_k \hat{b}_k^\dagger \hat{b}_k$, omitting the vacuum energy. The strength of the coupling between the system and the kth bath mode is determined by the coefficient g_k which is typically chosen to be real-valued. Since the interaction Hamiltonian is linear in the creation and annihilation operators, the odd moments of the interaction picture interaction Hamiltonian

$$\tilde{H}_I(t) = \hat{\tilde{S}}(t) \otimes \sum_k \left(g_k e^{i\omega_k t}\hat{b}_k^\dagger + g_k^* e^{-i\omega_k t}\hat{b}_k\right) \ , \tag{3.53}$$

vanish in a zero-mean Gaussian state (cf. Sec. 2.5.2). Note that the interaction picture representation of H_I is deduced using $\exp[itH_E]\hat{b}_k \exp[-itH_E] = \exp[-i\omega_k t]\hat{b}_k$

where $\hat{\tilde{S}}(t)$ refers to the interaction picture representation of the open system operator $\hat{S}$, i.e. $\hat{\tilde{S}}(t) = \exp[itH_S]\hat{S}\exp[-itH_S]$.

Due to these properties, the TCL 2 master equation for this model is indeed given by Eq. (3.51) where one has $\alpha = 1$ and ρ_E refers to a zero-mean Gaussian state. As a result of this thesis, it is shown that the criterion on the exactness for TCL 2 master equations corresponding to Hamilton operators (3.52) which was derived by Ban *et al.* (2010) for thermal environmental states actually extends to arbitrary zero-mean environmental Gaussian states.

Theorem 3.1. *The second-order TCL master equation associated with the Hamiltonian* (3.52) *and a zero-mean environmental Gaussian state is exact if and only if*

$$[\hat{\tilde{S}}(t), \hat{\tilde{S}}(t')] = 0 \tag{3.54}$$

holds for all times t and t'.

Proof. As said, for the particular choice of a thermal reference state (2.125) the statement has been proven by Ban *et al.* (2010) (see also Doll *et al.* (2008) for the sufficiency of Eq. (3.54)). However, the very same proof applies to any Gaussian state with vanishing means since the structure of the TCL 2 master equation as well as that of the characteristic function does not change. More specifically, one observes that the characteristic function (2.102) of an arbitrary zero-mean Gaussian state at $z_j = -i\int_0^t \mathrm{d}t'\,\alpha(t')g_j^*\exp[i\omega_j t']$ for some complex-valued function $\alpha(t) \in \mathbb{C}$ obeys

$$\chi_{\rho_E}^{t=\sqrt{2}}(\vec{z}) = \exp\left[-\int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{d}t''\ \alpha(t')\alpha(t'')C_R(t',t'')\right]. \tag{3.55}$$

Here, $C_R(t,s)$ defines the real part of the two-point reservoir correlation function $\langle\hat{X}(t)\hat{X}(s)\rangle_{\rho_E}$ where the operator is defined as $\hat{X}(t) = \sum_k g_k e^{i\omega_k t}\hat{b}_k + g_k^* e^{-i\omega_k t}\hat{b}_k^\dagger$. Note that the imaginary part of the correlation function is given by $C_I(t,s) = -\sum_k |g_k|^2 \sin\big(\omega_k(t-s)\big)$, irrespective of the choice of zero-mean Gaussian state.

Since Eq. (3.55) as well as the structure of the TCL 2 master equation are the only parts in the proof by Ban *et al.* (2010) where their particular choice of the environmental state enters, all arguments used by Ban *et al.* (2010) indeed apply for any zero-mean Gaussian state, too, which completes the proof. □

Note that the Eq. (3.54) provides a necessary and sufficient condition independent of the dimension of the open system's Hilbert space. It is obviously satisfied if $[H_S, \hat{S}] = 0$ holds, corresponding to a dynamics describing pure decoherence. As shown by Ban *et al.* (2010), this is yet not the full story – at least for infinite-dimensional open quantum systems. In fact, for $\dim\mathcal{H}_S = \infty$ there exist dissipative dynamics such that $[\hat{\tilde{S}}(t), \hat{\tilde{S}}(t')]$ vanishes for all times t and t' as a consequence of the canonical commutation relation (2.91). For finite systems, a vanishing commutator can indeed only be achieved for nondissipative dynamics as is shown by the following result of this thesis, providing a concise criterion for the exactness of TCL 2.

Lemma 3.1. *Let H_S and $\hat{S}$ be two Hermitian operators acting on a Hilbert space $\mathcal{H}_S$ of dimension $N_S < \infty$. The Heisenberg operator $\hat{\tilde{S}} = \exp[itH_S]\hat{S}\exp[-itH_S]$ satisfies*

$$[\hat{\tilde{S}}(t), \hat{\tilde{S}}(t')] = 0 \tag{3.56}$$

for all times t and t' if and only if

$$[H_S, \hat{S}] = 0 \ . \tag{3.57}$$

Proof. Clearly, if one has $[H_S, \hat{S}] = 0$, then $\hat{\tilde{S}}(t) = \hat{\tilde{S}}(0) = \hat{S}$ for all $t \in \mathbb{R}$ so that the constraint (3.56) is trivially satisfied. It thus remains to show the converse. Suppose that $[\hat{\tilde{S}}(t), \hat{\tilde{S}}(t')] = 0$ holds for all $t, t' \in \mathbb{R}$. As a consequence, the operator $\hat{X}_t \equiv \hat{\tilde{S}}(t)\hat{\tilde{S}}(0)$ is Hermitian for all times t and, therefore, the family of antihermitian operators

$$\Delta\hat{X}_t \equiv \hat{X}_t - \hat{X}_t^\dagger \tag{3.58}$$

vanishes. This is equivalent to the fact that the characteristic polynomial $p_{\Delta\hat{X}_t}(\lambda) = (-1)^{N_S}\sum_{k=0}^{N_S} c_k(t)\lambda^{N_S-k}$ (cf. Eq. (2.11)) of these finite-dimensional operators obeys $p_{\Delta\hat{X}_t}(\lambda) = (-1)^{N_S}\lambda^{N_S}$ for all $t \in \mathbb{R}$. Recall that the coefficients of the characteristic polynomial are recursively determined by (cf. Eq. (2.12))

$$k \cdot c_k(t) = -\sum_{j=1}^{k} c_{k-j}(t)\mathrm{Tr}\{(\Delta\hat{X}_t)^j\} \tag{3.59}$$

for $k \geq 1$ where $c_0 = 1$. Apart from the coefficient of the leading monomial, all other coefficients are thus linear combinations of terms $\mathrm{Tr}\{(\Delta\hat{X}_t)^j\}$ where, however, $\mathrm{Tr}\{\Delta\hat{X}_t\}$ vanishes for all t due to the cyclic property of the trace. Employing the Cauchy Schwartz inequality for the Hilbert-Schmidt scalar product, one furthermore shows for[5] $j \geq 3$ the relation

$$\begin{aligned}|\mathrm{Tr}\{(\Delta\hat{X}_t)^j\}| &= |\mathrm{Tr}\{(\Delta\hat{X}_t)^{j-1}(-\Delta\hat{X}_t)^\dagger\}| \\ &\leq \sqrt{\mathrm{Tr}\{(-\Delta\hat{X}_t)(-\Delta\hat{X}_t)^\dagger\}}\sqrt{\mathrm{Tr}\{(\Delta\hat{X}_t)^{j-1}(\Delta\hat{X}_t)^{j-1^\dagger}\}} \\ &= \sqrt{-\mathrm{Tr}\{(\Delta\hat{X}_t)^2\}}\sqrt{\mathrm{Tr}\{\Delta\hat{X}_t)^{j-1}(-\Delta\hat{X}_t)^{j-1}\}} \ ,\end{aligned} \tag{3.60}$$

where the real-valued square roots are well-defined due to the antihermiticity of ΔX_t. It follows that $\mathrm{Tr}\{(\Delta\hat{X}_t)^j\} = 0$ for all $j \geq 2$ if and only if one has $\mathrm{Tr}\{(\Delta\hat{X}_t)^2\} = 0$. It thus suffices to find the constraints on H_S and $\hat{S}$ imposed by the relation $\mathrm{Tr}\{(\Delta\hat{X}_t)^2\} = 0$ for all times t in order to obtain $c_k(t) = 0$ for any $k \geq 1$ and all times t.

Note that $c_k(t)|_{t=0} = 0$ for all $k \geq 1$ by the very definition. Looking at the derivatives of $\mathrm{Tr}\{(\Delta\hat{X}_t)^2\}$ with respect to time t at $t = 0$, one finds

$$(-\tfrac{1}{2}) \cdot \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Tr}\{(\Delta\hat{X}_t)^2\}\Big|_{t=0} = 0 \ , \tag{3.61}$$

$$\begin{aligned}(-\tfrac{1}{2}) \cdot \frac{\mathrm{d}^2}{\mathrm{d}t^2}\mathrm{Tr}\{(\Delta\hat{X}_t)^2\}\Big|_{t=0} &= \mathrm{Tr}\{H_S^2\hat{S}^4\} + 3\mathrm{Tr}\{H_S\hat{S}^2H_S\hat{S}^2\} \\ &\quad - 4\mathrm{Tr}\{H_S\hat{S}H_S\hat{S}^3\} \ ,\end{aligned} \tag{3.62}$$

[5] One has $j \geq 3$ if and only if $N_S \geq 3$ implying that the characteristic polynomial is at least of third order.

where the first derivative is zero as the trace is cyclic. The second derivative (3.62) can be expressed as

$$(-\tfrac{1}{2}) \cdot \frac{\mathrm{d}^2}{\mathrm{d}t^2}\mathrm{Tr}\{(\Delta\hat{X}_t)^2\}\Big|_{t=0} = \sum_{j>k} |\langle j|H_S|k\rangle|^2 (s_j - s_k)^4 \ , \tag{3.63}$$

employing the spectral decomposition of the operator $\hat{S}$, i.e.,

$$\hat{S} = \sum_{k=1}^{n_S} s_k |k\rangle\langle k| \ . \tag{3.64}$$

Since all contributions to the second derivative (3.63) are positive, each term must vanish separately in order to agree with $c_k(t) = 0$ for all k and t. If the eigenvalues of $\hat{S}$ are pairwise different, i.e., $\hat{S}$ has a nondegenerate spectrum, the transition matrix elements $\langle j|H_S|k\rangle$ must be zero for all integers $j \neq k$. This implies that H_S is diagonal[6] in the basis $\{|j\rangle\}$, too, which directly leads to the conclusion that Eq. (3.57) is satisfied. For a degenerate spectrum, there also exists a joint eigenbasis leading to $[H_S, \hat{S}] = 0$ since one has the freedom to change the basis spanning the degenerate subspaces so that H_S is diagonal in this case and, therefore, Eq. (3.57) is satisfied. □

By virtue of lemma 3.1 and theorem 3.1 one arrives at the following characterization for the exactness of TCL 2 master equations for finite-dimensional open quantum systems as a result of the present thesis.

Corollary 3.1. *For an open quantum system characterized by a Hilbert space* $\mathcal{H}_S$ *with* $\dim\mathcal{H}_S < \infty$*, the second-order TCL master equation associated with the Hamiltonian* (3.52) *and a zero-mean environmental Gaussian state is exact if and only if*

$$[H_S, \hat{S}] = 0 \ . \tag{3.65}$$

As condition (3.65) implies that the mean energy of the open quantum system is conserved, corollary 3.1 shows that the TCL 2 master equation is exact if and only if there is no exchange of energy with the bath corresponding to pure dephasing dynamics. However, there might still exist decoherence free subspaces, i.e., subspaces which are unaffected by the dynamics if the operator $\hat{S}$ is degenerate. The popular phase-noise models, describing pure decoherence (DiVincenzo, 1995; Palma *et al.*, 1996; Breuer and Petruccione, 2002), thus provide the sole finite-dimensional examples where the associated TCL 2 master equations are exact. Unfortunately, there is no immediate advantage as these models can also be solved exactly. In fact, if Eq. (3.65) holds, implying $\hat{\tilde{S}}(t) = \hat{S}$, the commutator of $\tilde{H}_I(t)$ and $\tilde{H}_I(t')$ (see Eq. (3.53)) for any two times t and t' obeys

$$[\tilde{H}_I(t), \tilde{H}_I(t')] = -2i\hat{S}^2 \sum_k |g_k|^2 \sin(\omega_k(t - t')) \ , \tag{3.66}$$

[6] Clearly, defining $H'_S \equiv H_S - \sum_j \Pi_j H_S \Pi_j$ where $\Pi_j = |j\rangle\langle j|$, one has $\langle j|H'_S|k\rangle = 0$ for all j, k which is equivalent to $H'_S = 0$, showing that H_S is diagonal with respect to basis $\{|j\rangle\}$.

that is, it is essentially proportional to the identity operator on the environmental Hilbert space. Due to this, the Baker-Campbell-Hausdorff formula can be used to eliminate the time-ordering in the propagator

$$\tilde{U}_I(t) = \mathrm{T}_{\leftarrow} \exp\left[-i \int_0^t \mathrm{d}s\ \tilde{H}_I(s)\right] \tag{3.67}$$

associated with the interaction Hamiltonian (cf. Eq. (3.8)). One thus obtains for the propagator (Breuer and Petruccione, 2002)

$$\begin{aligned}\tilde{U}_I(t) = \exp\left[-\frac{1}{2}\int_0^t \mathrm{d}s \int_0^t \mathrm{d}s' \,[\tilde{H}_I(s), \tilde{H}_I(s')]\Theta(s-s')\right] \\ \cdot \exp\left[-i \int_0^t \mathrm{d}s\ \tilde{H}_I(s)\right]\ ,\end{aligned} \tag{3.68}$$

where Θ denotes the Heaviside step function. While the first term yields solely a phase factor with respect to the bosonic environment as one deduces

$$\exp\left[-\frac{1}{2}\int_0^t \mathrm{d}s \int_0^t \mathrm{d}s' \,[\tilde{H}_I(s), \tilde{H}_I(s')]\Theta(s-s')\right] = \exp\left[i\hat{S}^2\phi(t)\right]\ , \tag{3.69}$$

where $\phi(t) \equiv \int_0^t \mathrm{d}s \int_0^s \mathrm{d}s' \sum_k |g_k|^2 \sin\bigl(\omega_k(s-s')\bigr) \in \mathbb{C}$, the second contribution can be written in terms of the Weyl displacement operator (2.103)

$$\exp\left[-i \int_0^t \mathrm{d}s\ \tilde{H}_I(s)\right] = D(\hat{S}\vec{z}(t)) \tag{3.70}$$

which is evaluated at

$$z_k(t) = (-i)\cdot \int_0^t \mathrm{d}s\ g_k \exp[i\omega_k s] = g_k\, \frac{1-\exp[i\omega_k t]}{\omega_k}\ . \tag{3.71}$$

Taking the free evolution of the open system into account and assuming factorizing initial conditions, one finds for the time evolution of the open quantum system with respect to the eigenbasis $\{|m\rangle\}$ of the system Hamiltonian $H_S = \sum_m E_m |m\rangle\langle m|$ (cf. Doll *et al.* (2008))

$$\begin{aligned}\langle m|\rho_S(t)|n\rangle &= e^{-i(E_m-E_n)t}\, \langle m|\mathrm{Tr}_E\{\tilde{U}_I(t)\rho_S(0)\otimes\rho_E\tilde{U}_I^\dagger(t)\}|n\rangle \\ &= \varrho_{mn}\, e^{-i(E_m-E_n)t}\, e^{i(S_m^2-S_n^2)\phi(t)}\langle D^\dagger(S_n\vec{z}(t))D(S_m\vec{z}(t))\rangle_{\rho_E} \\ &= \varrho_{mn}\, e^{-i(E_m-E_n)t}\, e^{i(S_m^2-S_n^2)\phi(t)}\chi_{\rho_E}^{\sqrt{2}}\bigl((S_m-S_n)\cdot\vec{z}(t)\bigr)\ ,\end{aligned} \tag{3.72}$$

where $\varrho_{mn} \equiv \langle m|\rho_S(t)|n\rangle$. To obtain this result, one employs the two relations $D(\vec{y})D(\vec{z}) = D(\vec{y}+\vec{z})\cdot\exp[i\sum_k \mathrm{Im}(y_k z_k^*)]$ and $D^\dagger(\vec{z}) = D(-\vec{z})$ for the displacement operator, where the additional phase factor of the former vanishes later on as the eigenvalues S_m are real-valued. One readily recognizes that the diagonal elements ρ_{mm} are constant, whereas the dynamics of the coherences in the energy eigenbasis is mainly governed by the characteristic function $\chi_{\rho_E}^{\sqrt{2}}$ of the environmental state ρ_E (cf. Eq. (2.102)).

As indicated previously, the set of dynamics for which TCL 2 is exact is in general larger than this simple dephasing dynamics. This is due to the fact that there

exist operators whose commutator is nonvanishing and proportional to the identity operator, i.e., one may have $[H_S, \hat{S}] = a\mathbb{1}_{\mathcal{H}_S} \neq 0$. In this case the Heisenberg operator $\hat{\hat{S}}$ differs by a time-dependent shift proportional to the identity operator from its counterpart in the Schrödinger picture for which reason Eq. (3.56) is trivially satisfied. However, such a commutation relation cannot be established in finite dimensions due to the cyclic property of the trace, implying that any nonzero commutator must have vanishing trace.

3.4 Divisibility of dynamical processes

The semigroup property (3.23) defines a very strong assumption so that most one-parameter families of CPT-maps, defining dynamical processes, usually do not satisfy it. The notion of divisibility of a dynamical map extends the strict condition of a semigroup by allowing the intermediate maps in Eq. (3.23) to be arbitrary completely positive and trace preserving maps that do not need to be part of the family of dynamical maps. The relaxation of complete positivity to just positivity of the intermediate maps provides a further generalization of the notion of divisibility. These concepts have recently received some attention in the classification of dynamical evolutions in terms of (non-)Markovian dynamics as is reviewed in Ch. 4.

To define this notion properly, suppose that the maps Φ_{t,t_0} comprising a dynamical process with initial time t_0 are invertible for all $t \geq t_0$ where the inverse shall be denoted by Φ_{t,t_0}^{-1}. One then defines a two-parameter family of maps by

$$\Lambda_{t,s} = \Phi_{t,t_0} \circ \Phi_{s,t_0}^{-1} \tag{3.73}$$

corresponding to any choice of parameters $t \geq s \geq t_0$. Clearly, the maps of this family satisfy $\Lambda_{t,t_0} = \Phi_{t,t_0}$ and $\Phi_{t,t_0} = \Lambda_{t,s} \circ \Phi_{s,t_0}$. Divisibility now deals with the properties of these maps concerning n-positivity (cf. definition 2.1).

Definition 3.1. *A dynamical process Φ is called n-divisible if and only if $\Lambda_{t,s}$ defines an n-positive map for all $t \geq s \geq t_0$. In particular, if $\Lambda_{t,s}$ is (completely) positive the dynamical process is said to be (C)P-divisible.*

If the dynamical process is CP-divisible[7] there thus exist CPT-maps connecting any pair of dynamical maps of the process. Clearly, for a semigroup dynamics associated with the Lindblad generator $\mathcal{K}_L$ (cf. Eq. (3.22)), the connecting maps $\Lambda_{t,s}$ are simply given by

$$\Lambda_{t,s} = \exp\left[\mathcal{K}_L(t-s)\right] \ , \tag{3.74}$$

and, therefore, are completely positive. In the general case of a time-dependent generator $\mathcal{K}_t$ as defined in Eq. (3.21), the maps of the two-parameter family read

$$\Lambda_{t,s} = \mathrm{T}_{\leftarrow}\exp\left[\int_s^t \mathrm{d}t' \ \mathcal{K}(t')\right] \ , \tag{3.75}$$

[7]Note that the present notion of CP-divisibility should not be confused with the identically called concept for single CPT-maps. Due to Wolf and Cirac (2008), a single CPT-map Λ is said to be CP-divisible if and only if there exist CPT-maps Λ_1 and Λ_2 such that $\Lambda = \Lambda_1 \circ \Lambda_2$, where neither Λ_1 nor Λ_2 are unitary since the required decomposition is otherwise trivial.

but n-divisibility is not guaranteed by the very structure of the generator.

The constraints for divisibility are, of course, trivially satisfied at the marginal times $t = s$ or $s = t_0$, but for arbitrary t and $s$the intermediate maps $\Lambda_{t,s}$ are generally not n-positive even though the dynamical maps are completely positive for all times. This is due to the fact that the inverse of a CP-map need not be positive as already touched upon in Sec. 3.3and, therefore, the above definition is indeed nontrivial. It is worth stressing though that the concept of divisibility relies on the existence of the two-parameter family which is limited to processes for which the inverse Φ_{t,t_0}^{-1} exists for all times. As already discussed in connection with time-local master equations (see Eq. (3.25)), this property is not warranted in general, thus making the concept of divisibility sometimes ill-defined.

Assuming that the inverse does indeed exist, which holds true apart from isolated points, the dynamics may thus be described in terms of a time-local master equation with generator $\mathcal{K}_t$ as was shown before (cf. Eq. (3.21)). As a consequence, the connecting maps $\Lambda_{t,s}$ are given by Eq. (3.75) and one obtains $\frac{\mathrm{d}}{\mathrm{d}t}\Lambda_{t,s}\,|_{t=s} = \mathcal{K}_s$ so that the condition of n-divisibility can then be traced back to features of the generator. In fact, Φ is n-divisible if and only if $\mathcal{K}_s$ generates an n-positive semigroup for any fixed $s \geq t_0$. By means of the famous Gorini-Kossakowski-Sudarshan-Lindblad theorem (Gorini *et al.*, 1976; Lindblad, 1976) and a result on generators of positive semigroups by Kossakowski (1972a) (cf. also the works by Kossakowski (1972b) and Ingarden and Kossakowski (1975)), one finally obtains a complete characterization of CP- and P-divisibility in terms of the rates and Lindblad operators of the generator, defining an important result of this thesis which has already been published (cf. Wißmann *et al.* (2015)).

Theorem 3.2. *The dynamics generated by a time-local generator $\mathcal{K}_t$ as given in Eq.* (3.21)

1. *is CP-divisible if and only if $\gamma_j(t) \geq 0$ holds for all j and $t \geq t_0$.*
2. *is P-divisible if and only if for all $n \neq m$*

$$\sum_j \gamma_j(t) |\langle m|A_j(t)|n\rangle|^2 \geq 0 \tag{3.76}$$

holds for any orthonormal basis $\{|n\rangle\}$ of $\mathcal{H}_S$ and all $t \geq t_0$.

Proof. The first statement is precisely the Gorini-Kossakowski-Sudarshan-Lindblad theorem (Gorini *et al.*, 1976; Lindblad, 1976) which was already touched upon in Sec. 3.3. The second claim can be derived from Kossakowski's result on generators of positive semigroups (Kossakowski, 1972a) (see also Ingarden and Kossakowski (1975)) that states: A dynamics generated by a generator $\mathcal{K}'$ is P-divisible if and only if for any set of projections $\Pi = \{\Pi_m\}_{m\in I}$ defining a discrete resolution of identity, i.e. one has $\Pi_m\Pi_n = \delta_{mn}\Pi_m$ and $\mathrm{Tr}_S\{\Pi_m\} < \infty$ for all $m, n \in I$ with $\sum_{m\in I}\Pi_m = \mathbb{1}_{\mathcal{H}_S}$, the following relations for $a_{mn}(\Pi) \equiv \mathrm{Tr}\{\Pi_m(\mathcal{K}'\Pi_n)\}$ are satisfied:

$$a_{mm}(\Pi) \leq 0\ , \quad m \in I\ , \tag{3.77}$$

$$a_{mn}(\Pi) \geq 0\ , \quad m \neq n \in I\ , \tag{3.78}$$

$$\sum_{m\in I} a_{mn}(\Pi) = 0\ , \quad n \in I\ . \tag{3.79}$$

It is easily seen that condition (3.79) correspond to trace preservation, which is always met for a generator of the form (3.21) by its very structure (cf. Eq. (3.20)). Rearranging terms, one then obtains from Eq. (3.79) the relation

$$a_{nn}(\Pi) = -\sum_{m\neq n} a_{mn}(\Pi) \tag{3.80}$$

for all $n \in I$, so $a_{mn}(\Pi) \geq 0$ for all $m \neq n$ already implies Eq. (3.77). The three constraints thus reduce to the single relation (3.78) which can additionally be restricted to sets of rank-one projections Π by virtue of linearity of the generator $\mathcal{K}_t$. Evaluating $a_{mn}(\Pi)$ for $m \neq n$ and rank-one projections associated with an orthonormal basis $\{|n\rangle\}$ of $\mathcal{H}$, one obtains

$$a_{mn}(\Pi) = \mathrm{Tr}\left\{|m\rangle\langle m|\mathcal{K}_t(|n\rangle\langle n|)\right\} = \sum_j \gamma_j(t)|\langle m|A_j(t)|n\rangle|^2 \ , \tag{3.81}$$

which precisely yields condition (3.76). □

Note that condition (3.76) only guarantees that the dynamics generated by $\mathcal{K}_t$ is positive. That is, it does not warrant complete positivity of the dynamics as required for dynamical maps (cf. Sec. 3.3). It is also worth stressing that the conditions for P- and CP-divisibility coincide for master equations with a single decay channel or identical rates for multiple channels (see Eq. (4.91) for an example of the latter case) as the transition matrix elements of the Lindblad operators are obviously always positive.

Besides relying on time-local generators, P-divisibility of a process can also be verified directly by means of the trace norm. As shown by Kossakowski (1972a,b), a trace preserving linear map Υ is positive if and only if it defines a contraction for any Hermitian operator X with respect to the trace norm, i.e., one has

$$\|\Upsilon X\|_1 \leq \|X\|_1 \ , \tag{3.82}$$

for all $X = X^\dagger$, in accordance with the previously stated contraction of the trace distance with respect to PT-maps (see Eq. (2.42)). By virtue of this contraction property, it is finally possible to link quantum Markovian behavior to P-divisibility of the underlying dynamical process as is shown in Sec. 4.4.

3.5 Open system dynamics for nonfactorizing initial conditions

When considering open quantum systems, factorizing initial conditions are typically assumed leading to the described family of completely positive and trace preserving linear maps for the open system's evolution as was shown in Sec. 3.2. However, the assumption of an open system that is statistically independent of its environment at the initial time is rather restrictive and clearly has strong influence on the dynamics of the open system (Romero *et al.*, 2004; Štelmachovič and Bužek, 2001, 2003; Grabert *et al.*, 1988; Royer, 1996; Smirne *et al.*, 2010), so one may not assume the absence of initial correlations in general. Since the mere

detection of correlations in a joint system-environment state is usually impossible because a full state tomography is far too complicated or the degrees of freedom of the environment are even inaccessible, the dynamics of an open quantum system eventually bears good prospects to determine whether or not such a composite system is correlated or not. In general, the dynamics of an open quantum system is described by (cf. Eq. (3.6))

$$\rho_S(t) = \mathrm{Tr}_E\{U(t,t_0)\rho_{SE}(t_0)U^\dagger(t,t_0)\} \ , \tag{3.83}$$

where the joint initial state of system and environment is given by $\rho_{SE}(t_0)$ and a unitary evolution of the total system is assumed. A lot of work has been spent on providing a treatment for such dynamics along with the study of its mathematical properties (see, e.g., Royer (1996), Shaji and Sudarshan (2005), Brodutch *et al.* (2013), Shabani and Lidar (2009), Liu and Tong (2014), Lu (2016), Dominy *et al.* (2016) and Dominy and Lidar (2016)). As a matter of fact, initial correlations often lead to a breakdown of complete positivity or even positivity of the subdynamics which may be employed to detect these correlations. In the following paragraph, this idea is made precise using distance measures that are contractive with respect to CPT-maps such as the trace distance, the Hellinger distance as well as the Bures metric and the Jensen-Shannon divergence (see Secs. 2.4.1 and 2.4.2 for their respective definitions). The results of this thesis presented in Sec. 3.5.2 suggest that the trace distance is the distance measure among these four quantifiers that is best suited to witness initial system-environment correlations.

3.5.1 Signatures of initial system-environment correlations

In fact, the distance of two open system states measured with respect to distance measures that are contractions under CPT-maps might increase above its initial value witnessing initial correlations or nonidentical reduced environmental states[8] as was first shown by Laine *et al.* (2010a). To obtain this result, one observes that, independent of correlations in the initial total state, the subdynamics (3.83) represents the action of a family of linear CPT-maps $\{\Lambda_{t,t_0}\}$ from the total state space $\mathcal{S}(\mathcal{H}_{SE})$ to the state space of the open system, i.e., one has $\rho_S(t) = \Lambda_{t,t_0}(\rho_{SE}(t_0))$ for any time $t \geq t_0$. For any distance measure $\mathcal{D}$ that is contractive with respect to CPT-maps (cf. Eq. (2.35)), one then obtains the inequality

$$\mathcal{D}(\rho_S^{(1)}(t), \rho_S^{(2)}(t)) \leq \ \mathcal{D}(\rho_{SE}^{(1)}(t_0), \rho_{SE}^{(2)}(t_0)) \tag{3.84}$$

for all times $t \geq t_0$ and any pair of initial states $\rho_{SE}^{(1)}(t_0)$ and $\rho_{SE}^{(2)}(t_0)$. That is, the distance between two time-evolved reduced states is upper bounded by the distance of their associated initial system-environment states. Note that the inequality can be tight as has, for example, been shown for the trace distance by Laine *et al.* (2010a). In addition, it reduces to the usual contraction property for dynamical maps associated with factorizing initial conditions, such that one has $\rho_{SE}^{(k)}(t_0) = \rho_S^{(k)}(t_0) \otimes \rho_E(t_0)$ in Eq. (3.84), if the distance measure is also subadditive

[8] Another local detection scheme is provided by applying local quantum operations to the open system and comparing the subsequent dynamics with the original one (Gessner and Breuer, 2011).

(2.39). When focusing on the variation of the distance of two open system states relative to their initial value, Eq. (3.84) implies that it may not be larger than

$$\mathfrak{I}(\rho_{SE}^{(1)}(t_0),\rho_{SE}^{(2)}(t_0)) = \mathcal{D}(\rho_{SE}^{(1)}(t_0),\rho_{SE}^{(2)}(t_0)) - \mathcal{D}(\rho_{S}^{(1)}(t_0),\rho_{S}^{(2)}(t_0)) \ , \tag{3.85}$$

which can be interpreted as quantifying the initial information lying outside the open system (Breuer *et al.*, 2016). This interpretation is particularly valid if the trace distance is employed having a clear operational meaning as a quantifier of the distinguishability of two states as was shown in Sec. 2.4.1.

The special role of initial correlations for a potential increase of the distance is most clearly revealed if the second state is chosen as $\rho_{SE}^{(2)}(t_0) = \rho_{S}^{(1)}(t_0) \otimes \rho_{E}^{(1)}(t_0)$ where $\rho_{S}^{(1)}(t_0) = \mathrm{Tr}_E\{\rho_{SE}^{(1)}(t_0)\}$ and $\rho_{E}^{(1)}(t_0) = \mathrm{Tr}_S\{\rho_{SE}^{(1)}(t_0)\}$ denote the marginals of the other initial total state. For this choice Eq. (3.84) reads

$$\mathcal{D}(\rho_{S}^{(1)}(t),\rho_{S}^{(2)}(t)) \leq \ \mathcal{D}(\rho_{SE}^{(1)}(t_0),\rho_{S}^{(1)}(t_0)\otimes\rho_{E}^{(1)}(t_0)) \ , \tag{3.86}$$

where the right-hand side determines how far apart the initial total state and its completely uncorrelated counterpart are, quantifying the amount of correlations in the system-environment state $\rho_{SE}^{(1)}(t_0)$. Because the initial open system states are the same by construction, any nonzero distance of their time-evolved counterparts indicates the presence of initial correlations in $\rho_{SE}^{(1)}(t_0)$. Moreover, the maximal increase is upper bounded by the amount of correlations measured by the distance of the initial total state to its completely uncorrelated counterpart.

In the general case, a similar inequality showing the effect of initial correlations in the total states can be derived if the distance measure is subadditive (2.39) and satisfies the triangle inequality (2.38). As was shown before, these properties are, e.g., satisfied by the trace distance (2.40), the Hellinger distance (2.56) and the Bures metric (2.62), whereas the Jensen-Shannon divergence (2.69) does not obey the triangle inequality in general so that the following treatment does not hold for this quantifier. Assuming that the triangle inequality and the subadditivity holds for the distance measure $\mathcal{D}$, one derives an upper bound for $\mathfrak{I}(\rho_{SE}^{(1)}(t_0),\rho_{SE}^{(2)}(t_0))$ by applying the former twice and then using the subadditivity. In fact, this finally yields the inequality

$$\begin{aligned}&\mathcal{D}(\rho_{S}^{(1)}(t),\rho_{S}^{(2)}(t)) - \mathcal{D}(\rho_{S}^{(1)}(t_0),\rho_{S}^{(2)}(t_0)) \\ &\leq \ \sum_{k=1}^{2} \mathcal{D}(\rho_{SE}^{(k)}(t_0),\rho_{S}^{(k)}(t_0)\otimes\rho_{E}^{(k)}(t_0)) + \mathcal{D}(\rho_{E}^{(1)}(t_0),\rho_{E}^{(2)}(t_0)) \ ,\end{aligned} \tag{3.87}$$

showing that an increase of the distance of the reduced states above their initial distinguishability implies that there must be either correlations in at least one initial total state or the environmental states must be different initially. To exclude the latter case, one may compare the time evolution of an open system state $\rho_{S}^{(1)}(t_0) = \mathrm{Tr}_E\{\rho_{SE}^{(1)}(t_0)\}$ to a reference state that is obtained by performing a local CPT-map on the total state $\rho_{SE}^{(1)}(t_0)$ so that the second reduced state is defined as $\rho_{S}^{(2)}(t_0) \equiv \mathrm{Tr}_E\{(\Lambda\otimes I_E)(\rho_{SE}^{(1)}(t_0))$ (Laine *et al.*, 2010a). Due to the local character of the quantum operation, the generated state $\rho_{SE}^{(2)}(t_0)$ is uncorrelated if $\rho_{SE}^{(1)}(t_0)$ is uncorrelated. Note that the reverse direction is not true in general as there exist,

e.g., local operations transforming zero discord states to states with nonvanishing discord as was shown by Gessner *et al.* (2012).

It is worth repeating that the stated treatment is independent of the chosen distance measure as long as it is contractive with respect to CPT-maps while subadditivity and the triangle inequality are additionally needed in order to arrive at relation (3.87). Despite this generality, most of the studies so far concerned the trace distance (see, e.g., Mazzola *et al.* (2012); Smirne *et al.* (2010) and Laine *et al.* (2010a)). Extending the comparative study of the performance of various distance measures given by Dajka *et al.* (2011), it will be shown that the trace distance has indeed a special status pertaining to the detection of initial system-environment correlations.

3.5.2 Detection of initial correlations: Performance of different distance measures

Motivated by the study of Dajka *et al.* (2011), the performance of the trace distance, the Bures metric (2.62), the Hellinger distance (2.56) and the Jensen-Shannon divergence (2.69) regarding the detection of initial system-environment correlations of the trace distance (2.40) is compared on the basis of two model systems. In fact, the frequency of an increase above the initial value for the different distance measures is determined for a spin star model with Heisenberg XY interaction and the pure dephasing dynamics (3.72) for a two-level system and initial states with tunable system-environment correlations where one of these states is chosen to be completely uncorrelated. As a consequence of this configuration of the considered states, the associated environmental states are nonequal unless both states are uncorrelated, implying a CPT-dynamics. However, the unambiguous connection of initial correlations and nonidentical environmental states still allows to infer the presence of the former from an increase of a contractive distance measure above its initial value. The present results of this thesis indicate that the trace distance is indeed the best choice for a distance measure to witness initial system-environment by virtue of the dynamics of the reduced states.

To start with, one considers a two-level system subject to decoherence as described by the coupling to a single-mode bosonic environment (cf. Eq. (3.52)) with free Hamiltonian $H_S = \epsilon\sigma_3$ and coupling $\hat{S} = \sigma_3$. More specifically, the dynamics of for initial system-environment states

$$|\Psi_V^\lambda(0)\rangle_{SE} = b_1 V|1\rangle \otimes |0\rangle_E + b_0 V|0\rangle \otimes |\Omega_\lambda\rangle_E \tag{3.88}$$

is studied, where the parameter λ obeys $0 \leq \lambda \leq 1$ and the complex-valued weights b_j satisfy $|b_1|^2 + |b_0|^2 = 1$. Moreover, the pure state $|1\rangle$ ($|0\rangle$) refers to the excited (ground) state of the two-level system as before and V represents a unitary operator on the Hilbert space $\mathbb{C}^2$. The field state $|\Omega_\lambda\rangle_E$ is given by the coherent superposition of the vacuum state $|0\rangle_E$ and a coherent state $|y \in \mathbb{C}\rangle_E$ of the bosonic field, i.e.

$$|\Omega_\lambda\rangle_E = C_\lambda^{-1}\left\{(1-\lambda)|0\rangle_E + \lambda|y\rangle_E\right\} \tag{3.89}$$

with normalization $C_\lambda = \sqrt{(1-\lambda)^2 + \lambda^2 + 2\lambda(1-\lambda)\mathrm{Re}\big({}_E\langle 0|y\rangle_E\big)}$, where that the scalar product of two coherent states reads ${}_E\langle x|y\rangle_E = \exp[-(|x|^2+|y|^2-2x^*y)/2]$. Clearly, if $|b_{1,0}| \notin \{0,1\}$, any nonzero value of the parameter λ results in an entangled and, therefore, correlated initial state $|\Psi_V^\lambda(0)\rangle_{SE}$. Furthermore, the correlations are monotonically increasing with respect to this parameter when quantified by the concurrence (2.77) as is, for example, shown by the black line in Fig. 3.4 for states corresponding to $V = \mathbb{1}_2$. Due to these features, one may assign the meaning of a correlation parameter to this quantity.

As the total system evolves according to the unitary dynamics that is generated by the Hamiltonian

$$H = H_S \otimes \mathbb{1}_E + \mathbb{1}_S \otimes H_E + \sigma_3 \otimes g(\hat{b}^\dagger + \hat{b}) \;, \tag{3.90}$$

with $H_S = \epsilon\sigma_3$ and $H_E = \omega\hat{b}^\dagger\hat{b}$ (cf. Eq. (3.52)), leading to unitaries

$$U(t) = e^{-i\epsilon\sigma_3 t} e^{i\phi(t)} D(\sigma_3 z(t)) \;, \tag{3.91}$$

where $z(t) = (g/\omega)(1-\exp[i\omega t])$ and $\phi(t) = \int_0^t \mathrm{d}s \int_0^s \mathrm{d}s' g^2 \sin\big(\omega(s-s')\big)$ (cf. Eq. (3.68)), the time-evolved total state $|\Psi_V^\lambda(t)\rangle_{SE}$ is found to obey

$$\begin{aligned} |\Psi_V^\lambda(t)\rangle_{SE} = e^{i\phi(t)} \sum_{m=0}^{1} \Big\{ & b_1 V_{m1} e^{i(-1)^m \epsilon t} |m\rangle \otimes D\big((-1)^m z(t)\big)|0\rangle_E \\ & + b_0 V_{m0} e^{i(-1)^m \epsilon t} |m\rangle \otimes D\big((-1)^m z(t)\big)|\Omega_\lambda\rangle_E \Big\} \;. \end{aligned} \tag{3.92}$$

Note that V_{mn} is defined as $V_{mn} = \langle m|V|n\rangle$. Employing that the displacement operator applied to an arbitrary coherent state $|y\rangle_E$ yields $D(z\in\mathbb{C})|y\rangle_E = \exp[i\mathrm{Im}(zy^*)]|z+y\rangle_E$, the reduced state of the open quantum system at time t is given by

$$\rho_S^\lambda(t) = \begin{pmatrix} p & e^{-2i\epsilon t} B_V^\lambda(t) \\ e^{+2i\epsilon t} B_V^\lambda(t)^* & 1-p \end{pmatrix} \;, \tag{3.93}$$

with respect to its energy eigenbasis. Here, the time-independent population p satisfies

$$\begin{aligned} p = {} & |b_1|^2 |V_{11}|^2 + |b_0|^2 |V_{10}|^2 \\ & + 2C_\lambda^{-1} \mathrm{Re}\Big(b_1 b_0^* V_{11} V_{10}^* \big[1 - \lambda + \lambda\, {}_E\langle y|0\rangle_E\big] \Big) \;, \end{aligned} \tag{3.94}$$

whereas the coherence factor $B_V^\lambda(t)$ is given by[9]

$$\begin{aligned} B_V^\lambda(t) = {}& {}_E\langle -z(t)|z(t)\rangle_E \cdot \\ & \cdot \Big\{ |b_1|^2 V_{11} V_{01}^* + \left(|b_0| C_\lambda^{-1}(1-\lambda)\right)^2 V_{10} V_{00}^* \\ & \quad + C_\lambda^{-1}(1-\lambda)\left[V_{11} V_{00}^* b_1 b_0^* + V_{10} V_{01}^* b_1^* b_0\right] \Big\} \\ & + {}_E\langle -z(t)|y+z(t)\rangle_E \cdot \lambda C_\lambda^{-1} A(t) V_{10} \\ & \cdot \Big\{ |b_0|^2 C_\lambda^{-1}(1-\lambda) V_{00}^* + b_1^* b_0 V_{01}^* \Big\} \\ & + {}_E\langle y-z(t)|y+z(t)\rangle_E \cdot \left(\lambda C_\lambda^{-1} A(t)|b_0|\right)^2 V_{10} V_{00}^* \\ & + {}_E\langle y-z(t)|z(t)\rangle_E \cdot \lambda C_\lambda^{-1} A(t) V_{00}^* \\ & \cdot \Big\{ |b_0|^2 C_\lambda^{-1}(1-\lambda) V_{10} + b_1 b_0^* V_{11} \Big\} \end{aligned} \tag{3.95}$$

and the time-dependent function $A(t)$ is defined by $A(t) = \exp[(z(t)y^* - z^*(t)y)/2]$. Note that the reduced dynamics is periodic with period given by $2\pi/\omega$ due to the single-mode environment. In the special case of $V = \mathbb{1}_2$, the cumbersome expression for the coherence factor reduces to

$$B_{\mathbb{1}_2}^\lambda(t) = \; b_1 b_0^* C_\lambda^{-1} e^{-R(t)} \cdot \Big\{ 1 - \lambda + \lambda e^{-2i\Lambda(t) + S(t)} \Big\} \,, \tag{3.96}$$

where

$$R(t) = 4(g/\omega)^2 \cdot \{1 - \cos(\omega t)\} \,, \tag{3.97}$$

$$S(t) = 2(g/\omega)\,|y| \cdot \{\cos(\varphi) - \cos(\omega t - \varphi)\} - \tfrac{1}{2}|y|^2 \,, \tag{3.98}$$

$$\Lambda(t) = (g/\omega)\,|y| \cdot \{\sin(\varphi) + \sin(\omega t - \varphi)\} \,, \tag{3.99}$$

using the definition $y = |y| \cdot \exp[i\varphi]$ (cf. the expression given by Dajka *et al.* (2011) where a minus sign in the second sine function of the phase factor $\Lambda(t)$ is, however, missing).

To compare the sensitivities of the trace distance $\mathcal{D}_T$, the Hellinger distance $\mathcal{D}_H$, the Bures metric $\mathcal{D}_B$ and the Jensen-Shannon divergence $\mathcal{D}_J$ regarding the detection of initial system-environment correlations, the time evolution of the respective distance measures for reduced states associated with an uncorrelated, corresponding to $\lambda = 0$, and a λ-correlated initial total state is considered as already mentioned in the introduction to this section. Note that one easily shows that the environmental state associated with the pure state $|\Psi_V^\lambda(0)\rangle_{SE}$ depends on the parameter λ. Thus, the two states differ not only in terms of system-environment correlations but also with respect to the marginal states describing the environment so that the upper bound (3.87), which is valid for the first three of the above distance measures, has actually two nonvanishing contributions. However, as correlations and nonidentical environmental states are unambiguously linked for this setup, one may still assign an increase of the distance measures above their initial value to the presence of initial correlations. Hence, if

$$\Delta\mathcal{D}_k(\lambda, t) \equiv \mathcal{D}_k\big(\rho_S^\lambda(t), \rho_S^0(t)\big) - \mathcal{D}_k\big(\rho_S^\lambda(0), \rho_S^0(0)\big) \tag{3.100}$$

[9] Note that there is a typo in the expression of the coherence factor in (Wißmann *et al.*, 2013). Similarly, the states $|\Psi_{V_S}^\lambda(0)\rangle_{SE}$ and $|\Psi_{V_X}^\lambda(0)\rangle_{SE}$ (cf. Eqs. (3.103) and (3.104)) are erroneously defined therein.

is positive for some time t and (nonzero) value of λ, the corresponding measure is interpreted to be able to reveal initial correlations in the total state $|\Psi_V^\lambda(0)\rangle_{SE}$ in the relative evolution of the reduced states ρ_S^λ and ρ_S^0.

Before turning to the generic case, the dynamics of the four quantities $\mathcal{D}_k$ for a subclass of initial states characterized by the unitary operator $V = \mathbb{1}_2$ and the choice of weights $b_1 = b_2 = 1/\sqrt{2}$ is studied. Without loss of generality, the energy splitting of the system, the frequency of the bosonic mode as well as the interaction strength of the linear coupling are set to $\epsilon = 1$, $\omega = 1$ and $g = 0.1$, respectively, in the sequel. In addition, one chooses the coherent state contained in the field state $|\Omega_\lambda\rangle_E$ (cf. Eq. (3.89)) to be given by $|y = 1\rangle_E$. The time evolutions[10] of the quantities $\mathcal{D}_k(\lambda, t)$ for parameters $\lambda = 0.1, 0.3, 0.6$ and $\lambda = 1$ are shown in Fig. 3.2. Surprisingly, the Bures metric and the Hellinger distance never increase above their initial values for the considered parameters λ and are thus not able to detect the initial correlations present in one of the total states. The same holds true for large values of λ for the two other distance measures. However, for sufficiently small λ, the trace distance and the Jensen-Shannon divergence increase above their initial values indicating the existing initial correlations. The transition is observed for values $\lambda^T_{\text{crit.}} \approx 0.4$ and $\lambda^J_{\text{crit.}} \approx 0.2$ for the trace distance and the Jensen-Shannon divergence, respectively.

This behavior is indeed universal meaning that it is solely related to the general structure of the initial state $|\Psi_{\mathbb{1}_2}^\lambda(0)\rangle_{SE}$ rather than to the particular choice of the weights of the superposition. One concludes this by recording the relative frequency for the occurrence of a positive value of $\Delta\mathcal{D}_k(\lambda, t)$ for randomly sampled pairs of amplitudes $\{b_1, b_2\} \in \mathbb{C}^2$ such that $\sum_j |b_j|^2 = 1$ holds. In fact, the fraction of 5×10^4 randomly generated pairs of weights, for which the distance measures increase above their initial values for at least a single time interval $[t_i^k, t_f^k]$, is presented in Fig. 3.3 **(a)** as a function of λ where a binning of size 0.01 with respect to this parameter, starting from $\lambda_{\text{ini}} = 10^{-5}$, has been used. The sampled data gives strong numerical evidence that the Bures metric and the Hellinger distance never increase above their respective initial values for any choice of amplitudes and values of λ. On the contrary, the Jensen-Shannon divergence and the trace distance indeed witness initial correlations if they are sufficiently weak. More specifically, they reveal the initial system-environment correlations almost with certainty for small parameters λ but fail to do so for larger values. While the transition from $\mathfrak{f}^{J,T} \approx 1$ to $\mathfrak{f}^{J,T} = 0$ as a function of the correlation parameter λ is very smooth for the Jensen-Shannon distance, it drops rapidly at $\lambda^T_{\text{trans}} \approx 0.4$ for the trace distance in accordance with the behavior found for the weights $b_1 = b_2 = 1/\sqrt{2}$.

In summary, the present study provides strong numerical evidence that the Bures metric and the Hellinger distance cannot detect the initial system-environment correlations present in any state $|\Psi_{\mathbb{1}_2}^\lambda(0)\rangle_{SE}$ in general contradicting the statement of Dajka *et al.* (2011). Note that the close relation of these quantifiers is not surprising due to their definitions (cf. Sec. 2.4.2). However, their complete insensitivity to initial correlations in the pure state $|\Psi_{\mathbb{1}_2}^\lambda(0)\rangle_{SE}$ astonishes, in particular, since the trace distance, which satisfies the same properties such as the triangle inequality and subadditivity, increases almost with certainty above its initial value

[10] Note that the plots provided by Dajka *et al.* (2011) differ substantially from the time evolutions shown in Fig. 3.2. Dajka *et al.* (2011) apparently plotted the absolute value of $\Delta\mathcal{D}_k(\lambda, t)$.

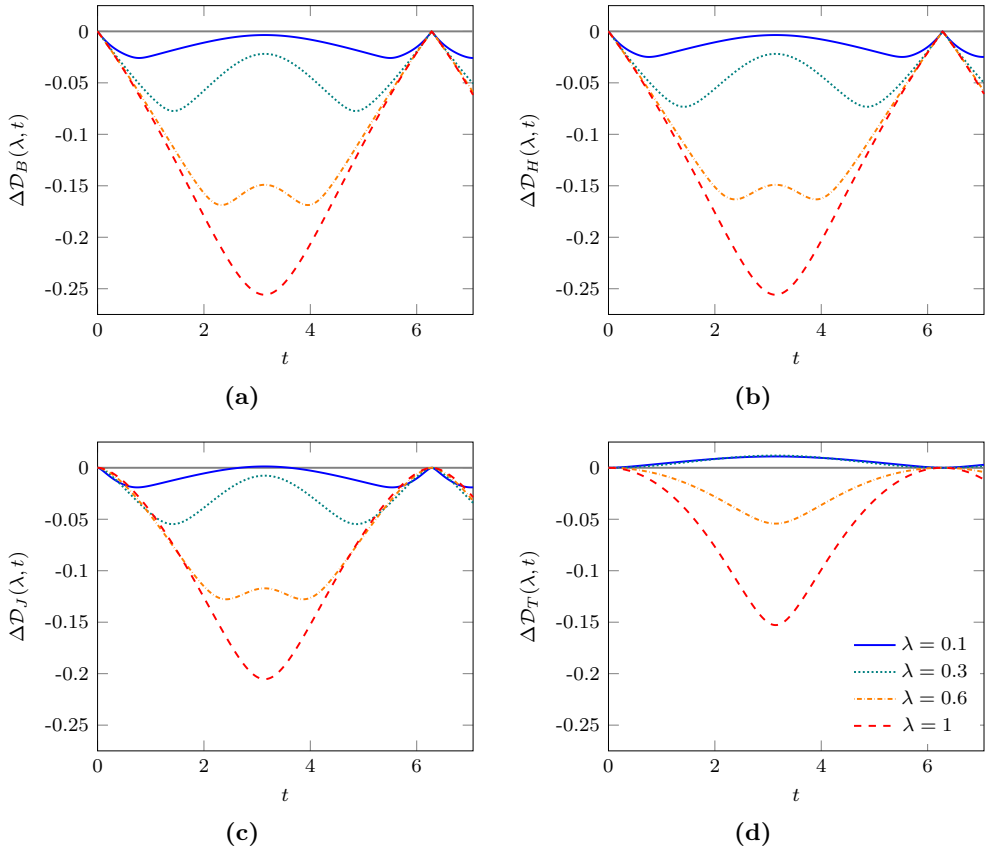

Figure 3.2 – Plot of $\Delta\mathcal{D}_k(\lambda,t)$ (cf. Eq. (3.100)) for $k = B, H, J$ and T (from **(a)** to **(d)**) as a function of time t for four particular values of the correlation parameter λ and an open system state obtained from the time-evolved pure state $|\Psi^{\lambda}_{\mathbb{1}_2}(0)\rangle_{SE}$ (cf. Eq. (3.92)) corresponding to the weights $b_1 = b_2 = 1/\sqrt{2}$ and the coherent state $|y = 1\rangle_E$ used to define $|\Omega_\lambda\rangle_E$ (see Eq. (3.89)). Note that time is dimensionless due to the choice of the other parameters which are set to $\epsilon = 1$, $\omega = 1$ and $g = 0.1$ (cf. Fig. 1 in Wißmann *et al.* (2013)).

for some time and sufficiently weak correlations. For large values of the correlation parameter, the trace distance and, similarly, the Jensen-Shannon divergence surprisingly loose their capability to witness initial correlations even though the strength of the initial correlations is monotonically increasing with respect to λ as is, for example, shown by means of the concurrence (cf. Fig. 3.4).

It is worth stressing that the transition of the trace distance cannot be explained in a satisfactory way by the lower and upper bounds for the change of this measure for two reduced states ρ_1 and ρ_2 at times t and s derived by Mazzola *et al.* (2012), Rodríguez-Rosario *et al.* (2012) and Smirne *et al.* (2013b). Only for very small values, these criteria provide some information indicating an increase of the trace distance above its initial value.

An intuitive understanding of the transition is, however, obtained by looking at the concurrence (2.77) of the total states. In fact, Fig. 3.4 shows this quantifier for bipartite entanglement of the pure state $|\Psi^{\lambda}_{\mathbb{1}_2}(t)\rangle_{SE}$ associated with weights $b_1 = b_2 = 1/\sqrt{2}$, revealing a similar threshold with respect to λ which in ad-

dition is close to the one found for the trace distance. More precisely, the blue line visualizes the change of behavior from an increasing concurrence from time zero to a monotonically decreasing dynamics from the initial time to $t = \pi$. This means that bipartite entanglement is solely increased during the time evolution for small values of λ, whereas it cannot be enhanced for parameters $\lambda \geq \lambda_{\text{crit.}} \approx 0.34$ causing the concurrence's decrease. Since the initial entanglement is monotonically increasing[11] as indicated by the black line in Fig. 3.4, this effect can be

[11] Note that the concurrence C_{gen} does not reach unity for $\lambda = 1$ at $t = 0$ because coherent states of a bosonic field are only approximately orthogonal (with an exponentially damped overlap) and, therefore, states $|\Psi_V^{\lambda=1}(t)\rangle_{SE}$ for $b_1 = b_0 = 1/\sqrt{2}$ do not define the Schmidt decomposition of a maximally entangled state of a two-level system and a single bosonic mode.

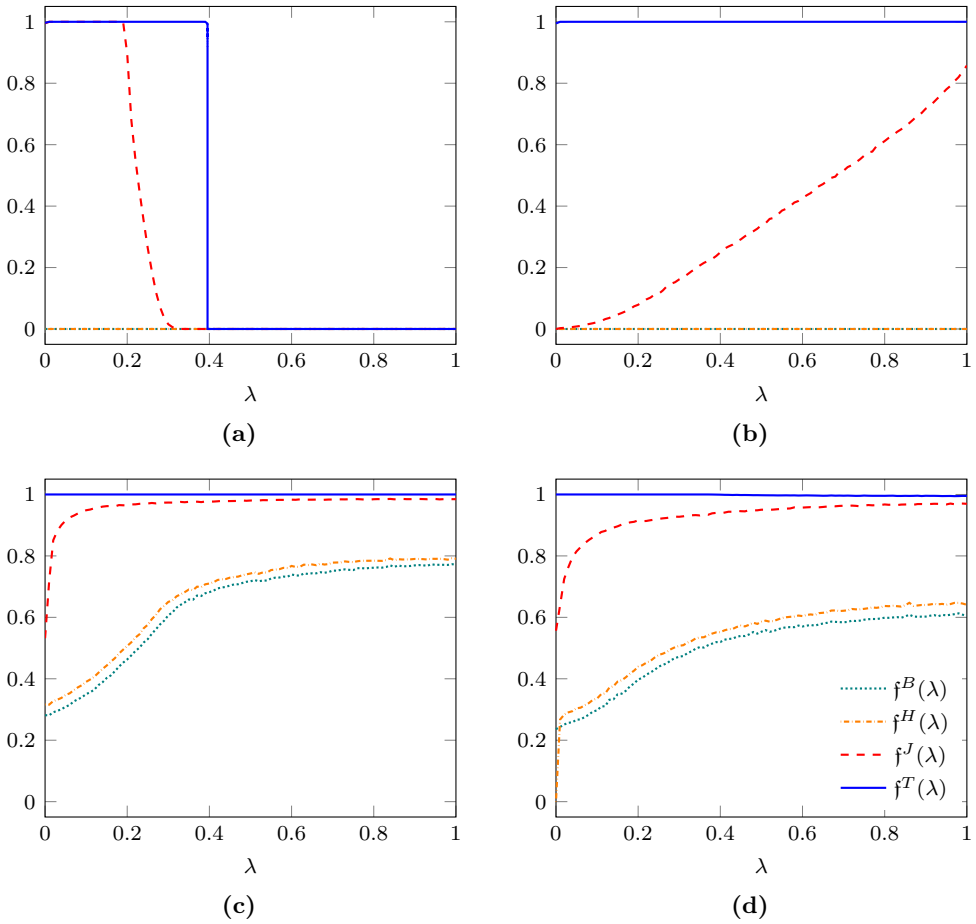

Figure 3.3 – Plot of the frequency of an increase $\mathfrak{f}^k(\lambda)$ above the initial value of the distance measures $\mathcal{D}_k$ $(k = B, H, J, T)$ for reduced states that correspond to $|\Psi^\lambda_{\mathbb{1}_2}(t)\rangle_{SE}$ **(a)**, $|\Psi^\lambda_{V_S}(t)\rangle_{SE}$ **(b)** (cf. Eq. (3.103)), $|\Psi^\lambda_{V_X}(t)\rangle_{SE}$ **(c)** (cf. Eq. (3.104)) and $|\Psi^\lambda_V(t)\rangle_{SE}$ **(d)** (see Eq. (3.92)). The lines show the fraction of states corresponding to 5×10^4 randomly sampled superposition amplitudes b_j, for which a positive quantity $\Delta\mathcal{D}_k(\lambda, t)$ occurred for each fixed λ in a binning with increment 0.01 and for at least one point in time $t \in [0, 2\pi)$. For $|\Psi^\lambda_V(t)\rangle_{SE}$ the sampling does not only comprise the weights but also the unitaries V that are distributed with respect to the Haar measure (cf. Figs. 2 and 3 in Wißmann *et al.* (2013)).

understood invoking the concept of entangling power of the unitary dynamics (Wißmann *et al.*, 2013). That is, the higher the initial entanglement the more unlikely the unitary dynamics can yield a target state which is more entangled than the initial one. In accordance with this intuitive idea, one observes that the maximal amount of correlations created by the dynamics, i.e., the largest value of $C_{\text{gen}}(|\Psi^{\lambda}_{\mathbb{1}_2}(t)\rangle_{SE}) - C_{\text{gen}}(|\Psi^{\lambda}_{\mathbb{1}_2}(0)\rangle_{SE})$ for some time $t \in [0, \pi)$ is obtained if λ is equal to zero which corresponds to a factorizing initial state. Due to this, it is reasonable to assume that the detected transition for the concurrence as well as the trace distance is attributed to the competition between initial entanglement and dynamically created correlations. One summarizes that the weaker the entangling power of the unitary dynamics the less frequently the trace distance will be capable to witness the initial system-environment correlations as only little further correlations are generated in time if they are yet not even diminished.

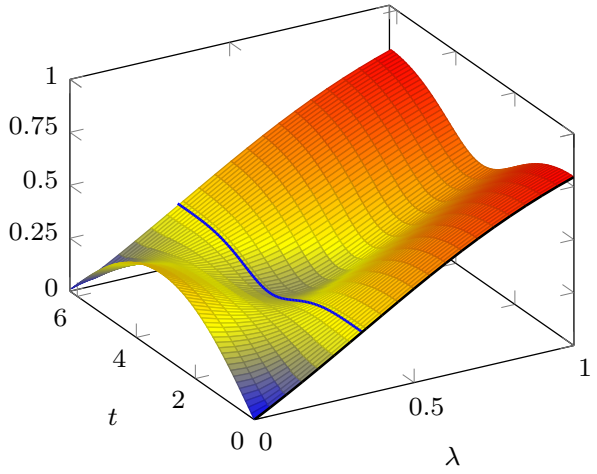

Figure 3.4 – Plot of the concurrence $C_{\text{gen}}(|\Psi^{\lambda}_{\mathbb{1}_2}(t)\rangle_{SE})$ (cf. Eq. (2.77)), quantifying the system-environment entanglement in $|\Psi^{\lambda}_{\mathbb{1}_2}(t)\rangle_{SE}$ (see Eq. (3.92)) with $b_1 = b_2 = 1/\sqrt{2}$, as a function of the correlation parameter λ and time t. The blue line indicates the transition where the concurrence never increases above its initial value during the time evolution (cf. Fig. 4 in Wißmann *et al.* (2013)).

The remarkable difference between the four distance measures regarding the capability of witnessing initial correlations in the present model is also observed for other types of initial total states associated with different unitaries V. Considering for example the initial states corresponding to the unitaries

$$V_S = \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{3.101}$$

$$V_X = \tfrac{1}{\sqrt{2}}(\sigma_1 + \sigma_3) = \tfrac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} , \tag{3.102}$$

one still concludes that the Jensen-Shannon divergence and the trace distance are far better suited to detect initial correlations when performing exactly the same analysis for these types of states as done for the pure state $|\Psi^{\lambda}_{\mathbb{1}_2}(t)\rangle_{SE}$ before (see Fig. 3.3 **(b)** and **(c)**). Note that the two unitaries specify superpositions that are characterized by contributions with very different mean energies in case of V_S, and

a completely different preparation of the two-level system for V_X which results in entanglement in the initial total state with respect to the eigenbasis of the Pauli spin operator σ_1. In fact, one finds

$$|\Psi^{\lambda}_{V_S}(0)\rangle_{SE} = b_1|0\rangle \otimes |0\rangle_E + b_0|1\rangle \otimes |\Omega_\lambda\rangle_E \tag{3.103}$$

and

$$|\Psi^{\lambda}_{V_X}(0)\rangle_{SE} = b_1|1_{\sigma_1}\rangle \otimes |0\rangle_E + b_0|0_{\sigma_1}\rangle \otimes |\Omega_\lambda\rangle_E \ , \tag{3.104}$$

where $|1_{\sigma_1}\rangle$ and $|0_{\sigma_1}\rangle$ refer to the eigenstates of σ_1, i.e., these states satisfy $\sigma_1|j_{\sigma_1}\rangle = (-1)^{j+1}|j_{\sigma_1}\rangle$. While the Bures metric and the Hellinger distance are also completely insensitive to initial correlations in the states $|\Psi^{\lambda}_{V_S}(0)\rangle_{SE}$, they are able to witness correlations for the other class of states. Nevertheless, the Jensen-Shannon divergence and the trace distance still increase more reliably above their initial values. More specifically, the frequency of an increase for the trace distance is constantly about unity for both classes of states, thus featuring no threshold as for the states $|\Psi^{\lambda}_{\mathbb{1}_2}(0)\rangle_{SE}$, whereas the Jensen-Shannon divergence shows a monotonic increase of its capability to witness the initial correlations for the states $|\Psi^{\lambda}_{V_X}(0)\rangle_{SE}$ as well as $|\Psi^{\lambda}_{V_S}(0)\rangle_{SE}$. For the former the frequency $\mathfrak{f}^J$ is close to unity already for very weak correlations as is shown in Fig. 3.3 **(c)**.

Note that the concept of entanglement capacity can also be used to explain the behavior for the states corresponding to the unitary V_S, whereas it fails to describe the findings for the states characterized by V_X as the concurrence is shown to decrease for all values of λ in the interval $[0, \pi]$ in this case. However, this does not sound the death knell for this intuitive concept as the initial state $|\Psi^{\lambda}_{V_X}(0)\rangle_{SE}$ for $b_0 = b_1 = 1/\sqrt{2}$ reads

$$|\Psi^{\lambda}_{V_X}(0)\rangle_{SE} = \frac{1}{2}\Big\{|1\rangle \otimes (|0\rangle_E + |\Omega_\lambda\rangle_E) + |0\rangle \otimes (|0\rangle_E - |\Omega_\lambda\rangle_E)\Big\} \ , \tag{3.105}$$

which yields a reduced state with vanishing coherences with respect to the basis $\{|j\rangle \,|\, j = 0, 1\}$ for all values of λ as the environmental states $|0\rangle_E + |\Omega_\lambda\rangle_E$ and $|0\rangle_E - |\Omega_\lambda\rangle_E$ are orthogonal for the chosen coherent state $|y = 1\rangle_E$ as one easily verifies. Clearly, states of a two-level system with fixed populations are most entangled if their coherences vanish (cf. the concurrence's definition for pure states (2.77)). As the unitary dynamics results in a pure dephasing process for the open system with respect to the eigenbasis of the Pauli matrix σ_3, coherences are created by the dynamics leading to a decrease of the entanglement. The initially saturated concurrence may thus only decrease for such a state.

Finally, the observed behavior for the second class of states (3.104) seems to represent the generic situation concerning the capability to witness initial correlations for the four measures as Fig. 3.3 **(d)** shows. Sampling not only the weights of the superposition but at the same time the unitary V from the set of unitaries distributed with respect to the Haar measure, the recorded relative frequency of increasing distance measures follows closely the behavior obtained for these states. Hence, the dynamics obtained for states $|\Psi^{\lambda}_{V}(0)\rangle_{SE}$ with unitaries $V = \mathbb{1}_2$ and $V = V_S$ may be seen as an exceptional case. Nonetheless, the results for arbitrary unitaries V still confirm that the trace distance and the Jensen-Shannon distance

are better suited to detect initial correlations in the present model for the considered initial states $|\Psi_V^\lambda(t)\rangle_{SE}$ in comparison with the Bures metric and the Hellinger distance.

The same observation is made if the bosonic environment is replaced by a spin bath. More specifically, let the open system's environment be given by N spin-$\frac{1}{2}$ particles labeled by the index k with associated Pauli operators $\sigma_j^{(k)}$. Assuming that they couple to the open system via a uniform Heisenberg XY interaction (Prokof'ev and Stamp, 2000), which has been found to provide an effective description for quantum dots (Imamoglu *et al.*, 1999) and cavity QED (Zheng and Guo, 2000), the system is thus described by the Hamiltonian

$$H = g \sum_{k=1}^{N} \left\{ \sigma_+ \sigma_-^{(k)} + \sigma_- \sigma_+^{(k)} \right\} \ , \tag{3.106}$$

where a free evolution of the system and the environment is omitted. Here, the interaction strength g is supposed to be real-valued and the operators $\sigma_{+(-)}$ and $\sigma_{+(-)}^{(k)}$ define the raising (lowering) operators of the central spin and the kth bath spin, respectively. This type of system is referred to as spin star model where the central spin now defines the open system. In the context of initial system-environment correlation, this exactly solvable model (see Appendix E) was first considered by Laine *et al.* (2010a). To perform the same study for the spin star model as for the single-mode bosonic bath before, one considers the pure states

$$|\xi_V^\lambda(0)\rangle_{SE} \equiv b_1 V|1\rangle \otimes |\chi_+\rangle_E + b_0 V|0\rangle \otimes |\tilde{\Omega}_\lambda\rangle_E \ , \tag{3.107}$$

where the environmental state is given by

$$|\tilde{\Omega}_\lambda\rangle_E = \tilde{C}_\lambda^{-1} \left\{ (1-\lambda)|\chi_+\rangle_E + \lambda |\chi_-\rangle_E \right\} \ , \tag{3.108}$$

with $\tilde{C}_\lambda = \{\lambda^2 + (1-\lambda)^2\}^{1/2}$ and

$$|\chi_+\rangle_E = \bigotimes_{k=1}^{N} |1\rangle \ , \qquad |\chi_-\rangle_E = \frac{i}{\sqrt{N}} \sum_{k=1}^{N} \sigma_-^{(k)} |\chi_+\rangle_E \ , \tag{3.109}$$

defining initial total states with system-environment correlations that are controlled by the parameter λ. Note that the states $|\chi_\pm\rangle_E$ define joint eigenstates of the total spin angular momentum of the bath $\vec{J}^2$ and its 3-component J_3 where $\vec{J} = \frac{1}{2}\sum_{k=1}^{N} \vec{\sigma}^{(k)}$ with $\hbar = 1$. In fact, one shows[12] that these two states are given by $|\chi_+\rangle_E = |\frac{N}{2}, \frac{N}{2}\rangle$ and $|\chi_-\rangle_E = i|\frac{N}{2}, \frac{N}{2} - 1\rangle$, respectively, so they are orthogonal at variance with the states contributing to the state $|\Omega_\lambda\rangle_E$ used for the bosonic environment (cf. Eq. (3.89)).

The detection of initial correlations with respect to the previously defined distance measures is then studied in the same way as for the first model. That is, the relative frequency $\mathfrak{f}^k$ of the occurrence of a positive quantity

$$\Delta\tilde{\mathcal{D}}_k(\lambda, t) \equiv \mathcal{D}_k\big(\tilde{\rho}_S^\lambda(t), \tilde{\rho}_S^0(t)\big) - \mathcal{D}_k\big(\tilde{\rho}_S^\lambda(0), \tilde{\rho}_S^0(0)\big) \ , \tag{3.110}$$

[12] Unfortunately, there is another typo in Ref. (Wißmann *et al.*, 2013): the imaginary unit i in the definition of $|\chi_-\rangle_E$ has been omitted in the mentioned published work.

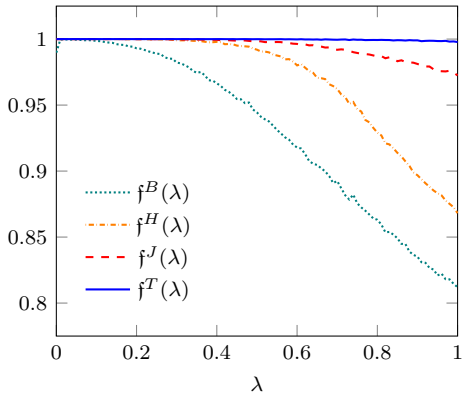

Figure 3.5 – Plot of the frequency of increase $\tilde{\mathfrak{f}}^k(\lambda)$ of the considered distance measures ($k = B, H, J$ and T) for the marginals of the states $|\xi_V^\lambda(t)\rangle_E$ (cf. Eq. (3.107)) with 5×10^4 randomly sampled superposition amplitudes b_j and unitaries V which have been distributed with respect to the Haar measure (cf. Fig. 5 in Wißmann *et al.* (2013)).

where $\tilde{\rho}_S^\lambda(t) = \mathrm{Tr}_E\{|\xi_V^\lambda(t)\rangle_{SE}\langle\xi_V^\lambda V(t)|\}$ refers to the central spin's reduced state, is determined for 5×10^4 random realizations of the weights b_j and the unitary V. Figure 3.5 shows that the trace distance is again best suited to detect the initial system-environment correlations present in these states as $\Delta\tilde{\mathcal{D}}_T(\lambda, t)$ is almost always positive at some time $t > 0$. However, the difference between the distance measures is diminished and, contrary to the first model (cf. Fig. 3.3 **(d)**), strong initial correlations, corresponding to large values of the parameter λ, are less reliably witnessed by all the distance measures even though the decrease for the trace distance is only tiny.

In summary, the results of the thesis presented is this section indicate that the trace distance represents the distance measure that is best suited to detect initial correlations in the joint state of an open quantum system and its environment in comparison to the Hellinger distance, the Bures metric as well as the Jensen-Shannon divergence.

Chapter 4

Non-Markovianity in the quantum regime

Over the past decades the notion of non-Markovian behavior has been frequently used in quantum mechanics to indicate the presence of memory effects in the time evolution of an open quantum system. The connotation of memory effects was rather loose though, without any strict definition, referring to the well-known concept of classical Markovian stochastic processes which are also interchangeably termed *memoryless* stochastic processes. However, the classical concept cannot be transferred to the quantum regime since it relies on the Kolmogorov hierarchy of n-point probability distributions which does not exist in quantum theory. Before turning to the different attempts to properly define quantum non-Markovianity, the classical concept is revisited and the impossibility for a transfer to quantum theory is highlighted.

4.1 Classical Markovian stochastic processes

Markovian processes in classical probability theory define a particular subclass of the set of stochastic processes which represent a one-parameter family of random variables where the parameter usually refers to time. More specifically, a stochastic process $\mathcal{Y}(t)$ is given by

$$\mathcal{Y}(t) = f(\mathcal{X}, t) \ , \tag{4.1}$$

where $\mathcal{X}$ refers to a random variable and f denotes an ordinary function depending on the realization of the stochastic process as well as the parameter t (van Kampen, 2007). Upon inserting a possible value x of the random variable $\mathcal{X}$, one thus obtains an ordinary function $\mathcal{Y}_x(t) = f(x,t)$ representing a so-called *realization* of the process. Recall that a random variable $\mathcal{X}$ is a measurable function from a probability space $\Xi = (I, \Sigma, \nu)$ – characterized by the triple of a set I, a σ-algebra over the sample space I and a probability measure[1] ν on Σ – to a measurable space (I', Σ'). For convenience, one assumes the sample space I' to be discrete with elementary events in the associated σ-algebra Σ' in the following.

[1] In addition to the properties of a measure $\nu : \Sigma \to [0,1]$ which satisfies $\nu(\emptyset) = 0$ and σ-additivity, i.e. $\nu(\bigcup_{j=1}^{\infty} \sigma_j) = \sum_{j=1}^{\infty} \nu(\sigma_j)$ for any countable collection $\{\sigma_j\}_{j=1}^{\infty}$ of pairwise disjoint elements of the σ-algebra Σ, a probability measure is characterized by the property $\nu(I) = 1$.

The probability distribution that the stochastic process takes on values y_j at time t_j for $j = 1, \ldots, n$ is then given by

$$P_n(y_n, t_n; \ldots; y_1, t_1) = \sum_{x \in I'} \prod_{m=1}^{n} \delta_{y_m, \mathcal{Y}_x(t_m)} \, \nu(\mathcal{X}^{-1}(\{x\})) \ , \tag{4.2}$$

as $\mu = \nu \circ \mathcal{X}^{-1}$ represents the probability measure[2] induced by the random variable on its image. The joint probability P_n can be seen as describing the fraction of realizations with values y_j at times t_j weighted by their occurrence. To support this interpretation, one typically assumes an ordered sequence of times $0 \leq t_1 < t_2 < \cdots < t_n$.

The hierarchy of these n-point probability distributions P_n completely characterizes the stochastic process since all averages may be determined from it according to

$$\langle \mathcal{Y}_\mathcal{X}(t_n) \cdots \mathcal{Y}_\mathcal{X}(t_1) \rangle = \prod_{j=1}^{n} \sum_{y_j \in f(I', t_j)} y_j P_n(y_n, t_n; \ldots; y_1, t_1) \ . \tag{4.3}$$

Clearly, the n-point probability distributions of any such hierarchy are positive and normalized, i.e.,

$$P_n(y_n, t_n; \ldots; y_1, t_1) \geq 0 \ , \tag{4.4}$$

$$\sum_{y_1 \in f(I', t_1)} P_1(y_1, t_1) = 1 \ , \tag{4.5}$$

and satisfies the consistency relation

$$\sum_{y_m \in f(I', t_m)} P_n(y_n, t_n; \ldots; y_m, t_m; \ldots; y_1, t_1) = P_{n-1}(y_n, t_n; \ldots; y_1, t_1) \tag{4.6}$$

for any index $1 \leq m \leq n$ linking the n-point and the $(n-1)$-point probability distributions. Quite interestingly, these constraints do not only provide necessary but also sufficient conditions, disregarding some mathematical subtleties, to specify a stochastic process as Kolmogorov (1956) has proven (see also Gardiner (2004) and van Kampen (2007)): any hierarchy of n-point probability distributions P_n with sample space I' obeying Eqs. (4.4)–(4.6) determines a stochastic process $\mathcal{Y}(t)$. The determination of the precise random variable and the function f (cf. Eq. (4.1)) corresponding to a given hierarchy is, however, challenging which is why stochastic processes are typically specified solely in terms of the probability distributions.

As a consequence of the consistency relation (4.6), one may omit any finite number of distributions without loosing information on the process. A Markovian stochastic process allows for an even more drastic reduction of the hierarchy. Indeed, a stochastic process $\mathcal{Y}(t)$ with values in I is said to be Markovian if and only if any conditional probability distribution

$$P_{1|n-1}(y_n, t_n | y_{n-1}, t_{n-1}; \ldots; y_1, t_1) \equiv \frac{P_n(y_n, t_n; y_{n-1}, t_{n-1}; \ldots; y_1, t_1)}{P_{n-1}(y_{n-1}, t_{n-1}; \ldots; y_1, t_1)} \tag{4.7}$$

[2] This is due to the fact that $\mathcal{X}$ is measurable, that is, for any $\sigma' \in \Sigma'$ one has $\mathcal{X}^{-1}(\sigma') \in \Sigma$. Note that the induced probability measure is also frequently denoted as $\mu = \mathrm{law}\mathcal{X}$ or $\mu = \mathcal{X}_\# \nu$, where the latter highlights that the measure on (I', Σ') can be seen as the push-forward of the random variable $\mathcal{X}$.

satisfies the relation (van Kampen, 2007)

$$P_{1|n-1}(y_n, t_n|y_{n-1}, t_{n-1}; \ldots; y_1, t_1) = P_{1|1}(y_n, t_n|y_{n-1}, t_{n-1}) \ . \tag{4.8}$$

For a Markovian process, the n-point probability distribution is then determined by

$$P_n(y_n, t_n; \ldots; y_1, t_1) = \prod_{j=1}^{n-1} P_{1|1}(y_{j+1}, t_{j+1}|y_j, t_j) P_1(y_1, t_1) \tag{4.9}$$

for $n \geq 2$, where the 1-point probability distribution obviously satisfies

$$P_1(y_2, t_2) = \sum_{y_1 \in I} P_{1|1}(y_2, t_2|y_1, t_1) P_1(y_1, t_1) \ , \tag{4.10}$$

due to the very definition of the conditional probability (4.7) and the consistency relation (4.6). Thus, the full hierarchy is completely determined by the 1-point probability distribution and the so-called transition probability $P_{1|1}$ which obviously simplifies the description of a stochastic process substantially. Apart from this implication, the classical Markov condition motivates the attribute the term *memoryless* to such a stochastic process. In fact, according to Eq. (4.8), the probability for a stochastic process $\mathcal{Y}(t)$ to take on the value y_n at time t_n, given that the values y_j have been observed at the earlier times t_j for $1 \leq j \leq n-1$, depends on the preceding value only and not on the remaining past. If the present state of the stochastic process is known, the past and the future are thus independent signifying a lack of memory. It is worth stressing that the Markov condition (4.8) holds for any value $n \geq 2$, imposing an infinite number of constraints on the conditional probabilities which is typically impossible to check for all practical purposes rendering it an abstract mathematical tool. Obviously, it does not suffice to consider some low-order distributions in order to verify the Markov condition (van Kampen, 2007).

For increasingly ordered times $t_1 \leq t_2 \leq t_3$, one derives the following relation for the transition probability from Eq. (4.9)

$$P_{1|1}(y_3, t_3|y_1, t_1) = \sum_{y_2 \in I} P_{1|1}(y_3, t_3|y_2, t_2) P_{1|1}(y_2, t_2|y_1, t_1) \ , \tag{4.11}$$

which is known as the *Chapman-Kolmogorov equation*. Just as Eqs. (4.4)–(4.6) for stochastic processes, this equation along with Eq. (4.10) for the 1-point probabilities completely characterize the 1-point and the transition probability[3] of a Markov process. That is, any two nonnegative functions satisfying Eqs. (4.10) and (4.11) unambiguously define a Markov process.

It is worth stressing that this does not mean that the Markovianity of a stochastic process is fully entailed by these equations providing a sufficient criterion and, thus, a reduction of the full Markov property. There are indeed stochastic processes that are not Markovian[4] but obey Eq. (4.11) (see Rivas *et al.* (2014) and

[3]Clearly, any transition probability must also be positive and satisfy $\sum_z P_{1|1}(z, t|y, s) = 1$ for any value y and times t and s.

[4]Stochastic processes with transition probabilities satisfying Eq. (4.11) are called *P-divisible* (see, e.g., Vacchini *et al.* (2011)).

Vacchini *et al.* (2011) for some examples). However, defining the full hierarchy associated with a stochastic process by means of Eq. (4.9) for these 1-point and transition probabilities, one obviously obtains a Markovian process that has the same 1-point and transition probabilities as the original non-Markovian process. Note that the Chapman-Kolmogorov equation may similarly be written as

$$\frac{\mathrm{d}}{\mathrm{d}t}P_{1|1}(y,t|x,s)=\sum_{z\in I}\Big[\mathcal{W}_{yz}(t)P_{1|1}(z,t|x,s)-\mathcal{W}_{zy}(t)P_{1|1}(y,t|x,s)\Big]\,, \tag{4.12}$$

provided the transition probability is differentiable with respect to time t (see, e.g., van Kampen (2007)). Here, $\mathcal{W}_{yz}(t)$ denotes the transition probability per unit time which is nonnegative and represents the probability for a transition to y given the classical state at time t was z. The differential Chapman-Kolmogorov equation, which is also called master equation (van Kampen, 2007), thus describes a loss and gain equation for the transition probabilities. It is clear that it solely characterizes the transition probability $P_{1|1}$, but a similar equation can be derived for the 1-point probability distribution

$$\frac{\mathrm{d}}{\mathrm{d}t}P_{1}(y,t)=\sum_{z\in I}\Big[\mathcal{W}_{yz}(t)P_{1}(z,t)-\mathcal{W}_{zy}(t)P_{1}(y,t)\Big]\,, \tag{4.13}$$

which is referred to as the Pauli master equation.

The main difficulty regarding an implementation of this well-established concept in quantum theory is given by the Kolmogorov consistency relation (4.6). It is, of course, possible to define a joint probability describing any sequence of measurement outcomes on a quantum system. However, these n-point distributions typically fail to satisfy the Kolmogorov condition (4.6). To illustrate this, assume for simplicity that a POVM $\{E_y\}$ with single Kraus operators Ω_y corresponding to these effects (see Sec. 2.4) is measured at the consecutive times $t_n\geq\cdots\geq t_1\geq 0$ on a closed system in the state $\rho_{SE}(0)$ which evolves according to the unitary operators $U(t)$. Applying Born's rule, the joint probability to obtain the sequence of outcomes y_j at t_j is then given by

$$P'_n(y_n,t_n;\cdots;y_1,t_1)=\mathrm{Tr}_{SE}\{\mathfrak{S}_{\Omega_{y_n}}\mathfrak{S}_{U(t_n-t_{n-1})}\cdots\mathfrak{S}_{\Omega_{y_1}}\mathfrak{S}_{U(t_1)}\rho_{SE}(0)\}\,, \tag{4.14}$$

where the notation $\mathfrak{S}_X\rho=X\rho X^\dagger$ has been employed. It is readily shown that P'_n is nonnegative and normalized for $n=1$ (cf. Eqs. (4.4) and (4.5)). However, unless the POVM $\{E_y\}$ defines a quantum non-demolition measurement (QND) which is characterized by the property $\sum_{y_1}\mathrm{Tr}\{\mathfrak{S}_{\Omega_{y_2}}\mathfrak{S}_{\Omega_{y_1}}\rho_{SE}(0)\}=\mathrm{Tr}\{\mathfrak{S}_{\Omega_{y_2}}\rho_{SE}(0)\}$ for any state $\rho_{SE}(0)$ (Breuer and Petruccione, 2002), one typically has

$$\sum_{y_m}P'_n(y_n,t_n;\ldots;y_m,t_m;\ldots;y_1,t_1)\neq P'_{n-1}(y_n,t_n;\ldots;y_1,t_1) \tag{4.15}$$

for any $1\leq m<n$. Hence, there does not exist a hierarchy of n-point probability distributions corresponding to measurements of quantum systems in general.

The violation of the Kolmogorov consistency relation may be summarized by the statement that any gain of information about a quantum system, realized by a measurement of it, typically disturbs the system, resulting in a fundamental change of its subsequent evolution (see Ch. 6 for a detailed discussion on this topic). The

effect of intermediate measurements is most easily observed when the POVM is assumed to describe a projective measurement with one-dimensional projections. In this case, the measurement completely removes quantum coherences and, therefore, erases quantum interference effects (Breuer *et al.*, 2016). Moreover, if the one-dimensional projections act only on the open system, the system-environment correlations are also fully eliminated by such a measurement which strongly influences the subsequent dynamics as already discussed in Sec. 3.5.

4.2 Concepts for quantum non-Markovianity

Since a hierarchy of n-point probability distribution functions, as used for the definition of a classical Markov process, does not exist for quantum systems, the fundamental questions emerge how to properly characterize memory effects in the dynamics of an open quantum systems, and how to quantify them. As a starting point for any attempt trying to answer these questions, one agrees on the facts that the property of a quantum process being Markov represents a fundamental feature of the open system dynamics which must be satisfied by any dynamics resulting from a master equation in Lindblad form (3.22), providing the prototype of a Markovian, memoryless dynamics. In particular, this means that the quantum Markov property cannot depend on the mathematical representation of the dynamics, such as a description in terms of a time-local master equation, but rather on features of the open system evolution which is completely described by a one-parameter family of dynamical maps (see Sec. 3.2). Advocating the open system point of view, memory effects should thus be based on the dynamics of individual open system states.

The last decade was shaped by an intense debate about the origin and the characterization of memory effects for quantum systems, following more or less the prescribed guideline. It culminated in several proposals for a definition of quantum non-Markovianity which can be approximately grouped into four different classes: first, proposals that rely on the divisibility (see Sec. 3.4) of the quantum dynamical process (Rivas *et al.*, 2010; Hou *et al.*, 2011; Chruściński and Maniscalco, 2014; Hall *et al.*, 2014), secondly, those which employ the concept of an information flow quantified by the distinguishability of states (Breuer *et al.*, 2009; Laine *et al.*, 2010b; Vasile *et al.*, 2011; Chruściński *et al.*, 2011; Chruściński and Kossakowski, 2012; Wißmann *et al.*, 2015), thirdly, the category of approaches which depend on the nonmonotonic behavior of other quantities invoking mostly concepts from quantum information theory (Rivas *et al.*, 2010; Lu *et al.*, 2010; Rajagopal *et al.*, 2010; Chruściński and Kossakowski, 2012; Luo *et al.*, 2012; Lorenzo *et al.*, 2013; Bylicka *et al.*, 2014; Fanchini *et al.*, 2014; Haseli *et al.*, 2014; Song *et al.*, 2015; Dhar *et al.*, 2015; Souza *et al.*, 2015) and, fourthly, the class directly quantifying deviations from semigroup dynamics (Wolf *et al.*, 2008; Ali *et al.*, 2015; Hou *et al.*, 2015).

The hitherto most promoted approaches are certainly given by the first two classes. The first category is motivated by the fact that the notion of CP-divisibility may be interpreted as the direct generalization of the semigroup property (see Sec. 3.4) as well as the Chapman-Kolmogorov equation (4.11). More precisely,

defining matrices $\Lambda_{t,r}$ whose elements are given by the transition probabilities, i.e. $(\Lambda_{t,r})_{yx} \equiv P_{1|1}(y,t|x,r)$, the Chapman-Kolmogorov equation can be written as

$$\Lambda_{t,r} = \Lambda_{t,s}\Lambda_{s,r} \ , \qquad t \geq s \geq r \geq t_0 \ , \tag{4.16}$$

which obviously has the same structure as the divisibility property for a dynamical process (cf. definition (3.1)). Clearly, this would suggest P-divisibility for an algebraic definition of quantum non-Markovianity in the first instance. However, since complete positivity is the relevant property for maps on quantum systems (cf. Sec. (2.4)), one may thus regard the replacement of the stochastic[5] matrices $\Lambda_{t,s}$ by completely positive maps as the natural quantum analog of the necessary condition (4.16) of a classical Markov process (Rivas *et al.*, 2014; Breuer *et al.*, 2016). This approach obviously respects quantum processes arising from a Lindblad master equation as prototypes of Markovian dynamics.

The usage of the concept of divisible quantum processes for the definition of quantum non-Markovianity has been first suggested by Rivas *et al.* (2010). In order to check the divisibility of the process, one would initially assume that the intermediate maps $\Lambda_{t,s}$ (cf. Eq. (3.73)) must be exactly known requiring the ability to perform process tomography. Knowing the full process, one may also determine the associated time-local master equation and check complete positivity by virtue of theorem 3.2. Besides the opportunity of a full process tomography, one can also limit resources to simple state tomography at the cost of being capable to prepare entangled states: the so-called Choi matrix $(\Lambda_{t,s}\otimes I_A)(|\Psi\rangle_{SA}\langle\Psi|)$ is positive if and only if $\Lambda_{t,s}$ is completely positivity (Choi, 1975), where $|\Psi\rangle_{SA}$ refers to a maximally entangled state between the open system and an ancilla describing a quantum system with Hilbert space dimension greater or equal than $\dim\mathcal{H}_S$. The apparent advantage of state tomography on an extended system is disproved by a close inspection of the scaling with respect to the Hilbert space dimension which is shown to be the same for both methods (Breuer *et al.*, 2016). The strength of the negativity of the Choi matrix (Rivas *et al.*, 2010) or the rates of the associated time-local master equation (Hall *et al.*, 2014), which exist whenever the notion of divisibility is well defined as was argued in Sec. 3.4, finally provide tools to measures the degree of non-Markovianity of a dynamical process as described by this criterion.

Returning to the first proposal for a "quantization" of the Chapman-Kolmogorov equation (4.16), that is, replacing the positive matrices $\Lambda_{t,s}$ by maps on the open system's state space that are at least positive, the quantum counterpart of equation (4.16) would accordingly be given by P-divisibility. This property is actually equivalent to a monotonically decreasing generalized trace distance and leads to rate equations for the eigenvalues of open system states that can be interpreted as Pauli master equations (4.13) of a classical Markov process, describing major results of this thesis which are presented in Sec. 4.4 (see also Wißmann *et al.* (2015)). In addition to providing an intrinsic definition of quantum non-Markovianity, the first characterization already has a classical analog which captures the features of a classical Markov process at the level of 1-point probability distributions. In fact,

[5] A positive semidefinite matrix $A = (a_{jk})$ is said to be stochastic if any of its columns sums to one, i.e., if one has $\sum_j a_{jk} = 1$ for all k. If the sum of any column and, in addition, any row is equal to unity, one speaks of a bistochastic matrix.

for any pair of 1-point probability distributions $P_1^{(k)}(r) = \{P_1^{(k)}(x,r)\}$ $(k = 1, 2)$ over the same sample space, which evolve according to $P_1^{(k)}(y,t) = \Lambda_{t,r} P_1^{(k)}(x,r)$, one has

$$\|q_1 P_1^{(1)}(t) - q_2 P_1^{(2)}(t)\|_{\ell^1} \leq \|q_1 P_1^{(1)}(s) - q_2 P_1^{(2)}(s)\|_{\ell^1} \tag{4.17}$$

for any binary probability distribution $\{q_j\}$ and any indices $t \geq s \geq r$, if and only if the maps $\Lambda_{t,r}$ obey the Chapman-Kolmogorov equation (4.16) (Breuer *et al.*, 2016). The lack of nonstochastic intermediate maps $\Lambda_{t,s}$, being detected by a nonmonotonic behavior of the generalized Kolmogorov distance (4.17), may therefore be used to quantify non-Markovian behavior of classical processes at the level of 1-point probability distributions as proposed by Smirne *et al.* (2013c).

However, a nonmonotonic behavior of the generalized trace distance can additionally be interpreted as a backflow of information due to the relation of this functional to ensemble discrimination which was pointed out in Sec. 2.4.1. The appealing idea that memory effects in the dynamics show up as a backflow of information into the open system also applies to any other distance measure that is contractive with respect to CPT-maps and invariant under unitary transformations, as the total information quantified by such measures is then preserved and they provide reasonable quantifiers for the distinguishability of quantum states, even though not in an operational setting in general such as the trace norm does (Breuer *et al.*, 2009; Laine *et al.*, 2010b; Vasile *et al.*, 2011; Chruściński *et al.*, 2011; Chruściński and Kossakowski, 2012). This sets the basis for the second category of approaches to quantum non-Markovianity which was brought up by Breuer *et al.* (2009) who studied the dynamical behavior of the trace distance. The details of this first attempt, combining a clear physical and operational interpretation and an intrinsic characterization of memory effects, are given in the next section along with a study of the associated measure.

To finish the introduction, the geometrical characterization of non-Markovianity is worth mentioning as it is also connected to P-divisibility of the process. Lorenzo *et al.* (2013) assign non-Markovian behavior to an intermediate growth of the volume of the open system state space, which is determined with respect to the parametrization obtained from the generalized Bloch representation (cf. Sec. 2.2). Another line of thought pursued in the third category is based on the evolution of correlations such as entanglement (Rivas *et al.*, 2010; Fanchini *et al.*, 2014; Haseli *et al.*, 2014) or the dynamics of the mutual information (Luo *et al.*, 2012) between the open system and an auxiliary system. While other concepts from quantum estimation and information theory like the quantum Fisher information (Lu *et al.*, 2010; Song *et al.*, 2015), the infometric power (Dhar *et al.*, 2015; Souza *et al.*, 2015) or means measuring the capacity of quantum channels (Bylicka *et al.*, 2014) have additionally been proposed, there is also the most strict school advocating the classification in terms of deviations from signatures of the semigroup such as the quantum regression theorem (Ali *et al.*, 2015) or the snapshot method (Wolf *et al.*, 2008).

4.3 Quantum non-Markovianity and the information flow

The trace distance, as well as its generalization, defines a measure for the distinguishability of quantum states equipped with an operational meaning as was shown in Sec. 2.4.1. It is therefore natural to interpret a dynamical change of the trace distance of two open system states as a flow of information between the open system and its environment. This interpretation is supported by the observation that the trace distance's contractivity for positive, trace preserving linear maps (see Eq. (2.42)) yields an upper bound for the distinguishability of two states $\rho_S^{(1,2)}(t)$ evolving with respect to a dynamical process $\Phi = \{\Phi_{t,t_0} \,|\, t \geq t_0\}$. In fact, one obtains

$$\mathcal{D}_T(\rho_S^{(1)}(t), \rho_S^{(2)}(t)) \leq \mathcal{D}_T(\rho_S^{(1)}(t_0), \rho_S^{(2)}(t_0)) \tag{4.18}$$

and the preservation of distinguishability in closed systems due to the unitary invariance of the trace norm reinforces the suggested interpretation, too. Note that the Eq. (4.18) does not prohibit a nonmonotonic behavior of the distinguishability but bounds the maximal gain of information. Indeed, the distinguishability cannot exceed its initial value. The loss of information, ascribed to a decrease of the distinguishability, may thus be accompanied by revivals of trace distance that are interpreted as a backflow of information from the environment to the open system.

It is worth stressing that the swap of information refers to the information which is accessible by measurements on the open quantum system's degrees of freedom only. Thus, information can also be carried by system-environment correlations. This can, for example, be seen by virtue of the quantities

$$\mathfrak{I}_{\text{int}}(t) = \mathcal{D}_T(\rho_S^{(1)}(t), \rho_S^{(2)}(t)) \ , \tag{4.19}$$

and

$$\mathfrak{I}_{\text{ext}}(t) = \mathcal{D}_T(\rho_{SE}^{(1)}(t), \rho_{SE}^{(2)}(t)) - \mathcal{D}_T(\rho_S^{(1)}(t), \rho_S^{(2)}(t)) \ , \tag{4.20}$$

where the latter has already been introduced in general terms in the study of initial system-environment correlations given in Sec. 3.5.1. Following the previous discussion, $\mathfrak{I}_{\text{int}}(t)$ represents the distinguishability of the open system at time t, whereas $\mathfrak{I}_{\text{ext}}(t)$ describes the gain of information when the total system is accessible instead of the open system only. Both quantities are positive and the unitary invariance of the trace norm along with the factorization of the initial total states implies that $\mathcal{D}_T(\rho_{SE}^{(1)}(t), \rho_{SE}^{(2)}(t)) = \mathcal{D}_T(\rho_S^{(1)}(t_0), \rho_S^{(2)}(t_0))$ holds for all times $t \geq t_0$ and, therefore, one has $\mathfrak{I}_{\text{ext}}(t_0) = 0$. The internal and external information thus obey (Breuer *et al.*, 2016)

$$\mathfrak{I}_{\text{int}}(t) + \mathfrak{I}_{\text{ext}}(t) = \mathfrak{I}_{\text{int}}(t_0) \ , \tag{4.21}$$

which clearly expresses the idea of an exchange of information between the open system and the environment as an increase of $\mathfrak{I}_{\text{ext}}$ necessarily forces $\mathfrak{I}_{\text{int}}$ to decrease. Employing the upper bound (3.87), system-environment correlations must be build up or the environmental states have to be different in order to achieve $\mathfrak{I}_{\text{ext}} > 0$.

This clearly shows that the lost information is inaccessible by measurements on the open system and, moreover, the recovery of lost information, corresponding to an intermediate increase of $\mathfrak{I}_{\text{int}}$, is due to the existence of correlations or different environmental states at some point of the evolution (Breuer *et al.*, 2016).

In view of the previous considerations, one now defines non-Markovianity in the following way: a dynamical process given by a one-parameter family of dynamical maps $\Phi = \{\Phi_{t,t_0} \,|\, t \geq t_0\}$ is said to be non-Markovian if and only if there exists a pair of initial states $\rho_S^{(1)}(t_0)$ and $\rho_S^{(2)}(t_0)$ such that

$$\sigma(t, \rho_S^{(j)}) \equiv \frac{\mathrm{d}}{\mathrm{d}t} \mathcal{D}_T(\rho_S^{(1)}(t), \rho_S^{(2)}(t)) > 0 \tag{4.22}$$

for some time $t > t_0$, where the time-evolved states read $\rho_S^{(j)}(t) = \Phi_{t,t_0}(\rho_S^{(j)}(t_0))$. Hence, non-Markovian behavior can be experimentally witnessed if state tomographic measurements of different initial states at different times can be realized as will be demonstrated for a photonic setup in Sec. 4.3.2. Because memory effects should define an intrinsic feature of the dynamical process, whose existence is basically the only prior information one requires, a state independent quantifier for the information flow must be established. An obvious solution for this problem is to sum up all revivals of the trace distance, that is, to sum up all contributions for which one has $\sigma > 0$, and to maximize over all pairs of initial states.

Definition 4.1. *A measure $\mathcal{N}(\Phi)$ for the degree of memory effects of a quantum process Φ is given by*

$$\mathcal{N}(\Phi) = \max_{\rho_S^{(1,2)} \in \mathcal{S}(\mathcal{H}_\mathcal{S})} \int_{\sigma>0} \mathrm{d}t \; \sigma(t, \rho_S^{(j)}) \in [0, \infty] \; . \tag{4.23}$$

A quantum process Φ is called non-Markovian if and only if $\mathcal{N}(\Phi) > 0$ (Breuer et al., 2009; Laine et al., 2010b).

Clearly, this definition of a measure for non-Markovianity is in prefect accordance with semigroup dynamics leading to a continuous loss of distinguishability just as any P-divisible quantum process. However, the converse is not true, that is, non-P-divisible processes Φ may still yield $\mathcal{N}(\Phi) = 0$ (see, e.g., Mazzola *et al.* (2010), Chruściński *et al.* (2011), Chruściński and Wudarski (2013) and Hall *et al.* (2014) for explicit examples). Summarizing, the lack of P-divisibility is just necessary but not sufficient for non-Markovianity.

As a P-divisible quantum process is not necessarily CP-divisible, it is evident that this concept is fundamentally different from the approaches based on CP-divisibility. Chruściński *et al.* (2011) proposed an approach reconciling the idea of an information flow with CP-divisibility which also inspired the generalization of definition 4.1 to a measure enjoying the interpretation of non Markovianity in terms of an information flow and equivalence to P-divisibility, which will be introduced in Sec. 4.4.

It is worth stressing that the maximum in Eq. (4.23) does not exist in general, independent of the dimension of the Hilbert space of the open quantum system. Of course, infinite systems describe the generic case where no maximizing pair exists, but also the integration which formally ranges to infinity is problematic in this

respect. To deal with these mathematical subtleties, the maximum must actually be replaced by the supremum so that there is a sequence of state pairs approaching $\mathcal{N}(\Phi)$. Apart from this problem, the maximization by itself is challenging as the concerned set $\mathcal{S}(\mathcal{H}_\mathcal{S}) \times \mathcal{S}(\mathcal{H}_\mathcal{S})$ is of dimension $2(\dim\mathcal{H}_S)^2 - 2$ and, thus, increases rapidly with the size of the Hilbert space. Significant progress concerning this difficulty is made by characterizing the set of maximizing states which, moreover, leads to a advantageous, local representation of the measure as will be shown in the following section.

4.3.1 Pairs of optimal states and the local representation

A pair of states $\rho_S^{(1)}$ and $\rho_S^{(2)}$ of the open quantum system is said to be optimal if and only if the maximum in Eq. (4.23) is attained for this pair, i.e., if it satisfies

$$\mathcal{N}(\Phi) = \int_{\sigma>0} \mathrm{d}t\ \sigma(t, \rho_S^{(j)})\ . \tag{4.24}$$

Of course, it may happen that there exist several maximizing pairs such as for the models leading to pure decoherence which were discussed in Sec. 3.3.2, or that the set of optimal states is empty. In addition, it is clear that the definition of optimal states is only reasonable if the dynamics is non-Markovian as for Markovian processes any pair of states is optimal by definition. Obviously, the states of an optimal pair, assuming its existence, must also be unequal.

Now, assuming that an optimal pair indeed exists, one shows that the optimal states must be orthogonal (Wißmann *et al.*, 2012) employing the Jordan-Hahn decomposition[6] (cf. lemma G.1). Optimal states, featuring a maximal backflow of information, thus obey the natural guess of having initially a maximal information content due to their perfect distinguishability at the initial time. Note that the result concerning optimality of states relies solely on the linearity of the dynamical maps, and therefore applies to open quantum systems of arbitrary dimension. The measure for quantum non-Markovianity thus reads

$$\mathcal{N}(\Phi) = \max_{\rho_S^{(1)} \perp \rho_S^{(2)}} \int_{\sigma>0} \mathrm{d}t\ \sigma(t, \rho_S^{(j)})\ . \tag{4.25}$$

Besides orthogonality of the states maximizing the backflow of information, no further characterization, such as their purity, is possible a priori. While the orthogonality of states indeed implies the purity of optimal states for two-level systems, this conclusion is in general wrong as was shown in Wißmann *et al.* (2012) by means of an example.

The orthogonality of optimal states may, however, be used to derive a local representation of the measure for quantum non-Markovianity for finite-dimensional systems as indicated before. By virtue of the Jordan-Hahn decomposition, one shows that the set of orthogonal states can be represented by states of an appropriate set and an arbitrary but fixed reference state of the state space's interior.

[6] An alternative proof for finite-dimensional open quantum systems is based on the joint translatability of two quantum states by traceless, Hermitian operators if they are not orthogonal (Wißmann, 2012).

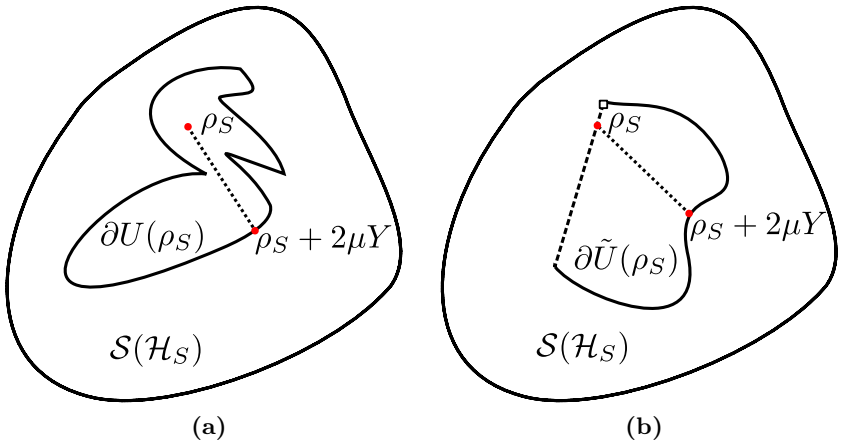

Figure 4.1 – Illustration of an enclosing surface with curved boundary **(a)** and of a hemispherical enclosing surface **(b)** for an inner point ρ_S (cf. Fig. 1 in Wißmann *et al.* (2015)).

The restriction to finite systems is readily understood as the interior is empty if one has $\dim\mathcal{H}_S = \infty$ (cf. Sec. 2.3). Because infinite quantum systems can often be accurately described by finite-dimensional Hilbert spaces for most practical purposes, this limitation is yet not as drastic as supposed. Apart from resolving the point of criticism that the maximization includes pairs of states, this representation highlights that non-Markovianity quantified by the measure $\mathcal{N}$ is a universal and intrinsic feature of the dynamical process appearing everywhere in the state space.

To establish the local representation, one first characterizes the mentioned, appropriate set of states over which the maximization has to be performed. Denoting the set of nonzero, Hermitian and traceless operators on the Hilbert space $\mathcal{H}_S$ by

$$\mathcal{E}_0(\mathcal{H}_S) = \{Y \in \mathcal{B}(\mathcal{H}_S) \mid Y \neq 0,\, Y = Y^\dagger,\, \mathrm{Tr}\{Y\} = 0\}\ , \tag{4.26}$$

one defines the following subset of the state space associated with an arbitrary reference state $\rho_S \in \mathring{\mathcal{S}}(\mathcal{H}_S)$ (Liu *et al.*, 2014; Wißmann, 2012):

Definition 4.2. *Let $\rho_S \in \mathring{\mathcal{S}}(\mathcal{H}_S)$ be an interior point of a finite-dimensional state space $\mathcal{S}(\mathcal{H}_S)$. A set $\partial U(\rho_0) \subset \mathcal{S}(\mathcal{H})$ not containing ρ_S is called an enclosing surface of ρ_S if and only if for any operator $Y \in \mathcal{E}_0(\mathcal{H})$ there exists a real number $\mu > 0$ such that*

$$\rho_S + 2\mu Y \in \partial U(\rho_S)\ . \tag{4.27}$$

An illustration of the definition is provided in Fig. 4.1 **(a)**. Clearly, one has $\rho_S \notin \partial U(\rho_S)$ and $\partial U(\rho_S) \subset \mathcal{S}(\mathcal{H}_S)$ by construction and the denomination is chosen as, according to the generalized Bloch representation (cf. Sec. 2.2), the set $\mathcal{E}_0(\mathcal{H}_S)$ is isomorphic to the perforated Euclidean space $\mathbb{R}^{N_S^2-1} \setminus \{0\}$ given an N_S-dimensional open quantum system, so that the inner point ρ_S is completely covered by any of its corresponding enclosing surfaces. The most simple instance of such a set is clearly given by a sphere contained in $\mathcal{S}(\mathcal{H}_S)$ which is centered around $\vec{v}_S$ specifying the inner point's Bloch vector. It is worth stressing that an enclosing

surface $\partial U(\rho_S)$ can be of any shape even though the previous example shows the existence of enclosing surfaces in general. In fact, by the very definition of the interior of the state space (cf. Sec. 2.3), there always exist such a sphere which thus proves that any inner point has an enclosing surface. Similarly, it follows that one cannot define such a set for any state on the boundary $\partial\mathcal{S}(\mathcal{H}_S)$ (cf. Eq. (2.17)) of the state space. Using this definition, one may prove the following theorem establishing the local representation (see Wißmann (2012) or Liu *et al.* (2014) for the proof):

Theorem 4.1. *For any dynamical process Φ for a finite-dimensional open quantum system, the measure for quantum non-Markovianity $\mathcal{N}$ defined in Eq.* (4.1) *admits a local representation, i.e., it can be determined as*

$$\mathcal{N}(\Phi) = \max_{\rho_S^{(2)} \in \partial U(\rho_S^{(1)})} \int_{\bar{\sigma}>0} \mathrm{d}t \; \bar{\sigma}(t, \rho_S^{(j)}) \tag{4.28}$$

with

$$\bar{\sigma}(t, \rho_S^{(j)}) \equiv \sigma(t, \rho_S^{(j)}) \cdot \mathcal{D}_T(\rho_S^{(1)}, \rho_S^{(2)})^{-1} \; , \tag{4.29}$$

where $\rho_S^{(1)} \in \mathring{\mathcal{S}}(\mathcal{H}_S)$ is any fixed state of the state space's interior and $\partial U(\rho_S^{(1)})$ refers to an arbitrary enclosing surface of $\rho_S^{(1)}$.

The non-Markovianity can thus be obtained by determining the information backflow of the trace distance between an arbitrary fixed state from the interior and the states of any of its enclosing surfaces at the cost of rescaling the information flux by the initial distinguishability. Considering a two-dimensional open quantum system for which the clear illustration in terms of the Bloch ball is available, one can easily understand this. In this case, the maximization in the original definition of $\mathcal{N}$ can be restricted to all pairs of antipodal states of the sphere due to the required orthogonality of optimal states as mentioned before. For a fixed point of the open unit ball and a set which encloses it – corresponding to an inner point ρ_S and an enclosing surface $\partial U(\rho_S)$, respectively – the straight line connecting states $\varrho_S \in \partial U(\rho_S)$ and ρ_S can be moved by parallel translation to be centered at the origin of the Bloch ball leaving the trace distance of the two states unaffected. Stretching the line by the inverse trace distance of the two involved states ρ_S and ϱ_S, the endpoints of the line correspond two antipodal points on the surface of the Bloch ball. Conversely, any pair of antipodal points can obviously be transformed in the same way to define the inner point ρ_S and a state of an enclosing surface $\partial U(\rho_S)$.

An inner point and any of its enclosing surfaces thus contain all directions covered by the difference of orthogonal states. However, the information provided by an inner point along with an enclosing surface is actually still overcomplete as the two-dimensional example already shows. First, the trace norm is not altered when the sign of the operator is changed, i.e., one has $\|Y\|_1 = \|Z\|_1$ for any operator Y where Z is defined according to $Z \equiv -Y$. And, secondly, the existence of a single parameter $\lambda > 0$ for any element in $\mathcal{E}_0(\mathcal{H}_S)$ in definition 4.2 actually suffices to deduce the non-Markovianity according to Eq. (4.28). Hence, theorem 4.1 can be rephrased in terms of hemispherical enclosing surfaces of an inner point which are

defined according to (see Fig. 4.1 **(b)** for an illustration): A set $\partial\tilde{U}(\rho_S) \subset \mathcal{S}(\mathcal{H})$ not containing ρ_S is said to be a hemispherical enclosing surface of an inner point ρ_S if and only if for any $Y \in \mathcal{E}_0(\mathcal{H}_S)$ there exists exactly one real number $\lambda > 0$ such that either $\rho_S + \lambda Y \in \partial\tilde{U}(\rho_S)$ or $\rho_S - \lambda Y \in \partial\tilde{U}(\rho_S)$ holds (Wißmann, 2012; Liu *et al.*, 2014).

Clearly, enclosing as well as hemispherical surfaces need neither be smooth nor connected which makes the local representation particularly convenient for noisy experiments. Apart from technical improvements for the precise determination of the measure for quantum non-Markovianity, this representation shows that it suffices to sample states locally and that the non-Markovianity of a dynamical process quantified by an information backflow defines a universal feature. The information about the non-Markovianity is thus contained and can be revealed in any part of the state space supporting the intuitive idea that quantum memory effects represent an intrinsic property of the dynamics. In the following section, the local representation and its functioning is illustrated by means of an all-optical setup, where the sampling conception as well as the data analysis and their representation represents a major result of this thesis.

4.3.2 The local representation in an all-optical setup

In order to highlight the relevance and feasibility of the local representation for experiments, it is applied to a photonic process (Liu *et al.*, 2014). The open quantum system is provided by the polarization degree of freedom of a single photon which is coupled to its frequency degree, representing the environment, by virtue of birefringent quartz plates. Unlike in many system-environment models, the system and the environment are thus not assigned to two physical entities but to different degrees of freedom of the same particle. Such a situation is in fact not uncommon for open quantum systems. The electronic degree of freedom of a trapped ion that is coupled to its motional degree of freedom provides another example (Gessner *et al.*, 2014b). Apart from the overall theoretical concept, the sampling conception as well as the data analysis of the experimental results obtained for the photonic process and, finally, their representation constitute the major achievement of this thesis that contributed to the work by Liu *et al.* (2014).

An all-optical setup has the distinguished features that it allows for a controlled system-environment interaction and, in addition, a selective and well-controlled state preparation. Due to this, such a system constitutes an ideal testbed for the study of fundamental aspects of the theory of open quantum systems. In the present experiment, the polarization state undergoes a dephasing process due to the insertion of birefringent quartz plates in the optical path. The differing propagation speed across the quartz plates leads to a coupling between the polarization and frequency degrees of freedom of the photon which finally results in the dephasing of superpositions of vertical and horizontal polarization states. In fact, the dephasing strongly depends on the structure of the frequency spectrum which can be efficiently manipulated by tilting a Fabry-Pérot cavity inserted into the optical path producing a bimodal spectrum as was considered by Liu *et al.* (2011) in the study of non-Markovianity. In the experiment memory effects are thus due to a structured environment representing a typical cause for non-Markovian behavior.

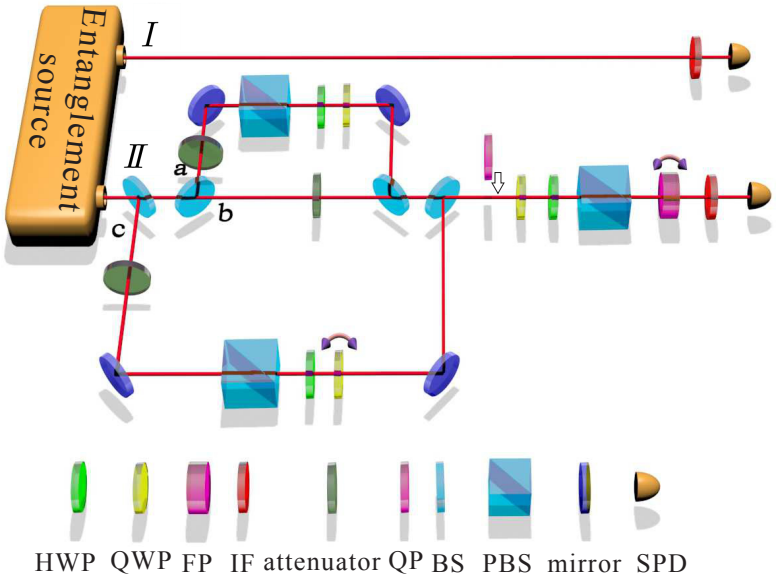

Figure 4.2 – Experimental setup for the studied photonic process. Key to the components: HWP – half-wave plate, QWP – quarter-wave plate, FP – Fabry-Pérot cavity, IF – interference filter, QP – quartz plate, (P)BS – (polarizing) beamsplitter, SPD – single photon detector (cf. Fig. 2 in Liu *et al.* (2014)).

A 0.1 mm thick, fused silica plate (layered with a partial reflecting coating of approximately 80 % reflectivity at 780 nm) now serves as the Fabry-Pérot cavity (FP) in the experiment which is additionally mounted on a rotator enabling to tilt it. The cavity and a consecutively placed interference filter (IF) (FWHM about 3 nm) single out two peaks near 780 nm of width $\sigma = 7.7 \times 10^{11}$ Hz each, which are separated by $\Delta\omega = 7.2 \times 10^{12}$ Hz corresponding to distances of 0.25 nm and 2.34 nm, respectively. While the relative amplitude A_α of the two peaks characterizing the bimodal spectrum depends on the tilt angle α significantly, the other quantities are approximately constant (see Liu *et al.* (2011)). The experimental setup is depicted in Fig. 4.2.

The entanglement source, producing the state $(|H,V\rangle - |V,H\rangle)/\sqrt{2}$ where $|H\rangle$ and $|V\rangle$ denotes the horizontal and vertical polarization states, is given by a pulsed, frequency doubled and mode-locked Ti:sapphire laser (central wavelength 780 nm, pulse duration $2 - 3$ ps with a repetition rate of 76 MHz) that pumps two 1 mm thick β-barium borate (BaB_2O_4 – abbr.: BBO) crystals which are located next to each other. The optic axis of the crystals are in the horizontal plane, but mutually twisted by 180° around the pump direction, so that they make an angle of 48.3° with the pump beam (Niu *et al.*, 2008; Kim, 2003). This special orientation of each of the crystals is also referred to as beamlike type-II phase-matching condition, yielding the particular type-II spontaneous parametric downconversion (SPDC) in any of the crystals (Kurtsiefer *et al.*, 2001; Takeuchi, 2001) where signal-idler photon pairs are emitted as two circular beams rather than two diverging cones as for usual type-II downconversion[7] (cf. Fig. 4.3). It thus follows that beamlike

[7]Such a process is obtained for the slightly larger angle $\theta_{PO} = 49.2°$ between the optic axis and the pump beam.

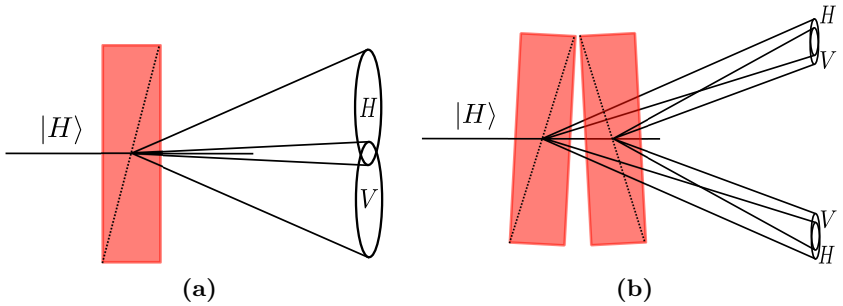

Figure 4.3 – The emission profile, viewed from the top, for type-II **(a)** and beam-like type-II **(b)** spontaneous downconversion processes in single and double crystal configuration, respectively. While the former, corresponding to an angle of 49.2° between the pump beam and the optical axis of the crystal, creates a double cone spatial emission profile of the downconverted photons, the latter emits the signal-idler photon pairs as two circular beams due to type-II phase matching $\theta_{PO} = 48.3°$ for each crystal.

type-II downconversion features a better pair detection efficiency since no small apertures selecting the intersections of the cones are required as for ordinary type-II and type-I SPDC which reduces the brightness of the source (Kim, 2003).

The concatenation of two crystals is then necessary to obtain maximally entangled photon states as a horizontally polarized pump beam only generates polarization product states. More precisely, one obtains photon pairs $|H, V\rangle$ or $|V, H\rangle$ depending on whether the first or the second crystal alone are pumped. Removing possible spatial and time information by means of suitable compensators, the photons created by the two concatenated crystals are solely distinguishable by their polarization, thus yielding the entangled state $(|H, V\rangle + |V, H\rangle)/\sqrt{2}$. By virtue of additional phase retarders such as (tiltable) half-wave plates or quarter-wave plates, any of the four maximally entangled two-qubit Bell state (cf. Eqs. (2.78)–(2.81)) may finally be prepared (Kim, 2003). Note that the generation of nonmaximally entangled states is difficult in this setup since, contrary two type-I downconversion, the weighting factors for each amplitude $|H, V\rangle$ and $|V, H\rangle$ cannot be simply adjusted by changing the polarization of the pump pulse.

The entangled two-photon state is used in the experiment to have a trigger for the single photon in arm *II* whose polarization and frequency degrees of freedom ultimately constitute the open quantum system and its environment. A direct detection of the photon in arm *I* using a single photon detector (SPD) causes photon *II* to be described by the maximally mixed state which represents the basic input for the creation of arbitrary polarization states via the optical setup in part *a*, *b* and *c* (see Fig. 4.2) needed for the sampling process. In fact, any single pure photon polarization state may be obtained in arm *IIc* using a polarizing beam splitter (PBS), a half-wave plate (HWP) and a tiltable quarter-wave plate (QWP) (Kwiat *et al.*, 1999). The transmitted part of photon *II* is again split by a beamsplitter (BS) to generate another pure state (*IIa*) which is finally recombined with the maximally mixed state (*IIb*) and the pure polarization state from arm *IIc* by virtue of several BS. Several tunable attenuators in each arm enable to adjust the relative amplitudes of the three different states. To ensure that the mixture of

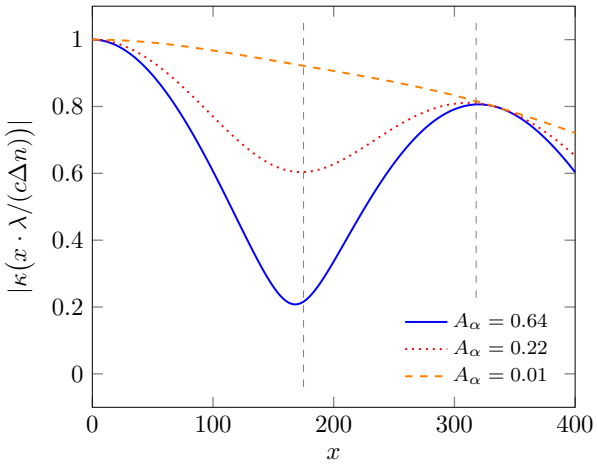

Figure 4.4 – Dynamics of the magnitude of the coherence factor $\kappa(t)$ (cf. Eq. (4.31)) as a function of the effective path difference $c\Delta n \cdot t$ in units of the central wavelength of the FP cavity for three different relative amplitudes of the peaks. The vertical lines indicate 175λ and 318λ which approximately define the minimum and the maximum for all considered values of A_α, respectively.

the three parts is classical, the path difference between each arm is set to about 25 mm, corresponding to a delay of 0.1 ns which is long compared with the single photon coherence length but, of course, shorter than the pulse spacing of the pump laser. The described setup conveniently allows to prepare any reference states as a result of the arms *IIa* and *IIb* together with arbitrary enclosing surfaces whose exact form is controlled by the attenuation of the pure states from arm *IIc* relative to the reference state. It is worth pointing out that the enclosing surfaces thus contain only mixed states unless the mixture is trivial.

After the preparation, photon *II* finally passes through birefringent quartz plates of variable thickness which finally cause the dephasing of superpositions of polarization states as was already discussed in the beginning of this section. The actual state is analyzed by standard single photon polarization state tomography[8] which is indicated by several phase retarders and an SPD at the end of arm *II* in Fig. 4.2. The errors of the state estimation for the experimental data are determined using Monte Carlo methods which depend on the photo counting rate and the integration time (Liu, 2014).

In the polarization basis $\{|H\rangle, |V\rangle\}$, the dynamics of the polarization state is found to obey (Liu *et al.*, 2011) (see also Appendix H)

$$\rho(t) = \begin{pmatrix} \rho_{VV}(0) & \kappa(t)\rho_{VH}(0) \\ \kappa(t)^*\rho_{HV}(0) & \rho_{HH}(0) \end{pmatrix} , \tag{4.30}$$

where the coherence factor is given by the Fourier transform of the photon's frequency distribution which can be well approximated by a sum of two Gaussians

[8]The polarization state of a photon can be reconstructed by maximum likelihood estimation from the photon counts measuring the four polarization bases $|H\rangle$, $|V\rangle$, $|D\rangle = (|H\rangle - |V\rangle)\sqrt{2}$, $|R\rangle = (|H\rangle - i|V\rangle)\sqrt{2}$ (James *et al.*, 2001). These bases single out linearly polarized photons in horizontal, vertical, diagonal (45°) and right-circular sense.

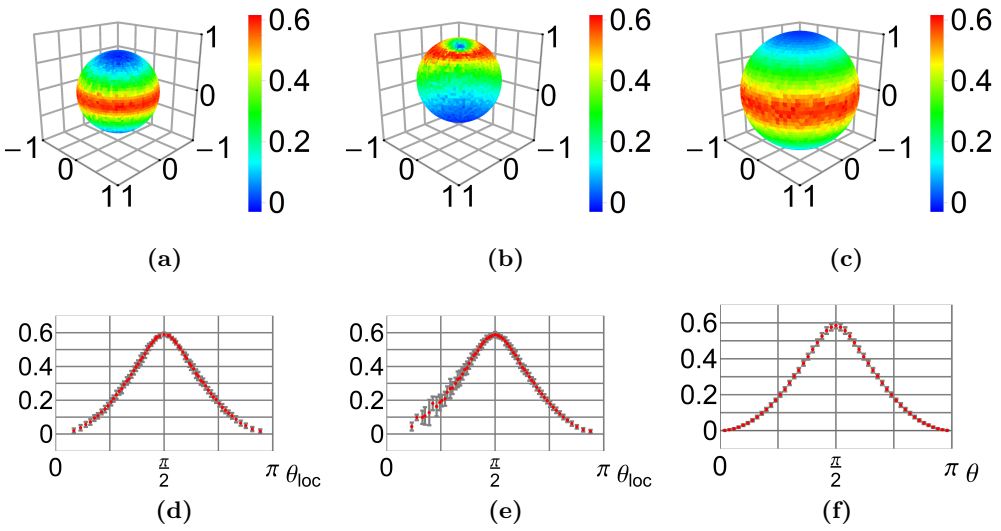

Figure 4.5 – Experimental results for the increase of the trace distance between 175λ and 318λ for a relative amplitude $A_\alpha = 0.64$ and states on the enclosing surface of reference state $\rho_0^{(1)}$ **(a)**, $\rho_0^{(2)}$ **(b)** as well as pairs of orthogonal states **(c)**. The experimental errors, not shown, are of the order of 2×10^{-2}. The corresponding ϕ_{loc}-averaged increase with respect to local spherical coordinates $(\phi_{\mathrm{loc}}, \theta_{\mathrm{loc}})$ is displayed in **(d)**, **(e)** and **(f)** where the error bars show the standard deviations (cf. Fig. 3 in Liu *et al.* (2014)).

corresponding to the peaks singled out by the FP cavity. One thus obtains for the modulus of the coherence factor (Liu *et al.*, 2011)

$$|\kappa(t)| = \frac{\exp\left[-\frac{1}{2}\sigma^2(\Delta n \cdot t)^2\right]}{1 + A_\alpha}\sqrt{1 + A_\alpha^2 + 2A_\alpha \cos(\Delta\omega\Delta n \cdot t)}\ , \tag{4.31}$$

where the birefringence Δn of the quartz used in the experiment is given by 8.9×10^{-3} at 780 nm. Note that the interaction time is related to the thickness L of the quartz plates according to well-known relation $t = L/c$ where c denotes the speed of light. Figure 4.4 shows the dynamics of the modulus of the coherence factor in terms of the effective path difference $L\Delta n$ in units of the central wavelength of the FP cavity ($\lambda = 780$ nm) for the three relative amplitudes $A_\alpha = 0.64$, 0.22 and 0.01, ranging from non-Markovian to Markovian evolutions (see below). It is clear that the experimental setup only allows to scan discrete evolution times as the thickness of the quartz plates cannot be adjusted arbitrarily. The simulated evolution times are finally fixed to 0λ, 75λ, 175λ, 275λ and 318λ where the modulus of the coherence factor increases from 175λ to 318λ for $A_\alpha = 0.64$ and 0.22 which, in addition, define good estimates of the minimal and maximal value of the modulus (cf. Fig. 4.4). It is thus reasonable to associate the degree of non-Markovianity of the three dynamics, which is determined experimentally employing the local representation, to the change of the trace distance between these two lengths of the quartz plates.

The local representation is finally applied to two reference states for the three dynamics characterized by the specified relative amplitudes, and the results are

compared with the outcome for pairs of orthogonal initial states. The two reference states $\rho_0^{(1)}$ and $\rho_0^{(2)}$ are characterized by

$$\mathbf{r}_0^{(1)} = (0.20, \tfrac{1}{2}\pi, \tfrac{13}{50}\pi) \ , \qquad \mathbf{r}_0^{(2)} = (0.88, \tfrac{8}{50}\pi, \tfrac{13}{50}\pi) \ , \tag{4.32}$$

employing the Bloch representation (cf. Sec. 2.2) which allows for a parametrization of the set of polarization states in terms of spherical coordinates $\mathbf{r} = (r, \theta, \phi)$. Reference state $\rho_0^{(1)}$ is thus located inside the equatorial plane, whereas the second reference state lies in the northern hemisphere close to the boundary. As indicated previously, the enclosing surfaces are determined by mixing the reference states and any pure state ρ prepared in arm IIc. The convex combination used in the experiment is set to $0.3 \cdot \rho_0^{(1,2)} + 0.7 \cdot \rho$ and, moreover, a total of 5000 pure states for each reference state are prepared. The associated azimuthal and polar angles (θ and ϕ, respectively), characterizing the pure states completely, are chosen to be on a lattice with equal spacing of $2\pi/100$ (Liu *et al.*, 2014).

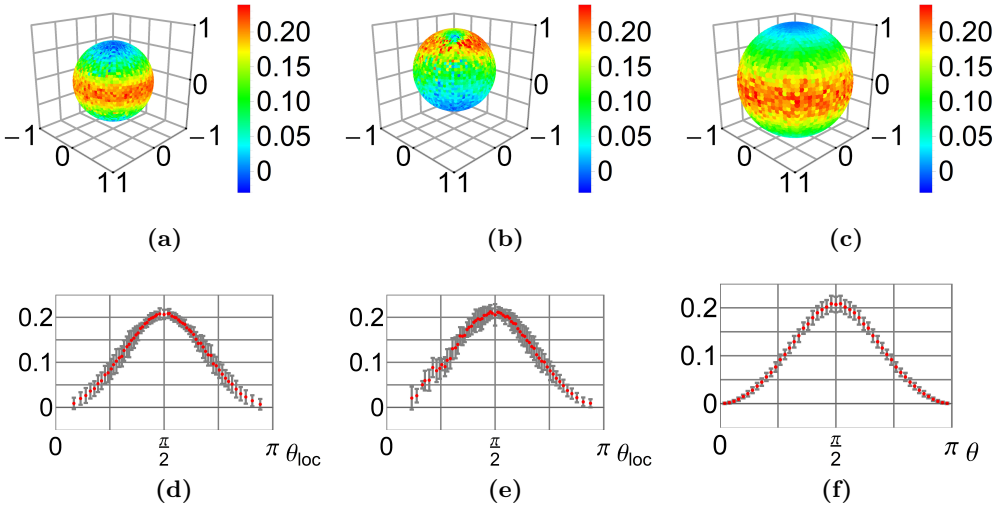

Figure 4.6 – The same as Fig. 4.5 for a relative amplitude $A_\alpha = 0.22$ (cf. Fig. 4 in Liu *et al.* (2014)).

The outcomes of the measurements are presented in Figs. 4.5, 4.6 and 4.7, where the increase of the trace distance between 175λ and 318λ for any state on the enclosing surface for the two reference states is shown in Figs. 4.5 **(a)**–4.7 **(a)** and 4.5 **(b)**–4.7 **(b)** using color coding and omitting the experimental errors, which are of the order of 2×10^{-2}. Note that the colored surfaces in these figures are neither spherical nor centered at the origin. By contrast, Figs. 4.5 **(c)**–4.7 **(c)** show ordinary Bloch spheres representing the measurement outcomes for pairs of orthogonal initial states. The photon count rate and integration time used to measure the reference states as well as orthogonal states and the states of the enclosing surfaces are summarized in Tabs. F.1 and F.2 in Appendix F.

A major result of this thesis is the representation of the experimental data for the reference states with respect to local spherical coordinates. In fact, denoting the spherical coordinates which are defined with respect to local coordinate systems centered at the position of the two reference states by $\mathbf{r}_{\text{loc}} = (r_{\text{loc}}, \theta_{\text{loc}}, \phi_{\text{loc}})$,

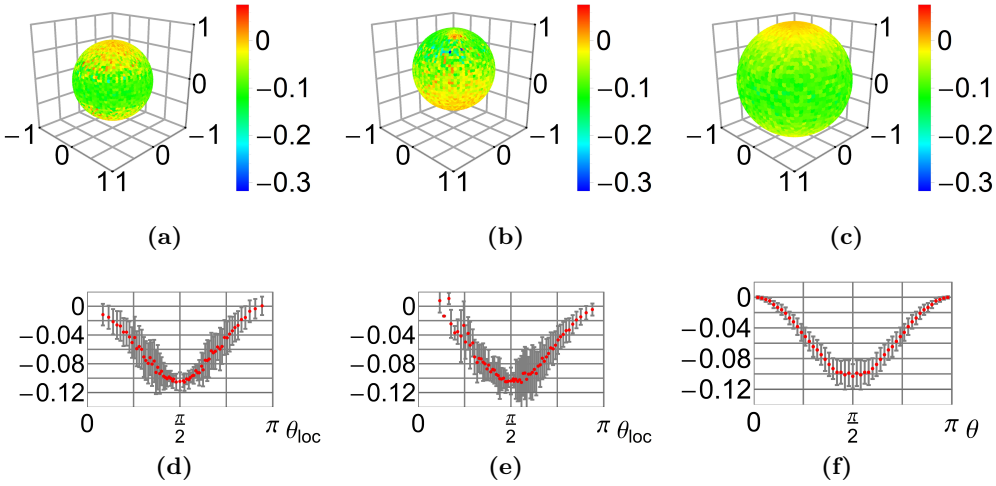

Figure 4.7 – The same as Fig. 4.5 for a relative amplitude $A_\alpha = 0.01$ (cf. Fig. 5 in Liu *et al.* (2014)).

one recovers the polar symmetry present for pairs of orthogonal states as one may see by looking at Figs. 4.5 **(a)**-**(c)**. In this case, it makes sense to average the outcomes over the polar angle ϕ_{loc} along lines of latitude in order to obtain a proper estimate for the degree of non-Markovianity of the process. As the local azimuthal angles are not uniformly distributed with respect to rotations around the z-axis, one must first introduce an appropriate binning on the z-axis before determining the average value. The average increase in any bin is then assigned to the azimuthal angle θ_{loc} associated with the mean z-value in the bin. In addition, one allocates the standard deviation to each of the averaged outcomes which is typically much larger than the averaged experimental errors. The resulting data are depicted in Figs. 4.5 **(d)**–4.7 **(d)** and 4.5 **(e)**–4.7 **(e)**, showing the same characteristics as the ϕ-averaged increase of pairs of orthogonal states displayed in Figs. 4.5 **(f)**–4.7 **(f)**. From these plots one also nicely sees the directional dependence of the trace distance, i.e., the bare dependence on traceless, Hermitian operators corresponding to vectors in Euclidean space.

The maximal increase of the trace distance for the two reference states obtained from the ϕ_{loc}-averaged data as well as for pairs of orthogonal states are given in Tab. 4.1. These values are in very good agreement with the predictions of the theoretical model, which is given by the value of $|\kappa(175\lambda/(c\Delta n)| - |\kappa(318\lambda/(c\Delta n)|$ for the specified parameters, demonstrating the experimental feasibility and the accuracy of the method. Thus, the local representation of the measure can indeed be efficiently applied to an arbitrary neighborhood of a fixed state in the interior of the state space. In particular, apart from illustrating the locality and the universality of the derived representation, the photonic experiment shows that optimal quantum states, featuring the maximal backflow of information, can always be represented by mixed states.

A_α	$\mathcal{N}_{\text{theo}}$	$\mathcal{N}_{\mathbf{(a)}}$	$\mathcal{N}_{\mathbf{(b)}}$	$\mathcal{N}_{\mathbf{(c)}}$
0.64	0.59	0.59 ± 0.01	0.59 ± 0.02	0.59 ± 0.02
0.22	0.21	0.21 ± 0.01	0.21 ± 0.02	0.21 ± 0.02
0.01	0	0.001 ± 0.013	-0.005 ± 0.008	-0.0002 ± 0.0015

Table 4.1 – The degree of quantum non-Markovianity measured by $\mathcal{N}$ for the three dynamics obtained from the averaged experimental data in comparison to the theoretical value determined by $|\kappa(175\lambda/(c\Delta n)| - |\kappa(318\lambda/(c\Delta n)|$ for the specified parameters (cf. Tab. 1 in Liu *et al.* (2014)).

4.4 Generalization of the trace-distance-based measure

This section focuses on the previously mentioned generalization of the trace-distance-based measure for quantum non-Markovianity, representing another major result of the present thesis which was already published in (Wißmann *et al.*, 2015). This extension of the previous approach to non-Markovianity features the very same interpretation as the original trace-distance based measure and provides, in addition, a clear-cut connection to classical Markovian stochastic processes. Furthermore, the associated measure has mathematical features and representations similar to those found for the original approach. That is, optimal initial states for non-Markovian dynamics must again be orthogonal, and the measure also admits an equivalent local representation. The generalized criterion thus combines a physical interpretation of quantum non-Markovianity, an intrinsic definition, showing locality and universality of memory effects, and a relation to the well-known classical definition. A similar approach was already proposed by Chruściński *et al.* (2011), but focusing on divisibility in terms of completely positive maps rather than P-divisibility which turns out to be equivalent to the definition considered here (see Sec. 4.4.1). Hence, CP-divisibility yields only a sufficient condition for this approach to quantum Markovianity, too.

The generalized trace-distance-based approach basically relies on the following natural and interesting generalization of the trace distance: interpreting the prefactor of the trace norm in $\mathcal{D}_T(\rho_1, \rho_2) = \frac{1}{2}\|\rho_1 - \rho_2\|_1$ as unbiased probability distribution, one generalizes the trace distance by allowing for arbitrary probability distributions $\{p_j\}$, i.e., instead of the trace distance one considers the quantity

$$\|p_1\rho_1 - p_2\rho_2\|_1 = \mathrm{Tr}\{|p_1\rho_1 - p_2\rho_2|\} \,, \tag{4.33}$$

which was first considered by Chruściński *et al.* (2011) in the context of non-Markovian dynamics. The Hermitian operator $\Delta = p_1\rho_1 - p_2\rho_2$ is known as Helstrom matrix (Helstrom, 1976; Holevo, 1972) and its trace norm describes the bias in favor for correct state discrimination in a one-shot, two state discrimination problem for states ρ_1 and ρ_2 with a priori probabilities p_1 and p_2, respectively, as was proven in Sec. 2.4.1. Thus, $\|\Delta\|_1$ defines a measure for the distinguishability of the two states, too.

Apart from this interpretation, the trace norm of Helstrom matrices has further properties in common with the trace distance such as the contraction under dy-

namical maps as well as the pairs of states yielding the minimal and maximal value of this quantifier. Clearly, linearity of dynamical maps Φ_{t,t_0} along with the fact that (C)PT-maps define contractions for the trace norm (cf. Eq. (3.82)) implies that

$$\|p_1\Phi_{t,t_0}(\rho_1) - p_2\Phi_{t,t_0}(\rho_2)\|_1 \leq \|p_1\rho_1 - p_2\rho_2\|_1 \tag{4.34}$$

holds for all t and any pair of states. Furthermore, applying the triangle inequality to the trace norm, one finds

$$|p_1 - p_2| \leq \|\Delta\|_1 \leq p_1 + p_2 = 1 \ , \tag{4.35}$$

where the bounds are attained for $\rho_1 = \rho_2$ and $\rho_1 \perp \rho_2$, respectively. This is directly shown by means of the characterization

$$\|\Delta\|_1 = 2\max_{\Pi} \mathrm{Tr}\{\Pi\Delta\} + p_2 - p_1 \ , \tag{4.36}$$

where the maximum is taken over all projection operators Π (see Appendix G for the proof).

A generalized criterion, which still relies on the concept of an information flow, is then obtained by adapting the previous characterization for quantum non-Markovianity (Wißmann *et al.*, 2015; Breuer *et al.*, 2016):

Definition 4.3. *A quantum process $\Phi = \{\Phi_{t,t_0}|t \geq t_0\}$ is said to be Markovian if $\|p_1\Phi_{t,t_0}(\rho_S^{(1)}(t_0)) - p_2\Phi_{t,t_0}(\rho_S^{(2)}(t_0))\|_1$ is a monotonically decreasing function of $t \geq 0$ for all sets $\{p_j, \rho_S^{(j)}(t_0)\}$ with $p_j \geq 0$ so that $p_1 + p_2 = 1$, and states $\rho_S^{(j)}(t_0) \in \mathcal{S}(\mathcal{H}_\mathcal{S})$.*

The associated measure is accordingly given by the summed maximal increase of a Helstrom matrix's trace norm, i.e., it reads

$$\tilde{\mathcal{N}}(\Phi) = \max_{\{p_j,\rho_S^{(j)}\}} \int_{\tilde{\sigma}>0} \mathrm{d}t \ \tilde{\sigma}(t, p_j, \rho_S^{(j)}) \tag{4.37}$$

with

$$\tilde{\sigma}(t, p_j, \rho_S^{(j)}) \equiv \frac{\mathrm{d}}{\mathrm{d}t}\|p_1\Phi_{t,t_0}(\rho_S^{(1)}(t_0)) - p_2\Phi_{t,t_0}(\rho_S^{(2)}(t_0))\|_1 \ , \tag{4.38}$$

where the integration is again constrained to all intervals in which the distinguishability increases. By definition, a process Φ is then said to be non-Markovian (with respect to the generalized criterion) if and only if $\tilde{\mathcal{N}}(\Phi) > 0$.

The previously developed explanation to substantiate the interpretation of quantum memory effects as an information backflow from the environment to the system (cf. Sec. 4.3) also applies here. Similarly to the quantities $\mathfrak{I}_{\mathrm{int}}(t)$ and $\mathfrak{I}_{\mathrm{ext}}(t)$ (cf. Eqs. (4.19) and (4.20) for their definition), one may define

$$\tilde{\mathfrak{I}}_{\mathrm{int}}(t) = \|p_1\rho_S^{(1)}(t) - p_2\rho_S^{(2)}(t)\|_1 \tag{4.39}$$

and

$$\tilde{\mathfrak{I}}_{\mathrm{ext}}(t) = \|p_1\rho_{SE}^{(1)}(t) - p_2\rho_{SE}^{(2)}(t)\|_1 - \tilde{\mathfrak{I}}_{\mathrm{int}}(t) \ , \tag{4.40}$$

representing the distinguishability of the open system at time t and the information on the total system which is not accessible by measurements on the open system only, respectively. By the very same argument for the original approach, one shows that these quantities satisfy

$$\tilde{\mathfrak{I}}_{\text{int}}(t) + \tilde{\mathfrak{I}}_{\text{ext}}(t) = \tilde{\mathfrak{I}}_{\text{int}}(t_0) = \text{const} \ . \tag{4.41}$$

However, the upper bounds for the external information $\tilde{\mathfrak{I}}_{\text{ext}}(t)$ do not allow for a clear interpretation in terms of formation of correlations between system and environment and changes in the environmental states as proven for the trace distance.

4.4.1 Equivalence to P-divisibility

The generalized criterion, still admitting an interpretation in terms of an information flux, has the nice feature that Markovianity is equivalent to P-divisibility of a quantum process as will be shown in the following. By contrast, this feature was only sufficient in the original definition. To show the equivalence, one first recognizes that the set of all Helstrom matrices is isomorphic to the real projective space of Hermitian operators. That is, any Hermitian operator can be written as scalar multiple of a Helstrom matrix.

Lemma 4.1. *For any Hermitian operator X, there exists a real number $\lambda > 0$ and a Helstrom matrix Δ such that $X = \lambda\Delta$.*

Proof. Let $X = X^\dagger$ be given. As the zero operator defines a Helstrom matrix, the trivial case, i.e. $X = 0$, is obviously satisfied for any choice of λ. Moreover, if $X \geq 0$, then $\rho_1 = (\text{Tr}\{X\})^{-1}X$ defines a state so that for $\lambda = \text{Tr}\{X\}$ the Helstrom matrix associated with $p_1 = 1$, $p_2 = 0$ and arbitrary second state ρ_2 proves the claim. Interchanging the roles of ρ_1 and ρ_2 then allows to treat the case $X \leq 0$, too.

Hence, suppose that X is indefinite. Employing the Jordan-Hahn decomposition (cf. lemma G.1), one thus obtains two nonzero and orthogonal operators $Y_1, Y_2 \geq 0$ such that $X = Y_1 - Y_2$ which yields $\text{Tr}\{|X|\} = \text{Tr}\{Y_1\} + \text{Tr}\{Y_2\} > 0$. The operators $\rho_j = (\text{Tr}\{Y_j\})^{-1}Y_j$ associated with Y_j clearly represent states and obey

$$X = \lambda(p_1\rho_1 - p_2\rho_2) \ , \tag{4.42}$$

for $\lambda = \text{Tr}\{|X|\}$ where the parameters p_j are defined as $p_j = \lambda^{-1}\text{Tr}\{Y_j\}$. In fact, these parameters are positive and sum to one by definition, thus, representing a probability distribution which concludes the proof. □

Since dynamical maps Φ_{t,t_0} as well as the trace norm are homogeneous with respect to real positive numbers, i.e., one finds $\|\Phi_{t,t_0}(X)\|_1 = \lambda\|\Phi_{t,t_0}(\Delta)\|_1$ for any Hermitian operator X, it thus suffices to apply Kossakowski's characterization of positivity given by Eq. (3.82) to Helstrom matrices which finally yields the equivalence of the generalized criterion to P-divisibility.

Theorem 4.2. *If the dynamical maps defining a process Φ are bijective, then Φ is Markovian if and only if it is P-divisible.*

Proof. One first notes that $p_1\Phi_{t,t_0}(\rho_S^{(1)}(t_0)) - p_2\Phi_{t,t_0}(\rho_S^{(2)}(t_0)) = \Phi_{t,t_0}(\Delta)$ holds for any probability distribution $\{p_j\}$ and pair of states $\rho_S^{(j)}$ due to linearity. The study of quantum Markovianity thus amounts to consider the time evolution of Helstrom matrices.

Suppose Φ is P-divisible (see definition 3.1). By definition of the intermediate maps $\Lambda_{t,s}$ (cf. Eq. (3.73)) and their positivity, it follows that

$$\|\Phi_{t,t_0}(\Delta)\|_1 = \|\Lambda_{t,s}(\Phi_{s,t_0}(\Delta))\|_1 \leq \|\Phi_{s,t_0}(\Delta)\|_1 \tag{4.43}$$

holds for all $t \geq s \geq t_0$ and Helstrom matrices Δ. Hence, $\|\Phi_{t,t_0}(\Delta)\|_1$ is a monotonically decreasing function of time for any Δ showing that the process Φ is Markovian.

In order to prove the converse, one first notes that the inverse Φ_{t,t_0}^{-1} exists for all $t \geq t_0$ as the dynamical maps are bijective on the set of Hermitian operators by assumption. One thus concludes that the intermediate maps $\Lambda_{t,s}$ exists for all $t \geq s \geq t_0$. Now, let the process be Markovian, i.e., one obtains $\|\Phi_{t,t_0}(\Delta)\|_1 \leq \|\Phi_{s,t_0}(\Delta)\|_1$ for all $t \geq s \geq t_0$ and Helstrom matrices Δ. This inequality may be rewritten as

$$\|\Lambda_{t,s}(\Phi_{s,t_0}(\Delta))\|_1 \leq \|\Phi_{s,t_0}(\Delta)\|_1 \ , \tag{4.44}$$

from which positivity of $\Lambda_{t,s}$ follows employing Kossakowski's criterion (3.82). More specifically, since Φ_{t,t_0} is bijective for all times t, lemma 4.1 along with the homogeneity of dynamical maps and the trace norm pertaining to positive numbers shows that $\Lambda_{t,s}$ defines a contraction with respect to the trace norm for any Hermitian operator. Kossakowski's criterion (3.82) then implies that $\Lambda_{t,s}$ is positive and, therefore, Φ is P-divisible. □

The generalized definition of Markovianity is thus equivalent to P-divisibility of a dynamical process Φ consisting of bijective maps. However, the associated measure (4.37) may be evaluated for any dynamical process independent of the fact that the notion of divisibility may be ill-defined, showing its great benefit. Chruściński *et al.* (2011) introduced a slightly different definition of quantum Markovianity employing Helstrom matrices of a dilated system, given by the open and an ancillary system. They thus considered the dilated process $\Phi_{t,t_0} \otimes I_{\mathcal{H}_A}$ in the same framework so that the definition suggested by Chruściński *et al.* (2011) is equivalent to CP-divisibility. But divisibility of quantum processes in terms of positive maps has a clear-cut connection to classical Markovian stochastic processes as will be shown in the subsequent section, representing an important result of this thesis.

4.4.2 Connections to the classical notion

P-divisible quantum processes provide the distinct feature of having a direct connection to classical Markov processes which can be established employing the characterization of P-divisible processes given in theorem 3.2. To show the connection, suppose that $\rho_S(t)$ denotes the solution of the time-local master equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_S(t) = \mathcal{K}_t\rho_S(t) \tag{4.45}$$

with initial state $\rho_S(t_0)$ where the generator $\mathcal{K}_t$ is in generalized Lindblad form (see Eq. (3.21)). Of course, the time-evolved state admits an instantaneous spectral decomposition

$$\rho_S(t) = \sum_m p_m(t)|\phi_m(t)\rangle\langle\phi_m(t)| \tag{4.46}$$

for any $t \geq t_0$ where $\{|\phi_m(t)\rangle\}$ defines an orthonormal basis on $\mathcal{H}_S$ and $\{p_m(t)\}$ represents a classical probability distribution. By virtue of the orthonormality of the eigenvectors, one shows that the eigenvalues $p_m(t) = \langle\phi_m(t)|\rho(t)|\phi_m(t)\rangle$ obey the closed differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t}p_m(t) = \sum_n \Big[W_{mn}(t)p_n(t) - W_{nm}(t)p_m(t)\Big] \,, \tag{4.47}$$

where the term with $m = n$ obviously drops out and the rates are given by

$$W_{mn}(t) = \sum_j \gamma_j(t)|\langle\phi_m(t)|A_j(t)|\phi_n(t)\rangle|^2 \,. \tag{4.48}$$

Given a solution of a quantum master equation, one thus obtains a classical jump process (cf. Eq. (4.13)). In fact, a quantum master equation and an initial state of the open quantum system uniquely determine a classical time-dependent master equation for the 1-point probability distribution given by the spectrum of the time-evolved state $\rho_S(t)$. Note that the resulting classical equation typically depends on the full information contained in the initial state. That is, the initial eigenbasis $\{|\phi_m(t_0)\rangle\}$ as well as the initial probability distribution $\{p_m(t_0)\}$ influence the rates $W_{mn}(t)$ in general since the solution of the master equation (4.45) is usually not convex. However, for a Lindblad master equation (3.22) obtained in the weak coupling limit with a nondegenerate Hamilton operator $H'_S = \sum_m \epsilon_m|m\rangle\langle m|$, there exists a distinguished basis such that the populations of any state with respect to this basis obey the same differential equation. Indeed, the dynamics of the coherences and the populations with respect to the eigenbasis of H'_S is decoupled, leading to a closed equation[9] for the populations $\langle m|\rho_S(t_0)|m\rangle$ for any initial open system state $\rho_S(t_0)$ (Breuer and Petruccione, 2002).

By comparison of Eq. (4.47) with the evolution equations for classical Markov processes, one concludes that it can be interpreted as Pauli master equation (4.13) for the 1-point probability distribution over the set $I = \{1, \ldots, \dim\mathcal{H}_S\}$ specified by spectrum of the open system states $\rho_S(t)$ if and only if

$$W_{mn}(t) = \sum_j \gamma_j(t)|\langle\phi_m(t)|A_j(t)|\phi_n(t)\rangle|^2 \geq 0 \tag{4.49}$$

holds for all $t \geq t_0$ and $m \neq n$. By virtue of Eq. (3.76), it follows that P-divisibility of the quantum process describes a sufficient condition to warrant positivity of the rates $W_{mn}(t)$ and, therefore, quantum non-Markovianity defined with respect to the generalized trace-distance-based approach allows for a connection to classical Markovian stochastic processes. Indeed, to any P-divisible dynamics, given as the

[9] This equation is also called Pauli master equation in the literature (see, e.g., Breuer and Petruccione (2002)).

solution of a time-local master equation generated by $\mathcal{K}_t$ of the form of Eq. (3.21) with Lindblad operators and rates satisfying constraint (3.76) for an initial state $\rho_S(t_0)$, one associates a classical Markov process that is determined by the solution of the classical master equation (4.47) with transition rates given by Eq. (4.48) and initial condition specified by the eigenvalues of $\rho_S(t_0)$.

As a matter of fact, P-divisibility of a quantum process even becomes necessary for the positivity of the rates $W_{mn}(t)$ if the quantum master equation has the property that the eigenbases $\{|\phi_n(t)\rangle\}$ of the time-evolved states $\rho_S(t)$ run over all orthonormal bases when varying the initial state $\rho_S(t_0)$. This means that all possible bases are encountered in the definition of the rates $W_{mn}(t)$ (cf. Eq. (4.48)) whose positivity is thus equivalent to the process being P-divisible according to theorem 3.2. For finite-dimensional open quantum systems, this condition is obviously satisfied if the maximally mixed state is in the image of the dynamical map Φ_{t,t_0} as any eigenbasis defines a resolution of identity. However, lemma 2.1, which could be proven in Sec. 2.3 of this thesis, also applies in this case since the image of a dynamical map $\mathrm{Im}\Phi_{t,t_0} = \{\Phi_{t,t_0}(\rho_S(t)) \,|\, \rho_S(t_0) \in \mathcal{S}(\mathcal{H}_\mathcal{S})\}$ represents a nonempty, convex and compact[10] set for any finite-dimensional Hilbert space due to linearity of Φ_{t,t_0} and convexity of the state space. It follows that $(1/N_S)\mathbb{1}_{N_S} \in \mathrm{Im}\Phi_{t,t_0}$ where $N_S = \dim\mathcal{H}_S$ is not only sufficient but also necessary to the requirement that any orthonormal basis represents an eigenbasis of some open system state at fixed time t. This is clearly true for the particular class of unital dynamical processes which are characterized by $\Phi_{t,t_0}((1/N_S)\mathbb{1}_{N_S}) = (1/N_S)\mathbb{1}_{N_S}$ for all $t \geq t_0$. However, due to continuity of a process and because $\Phi_{t_0,t_0} = I_{N_S}$ holds by definition, any quantum process actually satisfies this constraint for sufficiently small times.

Given that $(1/N_S)\mathbb{1}_{N_S} \in \mathrm{Im}\Phi_{t,t_0}$ holds for all $t \geq t_0$, one thus concludes that all classical processes derived from the quantum master equation are Markovian if and only if the quantum process is P-divisible. Hence, quantum non-Markovianity with respect to the generalized trace-distance-based measure merges the interpretation in terms of an information flow with a strict relation to divisibility which additionally allows for a clear-cut connection to classical Markovian stochastic processes for the first time. Due to these features, this ansatz for a definition of non-Markovianity is of great relevance for the study of quantum memory effects in the field of complex quantum systems and quantum information. Moreover, its experimental accessibility is further improved by the findings presented in the section.

4.4.3 Expressions for the generalized measure

Having stated the generalized definition for quantum non-Markovianity along with its interpretation and implications, the current section focuses on the expression of the associated measure. More specifically, its mathematical and physical features are addressed in the sequel. To begin with, one considers the maximization procedure contained in the quantifier for non-Markovianity (4.37) which, contrary to the original definition (Breuer *et al.*, 2009), now even requires to sample over

[10] Note that compactness follows from the fact that the state space for any finite-dimensional Hilbert space is compact and the fundamental result that the image of compact sets under continuous maps is again compact. However, this property is not required for lemma 2.1.

binary probability distributions. Fortunately, as a result of this thesis, a similar characterization of pairs of states maximizing Eq. (4.37) can be proven and yet a local representation is obtained simplifying the sampling significantly (see also Wißmann *et al.* (2015)).

Similarly as for the original definition (cf. Sec. 4.3.1), one first introduces the notion of optimality. In fact, one calls a set $\{p_j, \rho_S^{(1,2)}\}$, where $\rho_S^{(1)}$ and $\rho_S^{(2)}$ refer to states and $\{p_j\}$ defines a binary probability distribution, *optimal* if the maximum in Eq. (4.37) is attained for it. Again, the quantum states of an optimal set are necessarily nonequal as the dynamics of the trace norm of a nonindefinite Helstrom matrix under any dynamical map is trivial due to trace preservation and positivity of the map. Note that the reference to the initial time t_0 of a dynamical process is henceforth omitted for convenience. In addition, for a dynamical process consisting of dynamical maps Φ_{t,t_0}, the time-evolved initial state $\rho_S^{(j)}$ will be denoted as $\rho_S^{(j)}(t) = \Phi_{t,t_0}(\rho_S^{(j)})$.

Theorem 4.3. *The states of an optimal set must be orthogonal, i.e.*

$$\tilde{\mathcal{N}}(\Phi) = \max_{\{p_j, \rho_S^{(1)} \perp \rho_S^{(2)}\}} \int_{\tilde{\sigma}>0} \mathrm{d}t \; \tilde{\sigma}(t, p_j, \rho_S^{(j)}) \; . \tag{4.50}$$

Proof. Suppose $\{p_j, \rho_S^{(1,2)}\}$ is optimal but $\rho_S^{(1)} \not\perp \rho_S^{(2)}$. Along the lines of the proof of lemma 4.1, one then obtains a probability distribution $\{q_j\}$ and two orthogonal states $\varrho_S^{(1,2)}$ such that

$$p_1\rho_S^{(1)} - p_2\rho_S^{(2)} = \lambda(q_1\varrho_S^{(1)} - q_2\varrho_S^{(2)}) \tag{4.51}$$

holds, where the real-valued constant λ is given by $\lambda = \|p_1\rho_S^{(1)} - p_2\rho_S^{(2)}\|_1$. As one has $\rho_S^{(1)} \not\perp \rho_S^{(2)}$ by assumption and states of an optimal set are nonequal by definition, it follows from Eq. (4.35) that the parameter's range is given by $0 < \lambda < 1$. By means of linearity of the dynamical maps Φ_{t,t_0} and homogeneity of the trace norm with respect to positive numbers, one thus finds

$$\|q_1\varrho_S^{(1)}(t) - q_2\varrho_S^{(2)}(t)\|_1 = \frac{1}{\lambda}\|p_1\rho_S^{(1)}(t) - p_2\rho_S^{(2)}(t)\|_1 \tag{4.52}$$

for all $t \geq t_0$ where $\lambda^{-1} > 1$. This shows that any increase of $\|p_1\rho_S^{(1)}(t) - p_2\rho_S^{(2)}(t)\|_1$ is exceeded by the increase of $\|q_1\varrho_S^{(1)}(t) - q_2\varrho_S^{(2)}(t)\|_1$. Hence, the set $\{q_j, \varrho_S^{(1,2)}\}$ yields a non-Markovianity strictly larger than $\{p_j, \rho_S^{(1,2)}\}$ contradicting its optimality. □

As for the original trace-distance-based approach, states that feature a maximal backflow of information must initially be perfectly distinguishable, thus having a maximal information content, as a consequence of this result. By virtue of this property, one may moreover establish the analogous local representation for the generalized measure. To this end, one must, however, first prove the following characterization of enclosing surfaces (cf. definition 4.2) (see also Wißmann *et al.* (2015)).

Lemma 4.2. *Let* $\dim\mathcal{H}_S < \infty$. *A set* $\partial U(\rho_S) \subset \mathcal{S}(\mathcal{H}_S)$ *defines an enclosing surface for an inner point* $\rho_S \in \mathring{\mathcal{S}}(\mathcal{H}_S)$ *if and only if for any nonzero, Hermitian and indefinite operator* X *there exists a real number* $\lambda > 0$ *such that* $\lambda|\mathrm{Tr}\{X\}| < 1$ *holds and one has*

$$\frac{1}{p_-}\left\{p_+\rho_S - \mathrm{sgn}(\mathrm{Tr}\{X\})\lambda X\right\} \in \partial U(\rho_S) \ , \tag{4.53}$$

where $p_\pm \equiv \frac{1}{2}(1 \pm \lambda|\mathrm{Tr}\{X\}|)$ *and*

$$\mathrm{sgn}(x) = \begin{cases} -1 \ , & \textit{if } x \leq 0 \\ +1 \ , & \textit{else} \end{cases} \tag{4.54}$$

Proof. First, assume that $\partial U(\rho_S)$ denotes an enclosing surface of an inner point $\rho_S \in \mathring{\mathcal{S}}(\mathcal{H}_S)$. Given a nonzero, Hermitian and indefinite operator X,

$$Y \equiv \mathrm{sgn}(\mathrm{Tr}\{X\})\left[(\mathrm{Tr}\{X\})\,\rho_S - X\right] \tag{4.55}$$

defines a nonzero, Hermitian and traceless operator. By definition of an enclosing surface, there thus exists a real number $\mu > 0$ such that

$$\varrho_S \equiv \rho_S + 2\mu Y \in \partial U(\rho_S) \ . \tag{4.56}$$

One then defines a real number λ by means of the relation

$$\mu = \frac{\lambda}{1 - \lambda|\mathrm{Tr}X|} \ , \tag{4.57}$$

so that $\lambda = \mu/(1 + \mu|\mathrm{Tr}\{X\}|) > 0$ holds which clearly satisfies $\lambda|\mathrm{Tr}\{X\}| < 1$. Defining $p_\pm = \frac{1}{2}(1 \pm \lambda|\mathrm{Tr}\{X\}|)$, one finally obtains

$$\begin{aligned} \varrho_S &= \rho_S + \frac{2\lambda}{1 - \lambda|\mathrm{Tr}\{X\}|} \cdot \left\{\mathrm{sgn}(\mathrm{Tr}\{X\})\left[(\mathrm{Tr}\{X\})\rho_S - X\right]\right\} \\ &= \rho_S - \frac{\lambda}{p_-}\mathrm{sgn}(\mathrm{Tr}\{X\})X + \frac{p_+ - p_-}{p_-}\rho_S \\ &= \frac{1}{p_-}\left\{p_+\rho_S - \mathrm{sgn}(\mathrm{Tr}\{X\})\lambda X\right\} \ , \end{aligned} \tag{4.58}$$

which is Eq. (4.53).

Conversely, suppose that the states in $\partial U(\rho_S)$ are characterized by Eq. (4.53). For a nonzero, indefinite and Hermitian operator X one thus finds a real number $\lambda > 0$ such that $\lambda|\mathrm{Tr}\{X\}| < 1$ holds along with

$$\varrho_S \equiv \frac{1}{p_-}\left\{p_+\rho_S - \mathrm{sgn}(\mathrm{Tr}\{X\})\lambda X\right\} \in \partial U(\rho_S) \ , \tag{4.59}$$

where one has $p_\pm = \frac{1}{2}(1 \pm \lambda|\mathrm{Tr}\{X\}|)$. Now, consider the map

$$\Theta_{\rho_S}(X) \equiv \mathrm{sgn}(\mathrm{Tr}\{X\})\left[(\mathrm{Tr}\{X\})\,\rho_S - X\right] \ , \tag{4.60}$$

being defined on the set of nonzero, Hermitian and indefinite operators. An operator $Y = \Theta_{\rho_S}(X)$ is obviously traceless and Hermitian and, in addition, nonzero

as one has $Y = 0$ if and only if $(\mathrm{Tr}\{X\})\,\rho_s = X$ contradicting the fact that X is indefinite. Upon inserting the definition of the probabilities $p_\pm$, one rewrites Eq. (4.59), using $\mu \equiv \lambda/(2p_-) > 0$, as

$$\begin{aligned}\varrho_S &= \frac{1}{p_-}\left\{p_+\rho_S - \lambda\big[|\mathrm{Tr}\{X\}|\rho_S - Y\big]\right\} \\ &= \frac{p_+ - \lambda|\mathrm{Tr}\{X\}|}{p_-}\rho_S + \frac{\lambda}{p_-}Y \\ &= \rho_S + 2\mu Y \ , \end{aligned} \tag{4.61}$$

which is the form used to define enclosing surfaces. To complete the proof, it remains to show that Θ_{ρ_S} defines a surjection on the set of nonzero, Hermitian and traceless operators. However, this is obviously true as any traceless, nonzero and Hermitian operator Y is necessarily indefinite and Θ_{ρ_S} acts trivially on these operators, i.e. it satisfies $\Theta_{\rho_S}(Y) = Y$. Hence, the set $\partial U(\rho_S)$ indeed defines an enclosing surface. □

In order to derive the local representation for the generalized trace-distance-based measure, it actually suffices that an enclosing surface obeys the characterization (4.53) in terms of nonzero, Hermitian and indefinite operators as is shown now.

Theorem 4.4. *The generalized measure of quantum non-Markovianity $\tilde{\mathcal{N}}$ admits a local representation, i.e.*

$$\tilde{\mathcal{N}}(\Phi) = \max_{\{p_j\},\,\rho_S^{(2)}\in\partial U(\rho_S^{(1)})} \int_{\tilde{\tilde{\sigma}}>0} \mathrm{d}t\ \tilde{\tilde{\sigma}}(t, p_j, \rho_S^{(j)}) \tag{4.62}$$

with

$$\tilde{\tilde{\sigma}}(t, p_j, \rho_S^{(j)}) \equiv \frac{1}{\|p_1\rho_S^{(1)} - p_2\rho_S^{(2)}\|_1} \cdot \frac{\mathrm{d}}{\mathrm{d}t}\|p_1\rho_S^{(1)}(t) - p_2\rho_S^{(2)}(t)\|_1 \ , \tag{4.63}$$

where $\rho_S^{(1)} \in \mathring{\mathcal{S}}(\mathcal{H}_S)$ is any fixed inner point of the state space and $\partial U(\rho_S^{(1)})$ refers to an arbitrary enclosing surface of this state.

Note that $\tilde{\tilde{\sigma}}(t, p_j, \rho_S^{(j)})$ is well-defined for any state $\rho_S^{(2)} \in \partial U(\rho_S^{(1)})$ and probability distribution $\{p_j\}$ because one has $\rho_S^{(2)} \neq \rho_S^{(1)}$ by definition of an enclosing surface and, therefore, $0 < \|p_1\rho_S^{(1)} - p_2\rho_S^{(2)}\|_1$ according to Eq. (4.35).

Proof. Let $\partial U(\rho_S^{(1)})$ be an enclosing surface of an inner point $\rho_S^{(1)}$. Following the proof of theorem 4.3, one shows that the corresponding local representation is smaller than or equal to the original definition (4.50). That is, for a state $\rho_S^{(2)} \in \partial U(\rho_S^{(1)})$ and a probability distribution $\{p_j\}$ there exist two orthogonal states $\varrho_S^{(1)} \perp \varrho_S^{(2)}$ along with a probability distribution $\{q_j\}$ such that

$$p_1\rho_S^{(1)} - p_2\rho_S^{(2)} = \lambda(q_1\varrho_S^{(1)} - q_2\varrho_S^{(2)}) \tag{4.64}$$

holds with $\lambda = \|p_1\rho_S^{(1)} - p_2\rho_S^{(2)}\|_1 > 0$, employing the Jordan-Hahn decomposition (cf. lemma G.1). It then follows that one has

$$\tilde{\tilde{\sigma}}(t, p_j, \rho_S^{(j)}) = \tilde{\sigma}(t, p_j, \varrho_S^{(j)}) \tag{4.65}$$

for all times $t \geq t_0$ due to linearity of dynamical maps, and homogeneity of the trace norm and the derivative. One concludes that the right-hand side of Eq. (4.62) yields a value smaller than or equal to $\tilde{\mathcal{N}}(\Phi)$ as defined in Eq. (4.50).

Conversely, let $\varrho_S^{(1)} \perp \varrho_S^{(2)}$ be two orthogonal states and denote by $\{q_j\}$ a binary probability distribution. The Helstrom matrix $\Delta = q_1\varrho_S^{(1)} - q_2\varrho_S^{(2)}$ defines a nonzero, Hermitian and indefinite operator with $\|\Delta\|_1 = 1$ (see Eq. (4.35)). Thus, according to the characterization of an enclosing surface given in lemma 4.2, there exists a real number $\lambda > 0$ such that $\lambda|\mathrm{Tr}\{\Delta\}| < 1$ holds and one obtains

$$p_+\rho_S^{(1)} - p_-\rho_S^{(2)} = c\lambda\Delta \tag{4.66}$$

for some quantum state $\rho_S^{(2)} \in \partial U(\rho_S^{(1)})$ of the enclosing surface and the probabilities $p_\pm = \frac{1}{2}(1 \pm \lambda|\mathrm{Tr}\{\Delta\}|)$, where the parameter c is given by $c = \mathrm{sgn}(\mathrm{Tr}\{\Delta\})$. As $|c| = 1 = \|\Delta\|_1$, one finds $\|p_+\rho_S^{(1)} - p_-\rho_S^{(2)}\|_1 = \lambda > 0$ so that

$$\tilde{\tilde{\sigma}}(t, p_\pm, \rho_S^{(j)}) = \tilde{\sigma}(t, q_j, \varrho_S^{(j)}) \tag{4.67}$$

follows from linearity of dynamical maps along with homogeneity of the trace norm and the derivative. This shows that the original definition of $\tilde{\mathcal{N}}$ given in Eq. (4.50) leads to a value that is smaller than or equal to the right-hand side of Eq. (4.62) which concludes the proof. □

The maximization over an enclosing surface with an information flux rescaled by the initial distinguishability thus reproduces the memory effects present in pairs of orthogonal states. Based on the careful reformulation of an enclosing surface provided by lemma 4.2, one establishes an equivalent local representation of the generalized trace-distance-based measure showing that the novel characterization of quantum non-Markovianity is also a universal feature that is present everywhere in state space. Clearly, the local representation is indeed completely analogous to that for the original approach (cf. Eq. (4.28), simply replacing the trace distance by the trace norm of the associated Helstrom matrix as one readily sees.

Note that, again, no assumption on the enclosing surface concerning for example the shape or the smoothness is needed implying a great benefit for the analytical, numerical and experimental determination of the generalized measure. Moreover, reviewing the proof of lemma 4.2, one observes that it suffices if the defining relation for an enclosing surface, i.e. Eq. (4.53), holds for exactly one $\mu > 0$ as λ is uniquely determined by this parameter given a nonzero, Hermitian and indefinite operator. The further reduction to hemispherical surfaces (cf. Fig. 4.1 **(b)**), which was shown to be possible for the local representation of the original definition, cannot be deduced from the lemma's proof though. Apparently, biased probability distributions break the simple symmetry which is at the heart of hemispherical surfaces.

4.4.4 A paradigmatic model

The generalized definition is finally illustrated by means of examples which show the difference to the original characterization and other approaches to quantum non-Markovianity. Summarizing the results on the extended measure, the most important feature is that P-divisibility defines no longer solely a sufficient criterion for Markovianity. This fact is particularly apparent when uniform translations of states are encountered in the dynamics which do not describe positive maps but leave the trace distance unchanged (Liu *et al.*, 2013b). However, this insensitivity is cured choosing unequal weights p_j for the states, thus making it possible to expose this property of a dynamical process by virtue of the generalized definition.

To illustrate this effect, one considers a two-level open quantum system, i.e. $\mathcal{H}_S = \mathbb{C}^2$, undergoing the two-stage dynamics that is composed of an isotropic contraction of the state space followed by a uniform translation along the z-axis employing the Bloch representation (see Fig. 4.8). This kind of dynamics, which is assumed to range from t_0 to t_2 where the latter might be infinite, is described by a time-local master equation such as Eq. (4.45) with a generator $\mathcal{K}_t$ obeying

$$\mathcal{K}_t\rho_S(t) = \sum_{j=1}^{3} \frac{\gamma(t)}{4} \left[\sigma_j \rho_S(t) \sigma_j - \rho_S(t)\right] \tag{4.68}$$

for $t_0 \leq t \leq t_1 < t_2$ and

$$\begin{aligned} \mathcal{K}_t\rho_S(t) =& \frac{-b(t)}{2} \left[\sigma_- \rho_q S(t) \sigma_+ - \tfrac{1}{2}\{\sigma_+\sigma_-, \rho_S(t)\}\right] \\ &+ \frac{b(t)}{2} \left[\sigma_+ \rho_S(t) \sigma_- - \tfrac{1}{2}\{\sigma_-\sigma_+, \rho_S(t)\}\right] \end{aligned} \tag{4.69}$$

if $t_1 < t \leq t_2$ holds. Here, $\sigma_{+(-)}$ refers to the usual raising (lowering) operator with respect to the eigenstates $|j = 0, 1\rangle$ of the Pauli spin operator σ_3, and the rates $\gamma(t)$ and $b(t)$ are chosen to be positive for all t in their respective domains. Thus, the second phase of the process is neither CP- nor P-divisible. More specifically, for the eigenstates $|j\rangle$ one finds $(b(t)/2) \cdot \{|\langle 0|\sigma_+|1\rangle|^2 - |\langle 0|\sigma_-|1\rangle|^2\} = -b(t)/2 < 0$ for any $t \geq t_0$ thus violating condition (3.76) for P-divisibility[11] according to theorem 3.2. It is worth mentioning that this two-staged dynamical process exhibits the essential feature of the generalized amplitude damping channel studied by Liu *et al.* (2013b).

Returning to the Bloch representation, the present master equation is equivalently described by the following differential equation for the Bloch vector,

$$\frac{\mathrm{d}}{\mathrm{d}t}\vec{v}(t) = \begin{cases} A(t)\vec{v}(t)\ , & t_0 \leq t \leq t_1 < t_2 \\ \vec{b}(t)\ , & t_1 \leq t \leq t_2 \end{cases} \tag{4.70}$$

where one has $A(t) = \mathrm{diag}(-\gamma(t), -\gamma(t), -\gamma(t))$ and $\vec{b}(t) = \big(0, 0, b(t)\big)^T$. Hence, during the process' first phase the Bloch ball $B_1 = \{\vec{v}\,|\,\|\vec{v}\| \leq 1\}$ is isotropically contracted to the smaller ball $B_r = \{\vec{v}\,|\,\|\vec{v}\| \leq r\}$ with radius

$$r = \exp\left[-\int_{t_0}^{t_1} \mathrm{d}s\, \gamma(s)\right] \in (0, 1)\ , \tag{4.71}$$

[11] Obviously, the process is already not CP-divisible as a rate of $\mathcal{K}_t$ for $t \geq t_1$ is negative.

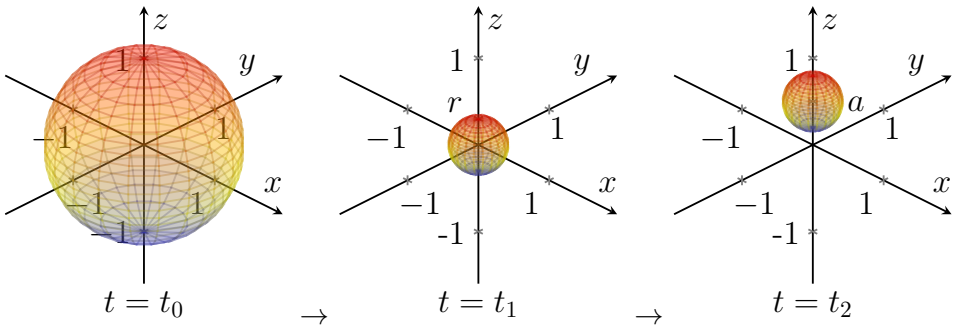

Figure 4.8 – Bloch sphere representation of the action of the dynamical map generated by the time-local generator $\mathcal{K}_t$ given in Eqs. (4.68) and (4.69) for the three times $t = t_0, t_1$ and t_2 (cf. Fig. 2 in (Wißmann *et al.*, 2015)).

which clearly is CP-divisible and therefore Markovian. Finally, the Bloch vectors are mapped to $\vec{v}(t_1) \mapsto \vec{v}(t_1) + \vec{a}(t)$ in the subsequent second phase where

$$\vec{a}(t) \equiv \big(0, 0, a(t)\big)^T \,, \qquad \text{with} \qquad a(t) = \int_{t_1}^{t} \mathrm{d}s\, b(s) > 0 \,, \tag{4.72}$$

thus corresponding to a uniform translation of the shrunk Bloch ball along the positive z-axis as mentioned before. Note that one must require $a(t_2) \leq 1 - r$ in order to maintain positivity of the dynamical map (cf. Fig. 4.8). It is easily shown that this condition is also necessary and sufficient for complete positivity of the process.

For two quantum states $\rho_S^{(1,2)} = \frac{1}{2}(\mathbb{1}_2 + \vec{v}_{1,2} \cdot \vec{\sigma})$ evolving according to the described dynamical map, the trace norm of the Helstrom matrix $\Delta = p_1\rho_S^{(1)} - p_2\rho_S^{(2)}$ at time t is found to obey

$$\|\Delta(t)\|_1 = \frac{1}{2}\{|p_1 - p_2 + \|\vec{w}(t)\|\,| + |p_1 - p_2 - \|\vec{w}(t)\|\,|\} \,, \tag{4.73}$$

where $\vec{w}(t) = p_1\vec{v}_1(t) - p_2\vec{v}_2(t)$. If the probability distribution is chosen as $p_1 = p_2 = 1/2$, then one has $\|\Delta(t)\|_1 = \frac{1}{2}\|\vec{v}_1(t) - \vec{v}_2(t)\|$, from which it is immediately clear that the original definition is unable to detect the non-Markovianity of the process resulting from the uniform translation.

Without loss of generality, one may assume $p_1 \geq p_2$ so that the trace norm of the Helstrom matrix is given by

$$\|\Delta(t)\|_1 = \begin{cases} p_1 - p_2 \,, & \text{if } p_1 - p_2 > \|\vec{w}(t)\| \\ \|\vec{w}(t)\| \,, & \text{if } p_1 - p_2 \leq \|\vec{w}(t)\| \,. \end{cases} \tag{4.74}$$

Due to theorem 4.3, one may furthermore restrict considerations to orthogonal states corresponding to antipodal unit vectors. That is, the Bloch vectors obey $\vec{v}_1 = -\vec{v}_2$ with $\|\vec{v}_1\| = 1$ which implies

$$\vec{w}(t) = \begin{cases} \vec{v}_1(t) \,, & \text{if } t_0 \leq t \leq t_1 \\ \vec{v}_1(t_1) + (p_1 - p_2)\,\vec{a}(t) \,, & \text{if } t_1 < t \leq t_2 \end{cases} \tag{4.75}$$

as $p_1+p_2=1$. It follows that $\|\Delta(t)\|_1$ is a monotonically decreasing function of t if the probability distribution is such that $p_1-p_2\geq\|\vec{w}(t)\|$ holds for all $t_1\leq t\leq t_2$. However, if this is not true so that in particular $\|\vec{v}_1(t_1)\|\leq p_1-p_2<\|\vec{w}(t_2)\|$ holds, then one deduces

$$\int_{\tilde{\sigma}>0}\mathrm{d}t\;\tilde{\sigma}(t)=\|\vec{w}(t_2)\|-(p_1-p_2)>0\;, \tag{4.76}$$

indicating non-Markovianity. The change of the trace norm is shown to increase with decreasing difference p_1-p_2, attaining its maximal value for $p_1-p_2=r=\|\vec{v}_1(t_1)\|$. In addition, the change of the trace norm for $p_1-p_2\leq r$ is given by

$$\|\Delta(t_2)\|_1-\|\Delta(t_1)\|_1=\|\vec{v}_1(t_1)+(p_1-p_2)\,\vec{a}(t_2)\|-\|\vec{v}_1(t_1)\|\;, \tag{4.77}$$

which is maximized if $p_1-p_2=r$ and $\vec{v}_1(t_1)$ is parallel to $\vec{a}(t_2)$, i.e., if one has $\vec{v}_1(t_1)=c\,\vec{a}(t_2)$ for some[12] $c>0$, leading to

$$\|\Delta(t_2)\|_1-\|\Delta(t_1)\|_1=r\cdot a(t_2)\;. \tag{4.78}$$

Obviously, the constraint on the probability distribution can only be satisfied by choosing $\{p_j\}=\{p_\pm=\frac{1}{2}(1\pm r)\}$ and the maximizing Bloch vector is given by $\vec{v}_1=(0,0,1)^T$ as the associated state must be pure. This simple example thus shows that, unlike the original definition, the generalized trace-distance-based measure is able to capture memory effects arising from uniform translations contained in the dynamical process.

The dynamics generated by $\mathcal{K}_t$ for $t_0\leq t\leq t_1$ (see Eq. (4.68)) for arbitrary final time t_1 provides yet the basis for a process highlighting the persistent difference between the trace-distance-based approach and its generalization compared to those that rely on CP-divisibility. Choosing the rates according to $\gamma_1(t)=\gamma_2(t)=1$ and $\gamma_3(t)=-\tanh(t)$ as proposed by Hall *et al.* (2014), the associated dynamical process is not CP- but P-divisible. Clearly, the former is not true due to theorem 3.2 as γ_3 is negative. In particular, there exists even no single interval for which CP-divisibility is restored as one has $\gamma_3(t)<0$ for all $t>t_0$ motivating the nomination "eternal non-Markovianity" (cf. Hall *et al.* (2014)). Another example featuring this property has been found by Vacchini *et al.* (2011). However, the dynamics is always P-divisible since

$$\Big(\sum_{j=0}^{1}|\langle m|\sigma_j|n\rangle|^2\Big)-\tanh(t)|\langle m|\sigma_3|n\rangle|^2 \tag{4.79}$$

is shown to be larger or equal to zero for all times $t\in[t_0,t_1]$ and unequal indices $m\neq n$ which is condition (3.76) of theorem 3.2. Hence, the trace-distance-based measure as well as its generalization are equal to zero for this dynamics, whereas measures for non-Markovianity that rely on CP-divisibility such as the proposals of Rivas *et al.* (2010), Chruściński *et al.* (2011) and Hall *et al.* (2014) do not vanish. This random unitary evolution (Vacchini, 2012; Chruściński and Wudarski, 2013) thus illustrates the persisting and significant difference between these two major approaches for the characterization of quantum non-Markovianity.

[12] From the relation $\vec{v}_1(t_1)=c\,\vec{a}(t_2)$ and $\|\vec{v}_1(t_1)\|=r$, one obtains $c=r/a(t_2)$ which amounts to $c\geq r/(1-r)$ since the function $a(t)$ must satisfy $a(t_2)\leq 1-r$.

4.5 Non-Markovianity of mixtures of dynamical processes

After having defined Markovian or non-Markovian dynamics leading to a partitioning of dynamical processes, it is natural to address the properties of the respective sets of processes which improves the understanding of memory effects. In particular, the convexity of these sets is an interesting problem as usual in quantum theory and because it proves or disprove the intuitive idea of the effect of mixing processes with or without memory. That is, one assumes, e.g., the convex mixture of two processes Φ and Φ' lacking memory to yield another Markovian process as there is no reason at first glance to interpret the mixing as a creation of memory effects. The study of convexity of the sets of Markovian and non-Markovian dynamical processes has already been addressed by Chruściński and Wudarski (2015) and Wudarski and Chruściński (2016). In fact, it has been shown by these authors by means of two examples that the mixing of CP-divisible processes may result in a solely P-divisible process (Chruściński and Wudarski, 2015) and that a CP-divisible dynamical process can be created out of the convex combination of non-P-divisible processes (Wudarski and Chruściński, 2016). As a result of this thesis, it is furthermore demonstrated that the mixture of CP-divisible processes may surprisingly result in a non-P-divisible process, too, thus showing that memory effects with respect to the generalized trace-distance-based approach can indeed be created by mixing Markovian dynamics. In the following, the three examples demonstrating the mentioned properties, i.e., that the set of CP-divisible processes is not convex with respect to P-divisible and non-P-divisible processes which, in addition, is shown to be neither convex by itself, are presented. For convenience, they are enumerated by ①, ② and ③, respectively.

① By means of a model closely related to the particular random unitary evolution studied in the preceding section, Chruściński and Wudarski (2015) have shown that CP-divisible processes are not convex with respect to the set of P-divisible maps (see also Wudarski and Chruściński (2016)). In fact, the unbiased convex combination of the semigroup dynamics for two-level systems generated by

$$\mathcal{K}_L^{(j)}\rho_S(t) = \frac{\gamma}{2}\big(\sigma_j\rho_S(t)\sigma_j - \rho_S(t)\big) \tag{4.80}$$

with a positive rate γ, yields a dynamical map $\Phi_{t,0} \equiv (1/2)\cdot\{\Phi_{t,0}^{(1)} + \Phi_{t,0}^{(2)}\}$ that is given by

$$\Phi_{t,0}(\rho_S) = \frac{1+e^{-\gamma t}}{2}\,\rho_S + \frac{1-e^{-\gamma t}}{4}\left(\sigma_1\rho_S\sigma_1 + \sigma_2\rho_S\sigma_2\right). \tag{4.81}$$

These dynamical maps are readily seen to describe the dynamics induced by the generator (4.68) for rates $\gamma_1(t) = \gamma_2(t) = \gamma/2$ and $\gamma_3(t) = -(\gamma/2)\tanh(\gamma t)$ exhibiting "eternal non-Markovianity" (Wudarski and Chruściński, 2016). However, the results of the previous section may also be applied directly, showing that this dynamical process is again P- but not CP-divisible.

② As indicated before, the convex combination of two semigroup dynamics may also result in a dynamical process that is even not P-divisible as is shown as

a result of this thesis, implying that the set of P-divisible and thus of Markovian processes is not convex. In fact, consider again a two-dimensional open quantum system along with two dynamical processes described by the generators in Lindblad form

$$\tilde{\mathcal{K}}_L^{(k)}\rho_S(t) = -i\Big[\frac{\lambda_k}{2}\sigma_3, \rho_S(t)\Big] + \frac{\gamma_k}{2}\big(\sigma_3\rho_S(t)\sigma_3 - \rho_S(t)\big) \tag{4.82}$$

for an arbitrary real-valued constant λ_k and positive rates γ_k. The corresponding dynamical processes for initial time $t_0 = 0$ are given by

$$\tilde{\Phi}_{t,0}^{(k)} = \mu_k(t) I_S + \big(1 - \mu_k(t)\big) \sum_{j=0}^{1} \mathfrak{S}_{|j\rangle\langle j|} \ , \tag{4.83}$$

where $\mu_k(t) = \exp[-(\gamma_k + i\lambda_k)t]$ and $\mathfrak{S}_{|j\rangle\langle j|}$ defines the projection superoperator on the eigenstate $|j\rangle$ of the Pauli spin operator σ_3, i.e., it obeys $\mathfrak{S}_{|j\rangle\langle j|}\rho_S = |j\rangle\langle j|\rho_S|j\rangle\langle j|$. This process describes a spiraling damping towards the z-axis in the Bloch picture with oscillation frequency λ_k, whereas the damping rate is given by γ_k. The convex combination $\tilde{\Phi}_{t,0} \equiv p\tilde{\Phi}_{t,0}^{(1)} + (1-p)\tilde{\Phi}_{t,0}^{(2)}$ for $0 \leq p \leq 1$ then leads to the time evolution of an open system state $\rho_S = (\rho_{S,jk} = \langle j|\rho_S|k\rangle) \in \mathcal{S}(\mathbb{C}^2)$ according to

$$\tilde{\Phi}_{t,0}(\rho_S) = \begin{pmatrix} \rho_{S,11} & \kappa(t)\rho_{S,10} \\ \kappa^*(t)\rho_{S,10}^* & \rho_{S,00} \end{pmatrix} \ , \tag{4.84}$$

where $\kappa(t) = p\mu_1(t) + (1-p)\mu_2(t)$. As Fig. 4.9 shows, the coherence factor $\kappa(t)$ has an oscillating modulus for certain choices of the parameters λ_k and γ_k, indicating an increasing trace distance[13] and, thus, non-Markovian dynamics. The necessary violation of P-divisibility also follows from theorem 3.2 as the rate $\gamma(t) = -\mathrm{Re}\big(\dot{\kappa}(t)/\kappa(t)\big)$ of the corresponding time-local generator, having the form (4.82) with [14] $\lambda(t) = -\mathrm{Im}\big(\dot{\kappa}(t)/\kappa(t)\big)$, is temporarily negative as can, e.g., be seen in Figs. 4.9 **(c)** and **(d)**. Hence, one concludes that memory effects can apparently be created by mixing two Markovian processes disproving the basic intuition about non-Markovianity.

③ Finally, Wudarski and Chruściński (2016) have shown that the set of non-P-divisible processes is not convex which one can easily imagine as the information backflow of two non-Markovian dynamics could be compensated when mixing two processes, thus resulting in a Markovian dynamics. In order to obtain an example showing this effect, Wudarski and Chruściński (2016) considered a set of projections $\Pi = \{\Pi_m\}_{m\in I'}$ defining a discrete resolution of identity. The associated superoperator $\hat{\mathfrak{S}}_\Pi \equiv \sum_{m\in I'} \mathfrak{S}_{\Pi_m}$ is completely positive and satisfies $\hat{\mathfrak{S}}_\Pi^2 = \hat{\mathfrak{S}}_\Pi$. In addition, it may be used to define a generator in Lindblad form according to

$$\mathcal{K}_L^\Pi \rho_S(t) = \Big[\hat{\mathfrak{S}}_\Pi - I_S\Big]\rho_S(t) = \sum_{m\in I'} \Pi_m\rho_S(t)\Pi_m - \rho_S(t) \ , \tag{4.85}$$

[13] Note that the trace distance of an orthogonal pair of states that is part of the equatorial plane in the Bloch picture is given by $|\kappa(t)|$.

[14] The shorthand logogram $\dot{\kappa}(t)$ represents the derivative with respect to t, i.e. $\dot{\kappa}(t) \equiv \frac{\mathrm{d}}{\mathrm{d}t}\kappa(t)$.

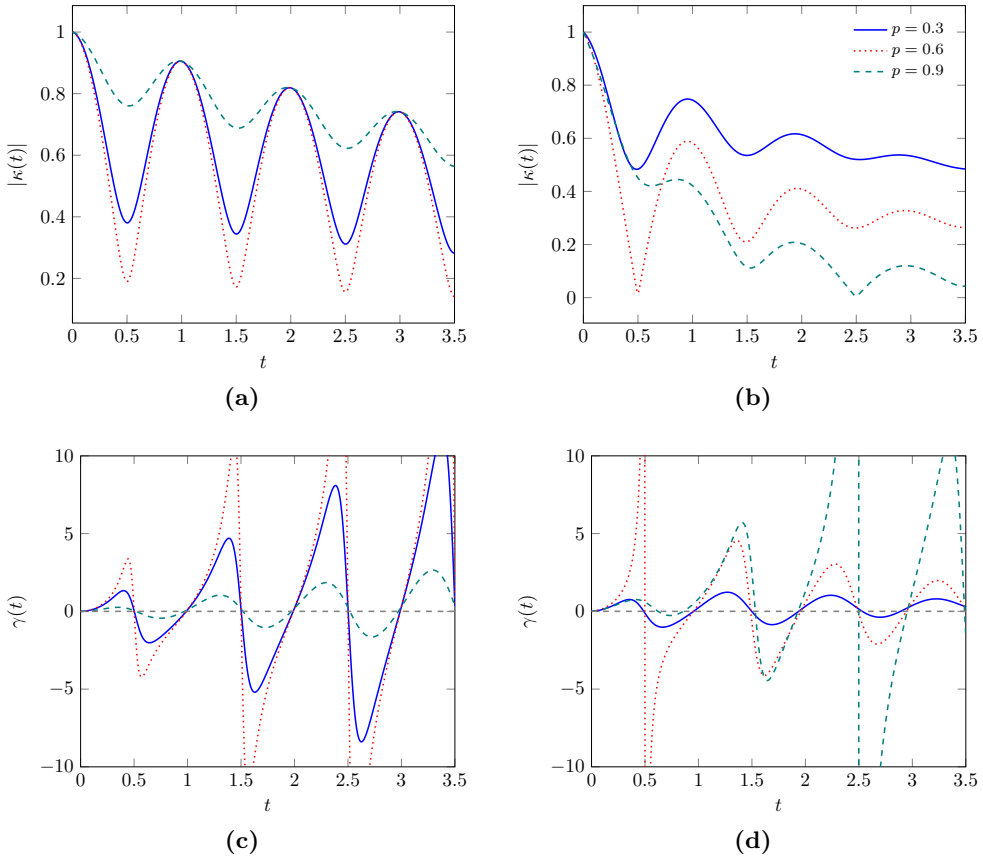

Figure 4.9 – The convex combination of two semigroup dynamics $\tilde{\Phi}_{t,0}^{(k)}$ defined by Eq. (4.83) yields a non-P-divisible dynamics as demonstrated by a nonmonotonic behavior of the modulus of the coherence factor $\kappa(t)$ or, equivalently, the (temporal) negativity of the rates $\gamma(t) = -\mathrm{Re}\big(\dot{\kappa}(t)/\kappa(t)\big)$ for γ_1=0.1 **(a)** & **(c)** and $\gamma_1 = 1$ **(b)** & **(d)** for several values of p. The other parameters are given by $\gamma_2 = 0.1$, $\lambda_2 = 2\pi$ and $\lambda_1 = 0$ in all plots.

having a single decay rate equal to unity for all channels. The dynamical semigroup that are generated by $\gamma\,\mathcal{K}_L^{\Pi}$ for some positive rate γ is found to be given by

$$\hat{\Phi}_{t,0} = \exp\left[\gamma t\,\mathcal{K}_L^{\Pi}\right] = e^{-\gamma t} I_S + (1 - e^{-\gamma t})\hat{\mathfrak{S}}_{\Pi}\ , \tag{4.86}$$

which can be written as convex combination $(0 < p < 1)$

$$\hat{\Phi}_{t,0} = p\,\hat{\Phi}_{t,0}^{(1)} + (1-p)\hat{\Phi}_{t,0}^{(2)} \tag{4.87}$$

of two dynamical maps $\hat{\Phi}_{t,0}^{(k)}$ induced by time-local generators $\gamma_k(t)\mathcal{K}_L^{\Pi}$ with time-dependent rates as Wudarski and Chruściński (2016) have shown. In fact, to warrant complete positivity of $\hat{\Phi}_{t,0}^{(k)} = \mu_k(t) I_S + [1 - \mu_k(t)]\hat{\mathfrak{S}}_{\Pi}$, the integrated rates $\Gamma_k(t) = \int_0^t \mathrm{d}s\,\gamma_k(s)$ must be positive which is equivalent to $0 < \mu_k(t) \equiv \exp[-\Gamma_k(t)] \leq 1$. Clearly, rates $\gamma_k(t)$ that are temporarily negative may also satisfy this condition thus yielding processes that are neither CP- nor P-divisible since

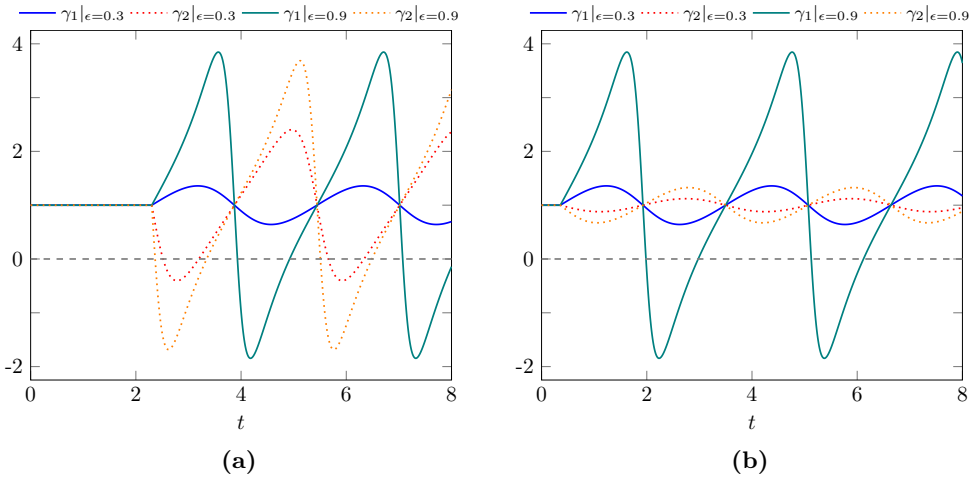

Figure 4.10 – Plot of the decay rates γ_1 (solid) and γ_2 (dotted) (cf. Eq. (4.91)) for $g(t)$ given by Eq. (4.90) with $\gamma = 1$ and several values of p and ϵ. The rates for $p = 0.9$ with $\epsilon = 0.9$ and $\epsilon = 0.3$ are depicted in **(a)** whereas **(b)** corresponds to $p = 0.3$ for values $\epsilon = 0.9$ and $\epsilon = 0.3$ (see also Fig. 1 in Wudarski and Chruściński (2016) for a different choice of the parameters).

there is only a single decay rate (cf. theorem 3.2). From the convex combination (4.87) one obtains the relation

$$e^{-\gamma t} = p\mu_1(t) + (1-p)\mu_2(t) \;, \tag{4.88}$$

which is for example satisfied by (Wudarski and Chruściński, 2016)

$$\mu_k(t) = \begin{cases} e^{-\gamma t} \;, & t \in [0, t_*] \\ e^{-\gamma t}\, \frac{1+(-1)^k\{1-2g(t)\}}{1+(-1)^k(1-2p)} \;, & t > t_* \end{cases} \tag{4.89}$$

where $t_* = (-1/\gamma)\ln(1-p)$ and the function $g(t)$ obeys

$$g(t) = p\left[1 - \epsilon \sin^2\big(\gamma(t-t_*)\big)\Theta(t-t_*)\right] \tag{4.90}$$

for $0 < \epsilon < 1$ and Θ denotes the Heaviside step function. Note that $\mu_k(0) = 1$ follows from $\hat{\Phi}^{(k)}_{0,0} = I_S$ and the exponential decay for $t \leq t_*$ finally guarantees that $0 < \mu_2(t) \leq 1$ holds as one has $g(t) \in (0, p]$. The corresponding decay rates are easily shown to be given by

$$\gamma_k(t) \equiv -\frac{\dot{\mu}_k(t)}{\mu_k(t)} = \gamma + (-1)^k \frac{\dot{g}(t)}{\frac{1}{2} + (-1)^k\{\frac{1}{2} - g(t)\}} \;, \tag{4.91}$$

which can be negative for some time and particular choices of parameters indicating non-Markovian behavior, irrespective of whether CP- or solely P-divisibility is used to define quantum Markovianity (see Fig. 4.10). In fact, choosing $\epsilon = p = 0.9$ and $\gamma = 1$, both rates $\gamma_k(t)$ are negative for some interval in time which shows that the semigroup dynamics $\hat{\Phi}$ (cf. Eq. (4.87)) can be obtained by mixing two non-P-divisible processes.

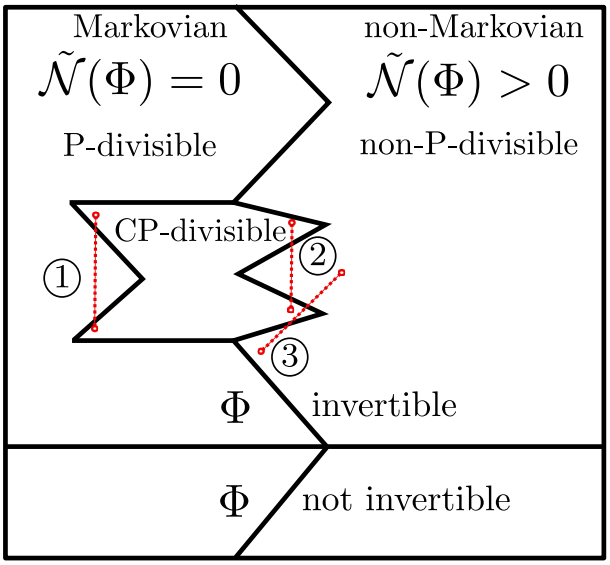

Figure 4.11 – Illustration of the set of dynamical processes and its subsets updating the schematic picture given by Breuer *et al.* (2016) (cf. Fig. 4 therein).

Summarizing, the set of non-Markovian processes characterized by $\tilde{\mathcal{N}}(\Phi) > 0$ as well as that of Markovian processes with its subset of CP-divisible dynamics are nonconvex as there exist examples showing that the convex combination of two

① CP-divisible processes gives a P-divisible but non-CP-divisible process.

② CP-divisible processes gives a non-P-divisible process.

③ non-P-divisible processes gives a CP-divisible process.

This is schematically depicted in Fig. 4.11 providing an update in view of the results ① and ② of the illustration of the set of dynamical processes given by Breuer *et al.* (2016) (cf. Fig. 4 therein). It remains open whether the mixing of P-divisible but not CP-divisible processes may also yield a non-Markovian process $\tilde{\mathcal{N}}(\Phi) > 0$ as indicated in Fig. 4.11. Further studies on this topic might clear this question.

Chapter 5

Nonlocal memory effects

The preceding section has shown that memory effects may be obtained by mixing two memoryless dynamical processes and, similarly, the convex combination of two non-Markovian dynamics can result in a process without memory. Apart from mixing dynamical processes, the additivity of memory effects with respect to the number of particles defining the open quantum system is an interesting topic. The influence of scaling up the number of particles is for example a central task in quantum information processing. Concerning quantum non-Markovianity, this question was studied by Addis *et al.* (2013, 2014) and Fanchini *et al.* (2013) for several approaches to quantify memory effects on the basis of particular models.

Here, the closely related problem of non-Markovian behavior for bipartite open quantum system obtained via local interactions is considered. That is, one studies the dynamics of a composite system which is described by

$$\begin{aligned}\rho_S^{(12)}(t) &= \Phi_{t,t_0}^{(12)}(\rho_S^{(12)}(t_0)) \\ &= \mathrm{Tr}_E\left\{U_{SE}^{(12)}(t,t_0)\rho_S^{(12)}(t_0)\otimes\rho_E^{(12)}(t_0)U_{SE}^{(12)^\dagger}(t,0)\right\}\,, \end{aligned} \tag{5.1}$$

where the joint unitary operator obeys $U_{SE}^{(12)}(t,t_0) = U_{SE}^{(1)}(t,t_0)\otimes U_{SE}^{(2)}(t,t_0)$ with local unitaries $U_{SE}^{(j)}(t,t_0)$ representing the local interaction between the open system S_j and its environment E_j. If this dynamical process factorizes, i.e., if one has $\Phi_{t,t_0}^{(12)} = \Phi_{t,t_0}^{(1)}\otimes\Phi_{t,t_0}^{(2)}$ for all times $t\geq t_0$ where the dynamical map $\Phi_{t,t_0}^{(1(2))}$ is defined by tracing over system $S_{2(1)}$ in Eq. (5.1), the dynamical process of the joint system S_1S_2 obviously inherits the non-Markovianity from its local parts, that is, that of the open systems S_1 and S_2, respectively. In general, the global dynamics is, however, not completely determined by the local subsystems and may thus display dynamical properties which are locally absent. Clearly, Eq. (5.1) represents a factorizing process if the initial environmental state $\rho_E^{(12)}(t_0)$ is described by the tensor product of two states for each local environment. Thus, correlations give rise to nonlocal processes of the global system. It is worth stressing though that this condition is only sufficient for a factorizing dynamics (see Appendix H for an example on the basis of the polarization dynamics employed in Sec. 4.3.2).

In the following, the appearance of memory effects in the global dynamics for locally Markovian processes is discussed by means of a generic model that additionally allows to address the question about the relevance of entanglement for this particular feature of bipartite open quantum systems. One considers two

qubits subject to pure decoherence due to the interaction with multimode bosonic fields. This type of non-Markovian process with memoryless local dynamics was first studied by Laine *et al.* (2012, 2013) along with a second model that was realized experimentally by Liu *et al.* (2013a) using a photonic system. Note that the phenomenon of nonlocal memory effects is rather surprising as it is in contrast to the standard situation in which a dynamical processes changes from being non-Markovian to Markovian when the open system is enlarged (cf. the study of Martinazzo *et al.* (2011) for the usual behavior) which is also observed for classical stochastic processes. Indeed, any non-Markovian process can be embedded in a Markovian one by suitably enlarging the number of random variables (see, e.g., van Kampen (2007)).

As previously indicated, the hitherto known dynamics leading to nonlocal memory effects are nondissipative processes for two qubits defining the open quantum system. That is, the bipartite open system state evolves according to (cf. Sec. 3.3.2)

$$\rho_S^{(12)}(t) = \begin{pmatrix} \varrho_{11,11} & \kappa_2(t)\,\varrho_{11,10} & \kappa_1(t)\,\varrho_{11,01} & \kappa_{12}(t)\,\varrho_{11,00} \\ & \varrho_{10,10} & \Lambda_{12}(t)\,\varrho_{10,01} & \kappa_1(t)\,\varrho_{10,00} \\ & & \varrho_{01,01} & \kappa_2(t)\,\varrho_{01,00} \\ \text{c.c.} & & & \varrho_{00,00} \end{pmatrix} , \tag{5.2}$$

resulting from local dephasing dynamics described by $U_{SE}^{(j)}$ where the coefficients $\varrho_{mn,rs}$ are determined as $\varrho_{mn,rs} = \langle mn|\rho_S^{(12)}(0)|rs\rangle$ and the free Hamiltonians are assumed to satisfy $H_S^{(j)} \sim \sigma_3^{(j)}$. The local unitaries $U_{SE}^{(j)}$ thus obey $[U_{SE}^{(j)}(t,t_0), \sigma_3^{(j)}] = 0$ for all times $t \geq t_0$. For such a process nonlocal memory effects show up as reviving nonlocal coherence factors κ_{12} or Λ_{12}, whereas all other quantities decay monotonically. Hence, such an open system can recover bipartite entanglement that has been lost in the meantime as all other quantum properties which follows from the characterization of the concurrence (2.85) shown in Sec. 2.4.3. The detrimental effect of the dephasing dynamics is thus reduced which has immediate application in noisy quantum information protocols, such as high fidelity quantum teleportation of mixed states (Laine *et al.*, 2014) and entanglement distribution (Xiang *et al.*, 2014), providing a hint of the usefulness of memory effects for quantum information tasks.

The generic model used to study nonlocal memory effects is derived from the nondissipative dynamics considered in the context of exact TCL 2 master equations (cf. Sec. 3.3.2). Describing each of the locally coupled qubits by the total Hamiltonian (3.52) with operators $\hat{S}^{(j)} = \sigma_3^{(j)}$ and $H_S^{(j)} = \epsilon_j \sigma_3^{(j)}$ for some $\epsilon_j \in \mathbb{R}$, the total system's dynamics is governed by the Hamiltonian

$$H_{\text{tot}}^{(12)} = \sum_{j=1}^{2} H_S^{(j)} + H_E^{(j)} + \chi_j(t)\,\sigma_3^{(j)} \otimes \sum_k \left(g_k^{(j)} \hat{b}_k^{(j)\dagger} + g_k^{(j)*} \hat{b}_k^{(j)} \right) , \tag{5.3}$$

where the free Hamiltonian of the environment reads $H_E^{(j)} = \sum_k \omega_k^{(j)} \hat{b}_k^{(j)\dagger} \hat{b}_k^{(j)}$. The real-valued function $\chi_j(t)$ characterizes the turning-on and -off of the presumably independently switchable interactions, i.e., one has

$$\chi_j(t) = \Theta(t - t_j^s)\Theta(t_j^f - t) = \begin{cases} 1\ , & t \in [t_j^s, t_j^f] \\ 0\ , & \text{else} \end{cases} \tag{5.4}$$

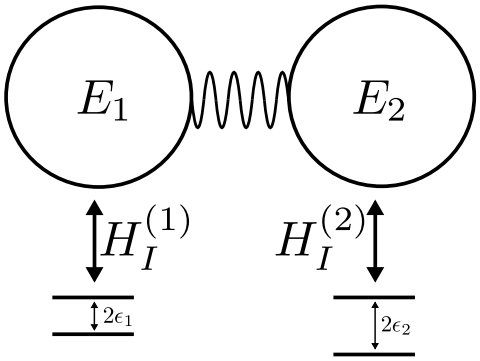

Figure 5.1 – Schematic picture of two qubit systems that are coupled to a correlated multimode environment with independently tunable local interactions. Later on, the initial state of the environment is assumed to be given by the product state of two-mode Gaussian states correlating pairs of modes of the two baths (cf. Fig. 1 in Wißmann and Breuer (2014)).

modelling a local interaction of subsystem j with its environment from time t_j^s to t_j^f. Because the duration as well as the starting time t_j^s can be varied independently for both subsystems, this setup allows to tune continuously from simultaneous to a successive application of the interactions. This is inspired by the idea of controllable quantum sensors which are brought in contact with a complex quantum system for some time, thereby acting as a quantum probe for properties of the complex system (see Ch. 6 for a further discussion on this topic).

Clearly, the choice of the total Hamiltonian $H_{\text{tot}}^{(12)}$ leads to a reduced dynamics of the two qubits given by Eq. (5.1) which can be solved exactly if $\rho_E^{(12)}(t_0)$ defines a Gaussian state (cf. Eq. (2.102)) as a result of this thesis which corrects and generalizes the results obtained by Laine *et al.* (2012) (cf. Laine *et al.* (2013)). Without loss of generality it is henceforth assumed that $t_1^s \leq t_2^s$ holds and that the coupling strengths are real-valued, i.e. one has $g_k^j \in \mathbb{R}$ for $j = 1, 2$ and any mode k. Finally, the source of nonlocal memory effects in this particular instance of the spin-boson model is studied for an initial state of the environment given by the tensor product of two-mode Gaussian states correlating pairs of modes.

5.1 Coherence factors for two-mode Gaussian states

In order to determine the reduced dynamics of the two qubits obtained for the Hamiltonian $H_{\text{tot}}^{(12)}$ (cf. Eq. (5.3)) and factorizing initial conditions, one simply employs the results of the preceding considerations on the exactness of a TCL 2 master equation (see Sec. 3.3.2). In fact, they obviously apply here as the annihilation and creation operators of the modes of the two bosonic baths satisfy the familiar commutation relation, i.e., these operators obey $[\hat{b}_k^{(i)}, \hat{b}_l^{(j)\dagger}] = \delta_{kl}\delta_{ij}$ and $[\hat{b}_k^{(i)}, \hat{b}_l^{(j)}] = [\hat{b}_k^{(i)\dagger}, \hat{b}_l^{(j)\dagger}] = 0$ (cf. Eq. (2.91)). According to Eq. (3.72), the time

evolution of the two two-level systems is characterized by[1]

$$\langle mn|\rho_S^{(12)}(t)|rs\rangle = \varrho_{mn,rs}\cdot e^{it\{[(-1)^m-(-1)^r]\epsilon_1+[(-1)^n-(-1)^s]\epsilon_2\}} \cdot \chi_{\rho_E}^{\sqrt{2}}\Big(([(-1)^r-(-1)^m]\vec{\beta}^{(1)}(t),[(-1)^s-(-1)^n]\vec{\beta}^{(2)}(t))\Big)\,, \tag{5.5}$$

where the components of $\vec{\beta}^{(j)}(t)$ read

$$\begin{aligned}\beta_k^{(j)}(t) &= (-i)\cdot\int_0^t \mathrm{d}s\;\chi_j(s)g_k^{(j)}\exp[i\omega_k^{(j)}s] \\ &= \frac{g_k^{(j)}}{\omega_k^{(j)}}\exp[i\omega_k^{(j)}t_j^s]\cdot\Big\{1-\exp[i\omega_k^{(j)}t_j(t)]\Big\}\,,\end{aligned} \tag{5.6}$$

introducing the effective interaction time $t_j(t)\equiv\int_0^t \mathrm{d}s\,\chi_j(s)$. By comparison with Eq. (5.2), it follows that the coherence factors are thus determined as

$$\kappa_1(t) = e^{-2i\epsilon_1 t}\cdot\chi_{\rho_E}^{\sqrt{2}}\Big((2\vec{\beta}^{(1)}(t),0)\Big)\,, \tag{5.7}$$

$$\kappa_2(t) = e^{-2i\epsilon_2 t}\cdot\chi_{\rho_E}^{\sqrt{2}}\Big((0,2\vec{\beta}^{(2)}(t))\Big)\,, \tag{5.8}$$

$$\kappa_{12}(t) = e^{-2it(\epsilon_1+\epsilon_2)}\cdot\chi_{\rho_E}^{\sqrt{2}}\Big((2\vec{\beta}^{(1)}(t),2\vec{\beta}^{(2)}(t))\Big)\,, \tag{5.9}$$

$$\Lambda_{12}(t) = e^{-2it(\epsilon_1-\epsilon_2)}\cdot\chi_{\rho_E}^{\sqrt{2}}\Big((2\vec{\beta}^{(1)}(t),-2\vec{\beta}^{(2)}(t))\Big)\,. \tag{5.10}$$

For an initial state of the environment ρ_E that is given by the tensor product of zero-mean two-mode Gaussian states correlating the kth modes of the two baths (cf. Sec. 2.5.2), i.e. $\rho_E=\bigotimes_k\rho_{\mathrm{G}}^k$, one may evaluate the coherence factors (5.7)–(5.10) explicitly, even for a continuum of modes. Clearly, in this case the characteristic function χ_{ρ_E} decomposes into a product of identical characteristic functions for each pair of modes, i.e., it obeys

$$\begin{aligned}&\chi_{\rho_E}^{\sqrt{2}}\Big(([(-1)^r-(-1)^m]\vec{\beta}^{(1)}(t),[(-1)^s-(-1)^n]\vec{\beta}^{(2)}(t))\Big) \\ &=\prod_k\chi_{\rho_{\mathrm{G}}^k}^{\sqrt{2}}\Big(([(-1)^r-(-1)^m]\beta_k^{(1)}(t),[(-1)^s-(-1)^n]\beta_k^{(2)}(t))\Big)\,,\end{aligned} \tag{5.11}$$

where $\chi_{\rho_{\mathrm{G}}^k}^{\sqrt{2}}$ is given by (cf. Eq. (2.102))

$$\chi_{\rho_{\mathrm{G}}^k}^{\sqrt{2}}\Big((\gamma_{k,rsmn}^{(1)}(t),\gamma_{k,rsmn}^{(2)}(t))\Big)=\exp\Big[-\vec{\mu}_{k,rsmn}(t)^T\boldsymbol{\sigma}_{\hat{X}_k,\rho_{\mathrm{G}}^k}\vec{\mu}_{k,rsmn}(t)\Big]\,, \tag{5.12}$$

with $\hat{X}_k=(\hat{q}_k^{(1)},\hat{p}_k^{(1)},\hat{q}_k^{(2)},\hat{p}_k^{(2)})^T$ and

$$\vec{\mu}_{k,rsmn}(t)=\begin{pmatrix}-\mathrm{Im}(\gamma_{k,rsmn}^{(1)}(t))\\ \mathrm{Re}(\gamma_{k,rsmn}^{(1)}(t))\\ -\mathrm{Im}(\gamma_{k,rsmn}^{(2)}(t))\\ \mathrm{Re}(\gamma_{k,rsmn}^{(2)}(t))\end{pmatrix}\,, \tag{5.13}$$

[1]Note that the additional phase factor $\exp[i(S_m^2-S_n^2)\phi(t)]$ equals unity as the eigenvalues S_m of the operator $\hat{S}=\sigma_3$ are given by ±1 (cf. Eq. (3.72)).

employing the definition $\gamma^{(j)}_{k,r_1r_2m_1m_2}(t) \equiv [(-1)^{r_j} - (-1)^{m_j}]\beta^{(j)}_k(t)$. Assuming moreover that the covariance matrices $\boldsymbol{\sigma}_{\hat{X}_k,\rho^k_{\mathrm{G}}}$ are identical for all modes k and in standard form (2.124), given by the 4×4-matrix

$$\boldsymbol{\sigma} = \begin{pmatrix} a_1 & 0 & c_1 & 0 \\ 0 & a_1 & 0 & c_2 \\ c_1 & 0 & a_2 & 0 \\ 0 & c_2 & 0 & a_2 \end{pmatrix} , \tag{5.14}$$

one obtains analytic expressions for the coherence factors in the continuum limit for ohmic spectral densities $J_j(\omega) = \alpha_j \omega \exp[-\omega/\omega_c]$ with equal cutoff frequency ω_c but arbitrary couplings α_j. More precisely, by means of the relations

$$\exp\left[\mathcal{L}\Big\{\frac{1-\cos(yt)}{t}\Big\}(s)\right] = \left[1 + \frac{y^2}{s^2}\right]^{\frac{1}{2}} , \tag{5.15}$$

$$\exp\left[\mathcal{L}\Big\{\sin(xt)\frac{\sin(yt)}{t}\Big\}(s)\right] = \left[\frac{(y+x)^2+s^2}{(y-x)^2+s^2}\right]^{\frac{1}{4}} \tag{5.16}$$

for the Laplace transform $\mathcal{L}$ evaluated at $s \neq 0$, one shows that the coherence factors obey (see Appendix I for a detailed derivation)

$$\kappa_1(t) = e^{-2i\epsilon_1 t}\left\{1 + \omega_c^2 t_1(t)^2\right\}^{-4a_1\alpha_1} , \tag{5.17}$$

$$\kappa_2(t) = e^{-2i\epsilon_2 t}\left\{1 + \omega_c^2 t_2(t)^2\right\}^{-4a_2\alpha_2} , \tag{5.18}$$

$$\kappa_{12}(t) = \kappa_1(t)\kappa_2(t)f(t) , \tag{5.19}$$

$$\Lambda_{12}(t) = \kappa_1(t)\kappa_2^*(t)f(t)^{-1} , \tag{5.20}$$

where the function f is given by

$$\begin{aligned} f(t) = &\left[\frac{\{1+\omega_c^2(t_1^s - t_2^s)^2\}\cdot\{1+\omega_c^2(t_1(t)+t_1^s-t_2(t)-t_2^s)^2\}}{\{1+\omega_c^2(t_1(t)+t_1^s-t_2^s)^2\}\cdot\{1+\omega_c^2(t_1^s-t_2(t)-t_2^s)^2\}}\right]^{4c_2\sqrt{\alpha_1\alpha_2}} \\ &\cdot\left[\frac{\{1+\omega_c^2(t_1^s+t_2^s)^2\}\cdot\{1+\omega_c^2(t_1^s-t_2(t)-t_2^s)^2\}}{\{1+\omega_c^2(t_1^s-t_2^s)^2\}\cdot\{1+\omega_c^2(t_1^s+t_2(t)+t_2^s)^2\}}\right. \\ &\quad\cdot\frac{\{1+\omega_c^2(t_1(t)+t_1^s-t_2^s)^2\}}{\{1+\omega_c^2(t_1(t)+t_1^s+t_2^s)^2\}} \\ &\quad\left.\cdot\frac{\{1+\omega_c^2(t_1(t)+t_1^s+t_2(t)+t_2^s)^2\}}{\{1+\omega_c^2(t_1(t)+t_1^s-t_2(t)-t_2^s)^2\}}\right]^{2(c_2-c_1)\sqrt{\alpha_1\alpha_2}} . \end{aligned} \tag{5.21}$$

One notes that the modulus of the coherence factors κ_j solely depend on the effective interaction time $t_j(t)$ and the variances of the position and momentum operators given by the diagonal elements of the covariance matrix $\boldsymbol{\sigma}$. On the contrary, κ_{12} and Λ_{12} are also influenced by the initial times t_j^s and the off-diagonal elements c_1 and c_2. Clearly, for $c_1 = c_2 = 0$, one has $f(t) = 1$ for all times t so that the dynamics factorizes. There is strong evidence that f is only equal to unity if and only if $\boldsymbol{\sigma}$ has vanishing off-diagonal elements corresponding to a completely

uncorrelated Gaussian state. Hence, the present bipartite process factorizes solely for a factorizing environmental state as is commonly expected (see Appendix H for a factorizing process associated with an correlated environment contradicting the common expectation).

Note that the present treatment can be easily extended to complex-valued coupling strengths $g_k^{(j)}$ and covariance matrices that are not in standard form by means of the techniques stated in Appendix I. Moreover, the scheme may be generalized to multiple interaction intervals as described by functions

$$\chi_j(t) = \sum_{m=1}^{n_j} \chi_{j,m}(t) \ , \tag{5.22}$$

where $n_j \geq 1$ and $\chi_{j,m}(t) = \Theta(t - t_{j,m}^s)\Theta(t_{j,m}^f - t)$ for times $t_{j,m}^s$ and $t_{j,m}^f$ satisfying $t_{j,m}^f < t_{j,m+1}^s$ for all $m \in \{1, \ldots, n_j - 1\}$ and $j = 1, 2$. Of course, the calculations are getting more and more involved for all these generalizations.

It is henceforth assumed for convenience that the initial time for subsystem S_1 is given by $t_1^s = 0$, implying the second line of Eq. (5.21) is equal to unity which thus simplifies the expressions for the nonlocal coherence factors. Further implications of this assumption are discussed below.

5.2 Role of entanglement for nonlocal memory effects

One now considers the non-Markovianity of the dynamics described by the coherence factors (5.17)–(5.20) for different two-mode Gaussian states. Focusing on subsequently applied local interactions of equal length, i.e. one sets $t_1^f = t_2^s$ and $\Delta t \equiv t_1^f = t_2^f - t_2^s$, one studies the dynamics of the two two-level systems for squeezed and mixed thermal states which were introduced in Sec. 2.5.4. In particular, the squeezed vacuum $\boldsymbol{\sigma}_{\hat{X},r}^{\mathrm{EPR}}$ (cf. Eq. (2.135)) and the special mixed thermal states $\boldsymbol{\sigma}_{\hat{X},r}^{\mathrm{MTS}}$ (cf. Eq. (2.145)), defining zero-mean two-mode Gaussian states that are entangled and separable for any value of r, respectively, provide a convenient tool to study the relevance of entanglement for the occurrence of nonlocal memory effects.

It is readily observed that the coherence factors $\kappa_1(t)$ and $\kappa_2(t)$ (cf. Eqs. (5.17) and (5.18), respectively) decay monotonically for any Gaussian state as the variances a_j are always positive. Thus, non-Markovian behavior is exclusively related to revivals of the nonlocal coherence factors $\kappa_{12}(t)$ and $\Lambda_{12}(t)$ (cf. Eqs. (5.19) and (5.20)), hence describing nonlocal memory effects as discussed before. In fact, only one of these coherence factors shows revivals for the considered setup. In view of the previous results about optimal states stated in Sec. 4.3.1, one thus concludes that the maximum for the measure $\mathcal{N}$ (and, similarly, for $\tilde{\mathcal{N}}$) is attained by one of the two pairs of Bell states (cf. Eqs. (2.78)–(2.80))

$$|\Psi_0\rangle = \frac{1}{\sqrt{2}}(|11\rangle + |00\rangle) \ , \qquad |\Psi_3\rangle = \frac{1}{\sqrt{2}}(|11\rangle - |00\rangle) \ , \tag{5.23}$$

or

$$|\Psi_1\rangle = \frac{i}{\sqrt{2}}(|01\rangle + |10\rangle) \,, \qquad |\Psi_2\rangle = \frac{i}{\sqrt{2}}(|01\rangle - |10\rangle) \,, \tag{5.24}$$

depending on whether κ_{12} or Λ_{12} revives, respectively. This is due to the fact that the trace distance of the time-evolved two-qubit states $\rho_{\Psi_j}(t)$ reads

$$\mathcal{D}_T\big(\rho_{\Psi_0}(t), \rho_{\Psi_3}(t)\big) = |\kappa_{12}(t)| \,, \tag{5.25}$$

$$\mathcal{D}_T\big(\rho_{\Psi_1}(t), \rho_{\Psi_2}(t)\big) = |\Lambda_{12}(t)| \,. \tag{5.26}$$

Since the modulus of the coherence factors describes also the entanglement in $\rho_{\Psi_j}(t)$ quantified by the concurrence C_2 as was shown in Eqs. (2.85) and (2.87), the non-Markovianity measured by a backflow of information is thus linked to revivals of entanglement of the Bell states subject to the considered dephasing dynamics.

Figure 5.2 shows the resulting dynamics of $|\Lambda_{12}(t)|$ for the Gaussian states corresponding to $\boldsymbol{\sigma}_{\hat{X},r}^{\mathrm{EPR}}$ and $\boldsymbol{\sigma}_{\hat{X},r}^{\mathrm{MTS}}$ for various values of the parameter r. Here, the time of the interaction Δt is given by 2.5×10^{-2} in units of the cutoff frequency ω_c which determines a natural time scale as its inverse defines the correlation time of the environment. Hence, one considers an interaction that is small compared to the correlation time of the environment. As will be shown later on, this configuration indeed needs to be chosen to observe revivals of coherence factors unless the free evolution of the bath modes is eliminated (see Sec. 5.3.1). For the considered setup one observes revivals of the coherence factor pointing to nonlocal memory effects in the considered model for both classes of zero-mean two-mode Gaussian states. These effects are getting stronger the bigger the parameter r. In fact, large values of this parameter enhance the decay and the subsequent revival for a fixed interaction length and coupling strength. Clearly, a boost of the coupling parameters α_j has the same effect, so one may choose them to be equal to unity for convenience. The most surprising fact exposed by Fig. 5.2 is that the variation of the coherence factor is enhanced for the mixed thermal states. Hence, one obtains stronger nonlocal memory effects for the separable Gaussian states characterized by $\boldsymbol{\sigma}_{\hat{X},r}^{\mathrm{MTS}}$ than for the highly entangled EPR state.

It is worth pointing out that the sign of c_1 determines which pair of Bell states is optimal for the two classes of two-mode Gaussian states. As shown by Fig. 5.2, for a positive cross-covariance c_1, the nonlocal coherence factor Λ_{12} increases during the interaction of the second subsystem with its environment whereas κ_{12} decays monotonically. In the opposite case, i.e. for a negative value of c_1, the roles of the two coherence factors are interchanged. By inspection of the cross-variances of the considered Gaussian states, it is thus clear that the maximal backflow of information is always given by the Bell states $|\Psi_1\rangle$ and $|\Psi_2\rangle$ independent of the sign of the parameter r for $\boldsymbol{\sigma}_{\hat{X},r}^{\mathrm{MTS}}$. However, this pair determines the non-Markovianity of the process solely for positive parameters r in the case of squeezed thermal states. On the contrary, for negative values the coherence factors κ_{12} increases, showing that the entanglement evolution of the Bell states $|\Psi_0\rangle$ and $|\Psi_3\rangle$ exhibits memory effects, as is readily understood due to the parity of sinh. Note that the non-Markovianity is yet independent of the sign of the squeezing parameter as a change of sign simply implies that the function $f(t)$ (cf. Eq. (5.21)) is inverted and, therefore, the coherence factors κ_{12} and Λ_{12} interchange their roles.

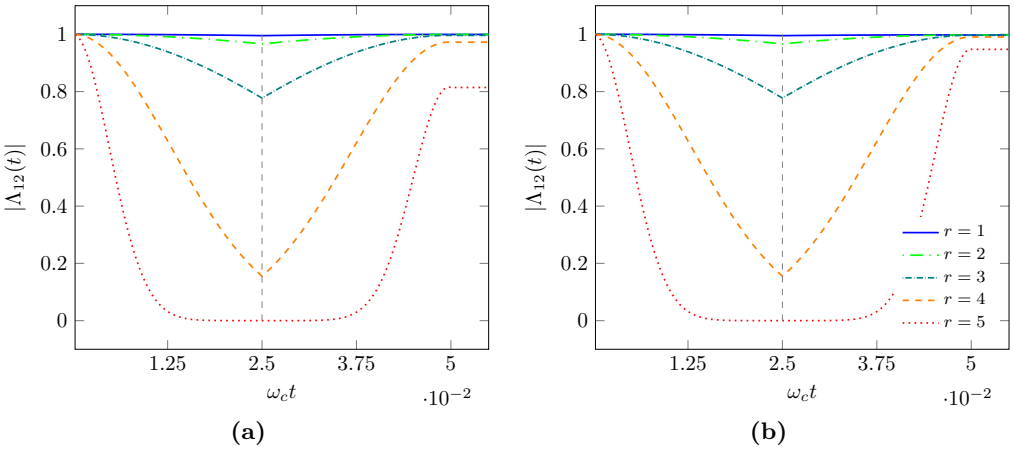

Figure 5.2 – The time evolution of the modulus of the coherence factor $\Lambda_{12}(t)$ (cf. Eq. (5.20)) for environmental states described by $\boldsymbol{\sigma}_{\hat{X},r}^{\mathrm{EPR}}$ **(a)** and $\boldsymbol{\sigma}_{\hat{X},r}^{\mathrm{MTS}}$ **(b)** (cf. Eqs. (2.135) and (2.145), respectively) in units of the environmental correlation time ω_c^{-1}. The coupling strengths are chosen as $\alpha_{1,2} = 1$, and the subsequently applied interactions are active for 2.5×10^{-2} units of time whose switch is indicated by the dashed vertical line. Several values of the parameter r are considered for which the non-Markovianity $\mathcal{N}$ (just as well as $\tilde{\mathcal{N}}$) is found to be given by: **(a)** 4×10^{-3} ($r = 1$), 3×10^{-2} ($r = 2$), 0.22 ($r = 3$), 0.82 ($r = 4$), 0.82 ($r = 5$); **(b)** 4×10^{-3} ($r = 1$), 3×10^{-2} ($r = 2$), 0.22 ($r = 3$), 0.84 ($r = 4$), 0.95 ($r = 5$) (cf. Fig. 2 in Wißmann and Breuer (2014)).

Nonlocal memory effects also persist for other values of Δt for the two classes of Gaussian states – unless the interaction is not too large in comparison with the environmental correlation time as shown in Fig. 5.3. In addition, the maximal increase of the coherence factor Λ_{12} distinguishes a unique interaction length maximizing the nonlocal memory effects. One observes that a large parameter r requires a small interaction time Δt in order to observe a completely decaying and subsequently reviving nonlocal coherence factor Λ_{12}. Thus, the optimal time Δt^*, yielding maximal memory effects, is a decreasing function of the squeezing parameter r (cf. Fig. 5.4). In the limit $\Delta t \to 0$ for finite squeezing, the non-Markovianity obviously tends to zero as the dynamical process gets trivial.

In summary, the strength of nonlocal memory effects in the present model depends on the magnitude of the cross-covariances and the chosen interaction time, and the optimal time $\omega_c \Delta t^*$ revealing the maximal non-Markovian behavior is a decreasing function of the magnitude of the former. This observation is confirmed if one considers truly squeezed thermal states (2.130) characterized by nonvanishing mean occupation numbers N_j and squeezing angles $\phi = 0$ or π. One sees that the larger the summed mean occupation number $N_\Sigma = \sum_j N_j$, the stronger the maximal nonlocal memory effects are and, moreover, the shorter the optimal interaction length becomes as the data depicted in Fig. 5.4 clearly shows. By looking at this figure, one also recognizes that the non-Markovianity of the process is unambiguously connected to the squeezing parameter of arbitrary squeezed thermal states with known mean occupation numbers. This suggests to use the dynamics of the open system to determine the squeezing parameter of an environment at

fixed and known temperature. The two locally interacting two-level systems may thus serve as a dynamical quantum probe for this environmental property.

To utilize the open system dynamics as a quantum probe experimentally, one must clearly be able to prepare the system in a state which has nonzero nonlocal coherences such as the maximally entangled Bell states and to couple it locally to the multimode field for different times, apart from knowing the mean occupation numbers. Clearly, there is no full state tomography needed since all the information about the squeezing is contained in the dynamics of the coherences which can be determined by measuring for example the correlations $\sigma_x^{(1)} \otimes \sigma_x^{(2)}$, $\sigma_y^{(1)} \otimes \sigma_y^{(2)}$, $\sigma_x^{(1)} \otimes \sigma_y^{(2)}$ and $\sigma_y^{(1)} \otimes \sigma_x^{(2)}$ on the two-qubit probe. Nonetheless, one must compare the magnitudes of the nonlocal coherences of a prepared state after the first and the second local interaction with their initial value for several durations of the interactions. Even though it actually suffices to consider only two different interaction lengths, the probing scheme thus still requires to measure the four correlations five times.

The proposed strategy might, however, still be useful for applications such as the determination of the squeezing in atomic Bose-Einstein condensates (Kuang *et al.*, 2003; Piovella *et al.*, 2003) by immersed atoms (Haikka *et al.*, 2011, 2013, 2012b) or any other system where no other reliable and easy method for this task is available. Of course, the generic example is given by the polarization degrees of freedom of photons that are used to determine the squeezing of their frequency states which might, for example, result from a downconversion process (see Sec. 4.3.2). In fact, the frequency degrees of freedom of downconverted photons are very well approximated by an EPR state (Lund *et al.*, 2014) if a nonlinear crystal is subject to a strong pump pulse. Note that this task is, however, rou-

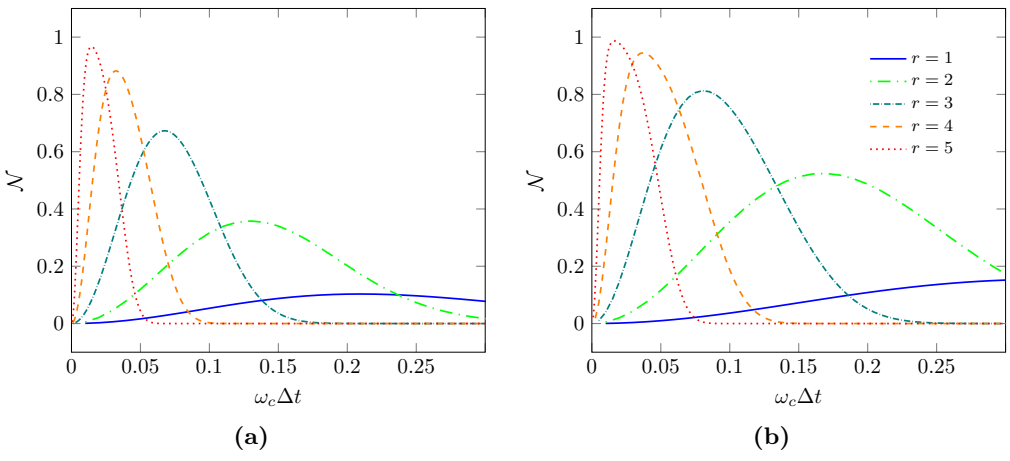

Figure 5.3 – The degree of non-Markovianity $\mathcal{N}$ of the quantum process characterized by Eqs. (5.17)–(5.20) for Gaussian states $\boldsymbol{\sigma}_{\hat{X},r}^{\mathrm{EPR}}$ **(a)** and $\boldsymbol{\sigma}_{\hat{X},r}^{\mathrm{MTS}}$ **(b)** (cf. Eqs. (2.135) and (2.145), respectively) as a function of the interaction length $\omega_c \Delta t$. The consecutively applied interactions have again the same length and the couplings are given by $\alpha_{1,2} = 1$. One clearly sees the unambiguous connection of the squeezing parameter and the non-Markovianity as a function of the interaction length (cf. Fig. 3 in Wißmann and Breuer (2014)).

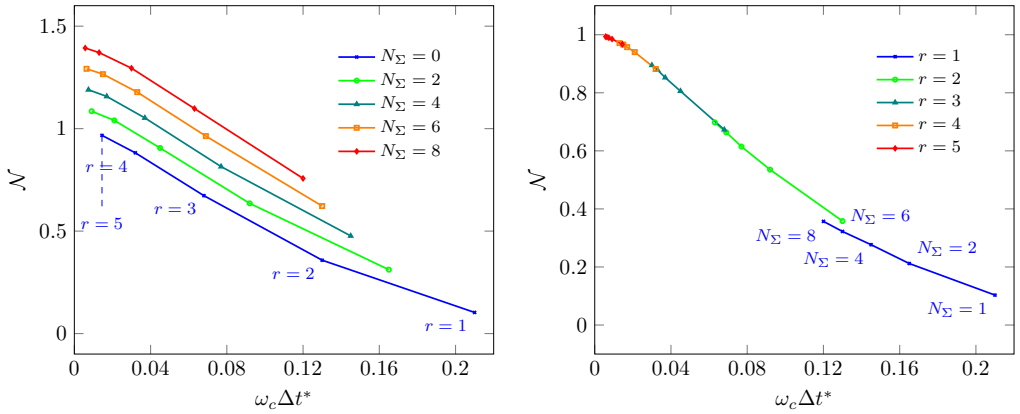

Figure 5.4 – The maximal non-Markovianity $\mathcal{N}$ obtained for the optimal interaction length Δt^* (in units of ω_c^{-1}) for different values of the summed mean occupation number $N_\Sigma = N_1 + N_2$ and squeezing parameters r for a squeezed thermal states $\boldsymbol{\sigma}^{\mathrm{STS}}_{\hat{X},r,\phi=0,N_j}$ (cf. Eq. (2.130)). The other configurations are the same as in Fig. 5.3. For the sake of clarity, a stacked plot adding a cumulative offset of 0.1 to each curve is presented in **(a)** (cf. Fig. 3 in Wißmann and Breuer (2014)).

tinely and reliably done by directly measuring the covariance matrix in quantum optical experiments. And, in addition, it is unclear how to establish the interaction required for the probing strategy (cf. Eq. (5.3)) in this setup.

It is worth mentioning that the unambiguous connection of the environmental properties and the rephasing of the nonlocal coherences is untouched by an imperfect realization of the local interactions, making the proposed probing strategy indeed applicable for experimental purposes. The topic of dynamical quantum probes will be further addressed in the second part of this thesis (see Ch. 6).

To complete the study of nonlocal memory effects in this model, it remains to evaluate the influence of the assumption that the first local interaction starts at $t_1^s = 0$. That is, what happens if one assumes arbitrary times for the inset t_1^s? It can be shown that the dynamics of $|\Lambda_{12}(t)|$ induced by the mixed thermal states (2.145) is independent of the instant of time at which the first interaction is turned on. For squeezed thermal states, the rephasing of the coherence factor is, however, reduced if the initial time t_1^s is nonzero. To explain these observations, one first notes that Gaussian states remain Gaussian under the free evolution of the bath modes, solely changing the argument of the characteristic function (2.115) according to

$$\vec{z} \;\mapsto\; \vec{z}\,' \equiv \left(\exp[i\omega_1 t]z_1, \ldots, \exp[i\omega_n t]z_n\right)^T , \tag{5.27}$$

where ω_j refers to the frequencies of the modes in the displacement operator (2.103). For the mixed thermal states (2.145) it is easy to prove that the phase factors $\exp[i\omega_j t]$ cancel out so that the characteristic function is in fact invariant under the free evolution. However, for squeezed thermal states, this is not true making the characteristic function depend on the frequencies of the modes and the elapsed time t prior to the interaction. It thus seems to be important to have identical Gaussian states for all pairs of modes when the open system starts to interact

with the bosonic modes in general. By means of this observation, a necessary and sufficient condition for the occurrence of nonlocal memory effects in general terms will be presented in the following section.

One finally concludes that there exist strong nonlocal memory effects in the present model, but entanglement in the initial state of the composite environment is not necessary to observe this phenomenon. The separable Gaussian states characterized by the covariance matrix $\boldsymbol{\sigma}_{\hat{X},r}^{\mathrm{MTS}}$ (cf. Eq. (2.145)) typically induce even stronger nonlocal memory effects in comparison to squeezed thermal states. Unfortunately, the studied system does not allow to reveal the relevance of quantum correlations in general as any two-mode Gaussian state with nonvanishing cross-covariances has nonzero quantum discord (cf. Sec. 2.5.3). Hence, the natural extension of this study, distinguishing the effect of classical and quantum correlations, is impossible on the basis of this model.

5.3 Explaining the nonlocal rephasing

The results presented in the previous section have shown that memory effects with respect to the revivals of nonlocal coherences are indeed observed in the present model for appropriately adjusted parameters and entangled as well as separable Gaussian states. To understand this effect better, an explanation for their occurrence in general terms is derived in this part of the thesis. In fact, apart from studying the main mechanism induced by the local interactions, a general dephasing model is used to derive a necessary and sufficient condition, solely based on the entries of the covariance matrix, which also explains the occurrence of nonlocal memory effects in the absence of entanglement. In addition, the correlations the different subsystems during the different stages of the local interaction dynamics are examined, also by means of a general model, showing that this effect cannot be traced back to the intermediate redistribution of bipartite correlations.

5.3.1 General dephasing model and approximate dynamics

The previous discussion has shown that a proper choice of two-mode Gaussian states along with suitably lasting local interactions are essential for the occurrence of nonlocal memory effects. For very short-time interactions the interesting coherence factor remains almost constant, whereas it decays irretrievably for long-lasting ones. Furthermore, the free evolution of the bath modes apparently leads to an irrecoverable displacement of the environmental states degrading the effect. In fact, a gap between the turning-off and on of the two local interactions, i.e. if one has for $t_1^f < t_2^s$, diminishes the revivals of the coherence factors which is also observed for squeezed thermal states if nonzero starting times of the first interaction are considered as reported previously.

In addition, the significance of the free evolution is confirmed by the second model presented by Laine *et al.* (2012) where the polarization and frequency degrees of freedom of a pair of photons define the open system and the environment, respectively, and the local interactions are again induced by quartz plates (cf. Ap-

pendix H). Clearly, there is no free evolution incorporated in this model, but one still observes nonlocal memory effects which, moreover, are amplified by the magnitude of the correlation coefficient $K = C_{12}/\sqrt{C_{11}C_{22}}$ quantifying the frequency correlations. Here, $C_{jk} = \langle\omega_j\omega_k\rangle - \langle\omega_j\rangle\langle\omega_k\rangle$ denotes the entries of the covariance matrix of the frequency distribution (Laine *et al.*, 2012). One also observes that the rephasing for subsequent interactions is independent of the actual length and a possible gap between the local interactions. It is worth noticing that the dynamics of the nonlocal coherence factors featuring revivals is trivial for simultaneously active interactions and perfectly anticorrelated frequency distributions, i.e. if the correlation coefficient satisfies $K = -1$. This is due to the fact that the associated environmental state defines an eigenstates of the interaction Hamiltonian.

Based on these observations, it suggests itself to explain the occurrence of nonlocal memory effects in the previous model by a modified ansatz, neglecting the free evolution of the bath modes. For the two-mode Gaussian states showing nonlocal memory effects, one thus expects to observe almost perfectly reviving coherence factors $\Lambda_{12}(t)$ or $\kappa_{12}(t)$ for consecutive interactions, while they should be almost constant if the interactions coexist under the approximate dynamics.

Indeed, erasing the free evolution of the bath modes and assuming a real-valued coupling strength $g_k^{(j)}$, the evolution of the kth bath mode is governed by the Hamiltonian (cf. Eq. (5.3))

$$H_{I,k}(t) = \sqrt{2}\sum_{j=1}^{2} g_k^{(j)}\chi_j(t)\,\sigma_3^{(j)} \otimes \hat{q}_k^{(j)} \;, \tag{5.28}$$

where $\hat{q}_k^{(j)}$ refers to the canonical position operator corresponding to the kth mode of subsystem j. Applying this Hamiltonian to the open system state $|11\rangle_{S_1S_2}$, one obtains that the dynamics of the environmental degrees of freedoms is described by the effective Hamiltonian

$$H_{I,k}^{|11\rangle}(t) = \sqrt{2}g_k(\chi_1(t)\,\hat{q}_k^{(1)} + \chi_2(t)\hat{q}_k^{(2)}) \;, \tag{5.29}$$

while one has

$$H_{I,k}^{|10\rangle}(t) = \sqrt{2}g_k(\chi_1(t)\,\hat{q}_k^{(1)} - \chi_2(t)\hat{q}_k^{(2)}) \;, \tag{5.30}$$

if $H_{I,k}(t)$ is applied to the state $|10\rangle_{S_1S_2}$ and one assumes equal coupling constants $g_k^{(1)} = g_k^{(2)} = g_k$. Similarly, one finds for the other two basis vectors $|00\rangle_{S_1S_2}$ and $|01\rangle_{S_1S_2}$,

$$H_{I,k}^{|00\rangle}(t) = -H_{I,k}^{|11\rangle}(t) \;, \qquad H_{I,k}^{|10\rangle}(t) = -H_{I,k}^{|01\rangle}(t) \;, \tag{5.31}$$

so the effective Hamiltonian basically depend either on the sum or the difference of the respective positions of particle 1 and 2 associated with the canonical operators $\hat{q}_k^{(j)}$.

If the unitary dynamics is exclusively generated by the approximated interaction Hamiltonian $H_I(t) \equiv \sum_k H_{I,k}(t)$, the time evolution of any environmental state given an open system state $|mn\rangle_{S_1S_2}$ is described by the operator $U_{|mn\rangle}(t) = \exp[-i\sum_k \int_0^t \mathrm{d}s H_{I,k}^{|mn\rangle}(s)]$. It then follows that the nonlocal coherence factors

$\tilde{\kappa}_{12}(t) \equiv \mathrm{Tr}_E\{U_{|00\rangle}(t)\rho_E U_{|11\rangle}(t)^\dagger\}$ and $\tilde{\Lambda}_{12}(t) \equiv \mathrm{Tr}_E\{U_{|01\rangle}(t)\rho_E U_{|10\rangle}(t)^\dagger\}$ are determined as

$$\tilde{\kappa}_{12}(t) = \mathrm{Tr}_E\left\{\exp\left[\sqrt{2}i\sum_k 2g_k(t_1(t)\hat{q}_k^{(1)} + t_2(t)\hat{q}_k^{(2)})\right]\rho_E\right\} \tag{5.32}$$

and

$$\tilde{\Lambda}_{12}(t) = \mathrm{Tr}_E\left\{\exp\left[\sqrt{2}i\sum_k 2g_k(t_1(t)\hat{q}_k^{(1)} - t_2(t)\hat{q}_k^{(2)})\right]\rho_E\right\} \ . \tag{5.33}$$

Choosing the environmental state ρ_E to be again given by the tensor product of identical zero-mean two-mode Gaussian states, one may apply the results of Sec. 5.1 to evaluate these expressions explicitly. In fact, for an ohmic spectral density $J(\omega) = \alpha\omega\exp[-\omega/\omega_c]$ with coupling strength α and cutoff frequency ω_c, the continuum limit results in $\sum_k g_k^2 \ \to \ \int_0^\infty \mathrm{d}\omega J(\omega) = \alpha\omega_c^2$ and, therefore, the coherence factors for the approximate dynamics in this limit read

$$\tilde{\kappa}_{12}(t) = \exp\left[-4\alpha\omega_c^2\Big\{a_1\big(t_1(t)^2 + t_2(t)^2\big) + 2c_1t_1(t)t_2(t)\Big\}\right] \ , \tag{5.34}$$

$$\tilde{\Lambda}_{12}(t) = \exp\left[-4\alpha\omega_c^2\Big\{a_1\big(t_1(t)^2 + t_2(t)^2\big) - 2c_1t_1(t)t_2(t)\Big\}\right] \ , \tag{5.35}$$

where it has been assumed that two-mode Gaussian state is given by the covariance matrix $\boldsymbol{\sigma}$ (cf. Eq. (5.14)) as before. Note that $\tilde{\kappa}_{12}(t)$ and $\tilde{\Lambda}_{12}(t)$ are real-valued for all times t.

Figure 5.5 depicts the dynamics of the nonlocal coherence factor $\tilde{\Lambda}_{12}(t)$ for successively acting local interactions and two-mode Gaussian states given by the squeezed vacuum and the particular mixed thermal state. For both classes of Gaussian states and sufficiently large parameter r, the approximate coherence factor displays an almost perfect decay and subsequent revival as conjectured. In particular, comparing the plots with the dynamics for the original model displayed in Fig. 5.2, the strong enhancement of nonlocal memory effects for an erased free evolution is obvious. These results clearly show the significance of the free evolution in the context of nonlocal memory effects.

It remains, however, to explain why large squeezing parameters are needed to observe substantial nonlocal memory effects in the previous models (cf. Figs. 5.2 and 5.5). To this end, one first studies the following general dephasing model that also comprises the approximated dynamics studied before: Suppose that the decoherence function $F(t)$ describing the dephasing process of the open system has the general structure

$$F(t) = \mathrm{Tr}_E\{\exp[iAt]\rho_E\} \ , \tag{5.36}$$

where A refers to a self-adjoint operator that is linear in the canonical operators. Clearly, this ansatz neglects any kind of free evolution of the environment and the open system as it was done for the approximated dynamics before. For a Gaussian state ρ_E this decoherence function is then completely characterized by the first two cumulants $\langle A\rangle_{\rho_E} = \mathrm{Tr}_E\{A\,\rho_E\}$ and $\langle\langle A\rangle\rangle_{\rho_E} = \langle A^2\rangle_{\rho_E} - \langle A\rangle_{\rho_E}^2$, as a cumulant expansion terminates at second order due to the linearity of A in the canonical variables. Hence, one finds

$$F(t) = \exp\left[i\langle A\rangle_{\rho_E}t - \frac{1}{2}\langle\langle A\rangle\rangle_{\rho_E}t^2\right] \ . \tag{5.37}$$

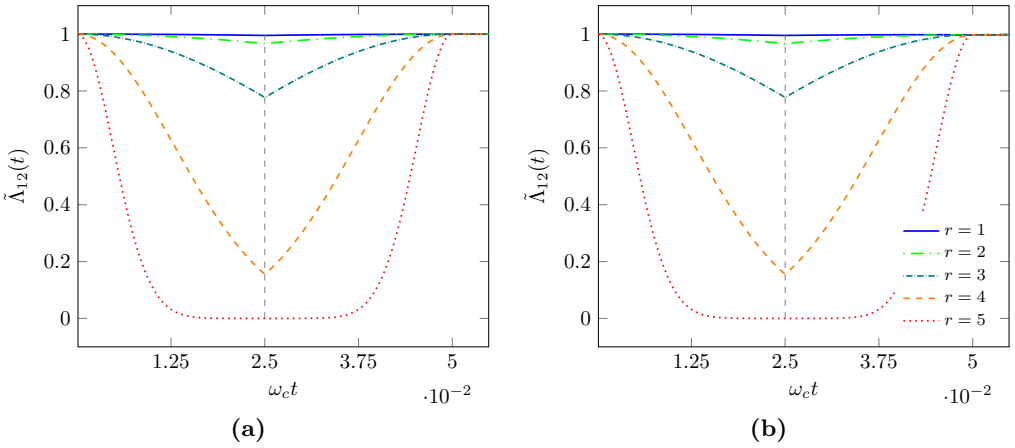

Figure 5.5 – The dynamics of the nonlocal coherence factor $\tilde{\Lambda}_{12}(t)$ (cf. Eq. (5.35)) obtained for environmental states given by $\boldsymbol{\sigma}_{\hat{X},r}^{\mathrm{EPR}}$ **(a)** and $\boldsymbol{\sigma}_{\hat{X},r}^{\mathrm{MTS}}$ **(b)** (cf. Eqs. (2.135) and (2.145), respectively). The parameters are chosen as in Fig. 5.2, that is, one considers squeezing parameter $r = 1, \ldots, 5$ for a coupling strength $\alpha = 1$ and subsequently applied interactions of length 2.5×10^{-2} in units of the environmental correlation time ω_c^{-1} (cf. Fig. 4 in Wißmann and Breuer (2014)).

It follows that $|F(t)| = 1$ holds for all times t if and only if the second cumulant vanishes, i.e., if one has

$$\langle\langle A \rangle\rangle_{\rho_E} = 0 \ , \tag{5.38}$$

which can, however, only be fulfilled if the environmental state ρ_E defines a dispersion free ensemble with respect to the operator A. That is, the support of the environmental state must not comprise elements of different eigenspaces of A. For a nondegenerate observable A, this results in $\rho_E = \Pi_a$, where Π_a refers to a one-dimensional projection onto the eigenspace associated with the eigenvalue a. Note that this condition is more strict than $[A, \rho_E] = 0$ which thus provides only a necessary but not sufficient condition for $|F(t)| = 1$. In fact, it is well-known that a vanishing commutator implies that A and ρ_E have a common eigenbasis $\{|j\rangle\}$ and, therefore, their spectral decompositions are given by $A = \sum_j a_j |j\rangle\langle j|$ and $\rho_E = \sum_j p_j |j\rangle\langle j|$. The decoherence function, however, reads

$$|F(t)| = \Big| \sum_j e^{i a_j t} p_j \Big| \tag{5.39}$$

for this state which can take any value between zero and one.

Now, adapting this general model to the setup of the original system, one assumes that the operator A is given by the difference of two local operators A_1 and A_2 which are linear in the canonical variables and may act independently of each other. One then distinguishes two cases: First, when both operators are simultaneously active and, secondly, when they act successively. In the former situation, one again obtains for the modulus of the coherence factor

$$|F(t)| = \exp\left[-\frac{1}{2} \langle\langle A \rangle\rangle_{\rho_E} t^2 \right] \tag{5.40}$$

with $A \equiv A_1 - A_2$, whereas the latter case implies

$$|F(t)| = \exp\left[-\frac{1}{2}\langle\langle A_1\rangle\rangle_{\rho_E} t^2\right] \tag{5.41}$$

during the first interaction.

Summarizing the observations about strong nonlocal memory effects, they occur within an appropriate time interval $[0,t]$ if and only if the reviving coherence factor is almost constant for simultaneously active interactions and decays rapidly within the first interaction period for subsequent interactions. Applying this to Eqs. (5.40) and (5.41), it thus follows that one must have $\langle\langle A\rangle\rangle_{\rho_E} \ll 1$ and $\langle\langle A_1\rangle\rangle_{\rho_E} \gg 1$ which can be combined leading to the following condition for the occurrence of strong rephasing effects in the general dephasing model:

$$\langle\langle A\rangle\rangle_{\rho_E} \ll \langle\langle A_1\rangle\rangle_{\rho_E} \ . \tag{5.42}$$

This condition can be rewritten if the second cumulants for the local operators A_1 and A_2 are equal. More specifically, if one has $\langle\langle A_1\rangle\rangle_{\rho_E} = \langle\langle A_2\rangle\rangle_{\rho_E}$, then Eq. (5.42) is reformulated as

$$2 \cdot \left\{\langle\langle A_1\rangle\rangle_{\rho_E} - \left(\tfrac{1}{2}\langle\{A_1, A_2\}\rangle_{\rho_E} - \langle A_1\rangle_{\rho_E}\langle A_2\rangle_{\rho_E}\right)\right\} \ll \langle\langle A_1\rangle\rangle_{\rho_E} \ , \tag{5.43}$$

so that one obtains

$$1 - K_{A_1,A_2}(\rho_E) \ll \frac{1}{2} \tag{5.44}$$

in terms of the correlation coefficient $K_{A_1,A_2}(\rho_E) = \left(\frac{1}{2}\langle\{A_1, A_2\}\rangle_{\rho_E} - \langle A_1\rangle_{\rho_E} \cdot \langle A_2\rangle_{\rho_E}\right)/\langle\langle A_1\rangle\rangle_{\rho_E}$ of the operators A_1 and A_2 (cf. Eq. (2.105)). In order to satisfy Eq. (5.44), it follows that the correlation coefficient must be positive and close to unity, corresponding to strongly correlated observables A_1 and A_2 in the environmental state ρ_E.

Note that the choice of a Gaussian state ρ_E along with environmental coupling operators A_j that are linear in the canonical observables (and have identical variances to end up with condition (5.44)) are essential for the distinct condition for the occurrence of strong nonlocal memory effects in the general dephasing model. For example for nonlinear couplings or non-Gaussian states, one obtains a more complicated set of conditions for the rephasing as the cumulant expansion will not truncate at second order. It is clear, however, that all these requirements are met for the original as well as the approximated model studied before so that it should apply in these cases.

To check this, one first observes that the approximated dynamics can indeed be described in terms of the general model. Clearly, the local interaction times $t_j(t)$ in the exponent of the coherence factors $\tilde{\kappa}_{12}$ and $\tilde{\Lambda}_{12}$ are proportional to t for any time $0 \leq t \leq t_1^f$ if one has simultaneously active local interactions corresponding to $t_2^s = 0$ and $t_1^f = t_2^f$. On the other hand, if the interactions act one after the other, assuming $t_1^f < t_2^f$ for convenience, one obtains $t_1(t) = t$ and $t_2(t) = 0$ for all $t \in [0, t_1^f]$. It follows that for $A_1 \equiv \sqrt{8}\sum_k g_k \hat{q}_k^{(1)}$ and $A_2 \equiv \mp\sqrt{8}\sum_k g_k \hat{q}_k^{(2)}$, the nonlocal coherence factors $\tilde{\kappa}_{12}(t)$ (for the choice $A_2 = -\ldots$) and $\tilde{\Lambda}_{12}(t)$ (for $A_2 = +\ldots$) are indeed described by the general dephasing model (5.36) within the time interval $[0, t_1^f]$.

For a Gaussian state ρ_E that is given by the tensor product of identical two-mode Gaussian states ρ_{G} with vanishing mean and equal diagonal entries such as the states $\boldsymbol{\sigma}_{\hat{X},r}^{\mathrm{EPR}}$ and $\boldsymbol{\sigma}_{\hat{X},r}^{\mathrm{MTS}}$ (cf. Eqs. (2.135) and (2.145), respectively), the correlation coefficient simplifies to $K_{A_1,A_2}(\rho_E = \bigotimes_k \rho_{\mathrm{G}}) = \langle A_1 A_2 \rangle_{\rho_E} / \langle A_1^2 \rangle_{\rho_E}$. The expectation values are found to obey

$$\langle A_1 A_2 \rangle_{\rho_E} = \mp 8 \sum_{k,k'} g_k g_{k'} \langle \hat{q}_k^{(1)} \hat{q}_{k'}^{(2)} \rangle_{\rho_E} = \mp 8 \alpha \omega_c^2 c_1 \ , \tag{5.45}$$

$$\langle A_1^2 \rangle_{\rho_E} = 8 \sum_{k,k'} g_k g_{k'} \langle \hat{q}_k^{(1)} \hat{q}_{k'}^{(1)} \rangle_{\rho_E} = 8 \alpha \omega_c^2 a \ , \tag{5.46}$$

in the continuum limit for an ohmic spectral density with cutoff frequency ω_c, since one has $\langle \hat{q}_k^{(j)} \hat{q}_{k'}^{(j')} \rangle_{\rho_E} = \delta_{k,k'} \langle \hat{q}_k^{(j)} \hat{q}_k^{(j')} \rangle_{\rho_{\mathrm{G}}}$ with $\langle \hat{q}_k^{(1)} \hat{q}_k^{(2)} \rangle_{\rho_{\mathrm{G}}} = c_1$ and $\langle (\hat{q}_k^{(1)})^2 \rangle_{\rho_{\mathrm{G}}} = a$ for any Gaussian states with covariance matrix given by Eq. (5.14) where $a_1 = a_2 = a$ holds. The correlation coefficient $K_{A_1,A_2}(\bigotimes_k \rho_{\mathrm{G}})$ is thus given by the quotient $\mp c_1/a$ and, therefore, the necessary and sufficient condition (5.44) reads

$$1 \pm \frac{c_1}{a} \ll \frac{1}{2} \ . \tag{5.47}$$

Hence, one should observe a strong rephasing of $\tilde{\Lambda}_{12}(t)$ if and only if $1 - c_1/a \ll 1/2$ is satisfied, whereas the approximate nonlocal coherence factor $\tilde{\kappa}_{12}(t)$ should revive if and only if one has $1 + c_1/a \ll 1/2$. Since c_1/a determines the correlation coefficient $K_{\hat{q}_1,\hat{q}_2}(\rho_{\mathrm{G}})$ between the canonical operators $\hat{q}_1$ and $\hat{q}_2$ for symmetric Gaussian states, it thus follows that strongly correlated positions, implying $K_{\hat{q}_1,\hat{q}_2}(\rho_{\mathrm{G}}) \approx 1$, should result in the rephasing of $\tilde{\Lambda}_{12}(t)$ within the second interaction period while anti-correlations of the observables $\hat{q}_1$ and $\hat{q}_2$ are supposed to yield a reviving coherence factor $\tilde{\kappa}_{12}(t)$.

Now, for the EPR state with covariance matrix $\boldsymbol{\sigma}_{\hat{X},r}^{\mathrm{EPR}}$ (cf. Eq. (2.135)), the correlation coefficient (2.140) reads

$$K_{\hat{q}_1,\hat{q}_2}(\rho_{|\psi_u\rangle}) = \frac{c_1}{a} = \tanh(2r) \ , \tag{5.48}$$

thus approaching ± 1 for $r \to \pm\infty$, which indeed explains the occurrence and the transition of the reviving coherence factor if the sign of the squeezing factor is changed. Moreover, for the particular two-mode mixed thermal state (2.145), the correlation coefficient is given by

$$K_{\hat{q}_1,\hat{q}_2}(\rho_{\boldsymbol{\sigma}_{\hat{X},r}^{\mathrm{MTS}}}) = 1 - \frac{1}{\cosh(2r)} \ , \tag{5.49}$$

which gets close to $+1$ for $|r| \to \infty$ coinciding with the previous observations, too. One concludes that the occurrence of nonlocal memory effects in the approximated model can indeed be explained by the constraint (5.44), which thus may be seen as a necessary and sufficient condition for the phenomenon of nonlocal non-Markovian behavior.

It is worth noticing that the necessary and sufficient condition (5.47) boils down to a constraint on the amount of entanglement contained in a pure Gaussian state. In fact, one easily shows that the generalized concurrence $C_{\mathrm{gen}}(\rho_E)$ (cf. Eq. (2.77))

for such states can be written as $C_{\mathrm{gen}}(\rho_{\mathrm{G}})^2 = 2(1-\sqrt{1-K_{\hat{q}_1,\hat{q}_2}(\rho_{\mathrm{G}})^2})$, employing the expression obtained for the EPR state in Eq. (2.139) and the fact that any pure two-mode Gaussian state is unitarily equivalent to this state (cf. Sec. 2.5.4). Hence, the more entangled the state, the stronger the nonlocal memory effects are. However, entanglement is not the only source for reviving nonlocal coherences as the particular mixed thermal state shows.

To understand the equivalence of entanglement and strong correlations, one needs to go back to the original version of the necessary and sufficient condition, i.e. Eq. (5.42). Applying it to the approximate dynamics, one finds

$$\langle(\hat{q}_1 \pm \hat{q}_2)^2\rangle_{\rho_{\mathrm{G}}} \ll \langle\hat{q}_1^2\rangle_{\rho_{\mathrm{G}}} \tag{5.50}$$

as constraint for the rephasing in terms of the canonical operators. Here, the minus (plus) sign corresponds to the coherence factor $\tilde{\Lambda}_{12}$ ($\tilde{\kappa}_{12}$). Based on the previous observations that the EPR state approximates an eigenstate of the operator $\hat{A}_{\mp} \equiv \hat{q}_1 \mp \hat{q}_2$ for $r \to \pm\infty$ (cf. Eq. (2.138)) whereas the expectation value of A_{-}^2 for the mixed thermal states is constant (cf. Sec. 2.5.4), it is clear that the two classes of Gaussian states use different mechanisms leading to nonlocal memory effects. While the left-hand side of Eq. (5.50) tends to zero for the squeezed vacuum in the appropriate limit, it remains constant for the mixed thermal states $\boldsymbol{\sigma}_{\hat{X},r}^{\mathrm{MTS}}$. For either states, however, the right-hand side diverges for $|r| \to \infty$, so that condition (5.50) is indeed satisfied.

So far the discussion focused on the approximate dynamics where the diminishing effect of the free evolution is not taken into account. Due to this, one cannot hope that the derived criterion (5.47) defines a sufficient[2] condition for nonlocal memory effects in case of the full dynamics. However, for sufficiently short interaction times $\omega_c \Delta t \ll 1$, the free evolution is almost negligible and, therefore, the criterion should still be reasonable. This is precisely confirmed by the results about the maximal non-Markovianity for all considered two-mode Gaussian states (cf. Figs. 5.3 and 5.4). One concludes that for interactions that are short compared to the environmental correlation time, Eq. (5.47) provides not only a necessary but also sufficient condition for the occurrence of nonlocal memory effects for the full dynamics. The rephasing of a nonlocal coherence factor is thus observed if and only if one has $\omega_c \Delta t \ll 1$ and the correlation coefficient of the canonical position operators satisfies

$$|K_{\hat{q}_1,\hat{q}_2}(\rho_{\mathrm{G}})| \approx 1 \; . \tag{5.51}$$

5.3.2 More than entanglement swapping

To extend the understanding of the phenomenon of nonlocal memory effects, it is worth considering the dynamics of correlations between the different parties for subsequently applied local interactions. Focusing on the original model showing nonlocal memory effects, the implication of the local interactions can be nicely illustrated if one assumes that the environment is given by a single pair of modes

[2] The necessity of the condition is obviously confirmed by the findings for the original model (cf. Sec. 5.2).

in the EPR state $|\psi_u\rangle_{E_1E_2} = \sqrt{1-u^2}\sum_{n=0}^{\infty} u^n|n,n\rangle_{E_1E_2}$ (cf. Eq. (2.136)). For this setup the state of the total system after the first interaction reads

$$|\Psi_{\mathrm{I}}\rangle_{SE} = \frac{1}{\sqrt{2}}\sum_{j=0}^{1}|jj\rangle_{S_1S_2}\otimes\left(V^{(j)}\otimes\mathbb{1}_{E_2}\right)|\psi_u\rangle_{E_1E_2}\ , \tag{5.52}$$

where the unitary $V^{(j)}$ are given by $V^{(j)} = D((-1)^{j+1}\beta_{E_1}(t))$ provided the open system was initially given by the Bell state $|\Psi_0\rangle$ (see Eqs. (2.78) and (5.23)). One then finds for the reduced state of the subsystems S_1 and E_1

$$\begin{aligned}\rho_{S_1E_1} &= \mathrm{Tr}_{S_2E_2}\left\{|\Psi_{\mathrm{I}}\rangle_{SE}\langle\Psi_{\mathrm{I}}|\right\}\\ &= \frac{1-u^2}{2}\sum_{m,n=0}^{\infty}\sum_{j=0}^{1}\gamma_{m,n}^{(j)}|j,n\rangle_{S_1E_1}\langle j,m|\ ,\end{aligned} \tag{5.53}$$

where $\gamma_{m,n}^{(j)} = \sum_{k=0}^{\infty}u^{2k}\langle n|V^{(j)}|k\rangle\langle k|V^{(j)\dagger}|m\rangle$. It is easily shown that $\gamma_{m,n}^{(j)}\to\delta_{m,n}$ for all j in the limit $u\to 1$ implying that the reduced state $\rho_{S_1E_1}$ approaches the maximally mixed state in the limit of infinitely strong squeezing. Thus, one concludes that there are still strong correlations between the two partitions S_1E_1 and S_2E_2, which agrees with the intuitive understanding that local unitary transformations cannot alter the entanglement in a bipartite system and, therefore, the initial correlations in the joint state of E_1 and E_2 cannot be diminished.

As a consequence of this result, one may also conclude that the occurrence of nonlocal memory effects cannot be explained by a swap of correlations. That is, the complete dephasing and subsequent rephasing of the Bell states $|\Psi_{0,3}\rangle$ or $|\Psi_{1,2}\rangle$ as observed for the dynamics generated by the Hamiltonian (5.3) is not due to the fact that the first local interaction leads to a state where each subsystem of the open system is solely correlated with its respective environment and the second interaction restores the initial configuration of a correlated open quantum system as well as environment. Obviously, such an effective dynamics would explain the disappearing and reviving nonlocal coherences factors (see, e.g., Fig. (5.5)). However, such an ansatz does not apply and can even be shown to do so in general by means of the following toy model which effectively describes the dynamics of the original model. Consider a bipartite four-dimensional open quantum system each interacting locally with the correlated environment according to the unitary map V as illustrated in Fig. 5.6 where N is arbitrary and may be even infinite (see below). Focusing initially on finite-dimensional environments, one would thus require in order to obtain nonlocal memory effects that the local interactions yield the state transformation

$$\left(V\otimes\mathbb{1}_{S_2E_2}\right)|\Psi\rangle_{S_1S_2}\otimes|\Phi\rangle_{E_1E_2} = |\zeta_1\rangle_{S_1E_1}\otimes|\zeta_2\rangle_{S_2E_2} \tag{5.54}$$

and

$$\left(\mathbb{1}_{S_1E_1}\otimes V\right)|\zeta_1\rangle_{S_1E_1}\otimes|\zeta_2\rangle_{S_2E_2} = |\tilde{\Psi}\rangle_{S_1S_2}\otimes|\tilde{\Phi}\rangle_{E_1E_2}\ . \tag{5.55}$$

Here, the states $|\Psi\rangle_{S_1S_2}$, $|\tilde{\Psi}\rangle_{S_1S_2}$, $|\Phi\rangle_{S_1S_2}$, $|\tilde{\Phi}\rangle_{S_1S_2}$ and $|\zeta_j\rangle_{S_jE_j}$ are assumed to be maximally entangled, where one additionally requires that the states $|\Psi\rangle_{S_1S_2}$ and $|\tilde{\Psi}\rangle_{S_1S_2}$ have a common Schmidt decomposition. By means of a detailed analysis of

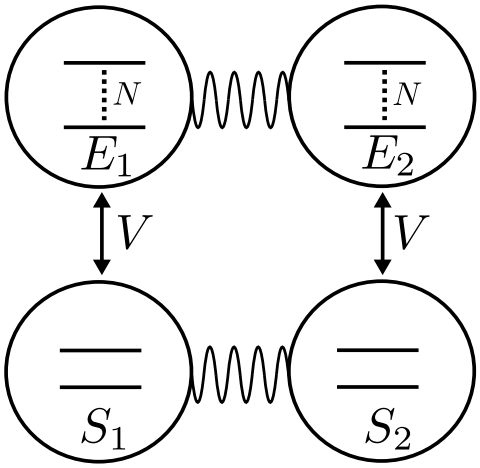

Figure 5.6 – Schematic plot of the open system given by two qubits that consecutively interact with their local N-dimensional environments described by the unitary V. The joint initial state of S_1 and S_2 as well as E_1 and E_2 is assumed to be maximally entangled.

the conditions imposed on the unitary V, it is shown in the following that a local interaction leading to the above state transformations does actually not exist.

First, note that one may assume without loss of generality that the open system's initial state is given by the Bell state $|\Psi_0\rangle$ since any maximally entangled state can be obtained by applying a local unitary to this state (Kok and Braunstein, 2000). The final maximally entangled state of system S_1 and S_2 must then be given by

$$|\tilde{\Psi}\rangle_{S_1S_2} = \frac{1}{\sqrt{2}}\left(e^{i\phi}|11\rangle_{S_1S_2} + |00\rangle_{S_1S_2}\right) \tag{5.56}$$

for some phase $\phi \in [0, 2\pi)$. Similarly, the other maximally entangled states may be written as

$$|\Phi\rangle_{E_1E_2} = (U \otimes \mathbb{1}_{E_2})|\Phi_{\max}\rangle_{E_1E_2} \ , \tag{5.57}$$

$$|\tilde{\Phi}\rangle_{E_1E_2} = (W \otimes \mathbb{1}_{E_2})|\Phi_{\max}\rangle_{E_1E_2} \ , \tag{5.58}$$

$$|\zeta_j\rangle_{S_jE_j} = (\mathbb{1}_{S_j} \otimes V_j)|\zeta_{\max}\rangle_{S_jE_j} \tag{5.59}$$

for unitary operators U, W and V_j on the N-dimensional environments and generic maximally entangled states

$$|\Phi_{\max}\rangle_{E_1E_2} \equiv \frac{1}{\sqrt{N}}\sum_{k=0}^{N-1}|kk\rangle_{E_1E_2} \ , \tag{5.60}$$

$$|\zeta_{\max}\rangle_{S_jE_j} \equiv \frac{1}{\sqrt{2}}\sum_{k=0}^{1}|k,k\rangle_{S_jE_j} \ , \tag{5.61}$$

where $\{|k\rangle_{E_j}\,|\,0 \leq k \leq N-1\}$ refers to some orthonormal basis of the environment E_j. To satisfy Eq. (5.54), the unitaries' entries must obey

$$\frac{1}{\sqrt{2N}}\sum_{k=0}^{N-1}V_{rtjk}U_{ku} = \frac{1}{2}\left(V_1\right)_{tr}\left(V_2\right)_{uj} \tag{5.62}$$

for all indices $j, r \in \{0, 1\}$ and $t, u \in \{0, \ldots, N-1\}$. This relation is obtained by expanding the left- and the right-hand side of Eq. (5.54) in the joint basis $\{|ij, kl\rangle_{SE} |\, 0 \leq i, j \leq 1\,,\, 0 \leq k, l \leq N-1\}$ and comparing the coefficients. In the same way, Eq. (5.55) is found to imply

$$\frac{1}{2}\left[\sum_{k=0}^{N-1}\sum_{j=0}^{1} V_{rtjk}(V_2)_{kj}\right](V_1)_{sl} = \frac{1}{\sqrt{2N}}\, W_{st}(\delta_{r,0} + e^{i\phi}\delta_{r,1}) \;, \tag{5.63}$$

where $l, r \in \{0, 1\}$ and $s, t \in \{0, \ldots, N-1\}$. One readily observes that Eq. (5.62) can be written as

$$U^T \begin{pmatrix} V_{rtj0} \\ \vdots \\ V_{rtj(N-1)} \end{pmatrix} = \sqrt{\frac{N}{2}} \cdot (V_1)_{tr} \begin{pmatrix} (V_2)_{0j} \\ \vdots \\ (V_2)_{(N-1)j} \end{pmatrix} \;, \tag{5.64}$$

where U^T refers to the transposed of U with respect to the basis $\{|k\rangle_{E_1}\}$, i.e. one has $(U^T)_{jk} = \langle k|U|j\rangle = U_{kj}$. As U is unitary by assumption, its transpose U^T is unitary, too, with inverse $\left(U^T\right)^\dagger = U^*$. One may then solve the set of equations (5.64) for V_{rtjk} which gives

$$V_{rtjk} = \sqrt{\frac{N}{2}} \cdot (V_1)_{tr} \sum_{m=0}^{N-1} U^*_{km}(V_2)_{mj} \;, \tag{5.65}$$

where the indices obey $j, r \in \{0, 1\}$ and $k, t \in \{0, \ldots, N-1\}$. Upon inserting this expression into Eq. (5.63), one finally obtains

$$\Delta_N (V_1)_{tr}(V_1)_{sl} = \; W_{st}\, \delta_{l,r}(\delta_{r,0} + e^{i\phi}\delta_{r,1}) \;, \tag{5.66}$$

with $l, r \in \{0, 1\}$ and $s, t \in \{0, \ldots, N-1\}$ as well as

$$\Delta_N \equiv \frac{N}{2} \cdot \sum_{k,m=0}^{N-1}\sum_{j=0}^{1} U^*_{km}(V_2)_{mj}(V_2)_{kj} \;. \tag{5.67}$$

Clearly, $\Delta_N = 0$ implies that $W = (W_{st}) = 0$ holds, which does not define a unitary operator. Therefore, one must have $\Delta_N \neq 0$ so that Eq. (5.66) implies

$$(V_1)^2_{tr} = W_{tt}\frac{1}{\Delta_N}(\delta_{r,0} + e^{i\phi}\delta_{r,1}) \tag{5.68}$$

for all indices $r \in \{0, 1\}$ and $t \in \{0, \ldots, N-1\}$. If $W_{tt} \neq 0$, it thus follows that $(V_1)_{t0}$ as well as $(V_1)_{t1}$ are nonzero. However, from Eq. (5.66) one deduces

$$(V_1)_{t0}(V_1)_{t1} = 0 \tag{5.69}$$

for any t, which cannot be satisfied for nonvanishing coefficients. Hence, one concludes that the diagonal elements of W must vanish, i.e. one has $W_{tt} = 0$ for all $t \in \{0, \ldots, N-1\}$. As this implies $(V_1)_{tr} = 0$ for any $r \in \{0, 1\}$, Eq. (5.66) gives

$$W_{st}\frac{1}{\Delta_N}(\delta_{r,0} + e^{i\phi}\delta_{r,1}) = (V_1)_{tr}(V_1)_{sr} = 0 \tag{5.70}$$

for all indices $s, t \in \{0, \ldots, N-1\}$ from which again $W = 0$ follows. One thus concludes that there does not exist a unitary operator V such that the entanglement swapping characterized by Eqs. (5.54) and (5.55) can be realized.

It is immediately observed that the preceding proof did not make use of the fact that W is unitary for which is reason this assumption may be relaxed. As a consequence, the above result extends to arbitrary final states $|\tilde{\Phi}\rangle_{E_1E_2}$ of the environment. Moreover, an imperfect rephasing of the open system state described by a final state

$$|\tilde{\Psi}'\rangle_{S_1S_2} = \sqrt{1-\epsilon}\,|\tilde{\Psi}\rangle_{S_1S_2} + \sqrt{\epsilon}\,\{a_0|01\rangle_{S_1S_2} + a_1|10\rangle_{S_1S_2}\} \tag{5.71}$$

for $0 < \epsilon \ll 1$ and $|a_0|^2 + |a_1|^2 = 1$ does neither allow to deduce a unitary operator V satisfying the sketched scheme for N-dimensional environments E_1 and E_2.

Finally, the above consideration may also be extended to initial states of the environment $|\Phi\rangle_{E_1E_2}$ that are obtained from $|\Phi_{\max}\rangle_{E_1E_2}$ (cf. Eq. (5.60)) by applying any properly normalized invertible operator U. More precisely, due to the fact that one has

$$\mathrm{Tr}_E\{|\Phi\rangle_{E_1E_2}\langle\Phi|\} = \sum_{j,k=0}^{N-1} |U_{jk}|^2\,, \tag{5.72}$$

the unitary U in Eq. (5.57) may be replaced by any invertible operator with Frobenius norm equal to unity. Clearly, the unitaries define a proper subset of this set, thus extending the developed treatment to a bigger class of initial states for the environment. An example for a state created by an invertible operator with Frobenius norm equal to one is provided by the finite-dimensional analog of the EPR state (2.136). Defining an operator U by

$$\langle j|U|k\rangle = \delta_{j,k}\sqrt{\frac{1-|u|^2}{1-|u|^{2N}}}\,u^j \tag{5.73}$$

for $j, k \in \{0, \ldots, N-1\}$ with parameter $u = \tanh r \in \mathbb{R}$, one easily verifies that it is invertible with inverse $\langle j|U^{-1}|k\rangle = \delta_{j,k}\sqrt{(1-|u|^{2N})/(1-|u|^2)}\,u^{-j}$ and has Frobenius norm equal to one which may be shown using the geometric series. As the corresponding state $|\Phi\rangle_{E_1E_2}$ yields the EPR state in the limit $N \to \infty$, the general considerations reflect the previous observations for the original model and show that the simple ansatz of entanglement swapping for nonlocal memory effects does not apply in general, that is, independent of the dimension of the environment.

5.4 Nonlocal memory effects for finite environments

The preceding sections have shown that nonlocal memory effects exist for the dynamics generated by the Hamiltonian (5.3) with a continuum of bosonic modes defining the environment, and revealed the conditions for their occurrence as well as the dynamics of correlations between the different partitions. Another question in the study of nonlocal memory effects concerns the significance of the environments. In fact, does the decay and the subsequent revival of a single nonlocal coherence factor of a bipartite open quantum system where all other coherences

get arbitrarily small as observed for the original model reflect the infinite dimensions of the bosonic environments? That is, can such a dynamics not be observed if the bosonic environments are replaced by finite-dimensional systems, thus allowing to obtain nonlocal memory effects by means of finite-dimensional systems?

To start revealing the role of the environmental dimension, finite-dimensional counterparts of the original model are considered in general terms in the following part of this thesis. Choosing the environments to be arbitrary finite-dimensional systems, the constraints on the local unitaries describing the local interactions are then determined if nonlocal memory effects are supposed to occur. Surprisingly, it turns out that the simplest case of environments, described by two-dimensional Hilbert spaces, is not possible, i.e., the derived constraints cannot be satisfied. For environments defined by two three-level instead of two-level systems, a solution can, however, be found but the determined example has the feature that both nonlocal coherence factors show substantial (intermediate) revivals during the second local interaction (see Fig. 5.7). In fact, the given example supports the conjecture that a dynamics where all but a single nonlocal coherence factor decays is obtained in the limit of an infinite-system. To prove this ultimately, further examinations of the derived constraints and their possible solutions are, however, necessary and may be carried out in the future. If the conjecture indeed proves to be true, one concludes that nonlocal memory effects as observed in the original model as well as in the second example provided in (Laine *et al.*, 2012) represent a clear signature of an environment described infinite-dimensional Hilbert spaces, which cannot be simulated via a finite-dimensional setup and, thus, could be used to probe the (effective) dimension of an open quantum system's environment.

As before, one assumes to have two N-dimensional environments E_1 and E_2 which are given in a state that is maximally entangled (cf. Fig. 5.6). In addition, the unitary dynamics is viewed as being effectively described by local unitaries $V^{(j)}$ acting on the environmental Hilbert spaces $\mathcal{H}_{E_k}$, so that the two-stage time evolution of the initial state of the total system $|\Psi_0\rangle_{S_1S_2} \otimes |\Phi\rangle_{E_1E_2}$ – where $|\Phi\rangle_{E_1E_2}$ is given by Eq. (5.57) and $|\Psi_0\rangle_{S_1S_2}$ refers to the Bell state (5.23) – is described as

$$|\Psi_{\mathrm{I}}\rangle_{SE} = \frac{1}{\sqrt{2}} \sum_{j=0}^{1} |jj\rangle_{S_1S_2} \otimes \left(V^{(j)} \otimes \mathbb{1}_{E_2}\right) |\Phi\rangle_{E_1E_2} \ , \tag{5.74}$$

and

$$|\Psi_{\mathrm{II}}\rangle_{SE} = \frac{1}{\sqrt{2}} \sum_{j=0}^{1} |jj\rangle_{S_1S_2} \otimes \left(V^{(j)} \otimes V^{(j)}\right) |\Phi\rangle_{E_1E_2} \ , \tag{5.75}$$

where the final state is additionally assumed to have the same structure of correlated bipartitions as the initial state. Due to this, it must be given by

$$|\Psi_{\mathrm{II}}\rangle_{SE} = \frac{1}{\sqrt{2}} \sum_{j=0}^{1} e^{i\phi_j} |jj\rangle_{S_1S_2} \otimes (W \otimes \mathbb{1}_{E_2}) |\Phi\rangle_{E_1E_2} \ , \tag{5.76}$$

where W denotes a unitary. That is, the state of the open system as well as the environment are maximally entangled. Expanding the two expression for $|\Psi_{\mathrm{II}}\rangle_{SE}$

in the joint basis $\{|ij,kl\rangle_{SE}|\,0\leq i,j\leq 1\,,\,0\leq k,l\leq N-1\}$ as before in Sec. 5.3.2, one obtains the following relation that determines the operator W:

$$e^{i\phi_j}\langle m|W|n\rangle = \langle m|V^{(j)}UV^{(j)T}|n\rangle\ , \tag{5.77}$$

for all $m,n\in\{0,\ldots,N-1\}$ where the transpose $V^{(j)T}$ is defined, as before, with respect to the basis $\{|j\rangle_{E_k}|\,0\leq j\leq N-1\}$. Note that the subscripts E_k have been omitted as the environments are isomorphic and may thus be identified with each other. Clearly, the operators $e^{-i\phi_j}V^{(j)}UV^{(j)T}$ are unitary so that there is no immediate contradiction. It thus remains to find unitaries U and $V^{(j)}$ and phases ϕ_j such that these operators are independent of the index j.

If the first part of the time evolution is supposed to result in a completely dephased state of the open system, i.e.

$$\rho^{\mathrm{I}}_{S_1S_2} = \mathrm{Tr}_E\{|\Psi_{\mathrm{I}}\rangle_{SE}\langle\Psi_{\mathrm{I}}|\} = \frac{1}{2}\sum_{j=0}^{1}|jj\rangle_{S_1S_2}\langle jj|\ , \tag{5.78}$$

then the local unitaries $V^{(j)}$ must additionally satisfy

$$\mathrm{Tr}_E\Big\{(V^{(j\neq k)\dagger}V^{(k)}\otimes\mathbb{1}_{E_2})|\Phi\rangle_{E_1E_2}\langle\Phi|\Big\} = 0\ . \tag{5.79}$$

Evaluating the left-hand side of Eq. (5.79), this condition is written as

$$\begin{aligned}
0 &= \mathrm{Tr}_E\Big\{(V^{(j\neq k)\dagger}V^{(k)}\otimes\mathbb{1}_{E_2})|\Phi\rangle_{E_1E_2}\langle\Phi|\Big\}\\
&= \frac{1}{N}\sum_{m,n,p,q=0}^{N-1}U_{pq}U^*_{mn}\,{}_{E_1E_2}\langle m,n|V^{(j\neq k)\dagger}V^{(k)}\otimes\mathbb{1}_{E_2}|p,q\rangle_{E_1E_2}\\
&= \frac{1}{N}\sum_{m,p=0}^{N-1}\left(\sum_{n=0}^{N-1}U_{pn}u^*_{mn}\right){}_{E_1}\langle m|V^{(j\neq k)\dagger}V^{(k)}|p\rangle_{E_1}\\
&= \frac{1}{N}\mathrm{Tr}_{E_1}\Big\{V^{(j\neq k)\dagger}V^{(k)}\Big\}\ .
\end{aligned} \tag{5.80}$$

Two unitaries satisfying Eq. (5.80) are for example given by the permutation matrices $V^{(j)}=\sum_{m=0}^{N-1}|\pi_j(m)\rangle_{E_1}\langle m|$ associated with permutations $\pi_j\in S_N$ of the set $\{0,\ldots,N-1\}$ where one has $\pi_0(m)\neq\pi_1(m)$ for any index m. For two-dimensional environments, i.e. $\mathcal{H}_{E_k}=\mathbb{C}^2$, the two unitaries

$$V^{(0)} = i\,\mathbb{1}_2 \qquad \text{and} \qquad V^{(1)} = i\,\sigma_1 \tag{5.81}$$

provide an explicit example for permutation matrices that obey Eq. (5.79). The unitary operators $\tilde{W}_j\equiv e^{-i\phi_j}V^{(j)}UV^{(j)T}$ are then given by

$$\tilde{W}_0 = -e^{-i\phi_0}U\ , \qquad\qquad \tilde{W}_1 = -e^{-i\phi_1}\sigma_1U\sigma_1\ , \tag{5.82}$$

which are equal if and only if the relation

$$\begin{pmatrix}U_{00} & U_{01}\\ U_{10} & U_{11}\end{pmatrix} = e^{-i(\phi_1-\phi_0)}\begin{pmatrix}U_{11} & U_{10}\\ U_{01} & U_{00}\end{pmatrix}\ , \tag{5.83}$$

holds. This equation is obviously satisfied by $U = \mathbb{1}_2$ and $\phi_1 = \phi_0 + 2\pi k$ for some $k \in \mathbb{N}_0$. However, evaluating the reduced state after the first and second interaction[3] for these unitaries and an initial state $|\Psi_{\text{ini}}\rangle_{SE} = \sum_{j,k=0}^{1} a_{jk}|jk\rangle_{S_1S_2} \otimes |\Phi\rangle_{E_1E_2}$ where $A = (a_{ij})$ refers to some 2×2-matrix with Frobenius norm equal to unity (cf. Eq. (5.72)), one finds

$$\begin{aligned}\tilde{\rho}^{\text{I}}_{S_1S_2} &= \text{Tr}_E\left\{(V \otimes \mathbb{1}_{S_2E_2})|\Psi_{\text{ini}}\rangle_{SE}\langle\Psi_{\text{ini}}|(V^\dagger \otimes \mathbb{1}_{S_2E_2})\right\} \\ &= \begin{pmatrix} |a_{11}|^2 & a_{11}a_{10}^* & 0 & 0 \\ a_{11}^*a_{10} & |a_{10}|^2 & 0 & 0 \\ 0 & 0 & |a_{01}|^2 & a_{01}a_{00}^* \\ 0 & 0 & a_{01}^*a_{00} & |a_{00}|^2 \end{pmatrix}\end{aligned} \tag{5.84}$$

and

$$\begin{aligned}\tilde{\rho}^{\text{II}}_{S_1S_2} &= \text{Tr}_E\left\{(V \otimes V)|\Psi_{\text{ini}}\rangle_{SE}\langle\Psi_{\text{ini}}|(V^\dagger \otimes V^\dagger)\right\} \\ &= \begin{pmatrix} |a_{11}|^2 & 0 & 0 & a_{11}a_{00}^* \\ 0 & |a_{10}|^2 & a_{10}a_{01}^* & 0 \\ 0 & a_{10}^*a_{01} & |a_{01}|^2 & 0 \\ a_{11}^*a_{00} & 0 & 0 & |a_{00}|^2 \end{pmatrix},\end{aligned} \tag{5.85}$$

which clearly shows that both nonlocal coherences rephase in contradiction to the observations for the original model.

To obtain a reduced dynamics that erases all but a single nonlocal coherence after the second interaction, one must furthermore require that the environmental states

$$|\Phi_{jk}\rangle_{E_1E_2} \equiv \sum_{m,n,p,q=0}^{N-1} U_{pq}\ {}_{E_1}\langle m|V^{(j)}|p\rangle_{E_1}\ {}_{E_2}\langle n|V^{(k)}|q\rangle_{E_2}\ \ |mn\rangle_{E_1E_2} \tag{5.86}$$

satisfy either

$${}_{E_1E_2}\langle\Phi_{jk}|\Phi_{rs}\rangle_{E_1E_2} = \delta_{j,k}\,\delta_{r,s} \tag{5.87}$$

or

$${}_{E_1E_2}\langle\Phi_{jk}|\Phi_{rs}\rangle_{E_1E_2} = \delta_{j,s}\,\delta_{k,r}\ , \tag{5.88}$$

depending on whether solely the coherences of $\tilde{\rho}^{\text{II}}_{S_1S_2}$ associated with $a_{11}a_{00}^*$ or $a_{10}a_{01}^*$ should be nonzero (see Eq. (5.85)). That is, condition (5.87) ensures that the reduced state for $|\Psi_{0(3)}\rangle$ (cf. Eq. (5.23)), attributed to κ_{12}, is invariant under the dynamics whereas Eq. (5.88) implies that the Bell states $|\Psi_{1(2)}\rangle$ (cf. Eq. (5.24)) are preserved, disregarding a shift of the relative phase as incorporated by the assumption on the final state (cf. Eq. (5.76)).

Without loss of generality, assume that the Bell state $|\Psi_{0(3)}\rangle$ revives. Using that the adjoint is obtained by taking the transpose and complex conjugation for

[3]Note that the corresponding total unitary dynamics describing these local unitaries reads $V = \exp\left[i\frac{\pi}{2}\left\{|0\rangle\langle 0| \otimes \mathbb{1}_2 + |1\rangle\langle 1| \otimes \sigma_x\right\}\right]$ which defines a CNOT-gate (Nielsen and Chuang, 2000).

operators on finite-dimensional Hilbert spaces, the associated condition (5.87) can be rewritten as

$$\begin{aligned} N \cdot \delta_{j,k}\, \delta_{r,s} &= \sum_{m,n=0}^{N-1} \left(V^{(j)} U V^{(k)T}\right)^*_{mn} \left(V^{(r)} U V^{(s)T}\right)_{mn} \\ &= \sum_{m,n=0}^{N-1} \left(\left(V^{(j)} U V^{(k)T}\right)^\dagger\right)_{nm} \left(V^{(r)} U V^{(s)T}\right)_{mn} \\ &= \sum_{m,n=0}^{N-1} \left(V^{(k)T^\dagger} U^\dagger V^{(j)\dagger}\right)_{nm} \left(V^{(r)} U V^{(s)T}\right)_{mn} \\ &= \mathrm{Tr}\left\{V^{(j)\dagger} V^{(r)} U V^{(s)T} V^{(k)T^\dagger} U^\dagger\right\} \ . \end{aligned} \tag{5.89}$$

In summary, the constraints on the unitaries $V^{(j)}$ and U are thus given by the three relations

$$\mathrm{Tr}\left\{V^{(1)\dagger} V^{(0)}\right\} = 0 \ , \tag{5.90}$$

$$\mathrm{Tr}\left\{V^{(1)\dagger} V^{(0)} U V^{(0)T} V^{(1)T^\dagger} U^\dagger\right\} = N \ , \tag{5.91}$$

$$\mathrm{Tr}\left\{V^{(1)\dagger} V^{(0)} U V^{(1)T} V^{(0)T^\dagger} U^\dagger\right\} = 0 \ , \tag{5.92}$$

as the other equations follow from complex conjugation.

Now, defining unitary operators $W_1 = V^{(1)\dagger} V^{(0)}$ and $W_0 = W_1^\dagger$, one observes that $W_1 \neq 0$ due to condition (5.91) but its eigenvalues $\exp[i\theta_j]$ (where $\theta_j \in [0, 2\pi)$) must sum to zero, i.e., they must obey

$$\sum_{j=0}^{N-1} e^{i\theta_j} = 0 \ , \tag{5.93}$$

due to Eq. (5.90). Moreover, since one has $X^\dagger = X^{*T} = X^{T*}$ for operators on finite-dimensional Hilbert spaces, one finds

$$V^{(0)T} V^{(1)T^\dagger} = \left(V^{(1)*^T} V^{(0)}\right)^T = W_1^T = W_0^* \ , \tag{5.94}$$

$$V^{(1)T} V^{(0)T^\dagger} = \left(V^{(0)*^T} V^{(1)}\right)^T = W_0^T = W_1^* \ , \tag{5.95}$$

so that Eqs. (5.91) and (5.92) can be rewritten in terms of the operators $R_j \equiv W_1 U W_j^T U^\dagger$ according to

$$\mathrm{Tr}\left\{R_j\right\} = N \cdot \delta_{j,1} \ . \tag{5.96}$$

Clearly, R_j define unitary operators and, therefore, their eigenvalues $\lambda_k^{(j)} \in \mathbb{C}$ are on the unit circle, i.e. one has $|\lambda_k^{(j)}| = 1$ for all $k \in \{0, \ldots, N-1\}$, and they need to satisfy $\sum_{k=0}^{N-1} \lambda_k^{(j)} = N \cdot \delta_{j,1}$ due to Eq. (5.96). Taking the real part and using linearity, one finally obtains

$$N = \sum_{k=0}^{N-1} \mathrm{Re}(\lambda_k^{(1)}) \leq \sum_{k=0}^{N-1} |\lambda_k^{(1)}| = N \ , \tag{5.97}$$

which implies $\mathrm{Im}(\lambda_k^{(1)}) = 0$ for all k and, therefore, $\lambda_k^{(1)} = 1$. Hence, $R_1 = W_1 U W_1^T U^\dagger$ is the unit operator which means that one has $W_1 U = U W_1^{T\dagger}$. By means of this relation, the trace of R_0 is finally deduced to obey

$$\mathrm{Tr}\{R_0\} = \mathrm{Tr}\left\{W_1^\dagger W_0\right\} = \mathrm{Tr}\left\{W_1^2\right\}^* , \tag{5.98}$$

where one additionally uses the cyclic property of the trace, its invariance under transposition, i.e. $\mathrm{Tr}\{A^T\} = \mathrm{Tr}\{A\}$, and the fact that $\mathrm{Tr}\{A^\dagger\} = \mathrm{Tr}\{A\}^*$ holds. Eq. (5.96) thus implies a second constraint on the eigenvalues of the unitary W_1. More precisely, they must then obey the two equations

$$\mathrm{Tr}\left\{W_1\right\} = \sum_{j=0}^{N-1} e^{i\theta_j} = 0 , \tag{5.99}$$

$$\mathrm{Tr}\left\{W_1^2\right\} = \sum_{j=0}^{N-1} e^{i2\theta_j} = 0 , \tag{5.100}$$

which cannot be satisfied simultaneously for two-dimensional environments E_1 and E_2. In fact, one concludes from Eq. (5.99) that the eigenvalues obey $\exp[i\theta_0] = -\exp[i\theta_1]$ so that their squares are equal, i.e. one has $\exp[i2\theta_0] = \exp[i2\theta_0]$ and, therefore, one obtains $\sum_{j=0}^{1} \exp[i2\theta_j] = 2\exp[i2\theta_0]$ which clearly violates Eq. (5.100) for any choice of θ_0.

As a consequence, the Hilbert space describing the environments E_k must be at least three-dimensional in order to observe nonlocal memory effects. Apart from Eqs. (5.99) and (5.100), the requirement $R_1 = \mathbb{1}_N$ imposes a condition on the operator W_1, too. If X denotes the unitary diagonalizing W_1 with respect to the basis $\{|j\rangle \,|\, 0 \leq j \leq N-1\}$, i.e. $W_1 = XDX^\dagger$ where $D = \sum_j \exp[i\theta_j]\,|j\rangle\langle j|$, then the relation $W_1 U = U W_1^{T\dagger}$ is found to be equivalent to

$$Y \;= DYD , \tag{5.101}$$

since D as well as $Y \equiv X^T U^\dagger X$ define unitaries. In particular, this equation implies

$$\langle j|Y|k\rangle = e^{i(\theta_j+\theta_k)}\langle j|Y|k\rangle \tag{5.102}$$

for all $j,k \in \{0,\ldots,N-1\}$. Hence, given a tuple of basis elements $|j\rangle$ and $|k\rangle$ such that $\langle j|Y|k\rangle \neq 0$ holds, Eq. (5.102) is satisfied if and only if one has

$$\theta_j + \theta_k = 2\pi \cdot f(j,k) , \tag{5.103}$$

where $f : \{0,\ldots,N-1\} \times \{0,\ldots,N-1\} \to \mathbb{Z}$ defines some integer-valued function. Clearly, nonzero transition matrix elements $\langle j|Y|j\rangle$ yield $\theta_j = \pi \cdot f(j,j)$ so that $\exp[i\theta_j] = \pm 1$. However, if all of these elements would be nonzero, then Eq. (5.100) cannot be satisfied. Thus, a finite-dimensional realization of nonlocal memory effects requires that the unitary operator Y is not diagonal in the basis with respect to which the maximally entangled state of the environment $|\Phi_{\max}\rangle_{E_1 E_2}$ (cf. Eq. (5.60)) is defined.

Before determining a unitary operator satisfying Eq. (5.102), one notes that such an operator on an N-dimensional Hilbert space must have at least N nonzero transition matrix elements with respect to any orthonormal basis. Clearly, this is equivalent to the existence of N orthonormal columns and rows which characterizes a unitary matrix. The eigenbasis of a unitary obviously provides such a basis with minimal amount of nonzero matrix elements. The previously considered permutation matrices corresponding to a fixed basis and permutation, i.e. $Y = \sum_{j=0}^{N-1} |\pi'(j)\rangle_{E_1}\langle j|$ for $\pi' \in S_N$, define an example for unitary operators with at least two bases with minimal amount of nonzero transition matrix elements. To minimizes the amount of constraints imposed by Eq. (5.102), it is thus convenient to consider the case that Y is described by such a permutation matrix. If one focuses on three-dimensional environments, possibly providing the simplest realization of nonlocal memory effects as two-level systems have been ruled out, one immediately recognizes that the permutation cannot be cyclic. In fact, any cyclic permutation defines a closed sequence of integers, e.g. $(0,1) \mapsto (1,2) \mapsto (2,0)$, so that Eq. (5.103) yields[4] $\theta_j = \pi \cdot g(j)$ for all j for some function $g : \{0, \ldots, N-1\} \to \mathbb{Z}$. So the eigenvalues of W_1 would again be given by ± 1 violating Eq. (5.100).

It follows that the nontrivial permutation must have a fixed point, i.e. it needs to obey $\pi'(j) = j$ for one index $j \in \{0,1,2\}$. Assuming $\pi'(2) = 2$ so that $Y = \left(\begin{smallmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{smallmatrix}\right)$, one may indeed find phases θ_j that are in accordance with the constraints imposed on Y. More specifically, Eq. (5.103) gives $\theta_1 = 2\pi f(0,1) - \theta_0$ and $\theta_2 = \pi f(2,2)$ where θ_0 and θ_2 must in addition satisfy Eqs. (5.99) and (5.100) which can be written as

$$e^{i\theta_2} + 2\cos(\theta_0) = 0 \ , \tag{5.104}$$

$$1 + 2\cos(2\theta_0) = 0 \ . \tag{5.105}$$

A solution is given by $\theta_0 = 2\pi/3$ if $\exp[i\theta_2] = 1$, whereas $\theta_0 = \pi/3$ solves these equations if one has $\exp[i\theta_2] = -1$. The triple of phases $(\theta_0, \theta_1, \theta_2) = (2\pi/3, 4\pi/3, 0)$ thus provides a choice of phases satisfying all requirements on the eigenvalues of W_1. Choosing $X = \mathbb{1}_3$ for simplicity, a unitary dynamics where the interaction on the open system is proportional to $\sigma_3^{(j)}$ as in the full model (cf. Eq. (5.3)), i.e. a dynamics that is described as $V(t) = \bigotimes_{j=0}^{1} \exp[-i\, t_j(t) \sigma_3^{(j)} \otimes H_I^{(j)}]$, is then obtained for the Hamiltonians

$$H_I^{(j)} = \frac{\pi}{3}|0\rangle_{E_j}\langle 0| + \frac{2\pi}{3}|1\rangle_{E_j}\langle 1| \ , \tag{5.106}$$

which shows nonlocal memory effects if the maximally entangled initial state of the environment is given by

$$|\Phi\rangle_{E_1E_2} = \frac{1}{\sqrt{3}}\{|1,0\rangle_{E_1E_2} + |0,1\rangle_{E_1E_2} + |2,2\rangle_{E_1E_2}\} \ . \tag{5.107}$$

Figure 5.7 shows the dynamics of the associated coherence factors for subsequent interactions of length $\Delta t = 1$. One observes that all but κ'_{12} are zero at

[4] For the permutation $\pi' \in S_3$ which implies the sequence $(0,1) \mapsto (1,2) \mapsto (2,0)$, Eq. (5.103) gives $\theta_1 = 2\pi f(0,1) - \theta_0$, $\theta_1 = 2\pi f(1,2) - \theta_2$ and $\theta_2 = 2\pi f(0,2) - \theta_0$. This can be solved leading to $\theta_0 = \pi\{f(0,1) - f(1,2) + f(0,2)\}$, $\theta_1 = \pi\{f(0,1) + f(1,2) - f(0,2)\}$ and $\theta_2 = \pi\{-f(0,1) + f(1,2) + f(0,2)\}$.

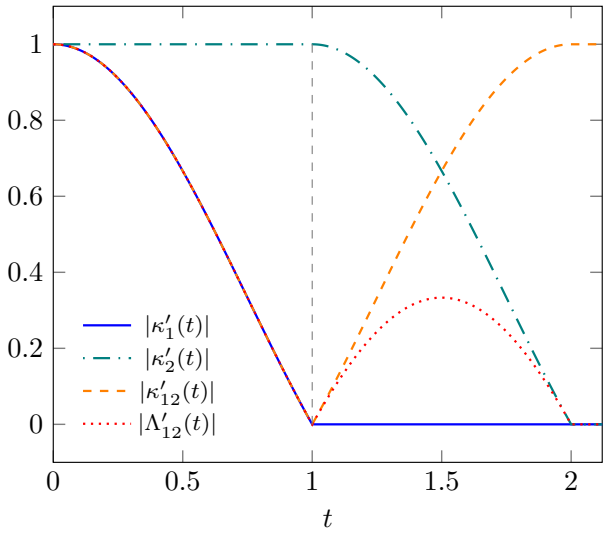

Figure 5.7 – Dynamics of the coherence factors for three-dimensional environments E_k with initial state $|\Phi\rangle_{E_1E_2}$ (cf. Eq. (5.107)) and an interaction described by $V(t) = \bigotimes_{j=0}^{1} \exp[-i\, t_j(t)\sigma_3^{(j)} \otimes H_I^{(j)}]$ with $H_I^{(j)}$ as defined in Eq. (5.106). Here, the interactions are again subsequently turned on and off for an interval $\Delta t = 1$ indicated by the vertical dashed line.

the end of the stepwise dynamics, but the nonlocal coherence factor Λ_{12}' has a revival up to a magnitude of $1/3$ during the second interaction at variance with the original model. The bump's magnitude immediately suggests a relation to the dimension of the environmental Hilbert spaces along with a reduction of the intermediate increase for higher-dimensional environments, finally approaching zero in the limit of infinite dimensions. To prove these conjectures, one must obviously determine solutions for higher-dimensional environments explicitly. However, a systematic approach to do this is not possible by means of the present ansatz using a permutation matrix with a single fix point as one easily shows. In fact, for the analogous permutation matrices with fixed point $\pi'(N-1) = N-1$, one deduces that Eqs. (5.99) and (5.100) read $1 + \sum_{j=0}^{N-2} \exp\left[i \cdot (-1)^{N-2-j} \alpha \cdot \theta_0\right] \stackrel{!}{=} 0$ for $\alpha = 1$ and $\alpha = 2$, respectively, which has no joint solution for $N > 3$.

It thus requires further studies of the constraints (5.99), (5.100) and (5.103) in order to fully reveal the role of the environmental dimension for nonlocal memory effects. This task is left for future studies.

Part II

Information extraction on quantum systems

Chapter 6

Indirect quantum measurement

Considering the generic situation of an open quantum system which interacts with its environment, one may ask which information on the environment can be inferred by measuring an observable on the open system at some instant of time? That is, the open system is used as a probe for the quantum system defining its environment where some features of the latter are deduced from a measurement of the former. Of course, the dynamics of an open quantum system may also carry information on its environment, so the open system bears the prospect of providing a new type of quantum sensors, allowing to gain information on quantum systems that may sometimes even be otherwise inaccessible. This investigation is motivated by the findings for the relation of nonlocal memory effects to the squeezing factor (see Sec. 5.2) and the correlation coefficient of photons (Laine *et al.*, 2012; Liu *et al.*, 2013a). Moreover, recent studies have highlighted a connection between non-Markovian behavior of an open system and environmental features such as angular correlations of pairs of entangled photons (Smirne *et al.*, 2013a), the effective dimension of ultracold bosonic gases (Haikka *et al.*, 2012b, 2013), the criticality of an Ising spin chain (Haikka *et al.*, 2012a) and a structural phase transition in an ion crystals (Borrelli *et al.*, 2013). However, there is also evidence that the dynamics of open quantum systems signifies other nontrivial environmental features including, for example, the critical point of a quantum phase transition (Gessner *et al.*, 2014a).

The inference of properties of a quantum system is generally of paramount interest for any use of quantum systems. Among other things, the theory of quantum measurements (see, e.g., Braginsky *et al.* (1992) and Busch *et al.* (1996)) examines the general question of how and what kind of information on a quantum system can be deduced using a quantum "apparatus", which is measured after some interaction to gather information on an object system. After a summary of the most important results of this theory concerning the information transmission on the apparatus relevant for the setup of an open quantum system which is given in Sec. 6.1, the study presented in this thesis focuses on means and relations quantifying an imperfect transmission and the thus-caused disturbance that are introduced and discussed in Sec. 6.2. The prospects of information extraction encoded into the dynamics of an open quantum system will later on be addressed in general terms in Secs. 6.3 and 6.4, completing the examination of open systems as quantum probes for their environments. In fact, the opportunity to extract information from the dynamics of the open system is studied on the basis of two approaches due to

Petersen (2014b) and Pollock *et al.* (2015) which are additionally generalized and applied to illustrate their functioning.

6.1 The theory of quantum measurements

The theory of quantum measurements characterizes in general terms how properties of observables on a quantum object are determined by means of the measurement of a second quantum system, the probe, thus defining an indirect measurement of the object system. In fact, the theory considers the situation presented in Fig. 6.1 where the measurement statistics of an observable A on the quantum object system is supposed to be deduced by means of a probe on which a von Neumann-Lüders measurement (von Neumann, 1932b; Lüders, 1950) associated with an observable B is performed. Of course, the measurement of B is first applied after an appropriate interaction between the two systems has taken place which is described by a positive and trace-preserving map Υ. The probe and the object are additionally assumed to be dynamically and statistically independent prior to that interaction so that the total initial state factorizes, i.e. one has $\rho_{OP} = \rho_O \otimes \rho_P$.

Clearly, the most prominent example for such a setup, which was already considered by von Neumann (1932b) (see also Braginsky *et al.* (1992) and Breuer and Petruccione (2002)), is certainly given by the measurement of the momentum operator $\hat{p}$ on a quantum probe $\mathcal{H}_P = \mathbb{L}_2(\mathbb{R})$ after a unitary state transformation corresponding to the interaction Hamiltonian

$$H_I(t) = g(t)A \otimes \hat{q} \tag{6.1}$$

has occurred. For a sufficiently strong interaction and a probe state with a narrow momentum distribution, the measurement statistics of A may be reliably inferred from the outcomes of the measurement of the probe's momentum. In the ideal case of a probe with an arbitrarily sharp momentum distribution, that is, a probe in a momentum "eigenstate", the probability distribution of A and $\hat{p}$ are deterministically related and, in addition, one may infer the final state of the object from the measured momentum of the probe (Breuer and Petruccione, 2002).

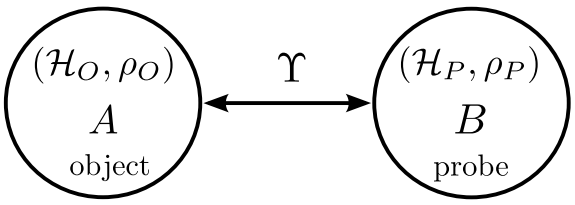

Figure 6.1 – Illustration of the probing scheme: Information about the quantum *object* with associated Hilbert space $\mathcal{H}_O$ is obtained by coupling it to a second quantum system, called the *probe*. The measurement statistics of the observable A on the object in a state ρ_O shall be reproduced by an ordinary measurement of an observable B on $\mathcal{H}_P$ in the state ρ_P after an appropriate interaction between the two quantum systems has taken place that is described by the positive and trace-preserving map Υ. Typically, this map refers to the unitary dynamics induced by some interaction Hamiltonian (cf. Eq. (6.1)), which thus is even completely positive.

In fact, assuming a discrete observable A with spectral decomposition $A = \sum_j a_j|\chi_j\rangle\langle\chi_j|$ and neglecting the free evolution of quantum object and probe so that the dynamics is solely governed by the interaction Hamiltonian (6.1), the probability density corresponding to the measurement of the momentum operator $\hat{p}$ at time $t^* > 0$ on the probe for a factorizing initial state $\rho_O \otimes \rho_P$ is given by (Breuer and Petruccione, 2002)

$$p_1(p, t^*) = \sum_j |\phi(p + G_{t^*} a_j)|^2 \langle\chi_j|\rho_O|\chi_j\rangle \ . \tag{6.2}$$

Here, $G_{t^*} = \int_0^{t^*} \mathrm{d}t\ g(t)$ defines the integrated interaction strength and one has $|\phi(p)|^2 \equiv \langle p|\rho_P|p\rangle$, determining the momentum distribution of the probe's initial state. For a sufficiently strong interaction and a probe state having a momentum distribution concentrated around its mean value, the function

$$f(p) = \frac{1}{G_{t^*}}\{\langle\hat{p}\rangle_{\rho_P} - p\} \tag{6.3}$$

represents a reliable estimator for the outcome of a potential measurement of A on the object given the probe was found to have momentum p. That is, one assigns the value $a = f(p)$ to the object if the momentum p is obtained when measuring the probe.

The associated probability density $p_1'(a, t^*) = (\mathrm{d}/\mathrm{d}a)P_1\big((-\infty, \langle\hat{p}\rangle_{\rho_P} - G_{t^*}a], t^*\big)$, where $P_1\big((-\infty, x], t\big)$ denotes the probability to measure a momentum smaller than or equal to $x \in \mathbb{R}$ on the probe, is determined by (Breuer and Petruccione, 2002)

$$p_1'(a, t^*) = \sum_j |G_{t^*}| \cdot |\phi(\langle\hat{p}\rangle_{\rho_P} - G_{t^*}(a - a_j))|^2 \langle\chi_j|\rho_O|\chi_j\rangle \ , \tag{6.4}$$

which yields the probability density of a measurement of the observable A in the limit of an arbitrarily sharp momentum distribution of ρ_P. Indeed, in the limit $|\phi(p)|^2 \to \delta(p - \langle\hat{p}\rangle_{\rho_P})$, Eq. (6.4) reduces to

$$p_1'(a, t^*) = \sum_j \delta(a - a_j)\langle\chi_j|\rho_O|\chi_j\rangle \ , \tag{6.5}$$

as the Dirac delta function scales as $\delta(\alpha x) = |\alpha|^{-1}\delta(x)$, and one finds

$$\begin{aligned} p_1(f^{-1}(a), t^*) &= \Big|\frac{d}{\mathrm{d}a} f^{-1}(a)\Big| \cdot \sum_j \delta\big(G_{t^*}\{f(f^{-1}(a)) - a_j\}\big)\langle\chi_j|\rho_O|\chi_j\rangle \\ &= p_1'(a, t^*) \end{aligned} \tag{6.6}$$

for any $a \in \mathbb{R}$. Thus, the two probability densities are deterministically related by means of the estimator (6.3) which therefore may also be called a pointer function (see below).

A systematic analysis of interactions leading to correlated probabilities is provided by the theory of quantum measurements (cf. Busch *et al.* (1996)). As a basic principle of this theory, measurements of an observable[1] A are characterized by five-tuples $\langle\mathcal{H}_P, B, \rho_P, \Upsilon, f\rangle$ satisfying the relation

$$\mathrm{Tr}_O\{E_A(X)\rho_O\} = \mathrm{Tr}_P\{E_B(f^{-1}(X))\mathrm{Tr}_O\{\Upsilon(\rho_O \otimes \rho_P)\}\} \tag{6.7}$$

[1]The consideration is actually not limited to self-adjoint operators but may be extended to any kind of generalized measurements represented by a POVM (cf. Sec. 2.4).

for any element X of the Borel σ-algebra $\mathfrak{B}(\mathbb{R})$ over the real line $\mathbb{R}$ and object state $\rho_O \in \mathcal{S}(\mathcal{H}_O)$. Here, E_K refers to the spectral projections of the observable $K = A$ and B, that is, one has $K = \int_{\mathbb{R}} x \, \mathrm{d}E_K(x)$ according to the spectral theorem (Rudin, 1991) (see also Eq. (6.9) for the spectral projections of discrete observables A and B). And Υ defines again a positive and trace-preserving map on the joint Hilbert space $\mathcal{H}_O \otimes \mathcal{H}_P$ which does not necessarily correspond to a unitary dynamics. As indicated before, the measurable function f is known as the pointer function whereas B defines the so-called pointer observable[2]. By means of a proper definition, the pointer function may obviously be absorbed in the definition of the latter. Relation (6.7) is known as probability reproducibility condition and a five-tuple satisfying it is said to define a premeasurement[3] of A (Busch *et al.*, 1996). By definition, given a five-tuple $\langle \mathcal{H}_P, B, \rho_P, \Upsilon, f \rangle$ representing a premeasurement of A, the measurement of the pointer observable on the probe in the evolved state $\mathrm{Tr}_O\{\Upsilon(\rho_O \otimes \rho_P)\}$ thus allows to fully reproduce the probability measure associated with the object observable. Note that one distinguishes various types of premeasurements regarding the induced correlations between quantities of the object and the probe, and the state change of the object state due to the measurement of the probe (see, e.g., Busch *et al.* (1996)).

An explicit construction of a premeasurement of a discrete observable has already been given by von Neumann (1932b). In general, a premeasurement of such an observable with spectral decomposition $A = \sum_{j=1}^{N_A} \sum_{k=1}^{n_j} a_j |\phi_{jk}\rangle\langle\phi_{jk}|$, allowing for degenerate eigenvalues as one may have $n_j \geq 1$ for any index j, is determined by the continuous linear or conjugate linear extension of the map[4]

$$U : |\phi_{jk}\rangle \otimes |\Phi\rangle \mapsto |\psi_{jk}\rangle \otimes |\Phi_j\rangle \ , \tag{6.8}$$

where the vectors $|\psi_{jk}\rangle$ are orthonormal with respect to the second index, i.e. one has $\langle\psi_{jk}|\psi_{jl}\rangle = \delta_{kl}$ for any index $j = 1, \ldots, N_A$ (Beltrametti *et al.*, 1990). Here, the pointer observable reads $B = \sum_{j=1}^{N_A} a_j |\Phi_j\rangle\langle\Phi_j|$ so that the pointer function is simply given by the identity map. In view of the consideration of open quantum systems, it is natural to focus on the unitary extension of Eq. (6.8) in the following. One readily concludes from the definition of the unitary operator that the probe's Hilbert space must be larger than or equal to the number of different eigenvalues of the observable A on the object which is to be determined. As the spectral projections read

$$E_A(X) = \sum_{\{j \,|\, a_j \in X\}} \sum_{k=1}^{n_j} |\phi_{jk}\rangle\langle\phi_{jk}| \ , \qquad E_B(X) = \sum_{\{j \,|\, a_j \in X\}} |\Phi_j\rangle\langle\Phi_j| \ , \tag{6.9}$$

[2]Note that it does not limit the treatment of (pre)measurements when the pointer observable is assumed to be a self-adjoint operator rather than a positive operator-valued measurement as was shown by Ozawa (1984). Moreover, one may restrict considerations to pure states of the probe without loss of generality.

[3]To define a measurement of an observable A, the so-called objectification requirement needs, however, to be satisfied by the five-tuple, too, which refers to the fact a measurement should lead to an objective, definite result.

[4]It is worth stressing that any such map U can always be extended by (conjugate) linearity to a (anti)unitary operator since the sets $\{|\phi_{jk}\rangle \otimes |\Phi\rangle\}$ and $\{|\psi_{jk}\rangle \otimes |\Phi_j\rangle\}$ may be extended to orthonormal bases on $\mathcal{H}_O \otimes \mathcal{H}_P$ (see also Appendix J).

where the first summation in each expression extends over all indices for which the associated eigenvalues a_j are in the Borel set X, the probability reproducibility condition[5] (6.7) is easily shown to be satisfied for the initial probe state $\rho_P = |\Phi\rangle\langle\Phi|$ and the state transformation Υ_U corresponding to the unitary extension of Eq. (6.8).

Note that the vectors $|\psi_{jk}\rangle$ need not be orthonormal in general. A particular and convenient choice of these vectors is clearly given by the set $\{|\phi_{jk}\rangle\}$ which yields a premeasurement of A that is termed *von Neumann-Lüders measurement*[6] (Beltrametti *et al.*, 1990). The resulting transformation of the object state coincides with the usual treatment of measurements of a quantum mechanical observable stated in standard textbooks (see, e.g., Breuer and Petruccione (2002)) which was first considered by von Neumann (1932b) and in greater detail by Lüders (1950). As shown in Appendix J, a unitary operator extending the map defined in Eq. (6.8) in case of a von Neumann-Lüders measurement is, for example, given by

$$U = \sum_{j,k=1}^{N_A} \sum_{l=1}^{n_{g(j,k)}} |\phi_{g(j,k)l}\rangle\langle\phi_{g(j,k)l}| \otimes |\Phi_j\rangle\langle\tilde{\Phi}_k| \,, \tag{6.10}$$

where the function $g : \{1, \ldots, N_A\}^2 \to \{1, \ldots, N_A\}$ refers to a symmetric function for which $g(\cdot, k)$ is bijective for any k and that satisfies $g(j,k) \neq j$ and $g(j,k) \neq g(j,l)$ for all j and pairwise different indices k and l. A possible choice for the function g is, for example, given by $g(j,k) = [j + k - 2]_{N_A}$ where $[\cdot]_{N_A}$ defines the coset with respect to division by N_A. Finally, the set $\{|\tilde{\Phi}_j\rangle\}$ denotes an orthonormal basis containing the initial probe state as first element, i.e. one has $|\tilde{\Phi}_1\rangle = |\Phi\rangle$.

It is worth pointing out that the unitary (6.10) and, similarly, any extension of the map (6.8) only characterizes a premeasurement of a discrete observable if the probe state is initially given by the pure state $|\Phi\rangle\langle\Phi|$. Moreover, it should be clear that applying projections $\mathbb{1}_O \otimes |\Phi_j\rangle\langle\Phi_j|$ to final states $U\rho_O \otimes |\tilde{\Phi}_k\rangle\langle\tilde{\Phi}_k|U^\dagger$ still implies a collapse of the object's quantum state. In fact, one easily deduces that the state of the quantum object is determined by $\sum_l^{n_{g(j,k)}} |\phi_{g(j,k)l}\rangle\langle\phi_{g(j,k)l}|$ in accordance with standard theory of measurements in quantum physics (see, e.g., (Breuer and Petruccione, 2002)). Thus, an indirect measurement of an observable A by means of the quantum probe after the interaction (6.10) does not represent a noninvasive strategy to gather information on the object system. To study the impact of an imperfect preparation of the probe, different means to compare the probability distribution of the pointer observable with that of the object observable are introduced in the following part of the thesis. In addition, several proposals for a relation between the gained information and the thus-induced disturbance on the quantum object are studied.

[5] Note that the specified premeasurement also satisfies the so-called *calibration condition*. That is, the measurement outcome of the probe shows a_j with certainty whenever this result was certain in the initial state of the object system (Busch *et al.*, 1996).

[6] Some authors such as Busch *et al.* (1996)) distinguish between a von Neumann and a Lüders measurement. Instead of considering a coarse grained observable B for the state transformation (6.8) as Lüders (1950) did, von Neumann (1932b) required that a measurement resolves the complete eigenbasis $\{|\phi_{jk}\rangle\}$ of the possibly degenerate observable A. Of course, this leads to a drastically different object states after the measurement of degenerate observables.

6.2 Information extraction and induced disturbance

As indicated before, a fixed state of the probe is the only choice of an initial state such that the extensions of the map (6.8) defines the correct state transformation satisfying the probability reproducibility condition (6.7) for the associated pointer and object observables. Due to this, one may ask what happens in case of an imperfect preparation of the probe state or of the state transformation which one certainly faces in any kind of experimental implementation. This directly leads to the question how to characterize the performance of an indirect measurement regarding the information transmission in general, thus taking into account imperfections. Clearly, for a given premeasurement $\langle \mathcal{H}_P, B, \rho_P, \Upsilon, f\rangle$ of an observable A, an imperfect preparation or state transformation yields a final state of the probe that is different from

$$\bar{\rho}_P \equiv \mathrm{Tr}_O\{\Upsilon(\rho_O \otimes \rho_P)\} \tag{6.11}$$

for which the probability reproducibility condition is known to be satisfied. One thus needs to quantify correlations of the probability measures (cf. Eq. (6.7))

$$P_{A,\rho_O}(X) \equiv \mathrm{Tr}_O\{E_A(X)\rho_O\} \;, \tag{6.12}$$

$$P_{B,\tilde{\rho}_P}(Y) \equiv \mathrm{Tr}_P\{E_B(Y)\tilde{\rho}_P\} \tag{6.13}$$

on the Borel σ-algebra over $\mathbb{R}$, where the final probe state $\tilde{\rho}_P$ results from an arbitrary state transformation and initial probe state. That is, one considers the final state to be associated with a state transformation Υ' and an initial probe state ρ'_P leading to

$$\tilde{\rho}_P = \mathrm{Tr}_O\{\Upsilon'(\rho_O \otimes \rho'_P)\} \;, \tag{6.14}$$

which is generally different from $\bar{\rho}_P$. There exist, of course, several approaches to determine correlations of these two probability measures. Some of the possible strategies require, however, that the joint probability distribution after the state transformation

$$P_{A\otimes B,\rho_O,\rho'_P}(X,Y) \equiv \mathrm{Tr}_O\{E_A(X)\otimes E_B(Y)\Upsilon'(\rho_O\otimes\rho'_P)\} \;, \tag{6.15}$$

has marginals $P_{A\otimes B,\rho_O,\rho'_P}(X,\mathbb{R})$ and $P_{A\otimes B,\rho_O,\rho'_P}(\mathbb{R},Y)$ given by Eqs. (6.12) and (6.13), respectively. Clearly, this requirement severely limits the possible state transformations. A transformation satisfying Eq. (6.15) is, for example, given by the unitary transformation induced by the interaction (6.1) for any evolution time as the observable A defines a constant of motion by construction.

Apart from the amount of information on the object observable obtained by measuring the probe, the disturbance of the object state due to the interaction as well as the measurement of the probe is an interesting quantity. In particular, one may ask whether the induced disturbance can be related to the amount of information gained via the indirect measurement. Such an information-disturbance relation would also clearly demonstrate that this type of information extraction on a quantum system is certainly not noninvasive as already argued for the state transformation (6.10) and initial probe states $|\tilde{\Phi}_k\rangle\langle\tilde{\Phi}_k|$ (see above). Therefore, it

does not disagree with Heisenberg's intuition of the nonexistence of a disturbance-free measurement of a quantum system which he illustrated by the well-known Gedankenexperiment of a γ-ray microscope (Heisenberg, 1927, 1930). Note that there exist various proposals for a general formulation capturing Heisenberg's intuition[7] (see, e.g., Maccone (2007), Maccone (2006), Buscemi (2007), Buscemi *et al.* (2014), Buscemi *et al.* (2008), Busch *et al.* (2013), Busch *et al.* (2014a) and Ozawa (2004) as well as references therein for different attempts).

Inspired by the works of Buscemi (2007) and Buscemi *et al.* (2014), entropic quantifiers are considered in the following that measure statistical correlations between the random variables (cf. Sec. 4.1) associated with the measurement of object and probe observables with probability measures given by Eqs. (6.12) and (6.13), respectively. Unfortunately, none of the information-disturbance relations given by Buscemi (2007) and Buscemi *et al.* (2014) can be applied to the discussed scenario of an indirect measurement as will be shown in this thesis. Another method to compare the probability distributions (6.12) and (6.13) employs the so-called Wasserstein metric which is known from the study of transportation problems (see, e.g., Villani (2003)). Contrary to the approach based on entropic quantifiers, the second ansatz is not limited to state transformations that yield a proper joint probability distribution (6.15). However, an information-disturbance relation could neither be established in this case so that the quest of establishing such a relation is generally open and left for future studies.

6.2.1 Entropic quantifiers

A central topic of classical information theory is to quantify the information content of random variables. Based on the Shannon entropy (2.64), where the logarithm is to the base 2, several quantifiers such as the mutual information and the conditional entropy determine how close two random variables are. More specifically, the Shannon entropy of a random variable $\mathcal{X}$ is defined as (Holevo, 1982)

$$H(\mathcal{X}) = -\sum_x P_{\mathcal{X}}(x) \log_2 P_{\mathcal{X}}(x) \ , \tag{6.16}$$

where $P_{\mathcal{X}}(x) = \nu(\mathcal{X}^{-1}(\{x\}))$ describes the probability to obtain the value $x \in I'$ for the random variable $\mathcal{X}$ from the probability space $\Xi = (I, \Sigma, \nu)$ to the measurable space (I', Σ') (cf. Eq. (4.2)). In information theory the Shannon entropy is interpreted as to quantify the amount information, measured in bits, acquired on the random variable if one knows one of its realizations. Equivalently, one may speak of the uncertainty of the random variable that is measured by $H(\mathcal{X})$ (Nielsen and Chuang, 2000).

For a pair of random variables $\mathcal{X}$ and $\mathcal{Y}$, one may similarly define the joined entropy $H(\mathcal{X}, \mathcal{Y})$ which refers to the Shannon entropy of the random variable $\mathcal{Z} = (\mathcal{X}, \mathcal{Y})$ with associated probability distribution $P_{\mathcal{X},\mathcal{Y}}(x, y)$ having marginals

[7] Heisenberg (1927) only achieved a rigorous relation for the momentum transfer of an electron due to a position measurement if it is assumed to be in a momentum "eigenstate". In this case the measurement-disturbance relation basically follows from the usual uncertainty relation for canonical operators (see Wiseman (1998)).

$P_{\mathcal{X}}(x)$ and $P_{\mathcal{Y}}(y)$. The relation between the information content of the two random variables is then quantified by the so-called conditional entropy

$$H(\mathcal{X}|\mathcal{Y}) \equiv H(\mathcal{X},\mathcal{Y}) - H(\mathcal{X}) \tag{6.17}$$

as well as the mutual information[8]

$$H(\mathcal{X}:\mathcal{Y}) \equiv H(\mathcal{X}) - H(\mathcal{X}|\mathcal{Y}) \tag{6.18}$$

in classical information theory. In fact, the former can be interpreted as the average uncertainty about the value of the random variable $\mathcal{X}$ if the value of $\mathcal{Y}$ is known, whereas the latter is said to quantify how much information the two random variables have in common (see, e.g., Nielsen and Chuang (2000)). Note that the mutual information is symmetric in its arguments and satisfies

$$0 \leq H(\mathcal{X}:\mathcal{Y}) \leq \min\{H(\mathcal{X}), H(\mathcal{Y})\} \;, \tag{6.19}$$

where the lower bound is attained if and only if $\mathcal{X}$ and $\mathcal{Y}$ are statistically independent, i.e. one has $P_{\mathcal{X},\mathcal{Y}}(x,y) = P_{\mathcal{X}}(x)P_{\mathcal{Y}}(y)$ for any x and y. On the contrary, the upper bound is realized if and only if the random variable $\mathcal{X}$ is a function of $\mathcal{Y}$ meaning that there exists a function f such that $\mathcal{X} = f(\mathcal{Y})$ holds (Nielsen and Chuang, 2000). In view of the probability reproducibility condition (6.7), one may call f a pointer function. Clearly, the conditional entropy satisfies $0 \leq H(\mathcal{X}|\mathcal{Y}) \leq H(\mathcal{X})$ where the upper and lower bound now correspond to statistically independent and deterministically related random variables, respectively. Note that the mutual information can be written as

$$H(\mathcal{X}:\mathcal{Y}) = \sum_{x,y} P_{\mathcal{X},\mathcal{Y}}(x,y) \log_2 \left(\frac{P_{\mathcal{X},\mathcal{Y}}(x,y)}{P_{\mathcal{X}}(x)P_{\mathcal{Y}}(y)} \right) \;, \tag{6.20}$$

where the right-hand side defines the relative entropy of the joint distribution and the product of its marginals (Nielsen and Chuang, 2000).

Now, returning to the problem of an indirect measurement, one may use the conditional entropy or the mutual information to quantify the correlations between the random variables associated with the measurement of the object and the probe observables. That is, let $P_{A,\rho_O}(\{a_j\})$ and $P_{B,\tilde{\rho}_P}(\{b_j\})$ (see Eqs. (6.12) and (6.13)) denote the probabilities corresponding to the von Neumann-Lüders measurement of the observable A in the object state ρ_O and B on the probe after the interaction, respectively, the entropic quantifiers may be used if the joint probability distribution (6.15) obeys

$$P_{A\otimes B,\rho_O,\rho'_P}(\{a_j\}, \mathrm{spec}(B)) = P_{A,\rho_O}(\{a_j\}) \;, \tag{6.21}$$

$$P_{A\otimes B,\rho_O,\rho'_P}(\mathrm{spec}(A), \{b_j\}) = P_{B,\tilde{\rho}_P}(\{b_j\}) \tag{6.22}$$

for all eigenvalues a_j and b_j, assuming discrete observables A and B for convenience. Note that the second equality is always satisfied by the very definition of

[8] Nielsen and Chuang (2000) also ascribe the expressions *entropy of $\mathcal{X}$ conditional on knowing $\mathcal{Y}$* and *mutual information content of $\mathcal{X}$ and $\mathcal{Y}$* to the conditional entropy and the mutual information, respectively.

$P_{B,\tilde{\rho}_P}(\{b_j\})$ (see Eq. (6.13)). For an interaction generated by some time-dependent Hamiltonian $H_I(t)$, one easily shows that the first relation implies, however, the constraint $[H_I(t), A] = 0$ for all times $t > 0$ which is known as back-action evasion condition (see, e.g., Breuer and Petruccione (2002)). Note that the Kraus operators Ω_j determining the state change of the object due to the interaction and the measurement of the observable $B = \sum_j b_j |\Phi_j\rangle\langle\Phi_j|$ on the probe with outcome b_j at time t are then determined through the relation (cf. Eq. (2.32))

$$\Omega_j \rho_O \Omega_j^\dagger = \mathrm{Tr}_P\{\mathbb{1}_O \otimes E_B(\{b_j\}) U(t) \rho_O \otimes \rho'_P U^\dagger(t)\} \ , \tag{6.23}$$

which yields

$$\Omega_j = \langle\Phi_j|U(t)|\Phi'\rangle \in \mathcal{B}(\mathcal{H}_O) \tag{6.24}$$

in case of a pure probe state $\rho'_P = |\Phi'\rangle\langle\Phi'|$.

To obtain an information-disturbance relation for the mutual information or the conditional entropy, it is worth considering the works by Buscemi (2007) and Buscemi *et al.* (2014) where such relations have been deduced for these two quantifiers. However, the results were obtained in a different setting which, unfortunately, is not compatible with the scenario of an indirect measurement as will be shown in the following. First, Buscemi (2007) considered the information transmission from a classical-quantum channel (see below) to a probe by means of a measurement of the latter. He derived the relation (cf. Eq. (5) in Buscemi (2007))

$$\mathcal{F}_e(\rho_O) \leq 1 - \frac{1}{4}\beta H(\mathcal{X} : \mathcal{Y}) \ , \tag{6.25}$$

where

$$\mathcal{F}_e(\rho_O) \equiv \mathrm{Tr}\{|\rho_O\rangle\langle\rho_O|(\mathcal{E} \otimes \mathbb{1})(|\rho_O\rangle\langle\rho_O|)\} \tag{6.26}$$

is called the entanglement fidelity (Schumacher, 1996; Schumacher and Nielsen, 1996). Here, $|\rho_O\rangle\langle\rho_O|$ refers to a purification of the state ρ_O and $\mathcal{E}$ represents the completely positive and trace-preserving map[9] induced by the (generalized) measurement on the probe, i.e., one has $\mathcal{E}(\rho_O) = \sum_j \Omega_j \rho_O \Omega_j^\dagger$ for some set of Kraus operators (cf. Eqs. (2.32) and (6.23)). Note that the entanglement fidelity is interpreted as measuring how coherently a state is preserved through a quantum channel $\mathcal{E}$ (Schumacher, 1996; Schumacher and Nielsen, 1996), thus defining a particular quantifier for the disturbance of a state. Clearly, it takes on values in the unit interval where one has $\mathcal{F}_e(\rho_O) \approx 1$ if $\mathcal{E}$ acts approximately like the identity channel on the support of the object state.

The mutual information in relation (6.25) determines the correlations between the random variables corresponding to the measurement of the probe and the information encoded into an object state by means of a classical-quantum channel. That is, a given state ρ_O is written as convex combination[10] of states $\rho_O^{(j)}$ with probabilities p_j, i.e. $\rho_O = \sum_j p_j \rho_O^{(j)}$, which represents the coding of a classical alphabet $\mathcal{A} = \{1, \ldots, N\}$ with associated a priori probability distribution $\{p_j\}$

[9] Note that such a map is typically called a *quantum channel* in the literature (see, e.g., Nielsen and Chuang (2000)).

[10] The convex decomposition can also be motivated by a measurement of a POVM on an ancilla by means of which the state ρ_O is purified before the object system is coupled to the probe (see, e.g., Buscemi *et al.* (2008)).

into quantum states according to the mapping $j \in \mathcal{A} \mapsto \rho_O^{(j)}$ (Holevo, 1977). Such a setup is known as classical-quantum channel in quantum communication theory (see, e.g., Helstrom (1976) and Holevo (1982)). The joint probability distribution is thus defined as

$$P_{\mathcal{X},\mathcal{Y}}(j,k) = p_j \mathrm{Tr}\{\Omega_k^\dagger \Omega_k \rho_O^{(j)}\} \ , \tag{6.27}$$

so that the marginals are found to be determined by $P_{\mathcal{X}}(j) = p_j$ and $P_{\mathcal{Y}}(k) = \mathrm{Tr}\{\Omega_k^\dagger \Omega_k \rho_O\}$. It follows that relation (6.25) can be interpreted as information-disturbance trade-off for the transmission of information encoded in the state ρ_O to the measurement of the probe. It is worth stressing that the disturbance is independent of the chosen coding scheme (Buscemi, 2007).

In trying to use this relation for the scenario of an indirect measurement of a constant of motion, one observes that the joint probability for outcomes a_j and b_k of a measurement of the object and probe observable at time t (cf. Eq. (6.15) for a unitary state transformation)

$$P_{A\otimes B,\rho_O,\rho'_P}(\{a_j\},\{b_k\}) = \mathrm{Tr}\big\{E_A(\{a_j\}) \otimes E_B(\{b_k\}) U(t) \rho_O \otimes \rho'_P U^\dagger(t)\big\} \tag{6.28}$$

can be rewritten as

$$P_{A\otimes B,\rho_O,\rho'_P}(\{a_j\},\{b_k\}) = \mathrm{Tr}\{\Omega_k^\dagger \Omega_k E_A(\{a_j\}) \rho_O E_A(\{a_j\})\} \ , \tag{6.29}$$

since one has $[E_A(\{a_j\}), U(t)] = 0$ for any index j and times t, where the Kraus operators are determined through Eq. (6.23). The essential difference between this expression and Eq. (6.27) is given by the fact that the states $\rho_O^{(j)}$ do not define a convex decomposition of the initial object state ρ_O in general. Clearly, one has

$$\rho_O^{(j)} = \frac{1}{p_j} E_A(\{a_j\}) \rho_O E_A(\{a_j\}) \in \mathcal{S}(\mathcal{H}_O) \tag{6.30}$$

with $p_j = \mathrm{Tr}\{E_O(\{a_j\})\rho_O\}$ so that the associated convex combination

$$\rho'_O \equiv \sum_j E_O(\{a_j\}) \rho_O E_O(\{a_j\}) \tag{6.31}$$

defines the final state of a nonselective measurement of A (see, e.g., Breuer and Petruccione (2002)) which is typically different from ρ_O unless this state is diagonal in the eigenbasis of the measured observable. Moreover, the operator $\rho_O - \rho'_O$ is indefinite in general as can be easily shown.

Lemma 6.1. *Let $\rho_O \in \mathcal{S}(\mathcal{H}_O)$ be a quantum state and denote by $\{\Pi_m\}_{m\in I}$ a set of orthogonal projections on $\mathcal{H}_O$ defining a resolution of identity (cf. theorem 3.2) where $[\Pi_m, \rho_O] \neq 0$ for at least one index $m \in I$. Then, the operator*

$$\rho_O - \sum_{m\in I} \Pi_m \rho_O \Pi_m \tag{6.32}$$

is indefinite.

Proof. Let ρ_O and $\{\Pi_m\}_{m\in I}$ be given satisfying $[\Pi_m, \rho_O] \neq 0$ for at least a single index $m \in I$. Since the projections define a resolution of identity, i.e. one has $\sum_{m\in I} \Pi_m = \mathbb{1}_O$, it is easily found that the Hermitian operator $\rho_O - \sum_{m\in I} \Pi_m \rho_O \Pi_m$ has zero trace which may be equivalently written as

$$\mathrm{Tr}\{(\rho_O - \sum_{m\in I} \Pi_m \rho_O \Pi_m)|\chi\rangle\langle\chi|\} = -\mathrm{Tr}\{(\rho_O - \sum_{m\in I} \Pi_m \rho_O \Pi_m)\Pi_\perp\} \; . \tag{6.33}$$

Here, $|\chi\rangle$ refers to an arbitrary element of $\mathcal{H}_O$ and $\Pi_\perp$ denotes the associated projection on the subspace orthogonal to it, i.e. the projection is defined by $\Pi_\perp = \mathbb{1}_O - |\chi\rangle\langle\chi|$. It thus follows that the two terms in Eq. (6.33) have alternating signs if they do not vanish. However, if the latter would be true for any element $|\chi\rangle \in \mathcal{H}_O$, one concludes that $\rho_O - \sum_{m\in I} \Pi_m \rho_O \Pi_m = 0$ holds (Rudin, 1991) which implies $[\Pi_m, \rho_O] = 0$ for all indices m in contradiction to the assumption.

Hence, there must exist a vector $|\chi\rangle$ such that $\langle\chi|\rho_O - \sum_{m\in I} \Pi_m \rho_O \Pi_m|\chi\rangle \neq 0$. Without loss of generality one may assume that the term is positive. Now, as the second term cannot vanish, there must exist at least a single pure state $|\psi\rangle \in \mathrm{Im}(\Pi_\perp)$ which yields

$$\langle\psi|\rho_O - \sum_{m\in I} \Pi_m \rho_O \Pi_m|\psi\rangle < 0 \; , \tag{6.34}$$

so that Eq. (6.33) is satisfied. Thus, $\rho_O - \sum_{m\in I} \Pi_m \rho_O \Pi_m$ is indeed indefinite. □

As a consequence of this lemma, the positive operator $\Lambda_j \equiv p_j \rho_O^{-1/2} \rho_O^{(j)} \rho_O^{-1/2}$, being defined on the support of the state ρ_O and trivially extended to $\mathcal{H}_O$ with p_j and $\rho_O^{(j)}$ as given by Eq. (6.30), is shown to have eigenvalues larger than unity so that one has

$$\mathbb{1}_O - \sum_j \Lambda_j \not\geqq 0 \; . \tag{6.35}$$

Positivity of this operator is, however, needed to arrive at inequality (6.25). More specifically, it is required to achieve a lower bound for the trace distance of two states by classical probability distributions corresponding to the measurement of a POVM $\{E_k\}$. In fact, the bound follows from the trace distance's characterization in terms of the Kolmogorov distance (see Eq. (2.44))

$$\mathcal{D}_T(\rho_1, \rho_2) = \max_{\{E_k\}} d_K(P_1, P_2) \; , \tag{6.36}$$

where the probability distributions $P_j = \{p_{j,k}\}$ are determined by $p_{j,k} = \mathrm{Tr}\{E_k \rho_j\}$ (Nielsen and Chuang, 2000). Even though one could also incorporate sets of positive operators in Eq. (6.36) that obey $\sum_k E_k < \mathbb{1}_O$, corresponding to unnormalized distributions P_j, the characterization of the trace distance may fail if the operator $\mathbb{1}_O - \sum_k E_k$ is indefinite.

In summary, inequality (6.25) can only be applied to the scenario of an indirect measurement if the object state is diagonal in the eigenbasis of the observable A which is to be estimated. This particular case obviously corresponds to an instance of the approach considered by Buscemi (2007) as one then has $\rho_O = \sum_j p_j \rho_O^{(j)}$.

Clearly, the requirement of a common eigenbasis represents a far reaching constraint for the use of the introduced means to quantify statistical correlations and the disturbance. It is also worth stressing that relation (6.25) is not very tight in general, since one obtains as a lower bound of the right-hand side

$$1 - \frac{1}{4}\beta H(\mathcal{X} : \mathcal{Y}) \geq 1 - \frac{1}{4d_O} \max_{j=O,P} \log_2 d_j \ , \tag{6.37}$$

where d_O and d_P refer to the number of states $\rho_O^{(j)}$ in the convex decomposition of ρ_O and the amount of elements of the POVM $\{\Omega_k^\dagger \Omega_k\}$, respectively. This follows from Eq. (6.19) and the facts that the Shannon entropy is bounded from above by $\log_2 d_j$, which is obtained for a uniform distribution, and one has $\beta \leq 1/d_O$ by definition. Assuming an equal amount of elements of the convex decomposition and the POVM which is, e.g., realized by the unitary premeasurements (6.8), the right-hand side of Eq. (6.37) is always larger than 0.9, thus corresponding to quantum channels that cause only a slight disturbance of the object state measured by the entanglement fidelity (6.26). A random sampling of channels and states shows, however, that it is rather unlikely to obtain an entanglement fidelity larger than 0.9 (see Fig. 6.2).

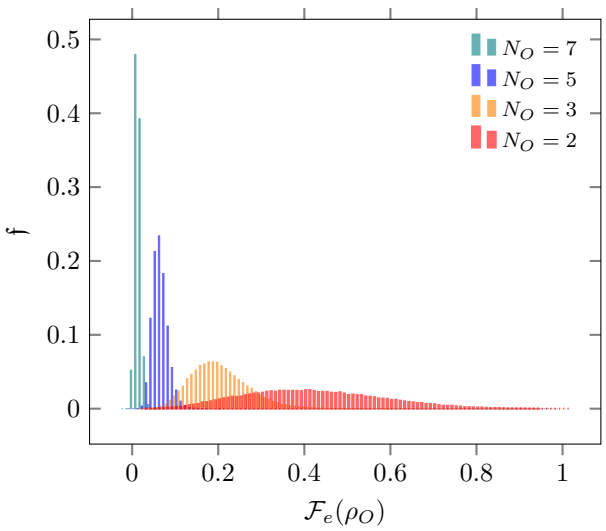

Figure 6.2 – Distribution of the entanglement fidelity $\mathcal{F}_e(\rho_O)$ (see Eq. (6.26)) for randomly drawn states $\rho_O \in \mathcal{S}(\mathcal{H}_O)$ and quantum channels for different dimension N_O of the Hilbert space $\mathcal{H}_O$. The plot shows the relative frequency $\mathfrak{f}$ of the values of the entanglement fidelity with respect to a binning of the unit interval with spacing $1/100$ and a sample size of $2.5 \times 10^4 \times N_O$ states and channels.

As indicated before, there exists yet another noise-disturbance relation for a similar setup which employs the relative entropy. In fact, for two nondegenerate observables A and A' on an N_O-dimensional Hilbert space with spectral decompositions

$$A = \sum_{j=1}^{N_O} a_j |\phi_j\rangle\langle\phi_j| \ , \qquad A' = \sum_{j=1}^{N_O} a'_j |\phi'_j\rangle\langle\phi'_j| \ , \tag{6.38}$$

Buscemi *et al.* (2014) determined the relation

$$H(\mathcal{X}|\mathcal{Y}) + H(\mathcal{X}'|\mathcal{Y}') \geq -2\log_2\big(\max_{j,k} |\langle\phi'_j|\phi_k\rangle|\big) \ , \tag{6.39}$$

where the relative entropy $H(\mathcal{X}|\mathcal{Y})$ is said to quantify the noise while $H(\mathcal{X}'|\mathcal{Y}')$ measures the disturbance. More precisely, the former is defined with respect to the joint probability distribution

$$P_{\mathcal{X},\mathcal{Y}}(j,k) = \frac{1}{N_O}\mathrm{Tr}\{\mathcal{E}_k(|\phi_j\rangle\langle\phi_j|)\} \ , \tag{6.40}$$

where $\mathcal{E}_k$ describes the state transformation (cf. Eq. (6.23)) due to the outcome k for the measurement of the probe, whereas the latter evaluates the correlations in the distribution

$$P_{\mathcal{X}',\mathcal{Y}'}(j,k) = \frac{1}{N_O}\mathrm{Tr}\{|\phi'_j\rangle\langle\phi'_j|(\mathcal{C}\circ\mathcal{E})(|\phi'_k\rangle\langle\phi'_k|)\} \ . \tag{6.41}$$

Here, $\mathcal{C}$ refers to a quantum channel correcting the action of the channel $\mathcal{E} = \sum_k \mathcal{E}_k$ associated with the measurement of the probe. The definition of noise is thus based on how well one is able to guess from the measurement statistics on the probe the input eigenstate $|\phi_j\rangle$ from a uniform distribution. And, similarly, the conditional entropy $H(\mathcal{X}'|\mathcal{Y}')$ quantifies to which extent the action of the corrected measurement channel reduces the information about which of the equally likely eigenstates $|\phi'_j\rangle$ of the observable A' was initially chosen.

To use this approach for the scenario of an indirect measurement of a nondegenerate object observable that defines a constant of motion as considered before, one first needs to specify the joint probability distributions characterizing the two conditional entropies. Clearly, the noise may again be simply related to the joint probability distribution (6.29), but there is a priori no second object observable A'. In the light of an indirect measurement, a natural choice to quantify the disturbance would certainly be given by the perturbation of the eigenbasis of the object state. That is, one considers the joint probability distribution

$$P_{\mathcal{X}',\mathcal{Y}'}(j,k) = \mu_j\mathrm{Tr}\{|\mu_k\rangle\langle\mu_k|\mathcal{E}(|\mu_j\rangle\langle\mu_j|)\} \ , \tag{6.42}$$

where μ_j and $|\mu_j\rangle$ refer to eigenvalues and eigenstates of the initial object state ρ_O, respectively. For convenience a correction of the quantum channel $\mathcal{E}$ has been omitted. The channel is induced by the measurement of the observable B on the probe, i.e., one has $\mathcal{E}(\rho_O) = \sum_j \Omega_j\rho_O\Omega_j^\dagger$ with Kraus operators characterized by Eq. (6.23).

It is readily observed that, at variance with the approach by Buscemi *et al.* (2014), the marginals $P_{A,\rho_O}(\{a_j\})$ and $P_{\mathcal{X}'}(j) = \sum_k P_{\mathcal{X}',\mathcal{Y}'}(j,k)$ of the two probability distributions (6.29) and (6.42), respectively, do not describe uniform distributions in general. In fact, this is only true if and only if the initial object state is maximally mixed. One may, however, show that uniformly distributed marginals are essential to arrive at a relation similar to inequality (6.39) as the entropic uncertainty relation due to Maassen and Uffink (1988), which is employed by Buscemi *et al.* (2014) to obtain the lower bound in Eq. (6.39), cannot be used in case of nonuniform distributions. More precisely, it is not possible to

use *Riesz's theorem*[11], on which the relation by Maassen and Uffink (1988) is essentially based, for such distributions as a consequence of the indefiniteness of the operator $\rho_O - \sum_{m\in I} \Pi_m \rho_O \Pi_m$ which has been proven in lemma 6.1 .

One thus concludes that none of the entropic information-disturbance relations due to Buscemi (2007) and Buscemi *et al.* (2014) may be used for the scenario of an indirect measurement in general. Besides the restriction to constants of motion that are supposed to be measured indirectly on the quantum object, relation (6.25) is only valid for object observables and states that commute, whereas one even needs to have a maximally mixed state of the object if inequality (6.39) shall be used to quantify the amount of gathered information and the thereby induced disturbance on the object by the measurement of a probe observable. Of course, these negative results do not imply that there does not exist information-disturbance relations (for constants of motion) at all. Further studies need, however, to be spent to derive such a relation, establishing a clear-cut connection between the information and the thus-caused disturbance by means of an indirect measurement which finally leads to a thorough understanding of these kind of measurement strategies for constants of motions.

6.2.2 Comparison of probability measures using the Wasserstein distance

In the previous section, the performance of indirect measurements has been characterized by means of entropic quantifiers determining how correlated the outcome distribution of a measurement on the probe and that of a direct measurement of the sought object observable are in terms of their joint distribution (6.15). Instead of relying on such a distribution, one could try to compare the measurement outcome distribution of the probe and the object directly. A prominent means of proximity of probability measures is given by the so-called Wasserstein α-distance which has been shown to be useful in probability theory (Villani, 2003; Gibbs and Su, 2002), in data analysis and pattern recognition (Peleg *et al.*, 1989; Rubner *et al.*, 2000; Rabin *et al.*, 2012). In addition, it is also closely related to the *Monge-Kantorovich functional*[12] known from the study of transportation problems (see, e.g., Villani

[11] *Theorem by Riesz (1927)*: Let $x = (x_1, \ldots, x_N)$ denote a sequence of complex numbers and $T \in \mathcal{B}(\mathbb{C}^N)$ an isometry such that $\sum_j |(Tx)_j|^2 = \sum_j |x_j|^2$ holds for all $x \in \mathbb{C}^N$. Defining $c = \max_{j,k}|T_{jk}|$ where $(Tx)_j = \sum_k T_{jk}x_k$, then one has

$$c^{1/b}\Big[\sum_j |(Tx)_j|^b\Big]^{1/b} \leq c^{1/a}\Big[\sum_j |x_j|^a\Big]^{1/a} , \tag{6.43}$$

for $1 \leq a \leq 2$ and $1/a + 1/b = 1$. The statement remains also valid if the condition on T is relaxed to $\sum_j |(Tx)_j|^2 \leq \sum_j |x_j|^2$ for all $x \in \mathbb{C}^N$ (Riesz, 1927).

[12] Kantorovich considered the minimization of the functional $I'[\kappa] \equiv \int_{\Omega_1\times\Omega_2} c(x,y)\,\mathrm{d}\kappa(x,y)$ over the set of joint probability distribution κ with fixed marginals μ and ν where $c : \Omega_1 \times \Omega_2 \to [0,\infty)$ represents a Borel measurable function over the sample spaces Ω_1 and Ω_2. This question generalizes the problem of minimizing $I[M] \equiv \int_{\Omega_1} c(x, M(x))\,\mathrm{d}\mu(x)$ for a given measurable map $M : \Omega_1 \to \Omega_2$ which was first studied by Gaspard Monge in his work *Mémoire sur la théorie des déblais et des remblais* in 1781 (Villani, 2003). In the literature, $I'[M]$ is said to represent the *total cost* associated with the *transference plan* κ between μ and ν – describing, e.g., a pile and the need of sand, respectively – for a *cost function* c.

(2003) and Rüschendorf (2005)).

Focusing on probability measures on the Borel σ-algebra over the real line $\mathbb{R}$, this distance measure is defined as[13] (Villani, 2009; van Gaans, 2011)

$$d_W^{(\alpha)}(\mu,\nu) = \left[\inf_{\kappa\in\Pi(\mu,\nu)} \int_{\mathbb{R}\times\mathbb{R}} |x-y|^\alpha \,\mathrm{d}\kappa(x,y)\right]^{1/\alpha} , \tag{6.44}$$

where $\alpha \in \mathbb{N}\cup\{\infty\}$ and $\Pi(\mu,\nu)$ refers to the set of probability measures on $\mathfrak{B}(\mathbb{R}\times\mathbb{R})$ with marginals μ and ν, that is, one has

$$\kappa(X,\mathbb{R}) = \mu(X) , \tag{6.45}$$

$$\kappa(\mathbb{R},X) = \nu(X) \tag{6.46}$$

for any Borel set $X \in \mathfrak{B}(\mathbb{R})$. Note that the so-called set of couplings $\Pi(\mu,\nu)$ is nonempty for any two measures as the product measure $\mu\otimes\nu$, which is defined on rectangles $X\times Y \in \mathfrak{B}(\mathbb{R})\times\mathfrak{B}(\mathbb{R})$ by $\mu\otimes\nu(X,Y) = \mu(X)\nu(Y)$ and then extended by Carathéodory's extension theorem to the Borel σ-algebra $\mathfrak{B}(\mathbb{R}\times\mathbb{R})$ (see, e.g., Elstrodt (2009)), represents an admissible, though trivial choice for a coupling. Clearly, definition (6.44) can be directly generalized to probability measures on $\mathbb{R}^N$ by inserting the corresponding Euclidean distance in the integral (van Gaans, 2011). The Wasserstein distance may, in general, even be defined for probability measures on the Borel σ-algebra of arbitrary metric spaces[14] $(\mathbb{V},d)$ and, moreover, it defines a metric for those probability measures for which the right-hand side of Eq. (6.44) is finite (Vasershtein, 1969). Note that the existence of a coupling minimizing the right-hand side depends on the structure of the metric space and the regularity of the probability measures. For Polish spaces[15] $(\mathbb{V},d)$ one shows that there exist an optimal coupling for any pair of probability measures μ and ν on the associated Borel σ-algebra (Villani, 2003). Any discrete finite and countable infinite set as well as $\mathbb{R}^n$ for any $n\in\mathbb{N}$ with its natural topology define, for example, Polish spaces (Elstrodt, 2009) so that this statement applies in particular to probability measures on the real line.

Even though the right-hand side relies on couplings, this does not mean that a proper joint probability distribution for the measurement of two quantum observables (cf. Eq. (6.15)) is needed when trying to use this distance for the problem of estimating the performance of an indirect measurement. That is, a coupling does not need to be induced by the projection-valued measure $E_A(X)\otimes E_B(Y)$ associated with observables A and B on the object and the probe in some joint

[13] Note that this metric is also frequently represented in terms of random variables which induce the considered probability measures. More precisely, one writes $d_W^{(\alpha)}(\mu,\nu) = \inf_{\mathcal{Z}} \mathbb{E}\big(d(\mathcal{X},\mathcal{Y})\big)$ where the infimum is taken over all pairs $\mathcal{Z}=(\mathcal{X},\mathcal{Y})$ of random variables $\mathcal{X}$ and $\mathcal{Y}$ with probability distributions μ and ν on $\mathfrak{B}(\mathbb{R})$, respectively (see, e.g., Villani (2003)).

[14] Interestingly, for an arbitrary metric spaces equipped with the discrete metric, i.e. one has $d(x,y)=\delta_{x,y}$ for all $x,y\in\mathbb{V}$, one obtains $d_W^{(\alpha)}(\mu,\nu)|_{\alpha=1} = \sup_{X\in\mathfrak{B}(\mathbb{V})}|\mu(X)-\nu(X)|$ as was shown by Dobrushin (1970), which is the Kolmogorov distance (cf. Sec. 2.4.1; see also Nielsen and Chuang (2000)).

[15] A Polish space $(\mathbb{V},d)$ represents a separable and completely metrizable topological space. Here, a space $\mathbb{V}$ is called separable if there exists a countable collection of sets which is dense, and it is completely metrizable if there exists a metric d which induces the topology (i.e. open sets can be defined as balls with respect to the metric). Finally, completeness refers, as usual, to the convergence of Cauchy sequences (Elstrodt, 2009; van Gaans, 2011).

state. As a consequence, one may apply this quantifier to observables A that do not define constants of motion, too. Moreover, the solution to the minimization over the convex set of all couplings is known: Vallender (1974) has shown that the Wasserstein 1-distance of any pair of probability measures μ and ν on the Borel σ-algebra on $\mathbb{R}$ is given by (see also Gibbs and Su (2002))

$$d_W^{(\alpha)}(\mu,\nu)\big|_{\alpha=1} = \int_{-\infty}^{\infty} \mathrm{d}x \; |F_\mu(x) - F_\nu(x)| \; , \tag{6.47}$$

where F_μ and F_ν denote the cumulative distributions corresponding to the probability measures μ and ν. That is, one has $F_\eta(x) = \eta((-\infty, x])$ for any $x \in \mathbb{R}$ and probability measure η on $\mathfrak{B}(\mathbb{R})$. In the realm of quantum mechanics, this distance measure was first used by Wiseman (1998) who determined the momentum transfer of a particle due to a position measurement. Recently, Busch *et al.* (2013) also employed it for their rigorous formulation of Heisenberg's statement concerning the relation between a quantum measurement and the caused disturbance (see also Busch *et al.* (2014b)).

Given characterization (6.47) of the Wasserstein 1-distance, it is obvious that one needs to know the probability distributions for the concerned observables as well as the pointer function (cf. Eq. (6.7)) if this concept should be applied to an indirect measurement. That is, it is only reasonable to compare the probability measures $P_{A,\rho_O}(X) \equiv \mathrm{Tr}\{E_A(X)\rho_O\}$ and $P^f_{B,\tilde{\rho}_P}(X) \equiv \mathrm{Tr}\{E_B(f^{-1}(X)\tilde{\rho}_P\}$ (cf. Eqs. (6.12) and (6.13), respectively) on the Borel σ-algebra $\mathfrak{B}(\mathbb{R})$ corresponding to an object observable A and a pointer observable B with pointer function f (see Sec. 6.1). This fact does, of course, not represent a drastic requirement as the pointer function should be known in advance in general. However, for object and probe observables with finite, discrete spectrum one may also establish a measure for proximity based on the Wasserstein distance which does not require knowledge about the pointer function.

Indeed, for discrete probability distributions $P_1 = \{p_{1,j}\}_{j\in I}$ and $P_2 = \{p_{2,j}\}_{j\in I}$ having a finite number of elements $I = \{1, \ldots, N\}$, one considers the Wasserstein α-distance for the probability measures

$$\mu_j = \frac{1}{N} \sum_{k=1}^{N} \delta_{p_{k,j}} \; , \tag{6.48}$$

where δ_q denotes the Dirac measure which is defined as $\delta_q(A) = 1$ if $q \in A$ holds, whereas one has $\delta_q(A) = 0$ if q is not an element of the set A. The probability measures (6.48) may thus be considered as random variables that map on a discrete probability distribution where each realization is equally likely, i.e. they satisfy $\mu_j(\{p_{j,k}\}) = 1/N$ for any $k \in I$ and index $j = 1, 2$. For such probability measures the set of couplings $\Pi(\mu_1, \mu_2)$ is given by the set of bistochastic $N \times N$-matrices $\mathcal{B}_N$ (see Eq. (4.16)) so that the Wasserstein α-distance is actually given by

$$d_W^{(\alpha)}(\mu_1, \mu_2)^{\,\alpha} = \frac{1}{N} \inf_{\pi \in \mathcal{B}_N} \sum_{j,k=1}^{N} \pi_{jk} |p_{1,j} - p_{2,k}|^\alpha \; , \tag{6.49}$$

representing a linear minimization problem over the convex set $\mathcal{B}_N$ which is known as Birkhoff polytope. The optimization problem is shown to be solved by the

extremal points of the Birkhoff polytope (Villani, 2003) that are given by the permutation matrices[16] according to the famous Birkhoff-von Neumann theorem (see, e.g., Villani (2003)). Thus, Eq. (6.49) then reads

$$d_W^{(\alpha)}(\mu_1,\mu_2)^{\,\alpha} = \frac{1}{N}\min_{\sigma\in\mathcal{S}_N}\sum_{j=1}^{N}|p_{1,j}-p_{2,\sigma(j)}|^{\alpha}\ . \tag{6.50}$$

Thus, for $\alpha = 1$ this distance is proportional to the minimal Kolmogorov distance (cf. Eq. (2.44)) of two discrete probability distributions with respect to reordering of the entries which represents an intuitive approach to compare discrete distributions. In particular, the distance measure vanishes for two discrete probability distributions corresponding to random variables that are related via a bijective map such as those obtained from premeasurements given by Eq. (6.8).

Note that this result actually holds true for arbitrary distance measures and for any discrete sets Ω_1 and Ω_2 of general vector spaces. Due to this, it may, e.g., be used to compare arbitrary point clouds. In fact, it provides a prominent tool for the comparison of histograms (see, e.g., Rubner *et al.* (2000)) as well as for image synthesis and retrieval (see the work by Rabin *et al.* (2012) and references therein). In addition, the optimization in Eq. (6.50) is solved by standard linear programming algorithms allowing for an efficient treatment (see, e.g., Burkard *et al.* (2009)). For a one-dimensional distribution of points, the minimizing solution is, however, even a priori known: Let $\sigma_j \in S_N$ denote the permutation such that the probabilities – and similarly for arbitrary one-dimensional point clouds – are arranged in increasing order, i.e. the permutation leads to $p_{j,\sigma_j(k)} \leq p_{j,\sigma_j(k+1)}$ for all $k = 1,\ldots,N-1$ and $j = 1,2$. The permutation minimizing Eq. (6.50) is then given by $\sigma^* \equiv \sigma_2 \circ \sigma_1^{-1}$ (Rabin *et al.*, 2012), that is, one has

$$d_W^{(\alpha)}(\mu_1,\mu_2)^{\,\alpha} = \frac{1}{N}\sum_{j=1}^{N}|p_{1,j}-p_{2,\sigma^*(j)}|^{\alpha}\ . \tag{6.51}$$

Hence, the probabilities $p_{1,j}$ and $p_{2,\sigma^*(j)}$ are assigned to each other by the quantifier (6.51). Contrary to the general expression requiring $\mathcal{O}(N^{5/2}\log(N))$ operations, the one-dimensional case can be computed by means of a fast sorting algorithm which only needs $\mathcal{O}(N\log(N))$ operations (Rabin *et al.*, 2012).

Now, this quantifier shall be employed to estimate the quality of an indirect measurement of an observable $A = \sum_{j=1}^{N_A}\sum_{k=1}^{n_j} a_j|\phi_{jk}\rangle\langle\phi_{jk}|$ ($n_j \geq 1$ for all j) on a finite-dimensional Hilbert space. Assuming that a nondegenerate pointer observable $B = \sum_{j=1}^{N_A} b_j|\Phi_j\rangle\langle\Phi_j|$ on the probe is to be measured in order to extract information on the observable A, the quantifier thus determines the proximity of the probability distributions (cf. Eqs. (6.12) and (6.13))

$$p_{1,j} \equiv \mathrm{Tr}_O\{E_A(\{a_j\})\rho_O\}\ , \tag{6.52}$$

$$p_{2,j} \equiv \mathrm{Tr}_P\{E_B(\{b_j\})\tilde{\rho}_P\}\ , \tag{6.53}$$

where $\tilde{\rho}_P$ refers to some probe state. Clearly, if the probe observable B is part of a five-tuple $\langle\mathcal{H}_P, B, \rho_P, \Upsilon_U, \mathrm{id}\rangle$ defining a premeasurement of the operator A where

[16] Given a permutation $\sigma \in S_N$, a permutation matrix is defined as the matrix whose entries are given by $\pi_{jk} = \delta_{j\sigma(k)}$.

the state transformation Υ_U is induced by a unitary U generated by a Hamilton operator H, then the probe state (cf. Eq. (6.11))

$$\tilde{\rho}_P = \mathrm{Tr}_O\{U\rho_O \otimes \rho_P U^\dagger\} \tag{6.54}$$

leads to perfectly correlated probability distributions $\{p_{1,j}\}$ and $\{p_{2,j}\}$ and, therefore, a vanishing Wasserstein distance (6.51). As no requirements on the state transformation needs to be made to employ this quantifier, it is thus possible to study not only the interesting question how the Wasserstein distance changes if the initial state ρ_P is perturbed but also the influence of imperfect unitary state transformations, leading to final probes states different from Eq. (6.54). A natural approach to study the impact of an imperfect state transformation is given by analyzing the effect of perturbations of the Hamilton operator H that generates the unitary U. That is, instead of the unitary $U = \exp[iH]$ which characterizes the ideal state transformation Υ_U, one considers transformations $\Upsilon_{U'}$ associated with the unitary $U' = \exp[iH']$. A convenient choice for the Hermitian operator H' is given by $H' = H + \tilde{H}$, so that the Hermitian operator $\tilde{H}$ can be interpreted as a perturbation of the ideal generator H.

Figure 6.3 shows the normalized Wasserstein 1-distance

$$\tilde{d}_W(\{p_{1,j}\}, \{p_{2,j}\}) \equiv \frac{1}{2}\sum_{j=1}^{N_A} |p_{1,j} - p_{2,\sigma^*(j)}| \tag{6.55}$$

of the probability distributions $\{p_{1,j}\}$ and $\{p_{2,j}\}$ for final states $\tilde{\rho}_P$ (cf. Eq. (6.54)) obtained for randomly sampled initial probe states ρ'_P (see Fig. 6.3 **(b)** & **(d)**) as well as randomly drawn perturbations $\tilde{H}$ (see Fig. 6.3 **(a)** & **(c)**) of the generator of the perfectly correlating unitary (6.10) (see also Appendix J). More specifically, the states as well as the Hamilton operators are randomly generated with respect to the Haar measure. The presented data corresponds to a randomly drawn state ρ_O and an arbitrary but fixed *nondegenerate* object observable A and an associated five-tuple $\langle \mathcal{H}_P, B, \rho_P, \Upsilon_U, \mathrm{id}\rangle$ for each of the different Hilbert spaces. It is, however, worth stressing that the displayed pattern has been reproduced for different choices of the object observable and a premeasurement, thus representing a somehow generic behavior. To visualize the effect of an improper preparation of the initial state or the unitary state transformation, the Wasserstein 1-distance (6.55) has been plotted in Fig. 6.3 as a function of the deviation of the sampled initial states ρ'_P to the ideal state ρ_P in terms of the trace distance (cf. Eq. (2.40)) and, similarly, for the Hermitian generators H'. Moreover, a two-dimensional binning has been used to represent the $2.5 \times 10^5 \times N_A$ sampled configurations.

As shown in Figs. 6.3 **(a)** & **(c)**, the proximity of the two probability distributions is only weakly disturbed by small perturbations of the ideal generator so that one may conclude that a premeasurement is rather stable with respect to the corresponding imperfection. Surprisingly, the influence of a perturbation of the generator on the proximity of the probability distributions (6.52) and (6.53) may also be small for large values of the trace distance and is generically even smaller for increasing dimension of the Hilbert space. On the contrary, an imperfect preparation of the initial probe state leads to large dissimilarities of the probability distributions which persist independent of the dimension. It is worth

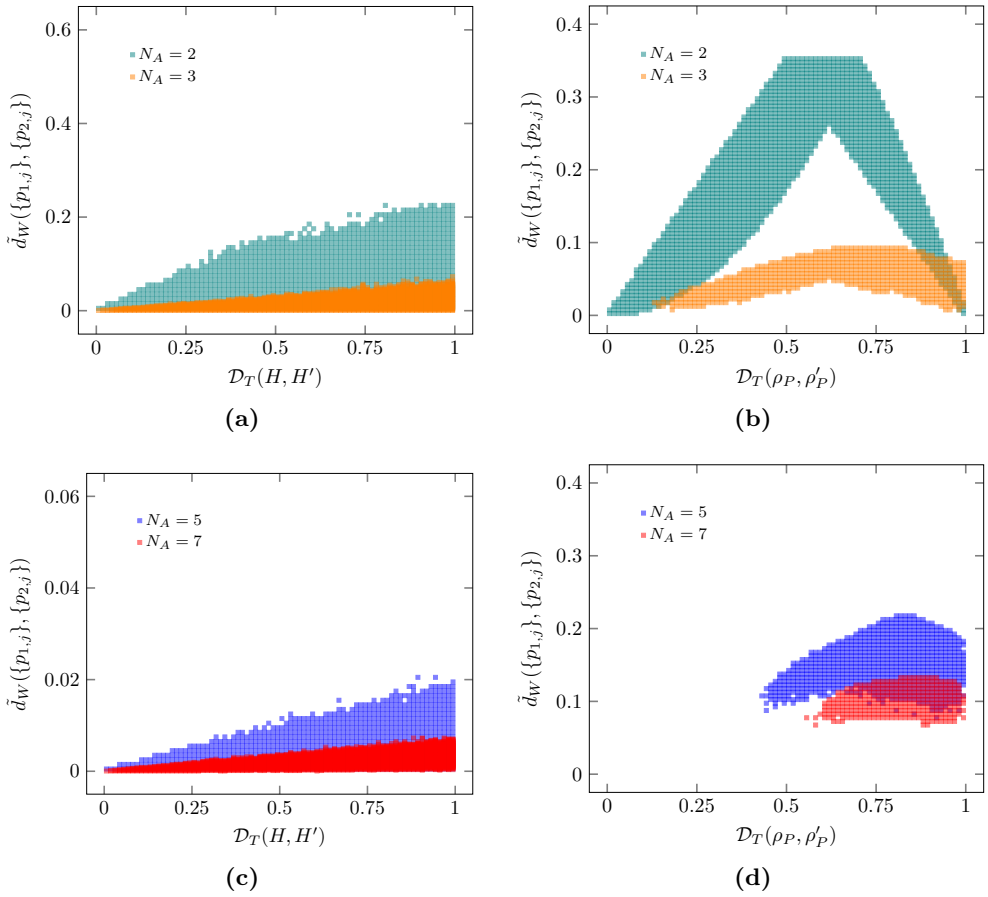

Figure 6.3 – Plot of the Wasserstein 1-distance $\tilde{d}_W(\{p_{1,j}\},\{p_{2,j}\})$ (cf. Eq. (6.55)) as a function of the deviations from the five-tuple $\langle \mathcal{H}_P, B, \rho_P, \Upsilon_U, \mathrm{id}\rangle$ defining a premeasurement of an arbitrary but fixed object observable A. Here, the ideal state transformation Υ_U is generated by the unitary extending Eq. (6.10). The proximity of the distributions as a function of the trace distance (cf. Eq. (2.40)) between randomly sampled initial probe states ρ'_P and the ideal state ρ_P is shown for different Hilbert spaces of the object in **(b)** & **(d)**. On the contrary, the effect of an imperfect generation of the ideal unitary state transformation Υ_U is depicted in **(a)** & **(c)** where randomly drawn perturbations $\tilde{H}$ of the generator H of the ideal unitary U (6.10) are considered leading to unitaries $U' = \exp[iH']$ with $H' \equiv H + \tilde{H}$. For all plots a two-dimensional binning has been used to represent the $2.5\times10^5\times N_A$ sampled states and Hamiltonians, respectively, which are randomly drawn with respect to the Haar measure.

pointing out that the Wasserstein 1-distance as a function of the trace distance for two-level systems shows an interesting behavior (cf. Fig. 6.3 **(b)**). Note that the proximity of the distributions obtained for initial states with unit trace distance is easily understood as these states are almost orthogonal to the ideal initial state ρ_P and should, therefore, work as initial states for perfect information transmission by construction of the unitary dynamics (cf. Eq. (J.9)), too. However, the observed sharp bounds as well as the apparent lack of symmetry of the Wasserstein 1-distance with respect to $\mathcal{D}_T(\rho_P,\rho'_P)$ is surprising and deserves further attention

in the future. So far no explanation for this behavior can be given which thus remains a challenging problem for future studies.

Another interesting task would be to establish a relation quantifying the information gain for the present approach and the thereby caused disturbance due to the indirect measurement as has already been tried for entropic quantifiers. Even though the Wasserstein 1-distance is closely related to Kolmogorov distance, which suggest the use of the trace distance in order to quantify the disturbance (cf. Eq. (2.43)), it was not possible to establish such a relation. Nonetheless, the Wasserstein 1-distance represents a promising tool to approach the question concerning what kind of information on an object system can be extracted by means of measuring a quantum probe as, contrary to the deployment of entropic quantifiers, no limitations are imposed regarding the (unitary) state transformation. So far this approach is still in its infancy and far-reaching further studies need to be performed. Besides the previously mentioned open problems, it might be worth studying which interaction yields the most reliable and stable information transmission for a given observable on the object system. Moreover, the Wasserstein 1-distance can be used to distinguish the role of interactions for which the object observable defines a constant of motion. This question is particularly interesting since there is numerical evidence[17] that the perfectly correlating unitary (6.10) is also generated by a Hermitian operator H that commutes with the target observable on the object system. Future studies will hopefully provide answers to these questions.

6.3 Nondissipative information extraction

In the preceding sections, the information gathered by an open system on its environment was determined on the basis of the measurement statistics of an observable at an arbitrary but fixed instant of time. In particular, the time evolution of the outcome statistics has thus not been considered. Due to the findings regarding nonlocal memory effects (cf. Sec. 5.2), it is, however, clear that the dynamics of the probability measures associated with some observables may also contain signatures of environmental properties. Clearly, as has been argued in Sec. 5.2, the squeezing factor of two-mode Gaussian states can, for example, be extracted by determining the probability measures associated with different observables, characterizing the nonlocal coherences, for (at least) three distinguished instants of time. Besides looking at the measurement statistics of observables on the open quantum system for different times, the full dynamics may additionally yield information on further features of the environment, too. Indeed, a first approach providing a particular, but nonetheless, systematic study of such a strategy is introduced and discussed in the following.

As shown by Petersen (2014a,b) for infinite and two-dimensional(!) object

[17] Numerical testing of the properties of the one-parameter group of unitaries, which are characterized by $U(t) = \exp[itH]$ where H refers to the generator of the randomly drawn perfectly correlating unitary U (see Eq. (6.10)), i.e. one has $U = \exp[iH]$, has shown that the object observable indeed defines a constant of motion. However, a rigorous proof of this fact, valid for all unitaries U on arbitrary Hilbert spaces, could not been derived so far.

systems, the dynamics of an infinite-dimensional quantum system that is equivalent[18] to the one-dimensional harmonic oscillator provides information on an object system when a linear interaction, leading to pure dephasing, is adjusted properly. More specifically, the time-averaged expectation value of an observable of the infinite-dimensional probe converges towards the first moment of a traceless Hermitian operator on the quantum object defining a constant of motion. Such a behavior is similar to the ergodic properties of stationary stochastic processes, stating that the time-average of such stochastic processes with appropriate two-time correlation functions converges to deterministic variables which are given by the respective means of the processes (Gardiner, 2004) (see below for more details).

The strategy is introduced and demonstrated in the present thesis for object systems that are described by arbitrary finite-dimensional Hilbert spaces, thus extending the study of Petersen (2014b) significantly. In addition, further details concerning the physical requirements of this approach are provided in the sequel. Since the quantum object may thus have arbitrary dimensions and any traceless constant of motion can be addressed, this strategy provides an interesting and powerful tool to gain information about a complex quantum system.

To begin with, one first recalls that for an object with N-dimensional Hilbert space $\mathcal{H}_O$ any Hamiltonian H_O may be written as (cf. Eq. (2.5))

$$H_O = \alpha_{H,0}\mathbb{1}_N + \sum_{j=1}^{N^2-1} \alpha_{H,j}\,\sigma_j \ , \tag{6.56}$$

employing the fundamental representation of the special unitary group which was introduced in Sec. 2.2. Note that the coefficients are given by $\alpha_{H,0} = (1/N)\mathrm{Tr}\{H_O\}$ as well as $\alpha_{H,j} = \sqrt{(N-1)/(2N)}\mathrm{Tr}\{H_O\sigma_j\}$. Without loss of generality, one may also assume that H_O is traceless as the contribution proportional to the unit operator solely adjusts the overall energy scale, leading to a global phase for the dynamics which cannot be observed. Grouping the coefficients $\alpha_{H,j}$ and the representatives of the SU(N)-generators σ_j into vectors $\vec{\alpha}_H \equiv (\alpha_{H,1},\ldots,\alpha_{H,N^2-1})^T$ and $\hat{\Sigma} \equiv (\sigma_1,\ldots,\sigma_{N^2-1})^T$, respectively, Eq. (6.56) is conveniently represented as

$$H_O = \vec{\alpha}_H^T\hat{\Sigma} \ . \tag{6.57}$$

Due to the sketched description of the probing strategy, it is clear that the dynamics for this probing scheme is conveniently described in terms of the Heisenberg picture. Moreover, employing the SU(N)-representation and linearity, it obviously suffices to determine the dynamics of the operator basis $\hat{\Sigma}$ in order to deduce the time evolution of any operator on the object system. Because the interaction considered later on is assumed to be linear in these operators, too, the time evolution of the operator basis is indeed sufficient to characterize the dynamics of the N-dimensional system. Note that the Heisenberg equations of the basis elements with respect to the Hamiltonian H_O can be summarized as (see Appendix K)

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\Sigma}(t) = -i[\hat{\Sigma}(t), H_O] = -2\Theta(\vec{\alpha}_H)\hat{\Sigma}(t) \ , \tag{6.58}$$

[18] The free evolution of the probe must be characterized by a Hamiltonian that is quadratic in the canonical operators, i.e. $H_P = (\hat{q},\hat{p})R(\hat{q},\hat{p})^T$, where the associated 2×2-matrix R is strictly positive. Such matrices are shown to be related to the one-dimensional quantum harmonic oscillator, for which one has $R = \mathbb{1}_2$, using symplectic transformations (see below).

since the generators do not explicitly depend on time (Breuer and Petruccione, 2002). Clearly, the commutator is understood component-by-component and the entries of the $(N^2-1)\times(N^2-1)$-matrix $\Theta(\vec{\alpha}_H)$ are determined by

$$\Theta(\vec{\alpha}_H)_{jk} = \sum_l f_{jkl}\alpha_{H,l} \ , \tag{6.59}$$

where f_{jkl} refers to the structure constants of the representation of SU(N) (cf. Sec. 2.2) which characterizes the commutation relation of the SU(N)-generators, i.e. (see Eq. (2.6))

$$[\sigma_j, \sigma_k] = 2i \sum_{l=1}^{N^2-1} f_{jkl}\, \sigma_l \ . \tag{6.60}$$

Thus, Θ defines a map from vectors in $\mathbb{R}^{N^2-1}$ to the $(N^2-1)\times(N^2-1)$-matrix with entries in $\mathbb{R}$, i.e.

$$\Theta : \vec{x} \in \mathbb{R}^{N^2-1} \mapsto \Big(\big(\sum_l f_{jkl} x_l\big)_{jk} \Big) \in \mathbb{R}^{(N^2-1)\times(N^2-1)} \ , \tag{6.61}$$

that encodes the commutation relation of the SU(N)-generators. Note that this map obeys $\Theta(\vec{\alpha})\vec{\alpha}' = -\Theta(\vec{\alpha}')\vec{\alpha}$ for any vectors $\vec{\alpha}, \vec{\alpha}' \in \mathbb{R}^{N^2-1}$ as the structure constants f_{jkl} defines a completely antisymmetric tensor. As a consequence, one thus has $\Theta(\vec{\alpha})\vec{\alpha} = 0$ for any $\vec{\alpha}$.

The Heisenberg equations of motion for the canonical operators $\hat{X} = (\hat{q}, \hat{p})^T$ (see Eqs. (2.92)) may also be represented as a linear differential equation (and similarly for any number of modes) if the dynamics is generated by a Hamiltonian that is quadratic in the canonical operators, i.e., it can be written as $H_P = \hat{X}^T R \hat{X}$ for a real-valued and symmetric 2×2-matrix R. Indeed, one deduces the equation (see Appendix K)

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{X}(t) = -i[\hat{X}(t), H_P] = 2\Omega_2 R \hat{X}(t) \ , \tag{6.62}$$

where Ω_2 refers to the symplectic form introduced in Sec. 2.5.1 (see Eq. (2.96)). Clearly, since $2\Omega_2 R$ defines an element of the Lie algebra $\mathfrak{sp}(2,\mathbb{R})$ (see Appendix A), the Hamiltonian H_P thus generates a symplectic transformation of the canonical operators which, of course, preserves the canonical commutations relation.

Now, suppose that information about the expectation value of some observable $A = \vec{\alpha}_A^T \hat{\Sigma}$ on $\mathcal{H}_O$ shall be obtained by measuring an operator $B = \vec{\beta}_B^T \hat{X}$ on the quantum probe (cf. Fig. 6.4). By definition of the representatives of the SU(N)-generators, the observable A is thus traceless and B represents a linear combination of the canonical operators $\hat{q}$ and $\hat{p}$. Assuming a linear[19] coupling between the quantum probe and the complex system, i.e. the interaction is represented by the interaction Hamiltonian $H_I = \vec{\alpha}_I^T \hat{\Sigma} \otimes \vec{\beta}_I^T \hat{X}$ for arbitrary[20] real-valued vectors

[19] Note that many important models in the theory of open quantum systems are based on linear interactions between the open system and its environment (cf. the models considered in Secs. 3.3.2 and 6.4.2).

[20] Note that the vectors $\vec{\alpha}_I$ and $\vec{\beta}_I$ may also be complex-valued if the matrix with entries $(\vec{\alpha}_I \vec{\beta}_I^T)_{jk}$ is still real-valued in order to warrant Hermiticity of the interaction Hamiltonian.

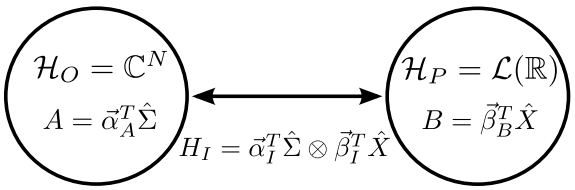

Figure 6.4 – Illustration of the setup for a dynamical probe trying to estimate the expectation value of an observable A on the object quantum system $\mathcal{H}_O$ by recording the evolution of the first moment of an observable B. Indeed, the time-averaged expectation value converges to $\langle A \rangle_{\rho_O}$ if the interaction H_I is appropriately adjusted (see Eq. (6.81)).

$\vec{\alpha}_I \in \mathbb{R}^{N^2-1}$ and $\vec{\beta}_I \in \mathbb{R}^2$, the evolution of the two interacting systems is thus governed by the total Hamiltonian

$$H = \vec{\alpha}_H^T \hat{\Sigma} \otimes \mathbb{1}_P + \mathbb{1}_O \otimes \hat{X}^T R \hat{X} + \vec{\alpha}_I^T \hat{\Sigma} \otimes \vec{\beta}_I^T \hat{X} \ . \tag{6.63}$$

The associated Heisenberg operators $\hat{\Sigma}(t)$ as well as $\hat{X}(t)$, which are understood as operators on $\mathcal{H}_O \otimes \mathcal{H}_P$, are then shown to be characterized by the equations (see Appendix K)

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\Sigma}(t) = -i[\hat{\Sigma}(t), H] = -2\{\Theta(\vec{\alpha}_H)\hat{\Sigma}(t) + \Theta(\vec{\alpha}_I)\hat{\Sigma}(t)(\vec{\beta}_I^T \hat{X}(t))\} \ , \tag{6.64}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{X}(t) = -i[\hat{X}(t), H] = 2\Omega_2 R \hat{X}(t) + (\vec{\alpha}_I^T \hat{\Sigma}(t))\Omega_2 \vec{\beta}_I \ , \tag{6.65}$$

which leads to the following evolution equations for the observables A and B due to linearity:

$$\frac{\mathrm{d}}{\mathrm{d}t}A(t) - 2\{\vec{\alpha}_A^T \Theta(\vec{\alpha}_H)\hat{\Sigma}(t) + \vec{\alpha}_A^T \Theta(\vec{\alpha}_I)\hat{\Sigma}(t)(\beta_I^T \hat{X}(t))\} \ , \tag{6.66}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}B(t) = 2\vec{\beta}_B^T \Omega_2 R \hat{X}(t) + (\vec{\beta}_B^T \Omega_2 \vec{\beta}_I)(\vec{\alpha}_I^T \hat{\Sigma}(t)) \ . \tag{6.67}$$

One immediately recognizes that A defines a constant of motion if the associated vector satisfies $\vec{\alpha}_A \sim \vec{\alpha}_H$ and $\vec{\alpha}_A \sim \vec{\alpha}_I$ as a result of the property of the map Θ shown before. Assuming that this holds true[21], the Heisenberg equation for the observable on the probe simplifies to

$$\frac{\mathrm{d}}{\mathrm{d}t}B(t) = 2\vec{\beta}_B^T \Omega_2 R \hat{X}(t) + \mu(\vec{\beta}_B^T \Omega_2 \vec{\beta}_I) A \otimes \mathbb{1}_P \ , \tag{6.68}$$

where the parameter μ is determined by $\vec{\alpha}_A = (1/\mu)\vec{\alpha}_I$. One easily deduces that Eq. (6.68) is solved by

$$B(t) = \mathbb{1}_O \otimes \vec{\beta}_B^T e^{2\Omega_2 R t} \hat{X} + \Big\{\mu \int_0^t \mathrm{d}s \ \vec{\beta}_B^T e^{2\Omega_2 R(t-s)} \Omega_2 \vec{\beta}_I\Big\} A \otimes \mathbb{1}_P \tag{6.69}$$

[21] The solution of the Heisenberg equation (6.65) for an observable A that does not define a constant of motion of the free evolution but is still proportional to the interaction, i.e. one has $\vec{\alpha}_A \sim \vec{\alpha}_I$ but $\vec{\alpha}_A \nsim \vec{\alpha}_H$, is found to be given by $\hat{X}(t) = e^{2\Omega_2 R t}\mathbb{1}_O \otimes \hat{X} + \int_0^T \mathrm{d}s \ e^{2\Omega_2 R(t-s)}\Omega_2 \vec{\beta}_I \big(\vec{\alpha}_A^T e^{-2\Theta(\vec{\alpha}_H)s}\hat{\Sigma}\big) \otimes \mathbb{1}_P$. The subsequent treatment developed for the choice $\vec{\alpha}_A \sim \vec{\alpha}_H$ can, however, not be applied in this case.

if the inverse of R exists which shall be denoted by R^{-1}. The solution may also be written as

$$B(t) = \mathbb{1}_O \otimes \vec{\beta}_B^T e^{2\Omega_2 R t}\hat{X} + \tfrac{1}{2}\mu\vec{\beta}_B^T\{e^{2\Omega_2 R t} - \mathbb{1}_2\}R^{-1}\vec{\beta}_I A \otimes \mathbb{1}_P \tag{6.70}$$

since one has $\Omega_2^{-1} = -\Omega_2$ so that one obtains

$$\int_0^t \mathrm{d}s\; e^{2\Omega_2 R(t-s)} = \tfrac{1}{2}\cdot\{\mathbb{1}_2 - e^{2\Omega_2 R t}\}R^{-1}\Omega_2\ . \tag{6.71}$$

The following lemma shows that the matrix exponential $\exp[2\Omega_2 R t]$ is upper bounded for all t with respect to the operator norm if the symmetric matrix R is not only invertible but also strictly positive, i.e. $R > 0$:

Lemma 6.2. *For any strictly positive matrix $X \in \mathcal{M}_{2n}(\mathbb{C})$, i.e. $X > 0$, the associated symplectic matrix $X_t' \equiv \exp[2t\Omega_n X]$ for arbitrary $t \in \mathbb{R}$ obeys*

$$\|X_t'\|_2 \leq \sqrt{\frac{\lambda_{\max}(X)}{\lambda_{\min}(X)}}\ . \tag{6.72}$$

Here, $\lambda_{\min}(X)$ and $\lambda_{\max}(X)$ refer to the smallest and largest eigenvalue of X, respectively, and $\|\cdot\|_2$ denotes the spectral norm on $\mathbb{C}^{2n}$, i.e.,

$$\|X_t'\|_2 \equiv \max_{\vec{y}\in\mathbb{C}^{2n}} \frac{\|X_t'\vec{y}\|}{\|\vec{y}\|}\ , \tag{6.73}$$

where $\|\cdot\|$ refers to the norm induced by the standard scalar product $(\cdot,\cdot)$ on the Hilbert space $\mathbb{C}^{2n}$.

Proof. Let $\vec{y} \in \mathbb{C}^{2n}$ be given and define $\vec{y}_t \equiv X_t'\vec{y}$ where $X_t' \equiv \exp[2t\Omega_n X]$ is associated with a strictly positive 2×2-matrix X. One easily shows that the derivative of the scalar product $(\vec{y}_t, X\vec{y}_t)$ with respect to the parameter t vanishes, implying that

$$(\vec{y}_t, X\vec{y}_t) = (\vec{y}, X\vec{y}) \tag{6.74}$$

holds for all t. Using this and the fact that the operators $X - \lambda_{\min}(X)\mathbb{1}_{2n}$ and $\lambda_{\max}(X)\mathbb{1}_{2n} - X$ are positive by definition, one deduces the relation

$$\lambda_{\min}(X)\|\vec{y}_t\|^2 \leq (\vec{y}_t, X\vec{y}_t) \leq \lambda_{\max}(X)\|\vec{y}\|^2\ , \tag{6.75}$$

which leads to

$$\lambda_{\min}(X)\cdot\|X_t'\|_2^2 \leq \lambda_{\max}(X)\ , \tag{6.76}$$

when taking the supremum over all vectors $\vec{y} \in \mathbb{C}^{2n}$ due to continuity of the square. Clearly, as $X > 0$ is equivalent to $\lambda_{\min}(X) > 0$, the inequality (6.76) may then be written as

$$\|X_t'\|_2 \leq \sqrt{\frac{\lambda_{\max}(X)}{\lambda_{\min}(X)}}\ , \tag{6.77}$$

which is exactly Eq. (6.72). □

Employing lemma 6.2, the operator norm of the time-averaged operator (6.71) for a strictly positive 2×2-matrix R can thus be bounded as

$$\begin{aligned}\frac{1}{t}\Big\| \int_0^t \mathrm{d}s\; e^{2\Omega_2 R t} \Big\|_2 &\leq \frac{1}{t}\{\|(2\Omega_2 R)^{-1} e^{2\Omega_2 R t}\|_2 + \|(2\Omega_2 R)^{-1}\mathbb{1}_2\|_2\} \\ &\leq \frac{1}{2t}\|R^{-1}\Omega_2\|_2 \cdot \{\|e^{2\Omega_2 R t}\|_2 + 1\} \\ &\leq \frac{1}{2t}\|R^{-1}\Omega_2\|_2 \cdot \{\sqrt{\lambda_{\max}(R)/\lambda_{\min}(R)} + 1\}\;, \end{aligned} \tag{6.78}$$

using, in addition, the triangle inequality and the fact that the operator norm is submultiplicative. As a consequence, the operator norm of the time-averaged operator (6.71) can be made arbitrarily small for sufficiently large times t. Note that this result is independent of the initial time of the time-averaging since lemma 6.2 holds for any choices of the parameter t. More specifically, for $\frac{1}{\Delta t}\int_{t'}^{\Delta t + t'} \mathrm{d}s\; e^{2\Omega_2 R s}$ where $t' \in \mathbb{R}$ is arbitrary, one similarly deduces

$$\frac{1}{\Delta t}\Big\| \int_{t'}^{\Delta t + t'} \mathrm{d}s\; e^{2\Omega_2 R s} \Big\|_2 \leq \frac{1}{\Delta t}\|R^{-1}\Omega_2\|_2 \cdot \sqrt{\lambda_{\max}(R)/\lambda_{\min}(R)}\;, \tag{6.79}$$

showing that the operator norm can also be made arbitrarily small for nonzero t' if the interval Δt is sufficiently large. Choosing $t' = (-1/2)\Delta t = -t$, one obtains the operator $\frac{1}{2t}\int_{-t}^{t} \mathrm{d}s\; e^{2\Omega_2 R s}$ which resembles the averaged random variable associated with a stationary stochastic process that is studied with respect to its ergodic properties (see, e.g., Gardiner (2004) and below for more details).

It is worth stressing that strict positivity of the symmetric square matrix R is essential for this result. For an invertible but indefinite matrix the operator norm of the associated time-averaged exponential does not converge to zero. As shown by Moshinsky and Winternitz (1980), all Hamiltonians of a one-dimensional particle that are quadratic in the canonical operators with strictly positive symmetric matrix R are related to the one-dimensional quantum harmonic oscillator by symplectic transformations. More specifically, the Lie algebra $\mathfrak{sp}(2, \mathbb{R})$ (which is given by elements of the kind $\Omega_2 R$, see Appendix A) has three conjugacy classes[22] with respect to the symplectic group $\mathrm{Sp}(2, \mathbb{R})$ which correspond to the repulsive harmonic oscillator, the free particle and the harmonic oscillator, respectively. As the elements of the Lie algebra corresponding to strictly positive matrices R are shown to be part of the latter class (see Moshinsky and Quesne (1971) and Moshinsky and Winternitz (1980)), any such 2×2-matrix can be represented as $R = \lambda \Omega_2 S S^T \Omega_2^T$ for some symplectic matrix $S \in \mathrm{Sp}(2, \mathbb{R})$ where the constant λ is determined by $\lambda = \det(R)$. This follows from the fact that the inverse of a symplectic matrix S is given by $S^{-1} = -\Omega_2 S^T \Omega_2$ (see Appendix A) and the harmonic oscillator is characterized by $R_{\mathrm{osc}} \sim \mathbb{1}_2$ so that one easily deduces the above expression for $\Omega_2^T S \Omega_2 R_{\mathrm{osc}} S^{-1}$ using the relation $\Omega_2^{-1} = -\Omega_2 = \Omega_2^T$.

Now, if R is assumed to be strictly positive, the time-averaged expectation value of B for an initial state ρ_{OP} of the quantum object and the probe

$$\overline{\langle B(t)\rangle}_{\rho_{OP}} \equiv \frac{1}{t}\int_0^t \mathrm{d}s\; \langle B(s)\rangle_{\rho_{OP}}\;, \tag{6.80}$$

[22] Note that two elements a, b of a group G are called *conjugate* if and only if there exists an element $g \in G$ such that $gag^{-1} = b$ holds. The conjugacy class of a contains all conjugates of this group element, i.e., it is defined as $\mathrm{Conj}_G(a) = \{b \,|\, \exists\, g \in G \,\mathrm{s.t.}\, b = gag^{-1}\}$ (Bosch, 2009).

where $\langle \hat{q}_k \rangle_{\rho_P}$ and $\langle \hat{p}_k \rangle_{\rho_P}$ with $\rho_P \equiv \mathrm{Tr}_O\{\rho_{OP}\}$ are assumed to exist, converges to the first moment of the observable A in the reduced state $\rho_O = \mathrm{Tr}_P\{\rho_{OP}\}$ on the object. That is, for any $\epsilon > 0$ and any total state ρ_{OP} with marginal ρ_P having finite expectation values for the position and momentum operator, there exists a time $t > 0$ such that the time-averaged expectation values $\overline{\langle B(t) \rangle}_{\rho_{OP}}$ satisfies

$$|\,\overline{\langle B(t) \rangle}_{\rho_{OP}} - \tau \langle A \rangle_{\rho_O}| < \epsilon \;, \tag{6.81}$$

where one defines $\tau = -\frac{1}{2}\mu(\vec{\beta}_B^T R^{-1} \vec{\beta}_I)$. Indeed, one deduces the inequality

$$\begin{aligned} |\,\overline{\langle B(t) \rangle}_{\rho_{OP}} - \tau \langle A \rangle_{\rho_O}| &\leq \sum_{j=1}^{2} \Big| \Big(\vec{\beta}_B^T \frac{1}{t} \int_0^t \mathrm{d}s \; e^{2\Omega_2 R s} \Big)_j \Big| \\ &\qquad \cdot \Big\{ |\langle \hat{X}_j \rangle_{\rho_P}| + |\tfrac{1}{2} (R^{-1} \vec{\beta}_I)_j \langle A \rangle_{\rho_O}| \Big\} \\ &\leq \max_j \Big| \Big(\vec{\beta}_B^T \frac{1}{t} \int_0^t \mathrm{d}s \; e^{2\Omega_2 R s} \Big)_j \Big| \\ &\qquad \cdot \sum_{k=1}^{2} \Big\{ |\langle \hat{X}_k \rangle_{\rho_P}| + |\tfrac{1}{2} (R^{-1} \vec{\beta}_I)_k \langle A \rangle_{\rho_O}| \Big\} \;, \end{aligned} \tag{6.82}$$

where the first factor can be related to the maximum absolute row sum norm[23] $\|A\|_\infty = \max_j \sum_{k=1}^n |a_{jk}|$ of an $m \times n$-matrix $A = (a_{jk})$ (Horn and Johnson, 1990). It thus follows that

$$\begin{aligned} \max_j \Big| \Big(\vec{\beta}_B^T \frac{1}{t} \int_0^t \mathrm{d}s \; e^{2\Omega_2 R s} \Big)_j \Big| &= \max_j \Big| \Big(-\frac{1}{t} \int_0^{-t} \mathrm{d}s \; e^{2\Omega_2 R s} \vec{\beta}_B \Big)_j \Big| \\ &\leq \Big\| -\frac{1}{t} \int_0^{-t} \mathrm{d}s \; e^{2\Omega_2 R s} \Big\|_\infty \cdot \|\vec{\beta}_B\|_\infty \;, \end{aligned} \tag{6.83}$$

employing the submultiplicativity of the norm $\|\cdot\|_\infty$. Here, $\|\vec{\beta}_B\|_\infty$ refers to the supremum norm on $\mathbb{C}^2$. As all norms on finite-dimensional vector spaces are equivalent (see, e.g., Rudin (1991)), the maximum absolute row sum norm can finally be related to the operator norm $\|\cdot\|_2$ studied before. That is, for any matrix $X \in \mathcal{M}_2(\mathbb{C})$ there exists a positive constant r such that one has $\|X\|_\infty \leq r \cdot \|X\|_2$. Applying this to the right-hand side of Eq. (6.83), one then obtains the following upper bound for Eq. (6.82):

$$\begin{aligned} |\,\overline{\langle B(t) \rangle}_{\rho_{OP}} - \tau \langle A \rangle_{\rho_O}| &\leq \frac{r}{2t} \|\vec{\beta}_B\|_\infty \|R^{-1} \Omega_2\|_2 \cdot \{ \|e^{2\Omega_2 R(-t)}\|_2 + 1 \} \\ &\qquad \cdot \sum_{k=1}^{2} \{ |\langle \hat{X}_k \rangle_{\rho_P}| + |\tfrac{1}{2} (R^{-1} \vec{\beta}_I)_k \langle A \rangle_{\rho_O}| \} \;. \end{aligned} \tag{6.84}$$

Obviously, the right-hand side can be made smaller than $\epsilon > 0$ for sufficiently large time t as the first moments $\langle \hat{X}_k \rangle_{\rho_P}$ are assumed to be finite.

As one immediately recognizes, this result is independent of the initial total state, solely requiring that the marginal state for the probe system has a well-defined position and momentum. The larger these expectation values, the longer

[23] This norm should not be interchanged with the operator norm defined via the Schatten p-norm (see Eq. (2.18) in Sec. 2.3).

the interval must be over which one must average to approximate the mean of observable on the object closely. Note that, for factorizing total states $\rho_{OP} = \rho_O \otimes \rho_P$ leading to a dynamical process Φ for the evolution of the probe due to the interaction with the finite-dimensional quantum object, the time-averaged expectation value (6.80) may be written as

$$\overline{\langle B(t)\rangle}_{\rho_O\otimes\rho_P} = \frac{1}{t}\int_0^t \mathrm{d}s \ \sum_{k=1}^{2} \beta_{B,k}\langle \hat{X}_k\rangle_{\Phi_{s,0}(\rho_P)} \ , \tag{6.85}$$

due to homogeneity and continuity of the trace. Hence, the time evolution of the probe's mean position and momentum provide the complete information to determine the expectation value of the object observable A on the quantum object. The pure dephasing dynamics of the probe, resulting from the Hamiltonian (6.63), may thus be used to estimate any traceless constant of motion of the object system independent of its initial state.

It is worth emphasizing that no assumption on the strength of the interaction has to be made, i.e., the vectors $\vec{\alpha}_I$ and $\vec{\beta}_I$ may have arbitrary norms. Due to this, the present strategy can be seen as the opposite limit of the standard approach used to describe indirect measurements which assumes a strong interaction between object and probe (see Eq. (6.1)). The speed of convergence depends, however, on the energy scale of the quadratic Hamiltonian. That is, the larger the eigenvalues of positive matrix R the faster the convergence is. To illustrate this effect, one considers again the dynamics of the particular spin-boson model studied in Ch. 5. The total Hamiltonian is thus given by

$$H = \epsilon\,\sigma_3 \otimes \mathbb{1}_P + \mathbb{1}_2 \otimes \omega(\hat{q}^2 + \hat{p}^2) + g\,\sigma_3 \otimes \hat{q} \tag{6.86}$$

for some real-valued and positive parameters ϵ, ω and g, which clearly describes a Hamiltonian of the kind given by Eq. (6.63). Indeed, the Hamiltonian H (6.86) is given by Eq. (6.63) for $\vec{\alpha}_H = (0,0,\epsilon)^T$, $R = \omega\mathbb{1}_2$, $\vec{\alpha}_I = (0,0,g)^T$ and $\vec{\beta}_I = (1,0)^T$ as one easily verifies. According to the above strategy, the time-averaged expectation value of an observable $B = \vec{\beta}_B^T\hat{X}$ in a state ρ_P converges to $\tau\langle\epsilon\sigma_3\rangle_{\rho_O}$ where τ is given by $\tau = \big(-g/(2\omega)\big)\cdot\beta_{B,1}$. Figure 6.5 shows the dynamics of the time-averaged expectation value of $B = \hat{q}$ in a thermal state $\rho_P = \rho_{\mathrm{th}}$ (see Eq. (2.125)) for different energy scales of the harmonic oscillator which are characterized by the frequency ω. Obviously, the larger this parameter the faster the time-averaged expectation value converges to multiples of the mean energy of the object.

Note that such an effect is closely related to the ergodic properties of stationary stochastic processes with appropriately decaying two-point correlation functions. In fact, let $\mathcal{Y}(t)$ denote such a stochastic process (see Sec. 4.1), the associated time-averaged random variable $\bar{\mathcal{Y}}(t) \equiv (1/2t)\int_{-t}^{t}\mathrm{d}s\ \mathcal{Y}(t)$ is shown to have a first moment identical to that of $\mathcal{Y}(t)$ and its variance tends to zero in the limit of $t\to\infty$ (see, e.g., Gardiner (2004)). Thus, $\lim_{t\to\infty}\bar{\mathcal{Y}}(t)$ represents a deterministic variable which equals $\langle\mathcal{Y}(t)\rangle$ for any t (due to stationarity), just as the time-averaged observable $\overline{\langle B(t)\rangle}_{\rho_{OP}}$ converges to the expectation value of the object observable in the limit of infinite times t. In analogy to the result for stationary process, it thus suffice to determine the mean of the observable B at successive times in order to reconstruct the first moment of a Hermitian operator on the object by means of time-averaging.

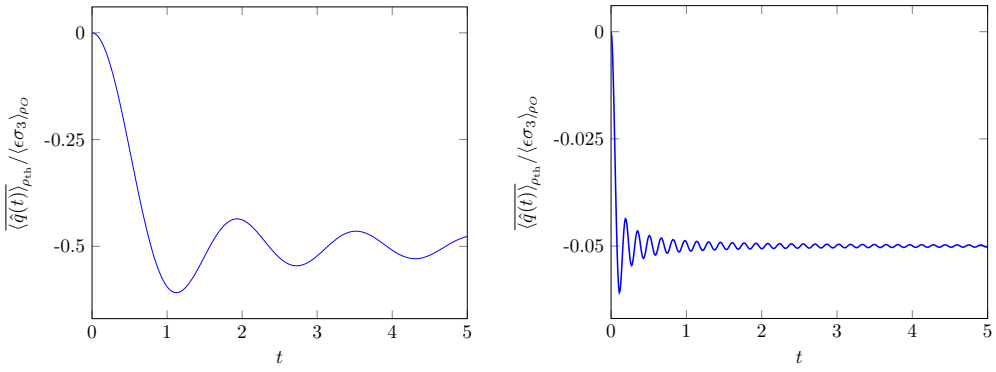

Figure 6.5 – The evolution of the time-averaged expectation value $\overline{\langle\hat{q}(t)\rangle}_{\rho_{\rm th}}$ in units of the object mean value $\langle\epsilon\sigma_3\rangle_{\rho_O}$ with respect to a thermal state with arbitrary temperature where the dynamics is induced by the Hamiltonian (6.86) for $\omega = 1$ **(a)** and $\omega = 10$ **(b)**. Since the coupling strength g is set to unity, the parameter τ is given by $-1/(2\omega)$ to which $\overline{\langle\hat{q}(t)\rangle}_{\rho_{\rm th}}$ obviously converges.

To employ this probing strategy for complex quantum system, full knowledge of the interaction is clearly required. That is, besides being able to measure an arbitrary but fixed observable on the probe at various times, one needs to know the linear interaction exactly in order to determine the precise expectation value of the traceless operator on the object. However, these requirements should not represent a major challenge for an experimental implementation of this strategy. A truly challenging task for any experimental use of this strategy is clearly given by the fact that one needs to perform frequent and close-by measurements of the observable B in order to determine the time-averaged mean from experimental data reliably. In particular, one has to prepare the quantum system again and again so that the observable on the probe system can be measured at successive times. An appropriate, close-by spacing of the instants of time where measurements are performed is especially important due to the highly oscillating behavior of the expectation values which one typically observes as the fast drop of the curves displayed in Fig. 6.5 and their oscillations shows. But, on the basis of the so far rapidly developing experimental techniques, it seems likely to assume that this task will be manageable in the nearby future.

6.4 Perturbative addressing of correlation functions

A second approach to gain information about a complex quantum system employing the dynamics of a quantum probe relies on the measurement of a coupled sensor system with variable energy splitting. In fact, the method which is presented in the following is exactly based on the idea that properties of a complex system are imprinted into the dynamics of a quantum probe to which it is brought into contact. To reveal the encoded information, it suffices to consider the outcome

statistics

$$p_t(\alpha,\beta) \equiv \mathrm{Tr}\{M_\beta \otimes \mathbb{1}_O U(t)\rho_P(\alpha)\otimes\rho_O U(t)^\dagger\}\ , \tag{6.87}$$

of the measurement of a POVM $\{M_\beta\}$ on the probe for different times and, additionally, several energy splittings of the free Hamiltonian, characterizing the quantum probe, which influences the unitary evolution. Clearly, the modulation of the free Hamiltonian of the probe may be interpreted as resulting from a control field such as a magnetic field that changes the Zeemann splittings of a particle with nonzero magnetic moment. To obtain the outcome's probability distribution, one must obviously assume that the probe can be brought into contact with the complex system for some period of time and be subsequently measured. Moreover, one supposes that this procedure can be repeated frequently – also for different energy splittings.

By varying the splitting, it is possible to separate different contributions of the measurement statistics (6.87) and, thus, to address the associated information about the complex system as has been first observed by Pollock *et al.* (2015) for two-level probes. Indeed, controlling the probe's energy splitting by a parameter λ, the probability distribution of the outcomes may be expanded in a power series with respect to $1/\lambda$, where the leading order terms are unambiguously determined by the preparation of the probe state and the measurement operators. That is, one may control the accessed information on the complex system by properly choosing the initial probe state $\rho_P(\alpha)$, parametrized by α, and the applied measurement for a given interaction. This can be nicely illustrated by looking at the resulting expansion of $p_t(\alpha,\beta)$ for a two-level probe with energy splitting $\lambda\epsilon$. As shown by Pollock *et al.* (2015), disregarding several typos, the probability distribution (6.87) is expanded as

$$\begin{aligned} p_t(\alpha,\beta) = \frac{q_{\alpha,\beta}}{2} &+ a_0^* a_1 b_0 b_1^* \zeta^{(1)}(\lambda) \\ &+ \frac{1}{\lambda\epsilon}\Big\{a_0 a_1^* \langle\sigma_3\rangle_\beta\, \zeta^{(1)}(\lambda) + b_0^* b_1 \sum_{k=0}^{1}(-1)^k |a_k|^2 \xi_k^{(1)}(\lambda)\Big\} \\ &- \frac{1}{(\lambda\epsilon)^2}\Big\{\frac{1}{2}\langle\sigma_3\rangle_\beta \cdot \sum_{k=0}^{1}(-1)^k |a_k|^2 \xi_k^{(2)}(\lambda) \\ &\qquad - b_0^* b_1 \big(a_0^* a_1 \zeta_0^{(2)} + a_0 a_1^* \zeta_1^{(2)}\big)\Big\} + \text{c.c.} \\ &+ \mathcal{O}(\lambda^{-3}) \end{aligned} \tag{6.88}$$

for a pure probe state $\rho_P(\alpha) \equiv |\alpha\rangle\langle\alpha|$ and a projective measurement $M_\beta \equiv |\beta\rangle\langle\beta|$ where a_k and b_k refer to the overlap of $|\alpha\rangle$ and $|\beta\rangle$, respectively, with eigenstates $|\pi_k\rangle$ of the free Hamiltonian of the probe. Hence, one has $a_k \equiv \langle\alpha|\pi_k\rangle$ and $b_k \equiv \langle\beta|\pi_k\rangle$ and, furthermore, the definitions $q_{\alpha,\beta} = |a_0^* b_0|^2 + |a_1^* b_1|^2$ and $\langle\sigma_3\rangle_\beta = |b_0|^2 - |b_1|^2$ are employed. The precise form of the functions $\zeta^{(j)}(\lambda)$ and $\xi_k^{(j)}(\lambda)$ can be found at the end of the subsequent section (see Eqs. (6.112)–(6.117)). Note that they depend on the free Hamiltonian of the complex system as well as the used interaction. Moreover, it is worth noticing that the energy splitting must be sufficiently large in comparison to the typical energies of the object influencing the probe's dynamics due to the interaction in order to obtain such an expansion

of the probability (6.87) in $1/\lambda$. As a consequence, the concerned probabilities $p_t(\alpha, \beta)$ are typically quite small.

Now, if, for example, neither the preparation nor the measurement of the probe are made in the energy eigenbasis $\{|\pi_k\rangle\}$ of the probe, then the coefficients of the terms in the first line of Eq. (6.88) are clearly nonzero and, thus, define the leading order contribution with respect to the energy splitting characterized by λ. On the contrary, when one prepares and measures an eigenstate of the probe's free Hamiltonian, i.e., one chooses $|\alpha\rangle = |\pi_k\rangle$ and $|\beta\rangle = |\pi_{k'}\rangle$ for some indices k and k', it is easily observed that only terms of the probability (6.88) survive that are in second order with respect to $1/\lambda$. The leading order contribution obtained for different preparations of $\rho_P(\alpha)$ and choices of the ensuing measurement is summarized in Tab. 6.1. In general, any of these terms represents a damped and oscillatory function of the scaling parameter as is easily seen by looking at Eqs. (6.112)–(6.117) (see the end of Sec. 6.4.1), i.e., one has

$$p_t(\alpha, \beta) \simeq \frac{1}{\lambda^n}\{a(t) + b(t)\cos(\lambda\epsilon t + \phi(t))\} \tag{6.89}$$

in leading order for sufficiently large energy splitting (cf. Eq. (6.118)). Different information on the complex system, such as the system's spectrum as well as its autocorrelation time and whether or not it is in thermal equilibrium, can then be deduced from the time evolution of the central value $a(t)$, the amplitudes $b(t)$ and the phase $\phi(t)$ as argued by Pollock *et al.* (2015). For example, if the central value of the leading contribution is independent of time for the configuration $|\alpha\rangle = |\pi_k\rangle$ and $|\beta\rangle \neq |\pi_0\rangle, |\pi_1\rangle$ (cf. Tab. (6.2)) and an interaction that is not diagonal in the probes energy eigenbasis, then one can conclude that the state ρ_O of the complex system is in thermal equilibrium.

Summarizing, the method requires to determine the probability (6.87) of a certain measurement outcome for a specific initial state of the probe as a function of the interaction time as well as the probe's energy splitting which finally allows to deduce the leading order contribution of the probability with respect to $1/\lambda$. A Fourier decomposition of the leading term then yields information on the object system. It is worth emphasizing that different properties can be accessed by changing the eigenbasis of the probe's Hamiltonian. The method allows to gain information by essentially post-processing the measurement statistics obtained for a given initial probe state and some measurement as, e.g., done in the full counting

	$\|\beta\rangle \neq \|\pi_0\rangle, \|\pi_1\rangle$	$\|\beta\rangle = \|\pi_j\rangle$
$\|\alpha\rangle \neq \|\pi_0\rangle, \|\pi_1\rangle$	$\mathrm{Re}\big(a_0^* a_1 b_0 b_1^* \zeta^{(0)}(\lambda)\big)$	$\mathrm{Re}\big((-1)^j a_0 a_1^* \zeta^{(1)}(\lambda)\big)/(\lambda\epsilon)$
$\|\alpha\rangle = \|\pi_k\rangle$	$\mathrm{Re}\big((-1)^k b_0 b_1^* \xi_k^{(1)}(\lambda)\big)/(\lambda\epsilon)$	$\mathrm{Re}\big((-1)^{j+k+1} \xi_k^{(2)}(\lambda)\big)/(\lambda\epsilon)^2$

Table 6.1 – The leading order terms of the probability $p_t(\alpha, \beta)$ with respect to $1/\lambda$ given in Eq. (6.88) for different choices of the preparation ($|\alpha\rangle$) and the measurement ($|\beta\rangle$) where possible constant contributions $q_{\alpha,\beta}$ have been omitted (cf. Tab. 1 in Pollock *et al.* (2015)). The damped oscillatory λ-dependence of these terms is apparent from the definition of the involved quantities (see Eqs. (6.112)–(6.117)).

statistics (Guarnieri *et al.*, 2016; Esposito *et al.*, 2009). Note that the method can also be seen as a generalized spectroscopic tool which is different from process tomography as information on quantities of the complex system is gained by varying the probe's energy scale for a fixed initial state and measurement.

Clearly, this strategy can similarly be extended to arbitrary measurements and quantum probes as well as multiple selective measurements. As a result of the latter, one may ultimately address higher-order contributions with respect to the inverse scaling $1/\lambda$ of the energy splitting, thus extending the work by Pollock *et al.* (2015) who solely considered the above setup. In the following section, the generalization to N_P-dimensional probes and arbitrary measurements is derived as a result of this thesis which eventually provides the basis for an extension to multiple measurements. From the derived general expressions, the terms for two-level probes are deduced (cf. Eqs. (6.88) and (6.112)–(6.117)) where some typos in the work by Pollock *et al.* (2015) are eventually identified. The prospects of the present scheme are finally illustrated by showing how the superfluid excitations in the Bose-Hubbard model can be obtained using this method which will be contrasted with a strategy suggested by Cosco *et al.* (2015) (see Sec. 6.4.2).

It must be stressed once more that, besides control over the interaction, the quantum probe's initial state and the performed measurement, the energy splitting needs to be sufficiently large so that the interaction of the probe with the quantum object only leads to virtual excitations of the former. Due to this, the considered transition probabilities (6.87) are typically quite small. Even though no assumptions on the object's state are required, the strategy is thus not completely universal, i.e., it may not be applied to any complex quantum system and interaction blindly, and requires a high resolution of the transition probabilities. As a consequence of the off-resonant coupling, very sensitive measuring devices and many repetitions are thus needed, imposing challenging requirements on a use of this strategy in experiments.

6.4.1 The method for N_P-dimensional quantum probes

The setup of this method is given by a quantum probe with free, nondegenerate Hamiltonian H_P, whose spectral decomposition reads

$$H_P = \lambda \sum_{j=0}^{N_P-1} \epsilon_j |\pi_j\rangle_P \langle \pi_j| \ . \tag{6.90}$$

The probe is eventually coupled to a complex system – the object with associated Hamiltonian H_O – via an interaction H_I. Here, all Hamiltonians are assumed to be time-independent and λ refers, as before, to a dimensionless constant whose magnitude controls the splitting of the energy levels. Note that the case $N_P = \infty$, i.e., a quantum probe that is characterized by an infinite-dimensional Hilbert space is not excluded in this approach (see Sec. 6.4.2 for an example). The power expansion of the probability (6.87) in powers of $1/\lambda$, as stated for two-level probes (cf. Eq. (6.88)), essentially relies on a Dyson expansion of the unitary propagator in the interaction picture which is defined with respect to the contributions of the interaction Hamiltonian that are not diagonal in the probe's energy eigenbasis.

Hence, the representation of the probability is exact for any pure dephasing dynamics. Expanding the total Hamiltonian $H = H_P \otimes \mathbb{1}_O + \mathbb{1}_P \otimes H_O + H_I$ in the eigenbasis $\{|\pi_j\rangle_P\}$, i.e.

$$\begin{aligned} H &= H_P \otimes \mathbb{1}_O + \sum_l S_l \otimes T_l \\ &= H_P \otimes \mathbb{1}_O + \sum_j \Big\{ |\pi_j\rangle_P\langle\pi_j| \otimes A_j + \sum_{k\neq j} |\pi_j\rangle_P\langle\pi_k| \otimes B_{jk} \Big\} \ , \end{aligned} \tag{6.91}$$

where one defines $A_j \equiv \sum_l \langle\pi_j|S_l|\pi_j\rangle T_l$ and $B_{jk} \equiv \sum_l \langle\pi_j|S_l|\pi_k\rangle T_l$ with $\sum_{k\neq j}$ denoting the summation over all indices k different from j, one considers the interaction picture with respect to the Hamiltonian

$$H_0 \equiv \frac{1}{\lambda}\Big[H_P \otimes \mathbb{1}_O + \sum_j |\pi_j\rangle_P\langle\pi_j| \otimes A_j \Big] \ . \tag{6.92}$$

Clearly, one has $A_j^\dagger = A_j$ and $B_{jk}^\dagger = B_{kj}$ as S_k and T_k are Hermitian. The interaction picture representation of the nondiagonal part of the interaction Hamiltonian $H_I' \equiv H - \lambda H_0$ is then found to be given by

$$\tilde{H}_I'(t) = \sum_j \sum_{k\neq j} e^{it(\epsilon_j - \epsilon_k)} |\pi_j\rangle_P\langle\pi_k| \otimes \tilde{B}_{jk}(t) \ , \tag{6.93}$$

where the operators $\tilde{B}_{jk}(t)$ are defined as

$$\tilde{B}_{jk}(t) = \exp\left[(it/\lambda)A_j\right] B_{jk} \exp\left[(-it/\lambda)A_k\right] \ . \tag{6.94}$$

One readily observes that the unitary propagator in the Schrödinger picture associated with H, i.e. $U(t) \equiv \exp[-itH]$, can be written as

$$U(t) = \exp\Big[-i\lambda t \left(H_0 + \frac{1}{\lambda} H_I'\right)\Big] \ , \tag{6.95}$$

so that the dissipative interaction H_I' can be seen as a perturbation of the free Hamiltonian H_0 which is evolved to an effective time λt. The relative scaling of the two parts is related to the approach concerning the derivation of a weak coupling master equation proposed by Davies (1976) (see also Pollock *et al.* (2015)). By means of the propagator that corresponds to the rescaled interaction Hamiltonian $(1/\lambda)\tilde{H}_I'(t)$, the unitary can finally be represented as

$$\begin{aligned} U(t) &= e^{-i\lambda t H_0}\, \mathrm{T}_{\leftarrow} \exp\Big[-i \int_0^{\lambda t} \mathrm{d}s\ \frac{1}{\lambda} \tilde{H}_I'(s)\Big] \\ &= e^{-i\lambda t H_0} \Big\{ \mathbb{1}_{PO} + \frac{1}{i\lambda} \int_0^{\lambda t} \mathrm{d}s\ \tilde{H}_I'(s) \\ &\qquad - \frac{1}{\lambda^2} \int_0^{\lambda t} \mathrm{d}s \int_0^s \mathrm{d}s'\ \tilde{H}_I'(s)\tilde{H}_I'(s') + \mathcal{O}(\lambda^{-3}) \Big\} \ , \end{aligned} \tag{6.96}$$

where the time-ordered exponential is expanded in a Dyson series in the last line. This expansion provides the starting point to represent the probability (6.87) associated with the outcome β, when measuring a POVM $\{M_\beta\}$ on the probe at time

t for an initial state $\rho_P(\alpha) \otimes \rho_O$, as a power series in $1/\lambda$. More precisely, upon inserting the time-ordered exponential (6.96) into Eq. (6.87), one firstly obtains

$$
\begin{aligned}
p_t(\alpha,\beta) = {} & \mathrm{Tr}\{M_\beta \otimes \mathbb{1}_O e^{-i\lambda t H_0} \rho_P(\alpha) \otimes \rho_O e^{i\lambda t H_0}\} && (6.97)\\
& + \frac{1}{i\lambda}\int_0^{\lambda t} \mathrm{d}s\, \mathrm{Tr}\{M_\beta \otimes \mathbb{1}_O e^{-i\lambda t H_0} [\tilde{H}'_I(s), \rho_P(\alpha)\otimes\rho_O] e^{i\lambda t H_0}\} && (6.98)\\
& + \frac{1}{\lambda^2}\int_0^{\lambda t}\mathrm{d}s \int_0^{\lambda t}\mathrm{d}s'\ \mathrm{Tr}\{M_\beta \otimes \mathbb{1}_O e^{-i\lambda t H_0} \\
& \qquad \cdot \tilde{H}'_I(s)\rho_P(\alpha)\otimes\rho_O \tilde{H}'_I(s') e^{i\lambda t H_0}\} && (6.99)\\
& - \frac{1}{\lambda^2}\int_0^{\lambda t}\mathrm{d}s \int_0^{s}\mathrm{d}s'\ \mathrm{Tr}\{M_\beta \otimes \mathbb{1}_O\, e^{-i\lambda t H_0} (\tilde{H}'_I(s)\tilde{H}'_I(s')\rho_P(\alpha)\otimes\rho_O \\
& \qquad + \rho_P(\alpha)\otimes\rho_O \tilde{H}'_I(s')\tilde{H}'_I(s)) e^{i\lambda t H_0}\} && (6.100)\\
& + \mathcal{O}(\lambda^{-3})\ .
\end{aligned}
$$

The integrals of the three terms (6.98)–(6.100) may, however, additionally be expanded in a power series with respect to the inverse energy scaling $1/\lambda$ in the limit of large energy splittings in comparison to the typical energies of the object that influence the dynamics of the probe. As the transition matrix elements $\langle\pi_k|\rho_P(\alpha)|\pi_l\rangle$ and $\langle\pi_m|M_\beta|\pi_n\rangle$ contained in the different terms (6.98)–(6.100) are yet the same for all contributions to the respective power series and they, together with the elements of Eq. (6.97), already cover all possible combinations of transition matrix elements (see below), the zeroth order terms of the three integrals along with Eq. (6.97) characterize the leading order contributions of the probability $p_t(\alpha,\beta)$ with respect to $1/\lambda$. It is clear that the leading order contribution to the probability depends again on the chosen initial probe state $\rho_P(\alpha)$ and the measurement $\{M_\beta\}$ as transition matrix elements may be zero for some choices (see Tab. 6.2 for the leading order dependence of $p_t(\alpha,\beta)$).

In the following, the lowest order contributions to the integrals in Eqs. (6.98)–(6.100) are explicitly determined in the previously mentioned limit. For the sake of clarity, the subscript P will be omitted for the Hilbert space elements and their duals in the sequel. To begin with, one recalls that the first term, i.e., Eq. (6.97)

$\langle\pi_n\|M_\beta\|\pi_m\rangle \neq 0$	$\langle\pi_k\|\rho_P(\alpha)\|\pi_l\rangle \neq 0$	
	$k = l$	$k \neq l$
$m = k \wedge n = l$	Eqs. (6.97)&(6.100)	Eq. (6.97)
$m \neq k \wedge n = l$	Eq. (6.98)	Eq. (6.98)
$m = k \wedge n \neq l$	Eq. (6.98)	Eq. (6.98)
$m, n \neq k, l$	Eq. (6.99)	Eq. (6.99)

Table 6.2 – Overview of the leading order dependence of the probability $p_t(\alpha,\beta)$ defined in Eq. (6.87). Clearly, the roles of m and n may be interchanged in the above columns. Note that Eq. (6.97) is independent of λ and t if one sets $k = l$, so the leading order term of Eq. (6.100) yields the dominating nonconstant term. In the same way, the lowest order approximations of Eqs. (6.98) and (6.99) characterize the leading order for the parameters specified in the second to fourth line.

yields

$$\begin{aligned}
&\mathrm{Tr}\{M_\beta \otimes \mathbb{1}_O e^{-i\lambda t H_0} \rho_P(\alpha) \otimes \rho_O e^{i\lambda t H_0}\} \\
&= \sum_{k,l} \langle \pi_k|\rho_P(\alpha)|\pi_l\rangle \mathrm{Tr}\{M_\beta \otimes \mathbb{1}_O e^{-i\lambda t H_0}|\pi_k\rangle\langle\pi_l| \otimes \rho_O e^{i\lambda t H_0}\} \\
&= \sum_{k,l} \langle \pi_k|\rho_P(\alpha)|\pi_l\rangle \langle \pi_l|M_\beta|\pi_k\rangle e^{-i\lambda t \Delta_{kl}} \langle e^{itA_l} e^{-itA_k}\rangle_{\rho_O} \ , \qquad (6.101)
\end{aligned}$$

where $\Delta_{kl} \equiv \epsilon_k - \epsilon_l$. Thus, this expression comprises constant terms associated with $k = l$ that specify the survival probability in the eigenstate $|\pi_k\rangle$. Similarly, upon inserting the definitions of the operators, the second term, i.e., Eq. (6.98) reads

$$\begin{aligned}
&\frac{1}{i\lambda} \int_0^{\lambda t} \mathrm{d}s \ \mathrm{Tr}\{M_\beta \otimes \mathbb{1}_O e^{-i\lambda t H_0} [\tilde{H}_I'(s), \rho_P(\alpha) \otimes \rho_O] e^{i\lambda t H_0}\} \\
=&\frac{1}{i\lambda} \sum_{k,l} \langle \pi_k|\rho_P(\alpha)|\pi_l\rangle \Big[\sum_{m\neq k} e^{-i\lambda t \Delta_{ml}} \langle \pi_l|M_\beta|\pi_m\rangle \\
&\qquad \cdot \int_0^{\lambda t} \mathrm{d}s \ e^{is\Delta_{mk}} \mathrm{Tr}\{e^{-itA_m} \tilde{B}_{mk}(s) \rho_O e^{itA_l}\} \\
&\qquad - \sum_{n\neq l} e^{-i\lambda t \Delta_{kn}} \langle \pi_n|M_\beta|\pi_k\rangle \\
&\qquad \cdot \int_0^{\lambda t} \mathrm{d}s \ e^{is\Delta_{ln}} \mathrm{Tr}\{e^{-itA_k} \rho_O \tilde{B}_{ln}(s) e^{itA_n}\} \Big] \ , \qquad (6.102)
\end{aligned}$$

where it now remains to evaluate the integrals. If the spectral decomposition of A_k is denoted by $A_k = \sum_j E_j^{(k)} |j_k\rangle\langle j_k|$, one deduces, for example,

$$\begin{aligned}
&\int_0^{\lambda t} \mathrm{d}s \ e^{is\Delta_{mk}} \mathrm{Tr}\{e^{-i\tau A_m} \tilde{B}_{mk}(s) \rho_O e^{itA_l}\} \\
&= \int_0^{\lambda t} \mathrm{d}s \ e^{is\Delta_{mk}} \mathrm{Tr}\{e^{-itA_m} e^{is/\lambda A_m} B_{mk} e^{-is/\lambda A_k} \rho_O e^{itA_l}\} \\
&= \sum_{a,b,c} e^{it(E_a^{(l)} - E_b^{(m)})} \langle a_l|b_m\rangle\langle b_m|B_{mk}|c_k\rangle\langle c_k|\rho_O|a_l\rangle \\
&\qquad \cdot \int_0^{\lambda t} \mathrm{d}s \ \exp\left[is\Big(\Delta_{mk} + \frac{E_b^{(m)} - E_c^{(k)}}{\lambda}\Big)\right] \ , \qquad (6.103)
\end{aligned}$$

and the remaining integral gives

$$\int_0^{\lambda t} \mathrm{d}s \exp\left[is\Big(\Delta_{mk} + \frac{E_b^{(m)} - E_c^{(k)}}{\lambda}\Big)\right] = \frac{e^{it(\Delta_{mk} + E_b^{(m)} - E_c^{(k)})} - 1}{i\Delta_{mk}\Big(1 + \frac{E_b^{(m)} - E_c^{(k)}}{\lambda\Delta_{mk}}\Big)} \ , \qquad (6.104)$$

as one has $m \neq k$ by construction. To obtain a power series in $1/\lambda$, one employs the Taylor expansion of the function $f(x) = 1/(1+x)$ at $x = 0$. The Taylor series is found to be given by $f_T(x) = \sum_{k\geq 0} (-x)^k$ which converges to the function f itself for $|x| < 1$ (Bronstein and Semendjajew, 1996). To apply this result to the factor in Eq. (6.104), one thus needs to have $\lambda\Delta_{mk} \gg E_b^{(m)} - E_c^{(k)}$ for all indices

m, k and b, c for which the transition matrix elements $\langle b_m|B_{mk}|c_k\rangle$ and $\langle c_k|\rho_O|a_l\rangle$ are nonzero, which leads to the previously mentioned constraint for the strategy.

In fact, by definition of the operator A_k, containing the free Hamiltonian of the object system, this condition obviously represents a far reaching constraint on the state or the interaction if the strategy shall be applied to an infinite-dimensional complex system that is characterized by a Hamiltonian H_O with unbounded spectrum such as the quantum harmonic oscillator. If no assumption on the state of the complex system is to be made, the interaction may thus only be weakly dissipative. This means that the interaction, specifying the operators B_{mk}, solely concerns states of the complex system that are energetically close compared to the probe's energy splitting, thus resulting in a slow change of the probe's energy as mentioned before. An example highlighting this property by means of coupled quantum mechanical oscillators defining the probe as well as the complex system is given by the superfluid Bose-Hubbard model with a coupled impurity atom that is studied in Sec. 6.4.2. Note that the constraint on the interaction can, in principle, always be satisfied for a sufficiently large energy splitting as one may very-well approximate any coupling by a Hamiltonian having finite support with respect to the energy eigenbasis of the quantum system. Obviously, a vast splitting also guarantees the validity of the expansion for any kind of finite-dimensional systems.

If $\lambda\Delta_{mk} \gg E_b^{(m)} - E_c^{(k)}$ holds for all indices m, k and b, c associated with nonzero transition matrix elements, then Eq. (6.103) is approximated as

$$\begin{aligned}
&\int_0^{\lambda t} \mathrm{d}s\; e^{is\Delta_{mk}} \mathrm{Tr}\{e^{-itA_m}\tilde{B}_{mk}(s)\rho_O e^{itA_l}\} \\
&\simeq \frac{1}{i\Delta_{mk}} \sum_{a,b,c} e^{it(E_a^{(l)}-E_b^{(m)})} \langle a_l|b_m\rangle\langle b_m|B_{mk}|c_k\rangle\langle c_k|\rho_O|a_l\rangle \left[e^{it(\Delta_{mk}+E_b^{(m)}-E_c^{(k)})} - 1\right] \\
&= \frac{i}{\Delta_{mk}} \left[\langle e^{itA_l}e^{-itA_m}B_{mk}\rangle_{\rho_O} - e^{it\lambda\Delta_{mk}}\langle e^{itA_l}B_{mk}e^{-itA_k}\rangle_{\rho_O}\right] , \qquad (6.105)
\end{aligned}$$

employing the zero order approximation of the function $1/(1+x)$ which is given by $1/(1+x)|_{x=0} \simeq 1$. Since the higher order corrections of the expansion are proportional to x^n for $n \in \mathbb{N}$, the additional terms in Eq. (6.105) are proportional to powers of $1/\lambda$ that do obviously not contribute to the leading order. The analogous evaluation of the second integral in Eq. (6.102) is abbreviated by the observation that the integral defines the complex conjugate of Eq. (6.103) if one additionally interchanges the indices according to $k \leftrightarrow l$ and $m \leftrightarrow n$. In summary,

one thus obtains for Eq. (6.98)

$$
\begin{aligned}
&\frac{1}{i\lambda}\int_0^{\lambda t}\mathrm{d}s\ \mathrm{Tr}\{M_\beta\otimes\mathbb{1}_O e^{-i\lambda t H_0}[\tilde{H}_I'(s),\rho_P(\alpha)\otimes\rho_O]e^{i\lambda t H_0}\}\\
&=\frac{1}{\lambda}\sum_{k,l}\langle\pi_k|\rho_P(\alpha)|\pi_l\rangle\\
&\quad\cdot\Bigg\{\sum_{m\neq k}\langle\pi_l|M_\beta|\pi_m\rangle\frac{1}{\Delta_{mk}}e^{-i\lambda t\Delta_{ml}}\\
&\qquad\cdot\Big[\langle e^{itA_l}e^{-itA_m}B_{mk}\rangle_{\rho_O}-e^{it\lambda\Delta_{mk}}\langle e^{itA_l}B_{mk}e^{-itA_k}\rangle_{\rho_O}\Big]\\
&\quad+\sum_{n\neq l}\langle\pi_n|M_\beta|\pi_k\rangle\frac{1}{\Delta_{nl}}e^{+i\lambda t\Delta_{nk}}\\
&\qquad\cdot\Big[\langle B_{ln}e^{itA_n}e^{-itA_k}\rangle_{\rho_O}-e^{-it\lambda\Delta_{nl}}\langle e^{itA_l}B_{ln}e^{-itA_k}\rangle_{\rho_O}\Big]\Bigg\}\\
&\quad+\mathcal{O}(\lambda^{-2})
\end{aligned}
\tag{6.106}
$$

for appropriately adjusted interaction and energy splitting of the probe.

Along the same lines one continues evaluating the other terms (Eqs. (6.99) and (6.100)) of the probability $p_t(\alpha,\beta)$. For Eq. (6.99) one finally determines

$$
\begin{aligned}
&\frac{1}{\lambda^2}\int_0^{\lambda t}\mathrm{d}s\int_0^{\lambda t}\mathrm{d}s'\ \mathrm{Tr}\{M_\beta\otimes\mathbb{1}_O e^{-i\lambda t H_0}\tilde{H}_I'(s)\rho_P(\alpha)\otimes\rho_O\tilde{H}_I'(s')e^{i\lambda t H_0}\}\\
&=\frac{1}{\lambda^2}\sum_{k,l}\langle\pi_k|\rho_P(\alpha)|\pi_l\rangle\sum_{m\neq k,n\neq l}\langle\pi_n|M_\beta|\pi_m\rangle e^{-i\lambda t\Delta_{mn}}\\
&\qquad\cdot\int_0^{\lambda t}\mathrm{d}s\int_0^{\lambda t}\mathrm{d}s'\ e^{is\Delta_{mk}}e^{is'\Delta_{ln}}\langle\tilde{B}_{ln}(s')e^{itA_n}e^{-itA_m}\tilde{B}_{mk}(s)\rangle_{\rho_O}\\
&=\frac{1}{\lambda^2}\sum_{k,l}\langle\pi_k|\rho_P(\alpha)|\pi_l\rangle\sum_{m\neq k,n\neq l}\langle\pi_n|M_\beta|\pi_m\rangle\frac{1}{\Delta_{mk}\Delta_{nl}}\\
&\qquad\cdot\Big\{e^{i\lambda t\Delta_{nm}}\langle B_{ln}e^{itA_n}e^{-itA_m}B_{mk}\rangle_{\rho_O}\\
&\qquad\quad-e^{i\lambda t\Delta_{nk}}\langle e^{itA_l}B_{ln}e^{-itA_m}B_{mk}\rangle_{\rho_O}\\
&\qquad\quad-e^{i\lambda t\Delta_{lm}}\langle B_{ln}e^{itA_n}B_{mk}e^{-itA_k}\rangle_{\rho_O}\\
&\qquad\quad+e^{i\lambda t\Delta_{lk}}\langle e^{itA_l}B_{ln}B_{mk}e^{-itA_k}\rangle_{\rho_O}\Big\}+\mathcal{O}(\lambda^{-3})\ .
\end{aligned}
\tag{6.107}
$$

Note that the sum contains terms that are proportional to $\langle\pi_k|\rho_P(\alpha)|\pi_l\rangle\langle\pi_k|M_\beta|\pi_l\rangle$ if the indices are chosen as $n=k$ and $m=l$ whenever one has $k\neq l$. These terms are, however, already contained in Eq. (6.101) (modulo partial complex conjugation, i.e. $\langle\pi_k|M_\beta|\pi_l\rangle\leftrightarrow\langle\pi_l|M_\beta|\pi_k\rangle$) for which reason these contributions to Eq. (6.107) are not in leading order and may thus be omitted when considering the leading contributions to the power expansion with respect to $1/\lambda$ (cf. Tab. 6.2).

Last but not least, the fourth term of the probability, i.e., Eq. (6.100) is found

to be given by

$$
\begin{aligned}
&-\frac{1}{\lambda^2}\int_0^{\lambda t}\mathrm{d}s\int_0^{s}\mathrm{d}s'\ \mathrm{Tr}\Big\{M_\beta\otimes\mathbb{1}_O e^{-i\lambda t H_0}\big(\tilde{H}_I'(s)\tilde{H}_I'(s')\rho_P(\alpha)\otimes\rho_O \\
&\qquad\qquad + \rho_P(\alpha)\otimes\rho_O\tilde{H}_I'(s')\tilde{H}_I'(s)\big)e^{i\lambda t H_0}\Big\} \\
&= -\frac{1}{\lambda^2}\sum_{k,l}\langle\pi_k|\rho_P(\alpha)|\pi_l\rangle \\
&\qquad\cdot\Bigg\{\sum_{m\neq k}\sum_{o\neq m}\langle\pi_l|M_\beta|\pi_o\rangle e^{-i\lambda t\Delta_{ol}} \\
&\qquad\quad\cdot\int_0^{\lambda t}\mathrm{d}s\int_0^{s}\mathrm{d}s'\ e^{is\Delta_{om}}e^{is'\Delta_{mk}}\cdot\langle e^{itA_l}e^{-itA_o}\tilde{B}_{om}(s)\tilde{B}_{mk}(s')\rangle_{\rho_O} \\
&\qquad+\sum_{n\neq l}\sum_{q\neq n}\langle\pi_q|M_\beta|\pi_k\rangle e^{-i\lambda t\Delta_{kq}} \\
&\qquad\quad\cdot\int_0^{\lambda t}\mathrm{d}s\int_0^{s}\mathrm{d}s'\ e^{is\Delta_{nq}}e^{is'\Delta_{ln}}\langle\tilde{B}_{ln}(s')\tilde{B}_{nq}(s)e^{itA_q}e^{-itA_l}\rangle_{\rho_O}\Bigg\}\ . \qquad (6.108)
\end{aligned}
$$

Before starting to evaluate the nested integrals, one first observes that most of the terms are not in leading order. More specifically, the transition matrix elements $\langle\pi_k|\rho_P(\alpha)|\pi_l\rangle\langle\pi_n|M_\beta|\pi_m\rangle$ encountered in Eqs. (6.97)–(6.100) are given by

$$
\begin{aligned}
\text{Eq. (6.97) (cf. Eq. (6.101))} &\ \leftrightarrow\ \langle\pi_l|M_\beta|\pi_k\rangle\ \textcircled{1}\ , \\
\text{Eq. (6.98) (cf. Eq. (6.102))} &\ \leftrightarrow\ \langle\pi_l|M_\beta|\pi_{m\neq k}\rangle\ \textcircled{2}\ \wedge\ \langle\pi_{n\neq l}|M_\beta|\pi_k\rangle\ \textcircled{3}\ , \\
\text{Eq. (6.99) (cf. Eq. (6.107))} &\ \leftrightarrow\ \langle\pi_{n\neq l}|M_\beta|\pi_{m\neq k}\rangle\ \textcircled{4}\ , \\
\text{Eq. (6.100) (cf. Eq. (6.108))} &\ \leftrightarrow\ \langle\pi_l|M_\beta|\pi_{o\neq m(\neq k)}\rangle\ \textcircled{5}\ \wedge\ \langle\pi_{q\neq n(\neq l)}|M_\beta|\pi_k\rangle\ \textcircled{6}\ ,
\end{aligned}
$$

where solely the part involving the measurement M_β is listed as the transition matrix element $\langle\pi_k|\rho_P(\alpha)|\pi_l\rangle$ is identical for all terms. Clearly, the contributions ⑤ and ⑥ are equal to those labeled by ② and ③ if one has $o\neq k$ and $q\neq l$, respectively, which thus determine the leading order with respect to $1/\lambda$ for the associated transition elements of ρ_O and M_β. Moreover, for indices $o=k$ and $q=l$, the transition matrix elements ⑤ and ⑥ are already encountered within Eq. (6.101). However, if one additionally has $k=l$ in this case, the corresponding terms of Eq. (6.101) are constant, so ⑤ and ⑥ ultimately characterize the first nonconstant contributions with respect to λ for the matrix elements $\langle\pi_k|M_\beta|\pi_k\rangle\langle\pi_k|\rho_P(\alpha)|\pi_k\rangle$. Note that these contributions are of second order and can be related to the quantum Zeno effect (Misra and Sudarshan, 1977) (cf. Monras *et al.* (2014)). The present observations regarding the contributions that characterize the leading order are in accordance with the summary given in Tab. 6.2.

Considering the contribution to Eq. (6.108) for $o=k=l=q$, one recognizes that the nested integrals can be disentangled into a double integral over the square

ranging from 0 to λt, i.e.

$$\begin{aligned}
&\int_0^{\lambda t} \mathrm{d}s \int_0^s \mathrm{d}s' \; e^{i\Delta_{km}(s-s')} \langle \tilde{B}_{km}(s) \tilde{B}_{km}(s')^\dagger \rangle_{\rho_O} \\
&\quad + \int_0^{\lambda t} \mathrm{d}s \int_0^s \mathrm{d}s' \; e^{-i\Delta_{km}(s-s')} \langle \tilde{B}_{km}(s') \tilde{B}_{km}(s)^\dagger \rangle_{\rho_O} \\
&= \int_0^{\lambda t} \mathrm{d}s \int_0^{\lambda t} \mathrm{d}s' \; e^{i\Delta_{km}(s-s')} \langle \tilde{B}_{km}(s) \tilde{B}_{km}(s')^\dagger \rangle_{\rho_O} \; . \qquad (6.109)
\end{aligned}$$

One may then proceed as before in order to determine the leading order contribution of Eq. (6.108) which finally gives

$$\begin{aligned}
&-\frac{1}{\lambda^2} \sum_k \langle \pi_k | \rho_P(\alpha) | \pi_k \rangle \langle \pi_k | M_\beta | \pi_k \rangle \sum_{m \neq k} \int_0^{\lambda t} \mathrm{d}s \int_0^{\lambda t} \mathrm{d}s' e^{i\Delta_{km}(s-s')} \langle \tilde{B}_{km}(s) \tilde{B}_{km}(s')^\dagger \rangle_{\rho_O} \\
&= -\frac{1}{\lambda^2} \sum_k \langle \pi_k | \rho_P(\alpha) | \pi_k \rangle \langle \pi_k | M_\beta | \pi_k \rangle \\
&\qquad \cdot \sum_{m \neq k} \frac{1}{\Delta_{km}^2} \Big\{ \langle B_{km} B_{km}^\dagger \rangle_{\rho_O} \\
&\qquad\qquad + \langle e^{itA_k} B_{km} B_{km}^\dagger e^{-itA_k} \rangle_{\rho_O} \\
&\qquad\qquad - e^{i\lambda t \Delta_{km}} \langle e^{itA_k} B_{km} e^{-itA_m} B_{km}^\dagger \rangle_{\rho_O} \\
&\qquad\qquad - e^{i\lambda t \Delta_{mk}} \langle B_{km} e^{itA_m} B_{km}^\dagger e^{-itA_k} \rangle_{\rho_O} \Big\} \\
&\quad + \mathcal{O}(\lambda^{-3}) \; . \qquad (6.110)
\end{aligned}$$

In summary, the probability (6.87) at leading order with respect to the inverse scaling parameter of the probe's energy splitting and the transition matrix elements

is thus given by (cf. Eqs. (6.101), (6.102), (6.107) and (6.110))

$$
\begin{aligned}
p_t(\alpha,\beta) = \sum_{k,l} & \langle \pi_k|\rho_P(\alpha)|\pi_l\rangle \\
& \cdot \Big\{ \langle \pi_l|M_\beta|\pi_k\rangle e^{-i\lambda t\Delta_{kl}} \langle e^{itA_l} e^{-itA_k}\rangle_{\rho_O} \\
& \quad + \frac{1}{\lambda}\Big[\sum_{m\neq k} \langle \pi_l|M_\beta|\pi_m\rangle \frac{1}{\Delta_{mk}} e^{-i\lambda t\Delta_{ml}} \\
& \qquad \cdot \big(\langle e^{itA_l} e^{-itA_m} B_{km}^\dagger\rangle_{\rho_O} - e^{i\lambda t\Delta_{mk}} \langle e^{itA_l} B_{km}^\dagger e^{-itA_k}\rangle_{\rho_O} \big) \\
& \qquad + \sum_{n\neq l} \langle \pi_n|M_\beta|\pi_k\rangle \frac{1}{\Delta_{nl}} e^{i\lambda t\Delta_{nk}} \\
& \qquad\quad \cdot \big(\langle B_{ln} e^{itA_n} e^{-itA_k}\rangle_{\rho_O} - e^{-i\lambda t\Delta_{nl}} \langle e^{itA_l} B_{ln} e^{-itA_k}\rangle_{\rho_O} \big) \Big] \\
& \quad + \frac{1}{\lambda^2}\Big[\tilde{\sum_{m\neq k, n\neq l}} \langle \pi_n|M_\beta|\pi_m\rangle \frac{1}{\Delta_{mk}\Delta_{nl}} \\
& \qquad\quad \cdot \big[e^{i\lambda t\Delta_{nm}} \langle B_{ln} e^{itA_n} e^{-itA_m} B_{km}^\dagger\rangle_{\rho_O} \\
& \qquad\qquad - e^{i\lambda t\Delta_{nk}} \langle e^{itA_l} B_{ln} e^{-itA_m} B_{km}^\dagger\rangle_{\rho_O} \\
& \qquad\qquad - e^{i\lambda t\Delta_{lm}} \langle B_{ln} e^{itA_n} B_{km}^\dagger e^{-itA_k}\rangle_{\rho_O} \\
& \qquad\qquad + e^{i\lambda t\Delta_{lk}} \langle e^{itA_l} B_{ln} B_{km}^\dagger e^{-itA_k}\rangle_{\rho_O} \big] \\
& \qquad - \sum_{m\neq k} \delta_{lk} \langle \pi_k|M_\beta|\pi_k\rangle \frac{1}{\Delta_{mk}^2} \\
& \qquad\quad \cdot \big[\langle B_{km} B_{km}^\dagger\rangle_{\rho_O} \\
& \qquad\qquad + \langle e^{itA_k} B_{km} B_{km}^\dagger e^{-itA_k}\rangle_{\rho_O} \\
& \qquad\qquad - e^{i\lambda t\Delta_{km}} \langle e^{itA_k} B_{km} e^{-itA_m} B_{km}^\dagger\rangle_{\rho_O} \\
& \qquad\qquad - e^{i\lambda t\Delta_{mk}} \langle B_{km} e^{itA_m} B_{km}^\dagger e^{-itA_k}\rangle_{\rho_O} \big] \\
& \quad + \zeta^{(2)}(\lambda) \Big] + \mathcal{O}(\lambda^{-3}) \,, \qquad (6.111)
\end{aligned}
$$

where $\tilde{\sum}_{m\neq k, n\neq l}$ refers to the sum over the indices m and n different from k and l, respectively, if one has $k = l$, whereas one must have $m \neq k, l$ and $n \neq k, l$ in case of unequal indices k and l. The function $\zeta^{(2)}(\lambda)$ contains all further terms in second order in the inverse scaling which, however, do not represent the leading contributions with respect to the transition matrix elements.

It is readily seen that for a two-level probe with eigenenergies $\epsilon_0 = -\epsilon_1 = \epsilon$ in a pure initial state $|\alpha\rangle\langle\alpha|$ and a (nontrivial) projection-valued POVM $\{|\beta\rangle\langle\beta|\}$, Eq. (6.111) is eventually equivalent to expression (6.88) where the functions $\zeta^{(j)}(\lambda)$

and $\xi_k^{(j)}(\lambda)$ are given by

$$\zeta^{(0)}(\lambda) = e^{-i\lambda\epsilon t}\langle e^{itA_1}e^{-itA_0}\rangle_{\rho_O} \ , \tag{6.112}$$

$$\zeta^{(1)}(\lambda) = \langle B\rangle_{\rho_O} - e^{i\lambda\epsilon t}\langle e^{itA_0}Be^{-itA_1}\rangle_{\rho_O} \ , \tag{6.113}$$

$$\xi_0^{(1)}(\lambda) = \langle e^{itA_0}B^\dagger e^{-itA_0}\rangle_{\rho_O} - e^{i\lambda\epsilon t}\langle e^{itA_0}e^{-itA_1}B^\dagger\rangle_{\rho_O} \ , \tag{6.114}$$

$$\xi_1^{(1)}(\lambda) = \langle e^{itA_1}B^\dagger e^{-itA_1}\rangle_{\rho_O} - e^{i\lambda\epsilon t}\langle B^\dagger e^{itA_0}e^{-itA_1}\rangle_{\rho_O} \ , \tag{6.115}$$

$$\begin{aligned}\xi_0^{(2)}(\lambda) = {} & \langle BB^\dagger\rangle_{\rho_O} + \langle e^{itA_0}BB^\dagger e^{-itA_0}\rangle_{\rho_O} \\ & - e^{i\lambda\epsilon t}\langle e^{itA_0}Be^{-itA_1}B^\dagger\rangle_{\rho_O} - e^{-i\lambda\epsilon t}\langle Be^{itA_1}B^\dagger e^{-itA_0}\rangle_{\rho_O} \ ,\end{aligned} \tag{6.116}$$

$$\begin{aligned}\xi_1^{(2)}(\lambda) = {} & \langle B^\dagger B\rangle_{\rho_O} + \langle e^{ittA_1}B^\dagger Be^{-itA_1}\rangle_{\rho_O} \\ & - e^{i\lambda\epsilon t}\langle B^\dagger e^{itA_0}Be^{-itA_1}\rangle_{\rho_O} - e^{-i\lambda\epsilon t}\langle e^{itA_1}B^\dagger e^{-itA_0}B\rangle_{\rho_O} \ .\end{aligned} \tag{6.117}$$

Note that the definitions of $\zeta^{(0)}(\lambda)$, $\xi_0^{(2)}(\lambda)$ and $\xi_1^{(2)}(\lambda)$ given by Pollock *et al.* (2015) are incomplete.

Returning to the general case, one directly recognizes from Eq. (6.111) that the leading order contribution of the probability distribution is again characterized by

$$p_t(\alpha,\beta) \simeq \frac{1}{\lambda^n}\sum_{k,l}\{a_{kl}(t) + b_{kl}(t)\cos(\lambda\Delta_{kl}t + \phi_{kl}(t))\} \ , \tag{6.118}$$

for sufficiently large energy splitting, describing a damped oscillation with respect to the parameter λ as for the case of a two-level probe (see Eq. (6.89)). The time-dependent coefficients $a_{kl}(t)$, $b_{kl}(t)$ and the phase $\phi_{kl}(t)$ then provide information on features of the complex system which may finally be resolved by fitting the measured data. Note that the coefficients in zeroth order with respect to $1/\lambda$ are, for example, found to be given by $a_{kl}(t) = \delta_{k,l}\langle\pi_k|\rho_P(\alpha)|\pi_k\rangle\langle\pi_k|M_\beta|\pi_k\rangle$ along with $b_{kl}(t) = |z(t)|$ and $\phi_{kl}(t) = -\arg(z(t))$ where the complex-valued function $z(t)$ is defined as $z(t) \equiv \langle\pi_k|\rho_P(\alpha)|\pi_l\rangle\langle\pi_l|M_\beta|\pi_k\rangle\langle e^{itA_l}e^{-itA_k}\rangle_{\rho_O}$.

It is worth emphasizing again that the present strategy requires full control over the quantum probe and the coupling to the complex system, similarly to the approach presented in the preceding section (see Sec. 6.3). Apart from being able to prepare arbitrary initial states of the probe for different energy splittings and to perform measurements on the evolved state, one must ensure that the typical energy scale of the probe is sufficiently large in comparison with the energy eigenstates of the complex system that are involved in the interaction in order to obtain the expansion (6.111). Thus, the probe is operated in a regime where only virtual excitations due to the coupling to the bath are possible, leading to small values for the considered probability. While this mode of operation can, in principle, be always fulfilled, it constrains the possible interactions for all practical purposes and, therefore, the set of operators T_k (see Eq. (6.91)) that can be probed. In addition, the strategy is obviously only applicable as long as the perturbative approach is accurate.

As mentioned before, for a pure dephasing dynamics (see, e.g., Sec. 3.3.2), there are no constraints and the leading order approximation of the probability (6.111) yields the exact transition probability, i.e.

$$p_t(\alpha,\beta)\Big|_{\text{deph.}} = \sum_{k,l}\langle\pi_k|\rho_P(\alpha)|\pi_l\rangle\langle\pi_l|M_\beta|\pi_k\rangle e^{-i\lambda t\Delta_{kl}}\langle e^{itA_l}e^{-itA_k}\rangle_{\rho_O} \ . \tag{6.119}$$

In this case one can thus solely extract the dynamics of the so-called *Loschmidt echo* $\langle e^{itA_l}e^{-itA_k}\rangle_{\rho_O}$ (see, e.g., Goussev *et al.* (2012)) by means of this method. A dissipative coupling of the probe to the object is thus required to resolve, e.g., the spectrum as is highlighted in the subsequent section. In fact, one may reveal the superfluid excitations of a Bose-Hubbard model measuring an immersed impurity atom by determining the phases $\phi_{kl}(t)$, whereas the time-dependent coefficients allow to obtain the Bose-Einstein distributions and, thus, the temperature of the condensate as will be illustrated in Sec. 6.4.2.

Extending the present treatment, one may apply it to expand the measurement statistics obtained for multiple, selective measurements on the probe (see Eq. (4.14)). This means that the previously developed treatment is applied to

$$p_n(\beta_n,t_n;\cdots;\beta_1,t_1;\alpha)=\mathrm{Tr}\{\mathfrak{S}_{\Omega_{\beta_n}}\mathfrak{S}_{U(t_n-t_{n-1})}\cdots\mathfrak{S}_{\Omega_{\beta_1}}\mathfrak{S}_{U(t_1)}\rho_P(\alpha)\otimes\rho_O\}\ , \tag{6.120}$$

which represents the joint probability to obtain the sequence of outcomes β_j at times t_j when the POVM $\{M_\beta\otimes\mathbb{1}_O\}$ is measured. Here, Ω_β refers to the Kraus operator associated with the outcome β_k of this POVM and the superoperators $\mathfrak{S}_X$ are defined as $\mathfrak{S}_X\rho=X\rho X^\dagger$ (cf. Eq. (4.14)). For projective measurements, it is, for example, possible to show that all combinations of transition matrix elements are encountered up to 4th order with respect to the inverse energy splitting for a total of 2 measurements. The lengthy proof of this statement has, however, been omitted in the present thesis. Note that the 4th order defines the leading order contribution to the probability corresponding to nonequal outcomes of successive measurements where the initial state of the probe additionally needs to define an eigenstate of the measured observable. There is strong evidence that the mentioned relationship remains true for an arbitrary number of measurements. That is, all combinations of transition matrix elements are contained in terms up to $(2n)$th order in case of n projective measurements, where the $(2n)$th order is eventually addressed for nonequal successive measurement outcomes. A rigorous proof of this conjecture could, however, not be achieved so far which is thus left for future studies.

Finally, it should be clear that the described technique, i.e., the particular Dyson expansion of the unitary propagator may not only be applied to probability distributions such as Eq. (6.120). A possible and interesting application is, for example, given by the resonance fluorescence spectrum. More specifically, the technique may be used to determine signatures of environmental properties in the two-time correlation function $\langle\sigma_+(t)\sigma_-(s)\otimes\mathbb{1}_O\rangle_{\rho_P\otimes\rho_O}$, specifying the resonance fluorescence spectrum of a two-level system that is coupled to an environment. The potential capacity of this application might be an objective of future studies, too.

6.4.2 Probing a superfluid Bose-Hubbard model

In the present section, the previously introduced probing scheme is applied to a one-dimensional Bose-Hubbard model in the superfluid phase in order to determine the frequencies of the Bogoliubov modes that characterize the system. Moreover,

the probing scheme is compared to the strategy suggested by Cosco *et al.* (2015) to extract the Bogoliubov dispersion relation by means of an immersed impurity atom. Obviously, the complex system in this case is described by an infinite-dimensional Hilbert space with a free Hamiltonian that is not upper bounded. Nevertheless, this system can be probed by the introduced strategy as the interaction only concerns neighboring energy levels of the 1D Bose-Hubbard Hamiltonian as will be shown.

Following Cosco *et al.* (2015) who suggested a slightly different kind of probing scheme for the Bogoliubov frequencies (see below), one considers a harmonically trapped impurity atom which is immersed into an ensemble of bosonic atoms and coupled to it by a local contact potential. If the bosonic ensemble is trapped in a one-dimensional lattice and cooled to the lowest Bloch band of the periodic potential, its dynamics is described by the well-known one-dimensional Bose-Hubbard model (Jaksch *et al.*, 1998; Sachdev, 2011)

$$H_{\mathrm{BH}} = -J \sum_{\langle j,k \rangle} \hat{a}_j^\dagger \hat{a}_k + \frac{1}{2} U \sum_j \hat{a}_j^\dagger \hat{a}_j^\dagger \hat{a}_j \hat{a}_j - \mu \sum_j \hat{a}_j^\dagger \hat{a}_j \ , \tag{6.121}$$

where the first sum is restricted to nearest neighbors and $\hat{a}_j^{(\dagger)}$ refers to local bosonic annihilation (creation) operator that are assigned to the lattice site j. Here, μ defines the chemical potential as the cold bosonic gas represents a grand-canonical ensemble. The relation between the hopping constant J and the on-site interaction U characterizes two regimes, differing in the static as well as the dynamical properties. In fact, the relation $J \ll U$ characterizes the Mott insulator phase, whereas the system is in the so-called superfluid phase if $J \gg U$ holds. In the latter case, one may apply the Bogoliubov approximation and transformation in order to diagonalize the Bose-Hubbard Hamiltonian which leads to (see, e.g., van Oosten *et al.* (2001))

$$H_{\mathrm{BH}} = \sum_{k \neq 0} \omega_k \hat{b}_k^\dagger \hat{b}_k \ , \tag{6.122}$$

where $\hbar = 1$ has been employed. Here, the energy of the phononic modes corresponding to the Bogoliubov annihilation (creation) operators $\hat{b}_k^{(\dagger)}$ is given by[24] $\omega_k = \sqrt{\epsilon_k(\epsilon_k + 2Un_0)}$ with the dispersion relation $\epsilon_k = 2J[1 - \cos(ka)]$. Note that a denotes the lattice constant and the sum runs over all k-vectors in the first Brillouin zone different from zero. For an odd[25] number of sites N_S one thus has

$$k \in \left\{ \frac{2\pi}{aN_S} \cdot j \,\middle|\, -(N_S-1)/2 \leq j \in \mathbb{Z} \leq (N_S-1)/2 \right\} \setminus \{0\} \ . \tag{6.123}$$

The density fraction of condensed atoms $n_0 \equiv N_0/N_S$ characterizes the relation between the amount of atoms N_0 in the zero-mode Bose-Einstein condensate and the number of lattice sites.

Assuming a contact potential for the immersed impurity and the cold bosonic system with coupling strength g, the interaction Hamiltonian for an impurity that is strongly localized at a site of the lattice is then shown to be given by (Cosco *et al.*, 2015) (see Appendix L)

$$H_I = g \sum_{\vec{m} \neq \vec{n} \in \mathbb{N}_0^3} \phi_{\vec{m}\vec{n}} |\vec{m}\rangle\langle\vec{n}| \otimes \left[n_0 + \sum_{k \neq 0} \beta_k (\hat{b}_k^\dagger + \hat{b}_k) \right] \ , \tag{6.124}$$

[24] This relation is also known as *Bogoliubov dispersion relation.*

[25] If N_S is even, one obtains $k \in \{(2\pi j)/(aN_S) \,|\, -(N_S/2-1) \leq j \in \mathbb{Z} \leq N_S/2\} \setminus \{0\}$.

where $\{|\vec{n} = (n_1, n_2, n_3)\rangle\}$ denotes the eigenbasis of the free Hamiltonian $H_P = \sum_{\vec{n}\in\mathbb{N}_0^3} \nu_{\vec{n}} |\vec{n}\rangle\langle\vec{n}|$ of the impurity, defining a three-dimensional quantum harmonic oscillator. Here, the effective coupling $\phi_{\vec{m}\vec{n}}$ between the modes and the impurity is determined by the overlap of the Wannier functions, describing the condensate at the different sites, and the impurity wave functions, so that $\phi_{\vec{m}\vec{n}}$ accounts for the exact shape of the probe's trapping potential as well as its location with respect to the lattice (Cosco *et al.*, 2015). In addition, the spectral function[26] is given by $\beta_k = \sqrt{n_0/N_S}\{|u_k| - |v_k|\}$ where $|u_k|$ and $|v_k|$ refer to the modulus of the coefficients of the Bogoliubov transformation which obey (van Oosten *et al.*, 2001)

$$|v_k|^2 = |u_k|^2 - 1 = \frac{1}{2}\Big\{\frac{\epsilon_k + Un_0}{\omega_k} - 1\Big\} , \tag{6.125}$$

and have the same phase (see Appendix L). Note that, placing the impurity between two sites, the effective coupling as well as the spectral function changes as the immersed atom then couples to two sites.

The contact potential thus leads to a dissipative coupling between the motional degrees of freedom of the immersed atom and the Bogoliubov modes, which may offer interesting information about the Bose-Hubbard model in the superfluid phase when using the trapped impurity atom as probe system for the probing strategy introduced in the preceding section. Clearly, the constraint on the energy scales of the probe and the complex system are not satisfied in general as the Bose-Hubbard Hamiltonian (6.122) has an unbounded spectrum. However, due to linearity of the interaction Hamiltonian with respect to the Bogoliubov mode operators, the energy levels influencing the time evolution of the probe are bounded. In fact, for the total Hamiltonian $H = H_P \otimes \mathbb{1}_O + \mathbb{1}_P \otimes H_{\mathrm{BH}} + H_I$ the operators $B_{\vec{m}\vec{n}}$ (cf. Eq. (6.91)) read

$$B_{\vec{m}\vec{n}} = g\phi_{\vec{m}\vec{n}}\Big[n_0 + \sum_{k\neq 0} \beta_k(\hat{b}_k^\dagger + \hat{b}_k)\Big], \tag{6.126}$$

whereas one finds $A_k = H_{\mathrm{BH}}$ for all indices k. It follows that the transition matrix elements of the operators $B_{\vec{m}\vec{n}}$ with respect to the Fock basis $\{|\vec{a}\,\rangle \,|\, a_k \in \mathbb{N}_0,\ k \neq 0\}$, describing the eigenbasis of the Bose-Hubbard Hamiltonian, obey $\langle\vec{a}|B_{\vec{m}\vec{n}}|\vec{b}\,\rangle \neq 0$ if and only if $|\vec{a}\,\rangle = |\vec{b}\,\rangle$ holds or one has

$$a_{k_0} = b_{k_0} \pm 1 , \tag{6.127}$$

for some mode k_0. Hence, the energy differences $|E_a^{(\vec{m})} - E_b^{(\vec{n})}|$, present in the leading order approximations (cf. Eq. (6.103)), are upper bounded by the maximal Bogoliubov frequency ω_k which must then be small compared to the transition frequencies $\Delta\nu_{\vec{m}\vec{n}} \equiv \nu_{\vec{m}} - \nu_{\vec{n}}$ of the impurity in order to apply the probing strategy to this setup. Note that the scaling parameter λ, which corresponds to a variable curvature of the harmonic potential of the impurity, has been absorbed in the energies $\nu_{\vec{m}}$ for convenience.

Now, suppose that the curvature of the potential is sufficiently large so that $\Delta\nu_{\vec{m}\vec{n}} \gg \max_k \omega_k$ holds true for any choice of the oscillator occupation "numbers"

[26] Note that Cosco *et al.* (2015) used an expression for β_k where the minus sign has been replaced by a plus sign which is, however, incorrect (see Appendix L for the derivation of the interaction Hamiltonian in terms of the Bogoliubov modes).

$\vec{m}$ and $\vec{n}$. According to Eq. (6.111), the leading order contribution of the transition probability $p_t(\vec{0},\vec{n})$ from the ground (associated with $\vec{0}$) to the excited state $\vec{n}$ at time t is given by

$$p_t(\vec{0},\vec{n}) = \frac{1}{\Delta\nu_{\vec{n}\vec{0}}^2}\Big[\langle B_{\vec{0}\vec{n}}B_{\vec{0}\vec{n}}^\dagger\rangle_{\rho_O} + \langle e^{itH_{\rm BH}}B_{\vec{0}\vec{n}}B_{\vec{0}\vec{n}}^\dagger e^{-itH_{\rm BH}}\rangle_{\rho_O} - e^{it\Delta\nu_{\vec{n}\vec{0}}}\langle e^{itH_{\rm BH}}B_{\vec{0}\vec{n}}e^{-itH_{\rm BH}}B_{\vec{0}\vec{n}}^\dagger\rangle_{\rho_O} - e^{-it\Delta\nu_{\vec{n}\vec{0}}}\langle B_{\vec{0}\vec{n}}e^{itH_{\rm BH}}B_{\vec{0}\vec{n}}^\dagger e^{-itH_{\rm BH}}\rangle_{\rho_O}\Big] . \quad (6.128)$$

Assuming that ρ_O defines a thermal state at inverse temperature β, i.e. one has $\rho_O = \rho_{\rm th} = e^{-\beta H_{\rm BH}}/{\rm Tr}\{e^{-\beta H_{\rm BH}}\}$, the expectation values may be evaluated explicitly. First, one obviously has $\langle B_{\vec{0}\vec{n}}B_{\vec{0}\vec{n}}^\dagger\rangle_{\rho_{\rm th}} = \langle e^{itH_O}B_{\vec{0}\vec{n}}B_{\vec{0}\vec{n}}^\dagger e^{-itH_O}\rangle_{\rho_{\rm th}}$ which, in addition, is found to be given by

$$\langle B_{\vec{0}\vec{n}}B_{\vec{0}\vec{n}}^\dagger\rangle_{\rho_{\rm th}} = g^2|\phi_{\vec{0}\vec{n}}|^2\Big[n_0^2 + \sum_{k\neq 0}\beta_k^2\{1+2n(\omega_k)\}\Big] , \quad (6.129)$$

employing the commutation relation $[\hat{b}_k,\hat{b}_l^\dagger] = \delta_{k,l}$ and the fact that $\langle\hat{b}_k^{(\dagger)}\rangle_{\rho_{\rm th}} = 0$ holds for any mode k. Here, $n(\omega_k) \equiv \langle\hat{b}_k^\dagger\hat{b}_k\rangle_{\rho_{\rm th}} = 1/(\exp[\beta\omega_k]-1)$ denotes the Bose-Einstein distribution of the kth mode at inverse temperature β.

The two remaining expectation values in Eq. (6.128) are related by complex conjugation and one deduces for the third term

$$\begin{aligned}&\langle e^{itH_{\rm BH}}B_{\vec{0}\vec{n}}e^{-itH_{\rm BH}}B_{\vec{0}\vec{n}}^\dagger\rangle_{\rho_{\rm th}}\\ &= g^2|\phi_{\vec{0}\vec{n}}|^2\Big[n_0^2 + \sum_k\beta_k^2\Big\{2\cos(\omega_k t)n(\omega_k) + e^{-i\omega_k t}\Big\}\Big] ,\end{aligned} \quad (6.130)$$

as one finds $e^{itH_{\rm BH}}\hat{b}_k e^{-itH_{\rm BH}} = e^{-i\omega_k t}\hat{b}_k$. Due to this, the sum of the two last contributions to Eq. (6.128) can be written as

$$\begin{aligned}&e^{it\Delta\nu_{\vec{n}\vec{0}}}\langle e^{itH_{\rm BH}}B_{\vec{0}\vec{n}}e^{-itH_{\rm BH}}B_{\vec{0}\vec{n}}^\dagger\rangle_{\rho_{\rm th}} + e^{-it\Delta\nu_{\vec{n}\vec{0}}}\langle B_{\vec{0}\vec{n}}e^{itH_{\rm BH}}B_{\vec{0}\vec{n}}^\dagger e^{-itH_{\rm BH}}\rangle_{\rho_{\rm th}}\\ &= -g^2|\phi_{\vec{0}\vec{n}}|^2\Big[n_0^2 2\cos(\Delta\nu_{\vec{n}\vec{0}}t) + \sum_k\beta_k^2\{4n(\omega_k)\cos(\omega_k t)\cos(\Delta\nu_{\vec{n}\vec{0}}t)\\ &\qquad + 2\cos((\Delta\nu_{\vec{n}\vec{0}}-\omega_k)t)\}\Big] .\end{aligned} \quad (6.131)$$

And using the relation $\cos(\alpha+\beta) = \cos(\alpha)\cos(\beta) - \sin(\alpha)\sin(\beta)$ one deduces

$$\begin{aligned}&4n(\omega_k)\{1-\cos(\omega_k t)\cos(\Delta\nu_{\vec{n}\vec{0}}t)\}\\ &= 2n(\omega_k)\Big\{[1-\cos((\Delta\nu_{\vec{n}\vec{0}}-\omega_k)t)] + [1-\cos((\Delta\nu_{\vec{n}\vec{0}}+\omega_k)t)]\Big\} ,\end{aligned} \quad (6.132)$$

by means of which the following expression for the transition probability (6.111) in leading order is finally obtained:

$$p_t(\vec{0},\vec{n}) = g^2|\phi_{\vec{0}\vec{n}}|^2\Big\{n_0^2\lambda(\Delta\nu_{\vec{n}\vec{0}},t) + \sum_k(\tilde{\Gamma}_k^+(\Delta\nu_{\vec{n}\vec{0}},t) + \tilde{\Gamma}_k^-(\Delta\nu_{\vec{n}\vec{0}},t))\Big\} , \quad (6.133)$$

where $\lambda(\omega,t) \equiv 2\{1-\cos(\omega t)\}/\omega^2$ and one defines

$$\Gamma_k^{\pm}(\omega,t) = \mu_k^{\pm}(\omega)^2\beta_k^2\,\lambda(\omega\pm\omega_k,t)\cdot\tfrac{1}{2}\{1\pm 1+2n(\omega_k)\}\ , \tag{6.134}$$

with $\mu_k^{\pm}(\omega) = (\omega\pm\omega_k)/\omega$.

One directly observes that the transition probability (6.133) defines the high probe transition frequency approximation of the result given by Cosco *et al.* (2015). This is readily understood as, contrary to the previous approach, the probing scheme of Cosco *et al.* (2015) relies on observing resonances in the transition probability of the impurity atom when the associated transition frequency matches that of a Bogoliubov mode. More specifically, the authors deduced for the transition probability at time t and at first order with respect to the weak coupling expansion of the unitary propagator (cf. Eqs. (6) and (7) in the work by Cosco *et al.* (2015))

$$\tilde{p}_t(\vec{0},\vec{n}) = g^2|\phi_{\vec{0}\vec{n}}|^2\left\{n_0^2\lambda(\Delta\nu_{\vec{n}\vec{0}},t)+\sum_k\big(\tilde{\Gamma}_k^{+}(\Delta\nu_{\vec{n}\vec{0}},t)+\tilde{\Gamma}_k^{-}(\Delta\nu_{\vec{n}\vec{0}},t)\big)\right\}\ , \tag{6.135}$$

where one has

$$\tilde{\Gamma}_k^{+}(\omega,t) = \beta_k^2\lambda(\omega+\omega_k,t)\{1+n(\omega_k)\}\ , \tag{6.136}$$

$$\tilde{\Gamma}_k^{-}(\omega,t) = \beta_k^2\tilde{\lambda}(\omega-\omega_k,t)n(\omega_k)\ , \tag{6.137}$$

and

$$\tilde{\lambda}(\omega-\nu,t) = \begin{cases}\lambda(\omega-\nu,t)\ , & \text{if } \omega\neq\nu\\ t^2\ , & \text{if } \omega=\nu\ .\end{cases} \tag{6.138}$$

Clearly, approximating $\Delta\nu_{\vec{n}\vec{0}}\pm\omega_k$ as

$$\Delta\nu_{\vec{n}\vec{0}}\pm\omega_k \approx \Delta\nu_{\vec{n}\vec{0}}\ , \tag{6.139}$$

if $\Delta\nu_{\vec{n}\vec{0}} \gg \omega_k$ holds true for all k, one has $\tilde{\Gamma}_k^{\pm}(\Delta\nu_{\vec{n}\vec{0}},t) \approx \Gamma_k^{\pm}(\Delta\nu_{\vec{n}\vec{0}},t)$ showing the relation between Eqs. (6.133) and (6.135). Contrary to the probability studied by Cosco *et al.* (2015), the transition probability (6.133) associated with the previous probing scheme clearly relies on virtual excitations of the impurity's motional degrees, thus leading to small values for the transition probability $p_t(\vec{0},\vec{n})$ (cf. Fig. 6.7).

To illustrate the probing scheme explicitly, one may, for example, consider the transition between the oscillator ground state and an excited state that is characterized by a single nonzero quantum number n_j corresponding to a direction x_j orthogonal to the optical lattice with frequency $\nu^{(j)}$. Henceforth, the excited state shall be simply abbreviated by the nonzero occupation number n_j. According to Cosco *et al.* (2015) the effective coupling $\phi_{\vec{0}n_j}$ for this configuration is given by

$$|\phi_{\vec{0}n_j}|^2 = g_{n_j}\nu^{(j)}\ , \tag{6.140}$$

where the constant term g_{n_j} depends on the spatial overlap of the impurity's wave functions for the different quantum numbers and the Wannier functions at the site at which the probe is localized. Changing the curvature of the trapping potential along the direction x_j thus alters the effective coupling, too. However, as kth

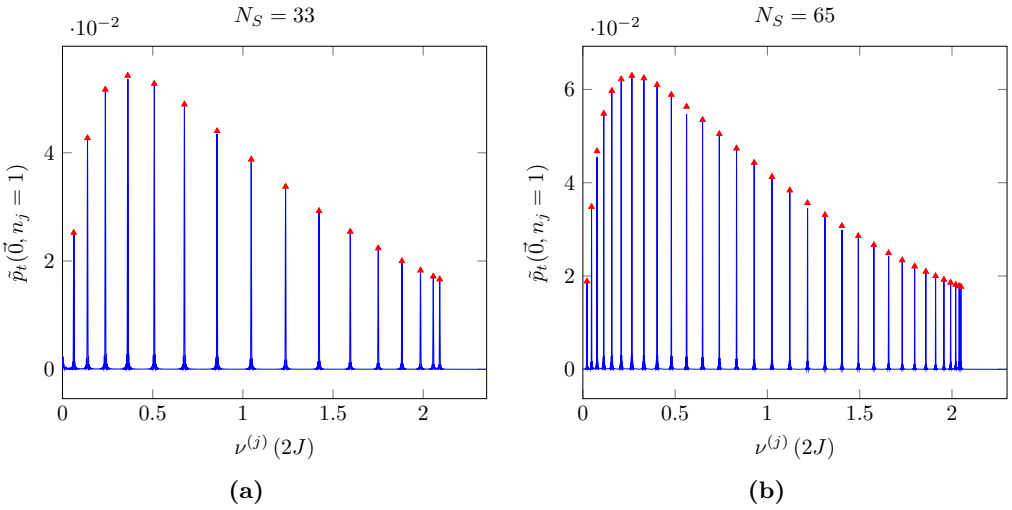

Figure 6.6 – The transition probability $\tilde{p}_t(\vec{0}, n_j = 1)$ (cf. Eq. (6.135)) as a function of the trap frequency $\nu^{(j)}$ (in units of $2J$) for $N_0 = 65$ atoms in the condensate in a lattice with $N_S = 33$ **(a)** and $N_S = 65$ **(b)** sites. The choice of the other parameters corresponds to that of Cosco *et al.* (2015). That is, one has $J/U = 10$ with $U = 8.5$, $\beta^{-1} = 1\text{nK}$ and a final time t obeying $g_{n_j} t = 0.15/n_0$ where one has $g_{n_j} = 10^{-3} U$ (Cosco, 2016). The red triangles depict the approximation (6.141) of the transition probability at resonance. Note that the nonmonotonic behavior of the peak's magnitude as a function of the frequency follows from the competition between the spectral density β_k^2 and the Bose-Einstein distribution $n(\omega_k)$. While the latter is a decreasing function of the frequency, the former is enhanced for modes at the boundary of the Brillouin zone (cf. Fig. 2 in the work by Cosco *et al.* (2015) which, however, looks different due to the missing minus sign in the definition of β_k – see Eq. (6.124)).

order terms in the power expansion (6.111) are proportional to the kth power of the effective coupling, this solely results in a reduction of the power of the inverse energy splitting for all contributions in the power series. Due to this, the probing scheme indicated before may still be applied to this configuration.

It is worth stressing that the constraints imposed on the number of condensate atoms in the zero-mode must yet be satisfied when evaluating the probabilities (6.133) and (6.135) explicitly. That is, to apply the Bogoliubov approximation, one must have $N_0 \gg 1$ (see Appendix L). As the interaction H_I (cf. Eq. (6.124)) is proportional to the density fraction of the condensate atoms n_0, the magnitude of the contributions in the power expansion is scaled up if the lattice comprises only a few sites for a constant number of atoms in the zero-mode. To determine the leading order contribution experimentally, the energy splitting must be varied over values that are sufficiently large in comparison with n_0. This practically limits the use of the probing strategy to rather large lattices as the confinement of the impurity cannot be reduced arbitrarily. Note that the same conclusion can be drawn for the probing scheme for the superfluid excitations in the Bose-Hubbard model introduced by Cosco *et al.* (2015): The larger the density fraction of the condensate the stronger the interaction is, limiting the validity of the weak coupling approximation which has been used to deduce Eq. (6.135) to extremely

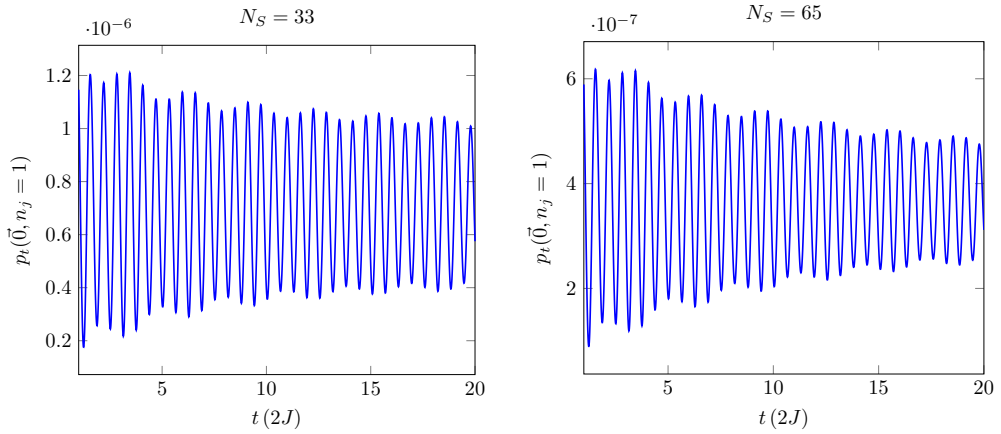

Figure 6.7 – The leading order contribution of the transition probability $p_t(\vec{0}, n_j = 1)$ (cf. Eq. (6.133)) as a function of time (in units of $2J$) at an energy splitting $\nu^{(j)} = 10 \cdot 2J$ for $N_0 = 65$ atoms in the condensate and lattices with $N_S = 33$ **(a)** and $N_S = 65$ **(b)** sites. The other parameters are chosen as in Fig. 6.6 .

short interaction times. Thus, possible limitations on the temporal resolution and control of the impurity-gas coupling then restrict the use of the approach by Cosco *et al.* (2015) to large lattices, too.

Figure 6.6 shows the transition probability $\tilde{p}_t(\vec{0}, n_j)$ (cf. Eq. (6.135)) from the vacuum to the excited state characterized by $n_j = 1$ as functions of the transition frequency $\nu^{(j)}$ (in units of $2J$). One clearly observes the enhancement for a transition to the excited state when the confinement of the trap matches a Bogoliubov mode for either length of lattices and a condensate of 65 atoms. For sufficiently large interaction times and a small density fractions, the transition probability $\tilde{p}_t(\vec{0}, n_j = 1)$ at resonance, i.e. for $\nu^{(j)} = \omega_k$ for some mode k, can be well approximated by

$$\tilde{p}_t(\vec{0}, n_j) \simeq 2(g_{n_j}\beta_k t)^2 n(\omega_k)\nu^{(j)} \ , \tag{6.141}$$

as shown by the red triangles in Figs. 6.6 **(a)** and **(b)** for the chosen configuration (cf. Cosco *et al.* (2015)). It is worth emphasizing that the peaks are extremely narrow (of the order of 10^{-3}) so that their detection as suggested in the probing scheme of Cosco *et al.* (2015) is experimentally challenging.

Instead of scanning the Bogoliubov modes directly, one may use the probing strategy developed before and determine the frequencies of the superfluid excitations in the Bose-Hubbard model by means of a Fourier analysis of the leading order contribution of $p_t(\vec{0}, n_j)$ which is shown for $n_j = 1$ as a function of time in Fig. 6.7. Clearly, from the Fourier coefficients one may also determine the Bose-Einstein distribution and, finally, the temperature of the cold gas by a fit of the exact expression (6.133) to the coefficients. As one can readily see from Fig. 6.7, the transition probability $p_t(\vec{0}, n_j)$ is quite small (of the order of 10^{-6}) for frequencies $\nu^{(j)}$ that are large compared to the Bogoliubov mode. In addition, the beat frequency of the leading order contribution is very light, thus requiring a

precise determination of the transition probability over a large interval of time in order to determine the Bogoliubov frequencies by means of a Fourier transform. Nonetheless, this seems to be feasible so that the present example illustrates the use of the discussed probing strategy for infinite-dimensional systems and dissipative couplings.

Chapter 7

Summary and conclusion

The present thesis has reviewed several recently discussed questions underlying the theory of open quantum systems, such as the role of initial system-environment correlations, the essence of memory effects in the quantum regime as well as their occurrence due to correlated environments, and the information content of open quantum systems regarding properties of the environment.

After an introduction of the basic notions used in the theory of open quantum systems such as dynamical maps and master equations, providing also an exhaustive and convenient characterization of the exactness of second order time-convolutionless master equations for zero-mean Gaussian environmental states and linear couplings, the detection of initial system-environment correlations by means of open system dynamics was addressed. Previous studies have shown that such correlations induce an information flow quantified by an increase of the trace distance of two evolving open systems states above its initial value. This effect essentially relies on the contractivity of the distance measure with respect to completely positive and trace-preserving linear maps which is, however, not only satisfied by the trace distance. Motivated by this fact, an extended comparative study, based on two exactly solvable models and initial states with tunable amount of correlations, of different distance measures on the state space has been performed in this thesis which indeed brought out a special role of the trace distance, being most sensitive to initial correlations.

Moreover, for the transfer of the well-established theory of Markovian stochastic processes to the quantum domain, which cannot be straightforwardly formulated by simply adapting the classical constraints on the conditional probabilities of the process due to the particular role of measurements in quantum theory, the trace distance was shown to be useful to describe memory effects in a physically and experimentally motivated, intuitive way. Assigning quantum non-Markovianity to a nonmonotonic behavior of the trace distance between pairs of states, memory effects may be interpreted as a backflow of information which has been previously lost, meaning that it was no longer locally accessible on the open system only. The result on the maximization contained in the associated quantifier measuring the degree of non-Markovianity has been reviewed along with the measure's local representation for finite open quantum systems that highlights the universality and locality of quantum non-Markovian behavior assigned to an information backflow in the quantum state space. The functioning and use of this representation has been demonstrated by means of an all-optical experiment where the measurement

strategy along with the data analysis and representation was developed as a part of this thesis. In fact, the photonic experiment has nicely shown that the degree of non-Markovianity can be efficiently obtained in an arbitrary neighborhood of any fixed inner state, that its determination solely requires a maximization over a single input state, and that those quantum states which feature a maximal backflow of information can just as well be represented by mixed states.

A fruitful extension of the trace-distance-based approach of quantum non-Markovianity is obtained in this thesis by defining memory effects with respect to the nonmonotonic dynamics of the trace norm of Helstrom matrices. It has been shown that this definition combines an interpretation in terms of an information flux and a clear-cut connection to classical Markov processes on the level of the rate equations for 1-point probabilities. Indeed, the extended approach leads to a definition of quantum Markovianity that has been proven to be equivalent to P-divisibility which finally ensures that the jump process associated with the eigenvalues of an evolving open system state is characterized by a Pauli master equation of a classical Markov process. For dynamical processes that have the maximally mixed state in their image, P-divisibility has, in addition, be shown to be not only sufficient but also necessary to warrant the connection of any rate equation obtained from a quantum master equation to a classical Markov process. This result mainly follows from an obtained characterization of the eigenbases of states defining a convex set. It is worth noticing that the generalized approach may also be applied when the notion of divisibility is ill defined.

Besides having the interpretation and the experimental feasibility in common with the trace-distance-based approach, the statements about optimal states, featuring a maximal backflow of information, and a local representation could be shown to hold true for the generalized measure, too. As a result, the analytical, numerical and experimental determination of the extended definition is drastically simplified. Moreover, it proves locality and universality of quantum non-Markovianity defined via the generalized criterion. Despite these nice features, the generalized approach does not reconcile with the other definitions of quantum Markovianity. The persisting difference with those approaches that are based on CP-divisibility has been highlighted by means of a particular model for two-level systems. Similarly, a paradigmatic model has been used to illustrate the essential feature of the generalized definition in comparison with the original definition, that is, the sensitivity to memory effects arising from uniform translations of the state space.

Addressing the mathematical structure of the space of non-Markovian quantum dynamical maps, it has been shown in the present thesis that the set of Markovian processes is not convex. In fact, a non-P-divisible dynamics has been obtained by mixing two particular CP-divisible processes. In conjunction with the recent results, obtained by other researchers, that the set of non-Markovian processes is neither convex and, within the set of Markovian dynamics, the mixing of CP-divisible processes can result in a process that is solely P-divisible, this provides far reaching advances in the understanding of the mathematical structure of the set of dynamical processes. To complete the picture, it remains, however, for future studies to consider the results of a mixing of P-divisible processes which finally uncovers the full structure of the sets of Markovian and non-Markovian dynamics.

This study may also lead to a complete understanding of non-Markovianity in the quantum domain and, therefore, the physical and mathematical causes of memory effects. Eventually, this might culminate in a complete theory of non-Markovian quantum dynamics providing, e.g., necessary and sufficient conditions for time-local master equations to yield a completely positive dynamics.

Apart from structured or finite reservoirs, low temperatures, and long-lasting, nonnegligible system-environment correlations, an initially correlated environment provides a particular source of memory effects which, in addition, typically leads to the counterintuitive phenomenon that enlarging a system turns the dynamics from being Markovian to non-Markovian, contrary to the standard situation. The role of entanglement for this phenomenon has been investigated in this thesis for a model of two qubits that are locally coupled to an environment being described by two-mode Gaussian states, leading to a pure dephasing dynamics which can be solved exactly even in the presence of a continuum of modes with an ohmic spectral density. For appropriately chosen subsequent local interactions (short with respect to the environmental correlation time), strong revivals of a nonlocal coherence factor, corresponding to the renascence of entanglement of a Bell state, have surprisingly been observed for separable as well as entangled Gaussian states that are characterized by correlation coefficients of the canonical operators with unit magnitude. Thus, entanglement in the environment is not the only source for such nonlocal memory effects.

While the requirement of a short interaction length has been shown to result from the detrimental effect of the free evolution of the bosonic baths, the constraint on the environmental state's correlation coefficient has been explained by means of a general pure dephasing dynamics with Gaussian states of the environment, from which a necessary and sufficient condition for the occurrence of nonlocal memory effects in terms of the magnitude of the correlation coefficient associated with the environmental coupling operators has been deduced. To deepen the study of nonlocal memory effects, it has been examined, besides the evolution of correlations between the different subsystems, whether or not they can effectively be observed with finite-dimensional environments in a maximally entangled state. As a consequence of the thus-obtained conditions on the local unitaries, each of the two quantum systems constituting the bipartite environment must at least be three-dimensional in order to find nonlocal memory effects for maximally entangled environments. A reasoning for the impossibility of two-level systems for the environments along with a systematic solution and analysis of the constraints is, however, still missing and remains an interesting task for future studies.

Due to the dependence of nonlocal memory effects for bosonic environments on the strength of correlations within the environment, it also provides an example for information on a complex system that can be obtained from the dynamics of another quantum system. In the last part of the present thesis, the possibilities and methods on information extraction about a quantum system by means of observing a second system that is coupled to it has been considered in general terms using different approaches. Inspired by the concept of premeasurements developed within the theory of quantum measurements, one approach to this question has been to compare probability distributions associated with observables on the probe and the object system. While for target observables on the object defining

constants of motion, such that a proper joint probability distribution with correct marginals exists, entropic quantifiers such as the conditional entropy and the mutual information may be used to determine how correlated the two distributions are, one needs tools for the general case allowing to compare the probability distributions directly. The Wasserstein distance has been shown to provide, e.g., a means to do this which has eventually been used for a first study of the fragility of a premeasurement of an observable on a finite-dimensional Hilbert space against imperfections. The revealed behavior of the distance as a function of imperfect state preparations and of perturbations of a perfectly correlating unitary dynamics deserves further studies in the future. Similarly, an interesting problem is given by the quest for a strict relation between the amount of information that is gained by measuring the probe system and the thus-induced disturbance on the object. Such an information-disturbance relation would provide an instance of Heisenberg's intuition on a quantum mechanical uncertainty principle. Several known tradeoff relations have been shown to be not applicable to the considered setup of an indirect measurement so that this interesting task is left for future studies.

Besides considering a single measurement, the information gain due to the dynamics of a probe system has also been considered on the basis of two general approaches. On the one hand, it has been shown how a pure dephasing dynamics of an open quantum system that is equivalent to a harmonic oscillator carries information on constants of motion of a finite-dimensional quantum object in the spirit of ergodic stationary stochastic processes. That is, the time-averaged expectation value of an observable linear in the canonical observables converges to the expectation value of a sought object observable for an appropriately adjusted interaction. On the other hand, for a dissipative coupling, it has been shown how information on an object system can be obtained from the time-dependent measurement statistics of a quantum probe having a variable energy splitting. In the limit of an off-resonant energy splitting, the probability distribution can be expanded in a power series of the inverse scaling of the energy splitting where each order provides some information on the object. As the leading terms are unambiguously determined and addressed by the preparation of the probe state and the applied measurement, different properties of the quantum object may then be inferred by post-processing the measurement statistics obtained for various values of the energy splitting. The prospects of this strategy, which may also be further extended to multiple selective measurements, have been illustrated by determining the superfluid excitations in the Bose-Hubbard model using a harmonically trapped impurity atom.

These two general approaches provide a first hint on the potential of such probing strategies, but a more systematic study needs to be done in the future in order to fully reveal their capabilities and limitations, finally establishing a new kind of sensors for complex quantum systems.

Appendix A

The symplectic group

In the present chapter it is shown that the set of symplectic matrices $\mathrm{Sp}(2n,\mathbb{R}) = \{S_n \in \mathcal{M}_{2n}(\mathbb{R}) | S_n \Omega_n S_n^T = \Omega_n\}$ defines a group with respect to ordinary matrix multiplication which, in addition, is closed under transposition. As $\mathrm{Sp}(2n,\mathbb{R})$ represents a subgroup of the set of invertible matrices $GL(2n,\mathbb{R})$ it also defines a Lie group, equipped with the standard Lie bracket $[A, A'] = AA' - A'A$, where the corresponding Lie algebra $\mathfrak{sp}(2n,\mathbb{R})$ is given by matrices satisfying $A\Omega_n + \Omega_n A^T = 0$. Note that the defining property for elements of the Lie algebra is equivalent to $\Omega_n A + A^T \Omega_n = 0$ as one has $\Omega_n^{-1} = -\Omega_n = \Omega_n^T$, and the exponential map, relating the Lie algebra to the Lie group, is given by the ordinary matrix exponential provided the element is sufficiently close to unity (Dragt, 2005).

Recall that a real $2n \times 2n$-matrix S is called symplectic if and only if

$$S\Omega_n S^T = \Omega_n \tag{A.1}$$

holds where $\Omega_n = \bigoplus_{j=1}^{n} \omega$ and $\omega = \left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$ (cf. Eq. (2.95)). To show the group property, one first recognizes that the neutral element of the matrix multiplication, i.e. $\mathbb{1}_{2n} = \mathrm{diag}(1, \ldots, 1)$ trivially satisfies (A.1) and for two symplectic matrices $S, R \in \mathrm{Sp}(2n,\mathbb{R})$ one finds

$$SR\Omega_n (SR)^T = SR\Omega_n R^T S^T = S\Omega_n S^T = \Omega_n \ . \tag{A.2}$$

Hence, $SR \in \mathrm{Sp}(2n,\mathbb{R})$ so that the set of symplectic matrices $\mathrm{Sp}(2n,\mathbb{R})$ is closed under matrix multiplication which is obviously associative. To complete the proof that $\mathrm{Sp}(2n,\mathbb{R})$ defines a group, it remains to show that any symplectic matrix is invertible with an inverse that is symplectic, too. For an element $S \in \mathrm{Sp}(2n,\mathbb{R})$ one considers

$$R \equiv \Omega_n S^T \Omega_n^T \ , \tag{A.3}$$

which obeys

$$SR = S\Omega_n S^T \Omega_n^T = \Omega_n \Omega_n^T = \mathbb{1}_{2n} \ , \tag{A.4}$$

and, therefore, defines the right inverse of the $2n \times 2n$-matrix S. However, the existence of left and right inverse goes hand in hand for square matrices as there are no one-sided inverses for square matrices. One concludes that $R = S^{-1}$ defines the unique inverse of S which is also symplectic since one deduces

$$R\Omega_n R^T = R\Omega_n(\Omega_n S \Omega_n^T) = -RS\Omega_n^T = -\Omega_n^T = \Omega_n \ , \tag{A.5}$$

which completes the proof that $\mathrm{Sp}(2n,\mathbb{R})$ defines a group.

Moreover, the symplectic group $\mathrm{Sp}(2n,\mathbb{R})$ is closed with respect to matrix transposition, i.e., one has $S \in \mathrm{Sp}(2n,\mathbb{R})$ if and only if $S^T \in \mathrm{Sp}(2n,\mathbb{R})$. In fact, given $S \in \mathrm{Sp}(2n,\mathbb{R})$ one finds

$$S^T\Omega_n(S^T)^T = -\Omega_n^2 S^T\Omega_n S = \Omega_n R S = \Omega_n \ , \tag{A.6}$$

so that $S^T \in \mathrm{Sp}(2n,\mathbb{R})$ and the same applies for the converse. Note that the symplectic group can thus be defined via the equation $S^T\Omega_n S = \Omega_n$, too.

Before turning to the associated Lie algebra, it is shown that symplectic matrices are unimodular, i.e., one has $\det(S) = +1$ for any $S \in \mathrm{Sp}(2n,\mathbb{R})$. Clearly, it follows from the symplectic property (A.1) that $\det(S) = \pm 1$ holds since $\det(\Omega_n) = 1$ and the determinant is multiplicative and invariant under matrix transposition. To exclude the case $\det(S) = -1$, one considers the Pfaffian

$$\mathrm{pf}(A)^2 = \det(A) \ , \tag{A.7}$$

that is defined for skew-symmetric matrices. By definition, it describes the square root of the polynomial representing the determinant of the concerned matrix. Note that the eigenvalues of skew-symmetric matrices come in pairs $\pm\lambda$ as A and A^T are similar. It follows that the determinant and, thus, the Pfaffian of any odd-dimensional skew-symmetric matrix vanishes as such a matrix must necessarily have at least one zero eigenvalue. Another intriguing property of the Pfaffian is given by the relation

$$\mathrm{pf}(BAB^T) = \det(B)\mathrm{pf}(A) \ , \tag{A.8}$$

for any $B \in \mathcal{M}_{2n}(\mathbb{R})$ where A denotes a skew-symmetric $2n \times 2n$-matrix. Applying this to the skew-symmetric matrix Ω_n and elements of the symplectic group $S \in \mathrm{Sp}(2n,\mathbb{R})$, one obtains

$$\mathrm{pf}(\Omega_n) = \mathrm{pf}(S\Omega_n S^T) = \det(S)\mathrm{pf}(\Omega_n) \ , \tag{A.9}$$

which is equivalent to $\det(S) = +1$ as one has $\mathrm{pf}(\Omega_n)^2 = \det(\Omega_n) = +1$.

To conclude the study on the symplectic group, one shows that the Lie algebra $\mathfrak{sp}(2n,\mathbb{R})$ associated with it is indeed defined by

$$\mathfrak{sp}(2n,\mathbb{R}) = \{A \in GL(2n,\mathbb{R}) \,|\, A\Omega_n + \Omega_n A^T = 0\} \ . \tag{A.10}$$

First, differentiating $\gamma(t)\Omega_n\gamma(t)^T$ at $t = 0$ where $\gamma(t) = \exp[At]$ represents a differentiable path for some $A \in \mathfrak{sp}(2n,\mathbb{R})$ satisfying $\gamma(0) = \mathbb{1}_{2n}$, one finds

$$\frac{\mathrm{d}}{\mathrm{d}t}\gamma(t)\Omega_n\gamma(t)^T\Big|_{t=0} = A\Omega_n + \Omega_n A^T \ . \tag{A.11}$$

Hence, the requirement $\gamma(t)\Omega_n\gamma(t)^T = \Omega_n$ implies $A\Omega_n + \Omega_n A^T = 0$. To show the converse, assume that a $2n \times 2n$-matrix A satisfies $A\Omega_n + \Omega_n A^T = 0$. Then, one

deduces

$$\begin{aligned}\exp[At]\Omega_n &= \Big(\mathbb{1}_{2n} + \sum_{k=0}^{\infty} \frac{t^k}{k!} A^k\Big)\Omega_n \\ &= \Omega_n + \sum_{k=1}^{\infty} \frac{t^k}{k!} A^{k-1}(-\Omega_n)A^T \\ &\vdots \\ &= \Omega_n + \sum_{k=1}^{\infty} \frac{(-t)^k}{k!} \Omega_n {A^T}^k = \Omega_n \exp[-A^T t] \ , \end{aligned} \tag{A.12}$$

which is equivalent to the defining property of the symplectic group and, thus, completes the proof. Note that any symmetric $2n \times 2n$-matrix R determines an element in $\mathfrak{sp}(2n, \mathbb{R})$ by means of $\Omega_n R$ or $R\Omega_n$ as one easily shows. Such a matrix is called Hamiltonian matrix (Dragt, 2005).

As indicated previously, any symplectic matrix S that is sufficiently close to unity can indeed be written as $\exp[A]$ for some unique element $A \in \mathfrak{sp}(2n, \mathbb{R})$ (Dragt, 2005). As a matter of fact, the matrix exponential is not surjective, but two factors suffice. That is, any symplectic matrix S can be written as $S = \exp[A]\exp[A']$ for two elements $A, A' \in \mathfrak{sp}(2n, \mathbb{R})$ due to the polar decomposition of the real symplectic group (Arvind *et al.*, 1995).

Appendix B

Uncertainty relation for covariance matrices

Here, the necessary and sufficient condition (cf. Eq. (2.106))

$$\boldsymbol{\sigma}_{\hat{X},\rho} + \frac{i}{2}\Omega_n \geq 0 \tag{B.1}$$

on the covariance matrix of the canonical operators for an n-mode continuous variable state ρ is derived. Starting from Schrödinger's uncertainty relation (see, e.g., Griffiths (2004)), any pair of operators satisfies

$$\langle\langle\hat{A}\rangle\rangle_\rho\langle\langle\hat{B}\rangle\rangle_\rho \geq \left|\frac{1}{2}\langle\{\hat{A},\hat{B}\}\rangle_\rho - \langle\hat{A}\rangle_\rho\langle\hat{B}\rangle_\rho\right|^2 + \left|\frac{1}{2i}\langle[\hat{A},\hat{B}]\rangle_\rho\right|^2 , \tag{B.2}$$

which for position and momentum operators reads

$$\langle\langle\hat{q}\rangle\rangle_\rho\langle\langle\hat{p}\rangle\rangle_\rho \geq \left|\frac{1}{2}\langle\{\hat{q},\hat{p}\}\rangle_\rho - \langle\hat{q}\rangle_\rho\langle\hat{p}\rangle_\rho\right|^2 + \frac{1}{4} . \tag{B.3}$$

Furthermore, as the anticommutator $\{\hat{q},\hat{p}\}$ is Hermitian, this can be conveniently written as

$$\det\boldsymbol{\sigma}_{\hat{X},\rho} \geq \frac{1}{4} , \tag{B.4}$$

where $\boldsymbol{\sigma}_{\hat{X},\rho}$ refers to the single mode covariance matrix whose positivity[1] directly follows from (B.4). Clearly, the well-known Heisenberg uncertainty principle, i.e., $\langle\langle\hat{q}\rangle\rangle_\rho\langle\langle\hat{p}\rangle\rangle_\rho \geq \frac{1}{4}$ is a simple consequence of this relation that actually characterizes the covariance matrix completely. This means that any 2×2-matrix satisfying condition (B.4) is physically realizable as the covariance matrix of a state $\rho \in \mathcal{S}\big(L^2(\mathbb{R})\big)$. As symplectic matrices are unimodular[2], condition (B.4) is furthermore invariant under symplectic transformations[3] so that it can be transformed

[1] As the covariance matrix is symmetric, it is diagonalizable and, therefore, the determinant is the product of the eigenvalues. It then follows from Eq. (B.4) that the eigenvalues must have the same sign. However, as the diagonal entries of the covariance matrix defining the variances are positive, one concludes that eigenvalues are indeed positive.

[2] In fact, the determinant of any element of the symplectic group is $+1$ (see Appendix A).

[3] Note that the symplectic transformation of the covariance matrix $S\boldsymbol{\sigma}_{\hat{X},\rho}S^T = \boldsymbol{\sigma}_{S\hat{X},\rho}$ amounts to the transformation $\rho(S) = U_S\rho U_S^\dagger$ of an arbitrary state by the unitary representative U_S corresponding to $S \in \mathrm{Sp}(2n,\mathbb{R})$. That is, one has $\boldsymbol{\sigma}_{\hat{X},\rho(S)} = \boldsymbol{\sigma}_{S\hat{X},\rho}$.

into $\det(\mathrm{diag}(\kappa,\kappa)) \geq \frac{1}{4}$ by applying Williamson's theorem (2.100) to the real symmetric and positive covariance matrix. Obviously, this is equivalent to

$$\kappa \geq \frac{1}{2} \,, \tag{B.5}$$

since the symplectic eigenvalues are strictly positive by definition.

If Williamson's theorem is in turn used for the covariance matrix of an n-mode continuous variable system, one recognizes that this yields uncoupled pairs of canonical operators. Hence, the general n-mode case reduces simply to n copies of the single mode example. A real symmetric and positive square matrix $V \in \mathcal{M}_{2n}(\mathbb{R})$ is thus a bona fide covariance matrix if and only if all of its symplectic eigenvalues satisfy

$$\kappa_j \geq \frac{1}{2} \,, \quad (1 \leq j \leq n) \tag{B.6}$$

As the eigenvalues of the matrix $\mathrm{diag}(\kappa_1,\kappa_1,\ldots,\kappa_n,\kappa_n) + (i/2)\Omega_n$ are given by $\kappa_j \pm \frac{1}{2}$ for all j, one rewrites condition (B.6) as $\mathrm{diag}(\kappa_1,\kappa_1,\ldots,\kappa_n,\kappa_n) + (i/2)\Omega_n \geq 0$. Finally, even though symplectic transformations do not represent similarity transformations in general, they preserve positivity of the concerned matrix because they are nonsingular (Simon *et al.*, 1994). Any real symmetric $2n \times 2n$-matrix V is thus a bona fide covariance matrix for an n-mode quantum system if and only if $V + (i/2)\Omega_n$ is positive semidefinite which is condition (B.1)

It is worth stressing that Eq. (B.1) implies already $V \geq 0$ since the sum of positive semidefinite matrices remains positive semidefinite, and one has $V + (i/2)\Omega_n \geq 0$ if and only if $V - (i/2)\Omega_n \geq 0$ due to the invariance of the spectrum under transposition. One observes moreover that states with minimal uncertainty are pure as the purity for Gaussian states is given by $P(\rho) = \mathrm{Tr}\{\rho^2\} = \left[2^n \sqrt{\det(\boldsymbol{\sigma}_{\hat{X},\rho})}\right]^{-1}$ (Olivares, 2012).

Appendix C

Two-mode squeezed vacuum

In the following, a detailed derivation of the position representation and the covariance matrix of the two-mode squeezed vacuum (2.135) is provided.

Recall that the state was defined with respect to the number bases as (cf. Eq. (2.136))

$$|\psi_u\rangle = \sqrt{1-u^2}\sum_{n=0}^{\infty} u^n |n\rangle \otimes |n\rangle \tag{C.1}$$

with $u = \tanh(r \in \mathbb{R})$. One readily checks using the geometric series that this state is normalized. In fact, one obtains

$$\langle\psi_u|\psi_u\rangle = (1-u^2)\sum_{n,m=0}^{\infty} u^{n+m}\big(\langle m|n\rangle\big)^2 = (1-u^2)\sum_{n=0}^{\infty}(u^2)^n = 1\ . \tag{C.2}$$

The position representation is then found to be given by

$$\psi_u(x,y) = \frac{1}{\sqrt{\pi}}\exp\left[-\frac{1}{4}\frac{1-u}{1+u}(x+y)^2 - \frac{1}{4}\frac{1+u}{1-u}(x-y)^2\right]\ , \tag{C.3}$$

and the associated covariance matrix of the canonical operators reads

$$\boldsymbol{\sigma}_{X,r}^{\mathrm{EPR}} = \frac{1}{2}\begin{pmatrix} \cosh(2r) & 0 & \sinh(2r) & 0 \\ 0 & \cosh(2r) & 0 & -\sinh(2r) \\ \sinh(2r) & 0 & \cosh(2r) & 0 \\ 0 & -\sinh(2r) & 0 & \cosh(2r) \end{pmatrix}\ . \tag{C.4}$$

Lemma C.1. *The wave function of the state $|\psi_u\rangle$ is given by $\psi_u(x,y)$, i.e.*

$$\psi_u(x,y) = \langle x,y|\psi_u\rangle\ . \tag{C.5}$$

Proof. By definition, one has

$$\langle x,y|\psi_u\rangle = \sqrt{1-u^2}\sum_{n=0}^{\infty} u^n \langle x|n\rangle\langle y|n\rangle\ , \tag{C.6}$$

where the position representation of the number states is determined by $\langle x|n\rangle = (\sqrt{\pi}2^n n!)^{-1/2} H_n(x)\exp[-\frac{1}{2}x^2]$. Here, H_n denotes the Hermite polynomial (for $\hbar = 1$ and $M\omega = 1$) of degree n which are defined as

$$H_n(x) = (-1)^n \exp[x^2]\,\frac{\mathrm{d}^n}{\mathrm{d}x^n}\exp[-x^2]\ . \tag{C.7}$$

Using the Fourier transform of Gaussian functions

$$\int_{\mathbb{R}} \mathrm{d}s \;\; \exp\left[isx - s^2/p^2\right] = p\sqrt{\pi}\exp[-\tfrac{1}{4}p^2x^2] \;, \tag{C.8}$$

the Hermite polynomials are equivalently written as

$$H_n(x) = \frac{\exp[x^2]}{2\sqrt{\pi}} \int_{\mathbb{R}} \mathrm{d}s \;\; (-is)^n \exp[isx - \tfrac{1}{4}s^2] \;. \tag{C.9}$$

By virtue of this representation, one explicitly determines the following series which is also known as Mahler's formula:

$$\begin{aligned}\sum_{n=0}^{\infty} u^n \frac{H_n(x)H_n(y)}{2^n n!} &= \frac{e^{x^2+y^2}}{4\pi} \int_{\mathbb{R}} \mathrm{d}s \int_{\mathbb{R}} \mathrm{d}t \; e^{i(sx+ty)-\frac{1}{4}(s^2+t^2)} \sum_{n=0}^{\infty} \frac{1}{n!}\left(-\frac{ust}{2}\right)^n \\ &= \frac{e^{x^2+y^2}}{4\pi} \int_{\mathbb{R}} \mathrm{d}s \int_{\mathbb{R}} \mathrm{d}t \; e^{i(sx+ty)-\frac{1}{4}(s^2+t^2)-\frac{1}{2}ust} \;. \end{aligned} \tag{C.10}$$

Changing variables to $\sigma \equiv \frac{1}{\sqrt{2}}(s+t)$ and $\tau \equiv \frac{1}{\sqrt{2}}(s-t)$ for which the determinant of the Jacobian has modulus 1, one finally obtains

$$\begin{aligned}\sum_{n=0}^{\infty} u^n \frac{H_n(x)H_n(y)}{2^n n!} &= \frac{e^{x^2+y^2}}{4\pi} \int_{\mathbb{R}} \mathrm{d}\sigma \, e^{\frac{1}{\sqrt{2}}i\sigma(x+y)-\frac{1}{4}(1+u)\sigma^2} \int_{\mathbb{R}} \mathrm{d}\tau \, e^{\frac{1}{\sqrt{2}}i\tau(x+y)-\frac{1}{4}(1-u)\tau^2} \\ &= \frac{e^{x^2+y^2}}{4\pi} \cdot \frac{2\sqrt{\pi}}{\sqrt{1+u}} \, e^{-\frac{(x+y)^2}{2(1+u)}} \cdot \frac{2\sqrt{\pi}}{\sqrt{1-u}} \, e^{-\frac{(x-y)^2}{2(1-u)}} \\ &= \frac{1}{\sqrt{1-u^2}} \cdot \exp\left[\frac{2u}{1+u}xy - \frac{u^2}{1-u^2}(x-y)^2\right] \;. \end{aligned} \tag{C.11}$$

With the help of this identity one can now evaluate (C.6). In fact, employing the relation

$$\begin{aligned} & -\frac{1}{2}(x^2+y^2) - \frac{u^2}{1-u^2}(x-y)^2 + \frac{2u}{1+u}xy \\ = \; & -\frac{1}{4}\frac{1-u}{1+u}(x+y)^2 - \frac{1}{4}\frac{1+u}{1-u}(x-y)^2 \;, \end{aligned} \tag{C.12}$$

one finally obtains

$$\begin{aligned}\langle x,y|\psi_u\rangle &= \sqrt{1-u^2} \cdot \frac{e^{-\frac{1}{2}(x^2+y^2)}}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{u^n}{2^n n!} H_n(x)H_n(y) \\ &= \frac{1}{\sqrt{\pi}} \exp\left[-\frac{1}{2}(x^2+y^2) - \frac{u^2}{1-u^2}(x-y)^2 + \frac{2u}{1+u}xy\right] \\ &= \frac{1}{\sqrt{\pi}} \exp\left[-\frac{1}{4}\frac{1-u}{1+u}(x+y)^2 - \frac{1}{4}\frac{1+u}{1-u}(x-y)^2\right] \;, \end{aligned} \tag{C.13}$$

which is the desired result, i.e. $\langle x,y|\psi_u\rangle = \psi_u(x,y)$.

□

Note that the converse statement follows from the following identity for Hermite polynomials (see, e.g., Schleich (2001, p. 126)):

$$\int_{\mathbb{R}} \mathrm{d}x \; H_n(\lambda x) e^{-(x-x_0)^2} = \sqrt{\pi}\,(1-\lambda^2)^{\frac{n}{2}}\, H_n\Big(\frac{\lambda}{\sqrt{1-\lambda^2}} x_0\Big) \; . \tag{C.14}$$

Lemma C.2. *The state with position representation given by Eq.* (C.3) *is* $|\psi_u\rangle$*, i.e., one has* $|\psi_u\rangle = \int_{\mathbb{R}} \mathrm{d}x \int_{\mathbb{R}} \mathrm{d}y \; \psi_u(x,y)|x,y\rangle$*.*

Proof. Employing the completeness of the number basis, one finds

$$\int_{\mathbb{R}} \mathrm{d}x \int_{\mathbb{R}} \mathrm{d}y \; \psi_u(x,y)|x,y\rangle = \sum_{n,m=0}^{\infty} f(n,m)|n,m\rangle \; , \tag{C.15}$$

where $f(n,m) \equiv \int_{\mathbb{R}} \mathrm{d}x \int_{\mathbb{R}} \mathrm{d}y \; \langle n|x\rangle\langle m|y\rangle \psi_u(x,y)$ can be written as

$$f(n,m) = \frac{1}{\pi\sqrt{2^n n! 2^m m!}} \int_{\mathbb{R}} \mathrm{d}x \int_{\mathbb{R}} \mathrm{d}y \, H_n(x) H_m(y) e^{-y^2} e^{-\left(\frac{x}{\sqrt{1-u^2}} - \frac{uy}{\sqrt{1-u^2}}\right)^2} \; , \tag{C.16}$$

using completion of the square. Changing variables to $\tilde{x} \equiv x/\sqrt{1-u^2}$ and employing identity (C.14) on Hermite polynomials, one retrieves

$$f(n,m) = \frac{\sqrt{1-u^2}}{\pi\sqrt{2^n n! 2^m m!}} \int_{\mathbb{R}} \mathrm{d}y H_m(y) e^{-y^2} \sqrt{\pi} u^n H_n(y) \; , \tag{C.17}$$

which can be further evaluated due to orthogonality of the Hermite polynomials with respect to the weight function $\exp[-y^2]$. In fact, due to the relation $\int_{\mathbb{R}} \mathrm{d}y H_m(y) H_n(y) e^{-y^2} = \delta_{n,m} 2^n n! \sqrt{\pi}$, one finally obtains

$$f(n,m) = \sqrt{1-u^2} u^n \delta_{nm} \; . \tag{C.18}$$

which thus leads to

$$\int_{\mathbb{R}} \mathrm{d}x \int_{\mathbb{R}} \mathrm{d}y \, \Psi_u(x,y)|x,y\rangle = \sqrt{1-u^2} \sum_{n=0}^{\infty} u^n |n,n\rangle \; , \tag{C.19}$$

showing that the position representation of $|\psi_u\rangle$ is indeed given by $\psi_u(x,y)$. □

Due to the fact that the wave function of the two-mode squeezed vacuum is a Gaussian function, the covariance matrix can easily be calculated directly. One recalls that the covariance matrix $\boldsymbol{\sigma}_{\hat{X},\rho}$ in a state ρ of a set of observables $\hat{X} = (\hat{X}_j)$ is defined as

$$\big(\boldsymbol{\sigma}_{\hat{X},\rho}\big)_{jk} = \tfrac{1}{2}\langle\{\hat{X}_j, \hat{X}_k\}\rangle_\rho - \langle\hat{X}_j\rangle_\rho \langle\hat{X}_k\rangle_\rho \; . \tag{C.20}$$

For $\hat{X} = (\hat{q}_1, \hat{p}_1, \hat{q}_2, \hat{p}_2)$ where the position representation of the canonical operators are given by

$$\langle\vec{x}|\hat{q}_j|\vec{y}\rangle = \delta(\vec{x}-\vec{y})\, x_j \; , \tag{C.21}$$

$$\langle\vec{x}|\hat{p}_j|\vec{y}\rangle = \delta(\vec{x}-\vec{y})\, (-i\hbar) \cdot \frac{\partial}{\partial x_j} \; , \tag{C.22}$$

the associated covariance matrix of the two-mode squeezed vacuum state can be determined by means of the following Gaussian integrals (Bronstein and Semendjajew, 1996): For any vectors $\vec{v}, \vec{w} \in \mathbb{R}^n$ and any $n \times n$-matrices $A, B, D, \Lambda \in \mathcal{M}_n(\mathbb{R})$ where A and B are symmetric and positive definite, one has

$$\int_{\mathbb{R}^n} \mathrm{d}^n\vec{x}\ \vec{x}^T D\vec{x} \exp\left[-\vec{x}^T A\vec{x} + \vec{v}^T\vec{x}\right] = \left[\vec{u}^T D\vec{u} + \tfrac{1}{2}\mathrm{Tr}\{DA^{-1}\}\right]\mathcal{M} \tag{C.23}$$

and

$$\begin{aligned}&\int_{\mathbb{R}^n} \mathrm{d}^n\vec{x}\ \exp\left[-\vec{x}^T B\vec{x} + \vec{w}^T\vec{x}\right]\left(-\frac{\partial}{\partial x}\Lambda\frac{\partial}{\partial x}\right)\exp\left[-\vec{x}^T A\vec{x} + \vec{v}^T\vec{x}\right]\\ &= \left[2\mathrm{Tr}\{B\Lambda AC^{-1}\} + 4\vec{z}^T B\Lambda A\vec{z} - 2\vec{z}^T(B\Lambda\vec{v} + A\Lambda\vec{w}) + \vec{w}^T\Lambda\vec{v}\right]\mathcal{M}\ ,\end{aligned} \tag{C.24}$$

where one has

$$\mathcal{M} = \sqrt{\pi^n/\det(A)}\ \exp\left[\tfrac{1}{4}\vec{v}^T A^{-1}\vec{v}\right]\ , \tag{C.25}$$

$$\vec{u} = (1/2)A^{-1}\vec{v}\ , \tag{C.26}$$

$$C = A + B\ , \tag{C.27}$$

$$\vec{y} = \vec{v} + \vec{w}\ , \tag{C.28}$$

$$\vec{z} = \frac{1}{2}C^{-1}\vec{y}\ . \tag{C.29}$$

Since the wave function of the two-mode squeezed vacuum may be written as

$$\psi_u(x,y) = \frac{1}{\sqrt{\pi}}\exp\left[-\tfrac{1}{2}(x,y)A_-(x,y)^T\right] \tag{C.30}$$

with

$$A_\pm = \begin{pmatrix}\cosh(2r) & \pm\sinh(2r)\\ \pm\sinh(2r) & \cosh(2r)\end{pmatrix}\ , \tag{C.31}$$

thus satisfying $A_-^{-1} = A_+$ and $\det(A_\pm) = 1$, one directly concludes from the absence of linear terms with respect to x and y that it has vanishing means. By virtue of Eqs. (C.23) and (C.24), the diagonal elements of the covariance matrix $\boldsymbol{\sigma}_{\hat{X},|\psi_u\rangle}$ ($\hbar = 1$) are eventually determined as

$$\left(\boldsymbol{\sigma}_{\hat{X},|\psi_u\rangle}\right)_{jj} = \int_{\mathbb{R}^2}\mathrm{d}^2\vec{x}\ \frac{1}{\pi}\vec{x}^T D_i\vec{x}\exp\left[-\vec{x}^T A_-\vec{x}\right] = \frac{1}{2}\mathrm{Tr}\{D_j A_+\} \tag{C.32}$$

for $j = 1, 3$ and

$$\begin{aligned}\left(\boldsymbol{\sigma}_{\hat{X},|\psi_u\rangle}\right)_{kk} &= \int_{\mathbb{R}^2}\mathrm{d}^2\vec{x}\ \frac{1}{\pi}\exp\left[-\frac{1}{2}\vec{x}^T A_-\vec{x}\right]\left(-\frac{\partial}{\partial x}\Lambda_k\frac{\partial}{\partial x}\right)\exp\left[-\frac{1}{2}\vec{x}^T A_-\vec{x}\right]\\ &= \frac{1}{2}\mathrm{Tr}(A_-\Lambda_k A_- A_+) = \frac{1}{2}\mathrm{Tr}\{A_-\Lambda_k\}\end{aligned} \tag{C.33}$$

for the indices $k = 2$ and 4, where the matrices D_j and Λ_k are defined as

$$D_j = \begin{pmatrix}\delta_{j,1} & 0\\ 0 & \delta_{j,3}\end{pmatrix}\qquad,\qquad \Lambda_k = \begin{pmatrix}\delta_{k,2} & 0\\ 0 & \delta_{k,4}\end{pmatrix}\ . \tag{C.34}$$

The diagonal entries of the covariance matrix are thus found to be given by

$$\left(\boldsymbol{\sigma}_{\hat{X},|\psi_u\rangle}\right)_{ll} = \frac{1}{2}\cosh(2r) \ , \qquad \forall\ l = 1,\ldots,4 \ , \tag{C.35}$$

and the off-diagonal entries are similarly determined which finally yields

$$\left(\boldsymbol{\sigma}_{\hat{X},|\psi_u\rangle}\right)_{13} \overset{(C.23)}{=} \frac{1}{2}\mathrm{Tr}\{CA_+\} = \frac{1}{2}\sinh(2r) \ , \tag{C.36}$$

$$\left(\boldsymbol{\sigma}_{\hat{X},|\psi_u\rangle}\right)_{24} \overset{(C.24)}{=} \frac{1}{2}\mathrm{Tr}\{A_-C\} = -\frac{1}{2}\sinh(2r) \ , \tag{C.37}$$

as $C = \left(\begin{smallmatrix} 0 & 1 \\ 0 & 0 \end{smallmatrix}\right)$, whereas the remaining entries are zero. Hence, the covariance matrix of the EPR state for $\hat{X} = (\hat{q}_1, \hat{p}_1, \hat{q}_2, \hat{p}_2)$ is indeed given by Eq. (C.4).

An alternative approach to obtain the covariance matrix of this two-mode Gaussian state is provided by a direct evaluation of the characteristic function (2.102). Defining $\vec{z} = \vec{x} + i\vec{y}$ for elements $\vec{x}$ and $\vec{y}$ of $\mathbb{R}^2$, one finds for the EPR state for this function

$$\chi^t_{|\psi_u\rangle}(\vec{z}) = \int_{\mathbb{R}^2} \mathrm{d}^2\vec{r} \int_{\mathbb{R}^2} \mathrm{d}^2\vec{s}\ \psi_u(\vec{r})^*\psi_u(\vec{s})\,\langle\vec{r}|\exp\Big[-it\sum_{k=1}^{2}(x_k\hat{p}_k - y_k\hat{q}_k)\Big]|\vec{s}\rangle \ . \tag{C.38}$$

The transition matrix element can be evaluated by means of the Campbell-Baker-Hausdorff formula

$$e^{\hat{X}+\hat{Y}} = e^{\hat{X}}e^{\hat{Y}}e^{-\frac{1}{2}[\hat{X},\hat{Y}]} \ , \tag{C.39}$$

and the identities $e^{iy\hat{q}}|x\rangle = e^{iyx}|x\rangle$ and $e^{iy\hat{p}}|x\rangle = |x-y\rangle$ for some real number y, which finally gives

$$\begin{aligned} &\langle\vec{r}|\exp\Big[-it\sum_{k=1}^{2}(x_k\hat{p}_k - y_k\hat{q}_k)\Big]|\vec{s}\rangle \\ &= \delta(\vec{r} - (t\vec{x} + \vec{s}))\cdot\exp\Big[it\sum_{j=1}^{2}y_js_j + \tfrac{1}{2}it^2\sum_{k=1}^{2}x_ky_k\Big] \ . \end{aligned} \tag{C.40}$$

Employing the result of a Gaussian integral

$$\int_{\mathbb{R}^n}\mathrm{d}^n\vec{\lambda}\ \exp\left[-\vec{\lambda}^TA\vec{\lambda} + \vec{\mu}^T\vec{\lambda}\right] = \sqrt{\frac{\pi^n}{\det(A)}}\cdot\exp\left[\tfrac{1}{4}\vec{v}^TA^{-1}\vec{v}\right] \ , \tag{C.41}$$

as well as $A_-^T = A_-$, the characteristic function is shown to obey

$$\begin{aligned} \chi^t_{|\psi_u\rangle}(\vec{z}) &= \frac{1}{\pi}\int_{\mathbb{R}^2}\mathrm{d}^2\vec{r}\int_{\mathbb{R}^2}\mathrm{d}^2\vec{s}\ e^{-\frac{1}{2}\vec{r}^TA_-\vec{r} - \frac{1}{2}\vec{s}^TA_-\vec{s}}\delta(\vec{r} - (t\vec{x} + \vec{s}))e^{it\vec{y}^T\vec{s} + \frac{1}{2}it^2\vec{y}^T\vec{x}} \\ &= \frac{1}{\pi}e^{-\frac{1}{2}t^2\vec{x}^TA_-\vec{x}}e^{\frac{1}{2}it^2\vec{y}^T\vec{x}}\int_{\mathbb{R}^2}\mathrm{d}^2\vec{s}\ e^{-\vec{s}^TA_-\vec{s}}e^{t(i\vec{y}^T - (A_-\vec{x})^T\vec{s})} \\ &= \exp\left[-\frac{t^2}{2}(x_1,x_2,y_1,y_2)A_- \oplus A_+(x_1,x_2,y_1,y_2)^T\right] \ . \end{aligned} \tag{C.42}$$

An easy transformation of the exponential function's argument then yields the common representation of the characteristic function proving that the two-mode squeezed vacuum is Gaussian with covariance matrix given by Eq. (C.4).

Appendix D

Position representation of two-mode Gaussian states

Besides the Husimi Q-function (Husimi, 1940) and the P-representation (Glauber, 1963; Sudarshan, 1963), the Wigner function provides another phase-space formulation of operators of a continuous variable system (Wigner, 1932; Glauber, 1963; Cahill and Glauber, 1969). Its inverse, assigning symmetrically ordered operators on $L^2(\mathbb{R}^n)$ to these phase-space distributions, is given by the so-called Weyl transform (Weyl, 1927; Moyal, 1949). Note that the ordering of the operators is an important feature which corresponds to the quantization rule applied for classical quantities in quantum theory.

The Weyl transform of an n-mode state ρ, providing the correct order of operators, is defined by

$$\mathcal{W}_\rho(P_\mathrm{p}\hat{X}, P_\mathrm{q}\hat{X}) \equiv \frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^n}\mathrm{d}^n\vec{x}\int_{\mathbb{R}^n}\mathrm{d}^n\vec{y}\; e^{+i/\hbar\,(\vec{x}^{\,T}P_\mathrm{o}\hat{X}+\vec{y}^{\,T}P_\mathrm{e}\hat{X})}\chi_\rho^{t=1}(\vec{y}-i\vec{x})\;, \tag{D.1}$$

where $\hat{X} = (\hat{q}_1, \hat{p}_1, \ldots, \hat{q}_n, \hat{p}_n)^T$ and the matrices $P_\mathrm{p} \equiv \mathrm{diag}(0, 1, \ldots, 0, 1)$ and $P_\mathrm{q} \equiv \mathrm{diag}(1, 0, \ldots, 1, 0)$ single out the canonical momentum and position operators, respectively. Thus, the function $\mathcal{W}_\rho$ represents the state ρ in terms of the canonical operators. Note that the connection to the Wigner function is established by virtue of Eq. (2.112).

Applying again the Campbell-Baker-Hausdorff formula (C.39), one finds for the position representation of the Weyl transform (with $\hbar = 1$)

$$\begin{aligned}\langle\vec{x}\,'|\mathcal{W}_\rho|\vec{y}\,'\rangle &= \frac{1}{(2\pi)^n}\int_{\mathbb{R}^n}\mathrm{d}^n\vec{x}\int_{\mathbb{R}^n}\mathrm{d}^n\vec{y}\;\delta(\vec{y}-(\vec{y}\,'-\vec{x}\,'))e^{\frac{i}{2}\vec{x}^{\,T}(2\vec{x}\,'+\vec{y})}\chi_\rho^{t=1}(\vec{y}-i\vec{x})\\ &= \frac{1}{(2\pi)^n}\int_{\mathbb{R}^n}\mathrm{d}^n\vec{x}\;e^{\frac{i}{2}\vec{x}^{\,T}(\vec{x}\,'+\vec{y}\,')}\chi_\rho^{t=1}(\vec{y}\,'-\vec{x}\,'-i\vec{x})\;.\end{aligned} \tag{D.2}$$

Upon inserting the characteristic function corresponding to a two-mode Gaussian state with vanishing means and covariance matrix in standard form (2.124), which reads

$$\chi_\rho^{t=1}(\vec{x}+i\vec{y}) = \exp\left[-\tfrac{1}{2}\,\vec{v}^{\,T}\begin{pmatrix} a\,\mathbb{1}_2 & \mathrm{diag}(c_1,c_2)\\ \mathrm{diag}(c_1,c_2) & b\,\mathbb{1}_2\end{pmatrix}\vec{v}\right]\;, \tag{D.3}$$

where $\vec{v} = (-y_1, x_1, -y_2, x_2)^T$, the position representation of the Weyl transform is finally evaluated to

$$\begin{aligned}\langle \vec{x}\,'|\mathcal{W}_\rho|\vec{y}\,'\rangle &= \frac{1}{(2\pi)^2}\, e^{-\frac{1}{2}(\vec{y}\,'-\vec{x}\,')^T B_2(\vec{y}\,'-\vec{x}\,')} \int_{\mathbb{R}^2} \mathrm{d}^2\vec{x}\; e^{\frac{i}{2}\vec{x}^T(\vec{x}\,'+\vec{y}\,')-\frac{1}{2}\vec{x}^T B_1 \vec{x}} \\ &= \frac{1}{(2\pi)^2}\, \exp\left[-\tfrac{1}{2}(\vec{y}\,'-\vec{x}\,')^T B_2(\vec{y}\,'-\vec{x}\,')\right] \\ &\qquad \cdot \sqrt{\frac{(2\pi)^2}{\det(B_1)}}\, \exp\left[-\tfrac{1}{8}(\vec{y}\,'+\vec{x}\,')^T B_1^{-1}(\vec{y}\,'+\vec{x}\,')\right] \;, \end{aligned} \tag{D.4}$$

using multidimensional Gaussian integration (C.41). Here, the matrices B_j are defined as

$$B_j = \begin{pmatrix} a & c_j \\ c_j & b \end{pmatrix} \;, \tag{D.5}$$

so that its inverse obeys

$$B_j^{-1} = \frac{1}{\det(B_j)} \begin{pmatrix} b & -c_j \\ -c_j & a \end{pmatrix} \;. \tag{D.6}$$

For the two-mode squeezed vacuum, the matrices B_j are found to be given by $\frac{1}{2}A_{(-1)^{j+1}}$ (cf. Eq. (C.31)) which implies that one has $\det(B_j) = \frac{1}{4}$ and the inverse obeys $B_j^{-1} = 2A_{(-1)^j}$. The Weyl transform (D.4) then reads

$$\begin{aligned}\langle \vec{x}\,'|\mathcal{W}_\rho|\vec{y}\,'\rangle = \frac{1}{\pi}\, \exp\Big[-\tfrac{1}{4}\{&(\vec{y}\,'-\vec{x}\,')^T A_+(\vec{y}\,'-\vec{x}\,') \\ &+ (\vec{y}\,'+\vec{x}\,')^T A_-(\vec{y}\,'+\vec{x}\,')\}\Big] \;, \end{aligned} \tag{D.7}$$

which is indeed equal to $\psi_u(\vec{x}\,')\psi_u(\vec{y}\,')^*$ (cf. Eq. (C.3)).

Appendix E

Dynamics for the spin star model

In the following, the exact dynamics for the initial state (cf. Eq. (3.107))

$$|\xi_V^\lambda(0)\rangle_{SE} = b_1 V|1\rangle \otimes |\chi_+\rangle_E + b_0 V|0\rangle \otimes |\tilde{\Omega}_\lambda\rangle_E \ , \tag{E.1}$$

describing the central spin along with the N-particle spin bath is solved and then used to determine the central spin's dynamics needed for the studies presented in Sec. 3.5.2.

Recall that the Hamiltonian for the Heisenberg XY interaction (3.106) can be written as

$$H = g\{\sigma_+ \otimes J_- + \sigma_- \otimes J_+\} \tag{E.2}$$

for a real-valued coupling g, where $J_\pm$ refer to the raising and lowering operators of the total spin angular momentum of the bath $\vec{J} = \frac{1}{2}\sum_{k=1}^N \vec{\sigma}^{(k)}$ (for $\hbar = 1$). Moreover, the environmental state $|\tilde{\Omega}_\lambda\rangle_E$ (see also Eq. (3.108)) is chosen to be a superposition of the states

$$|\chi_+\rangle_E = |\tfrac{N}{2}, \tfrac{N}{2}\rangle \ , \qquad |\chi_-\rangle_E = i|\tfrac{N}{2}, \tfrac{N}{2} - 1\rangle \ , \tag{E.3}$$

defining joint eigenstates[1] $|j, m\rangle$ of $\vec{J}^2$ and J_3 with eigenvalues $j(j+1)$ and m, respectively. Hence, the Hamiltonian (E.2) basically interchanges $|1\rangle \otimes |\frac{N}{2}, \frac{N}{2} - 1\rangle$ and $|0\rangle \otimes |\frac{N}{2}, \frac{N}{2}\rangle$, i.e., one finds

$$H|1\rangle \otimes |\tfrac{N}{2}, \tfrac{N}{2} - 1\rangle = g\sqrt{N}|0\rangle \otimes |\tfrac{N}{2}, \tfrac{N}{2}\rangle \ , \tag{E.4}$$

$$H|0\rangle \otimes |\tfrac{N}{2}, \tfrac{N}{2}\rangle = g\sqrt{N}|1\rangle \otimes |\tfrac{N}{2}, \tfrac{N}{2} - 1\rangle \ , \tag{E.5}$$

whereas the two other combinations of eigenstates of σ_3 and bath states $|\chi_\pm\rangle_E$ are in the kernel of H. Then, it follows that

$$H^{2n+1}|\xi_V^\lambda(0)\rangle_{SE} = (g\sqrt{N})^{2n+1}|\tilde{\xi}_V^\lambda(0)\rangle_{SE} \ , \tag{E.6}$$

$$H^{2n+2}|\xi_V^\lambda(0)\rangle_{SE} = (g\sqrt{N})^{2n+2}|\tilde{\tilde{\xi}}_V^\lambda(0)\rangle_{SE} \ , \tag{E.7}$$

[1] The assignment of these eigenstates by $|j, m\rangle$ is in general incomplete as the dimension of the eigenspaces corresponding to a given pair (j, m) of quantum numbers is given by $n(j, N) = \binom{N}{\frac{N}{2}-j} - \binom{N}{\frac{N}{2}-j-1}$ (see, e.g., Breuer *et al.* (2004)). In the present case where $j = N/2$, one thus finds $n(N/2, N) = 1$ so that no further index labeling the degenerate eigenstates is needed.

for all $n \in \mathbb{N}_0$ where

$$|\tilde{\xi}_V^{\lambda}(0)\rangle_{SE} \equiv \beta_V^{\lambda}|0\rangle \otimes |\tfrac{N}{2}, \tfrac{N}{2}\rangle + \alpha_V^{\lambda}|1\rangle \otimes |\tfrac{N}{2}, \tfrac{N}{2}-1\rangle \ , \tag{E.8}$$

$$|\tilde{\tilde{\xi}}_V^{\lambda}(0)\rangle_{SE} \equiv \alpha_V^{\lambda}|0\rangle \otimes |\tfrac{N}{2}, \tfrac{N}{2}\rangle + \beta_V^{\lambda}|1\rangle \otimes |\tfrac{N}{2}, \tfrac{N}{2}-1\rangle \ . \tag{E.9}$$

Here, the coefficients α_V^{λ} and β_V^{λ} are defined as

$$\alpha_V^{\lambda} = b_1 V_{01} + b_0 V_{00} \tilde{C}_{\lambda}^{-1}(1-\lambda) \ , \tag{E.10}$$

$$\beta_V^{\lambda} = i b_0 V_{10} \tilde{C}_{\lambda}^{-1} \lambda \ , \tag{E.11}$$

where V_{mn} refers to the transition matrix elements of the unitary V with respect to the eigenbasis of σ_3, i.e. one has $V_{mn} \equiv \langle m|V|n\rangle$. The time-evolved total state $|\xi_V^{\lambda}(t)\rangle_{SE} = \exp[itH]|\xi_V^{\lambda}(0)\rangle_{SE}$ is thus given by

$$|\xi_V^{\lambda}(t)\rangle_{SE} = |\xi_V^{\lambda}(0)\rangle_{SE} - i\sin(g\sqrt{N}t)|\tilde{\xi}_V^{\lambda}(0)\rangle_{SE} \tag{E.12}$$

$$+ \left[\cos(g\sqrt{N}t) - 1\right]|\tilde{\tilde{\xi}}_V^{\lambda}(0)\rangle_{SE} \ , \tag{E.13}$$

so that the reduced state of the central spin is easily shown to obey

$$\tilde{\rho}_S^{\lambda}(t) = \begin{pmatrix} p & c \\ c^* & 1-p \end{pmatrix} \tag{E.14}$$

where the populations and the coherences are given by

$$\begin{aligned} p = {} & |\alpha_V^{\lambda}|^2 \sin(g\sqrt{N}t)^2 + |\beta_V^{\lambda}|^2 \cdot \left(1 - \cos(g\sqrt{N}t)\right)^2 \\ & + 2\lambda \tilde{C}_{\lambda}^{-1} \mathrm{Im}(b_0 V_{10} \beta_V^{\lambda\,*}) \cdot \left(1 - \cos(g\sqrt{N}t)\right) \\ & + \mathrm{Im}(\alpha_V^{\lambda} \beta_V^{\lambda\,*}) \cdot \left(\sin(2g\sqrt{N}t) - 2\sin(g\sqrt{N}t)\right) \\ & - 2\lambda \tilde{C}_{\lambda}^{-1} \mathrm{Re}(b_0 V_{10} \alpha_V^{\lambda\,*}) \sin(g\sqrt{N}t) \\ & + |b_0 V_{10}|^2 + |b_1 V_{11}|^2 + 2(1-\lambda)\tilde{C}_{\lambda}^{-1} \mathrm{Re}(b_1 b_0^* V_{11} V_{10}^*) \ , \end{aligned} \tag{E.15}$$

and

$$\begin{aligned} c = {} & \cos(g\sqrt{N}t) \cdot \Big\{ |b_1|^2 V_{01}^* V_{11} + |b_0|^2 V_{00}^* V_{10} \\ & \qquad + (1-\lambda)\tilde{C}_{\lambda}^{-1}(b_1 b_0^* V_{11} V_{00}^* + b_1^* b_0 V_{01}^* V_{10}) \Big\} \\ & + \sin(g\sqrt{N}t) \cdot b_0^* \lambda \tilde{C}_{\lambda}^{-1} \Big\{ V_{10}^* \left[b_1 V_{11} + b_0(1-\lambda)\tilde{C}_{\lambda}^{-1} V_{10}\right] \\ & \qquad - V_{00} \left[b_1 V_{01} + b_0(1-\lambda)\tilde{C}_{\lambda}^{-1} V_{00}\right] \Big\} \ . \end{aligned} \tag{E.16}$$

Appendix F

Experimental details of the photonic process

Here, a summary of the photon counting rates as well as the integration times is given that were used in the all-optical experiment discussed in Sec. 4.3.2 to measure the polarization states. The reference states and, similarly, the initial polarization states on the enclosing surfaces are more accurately determined due to their relevance in the local representation (4.28) (cf. Tabs. F.1 and F.2). In addition, to improve the accuracy of the measured degree of non-Markovianity, the integration times for states of the enclosing surfaces that are close to the plane which is parallel to the equatorial plane of the Bloch ball are increased, too.

	$\rho_0^{(1)}$		$\rho_0^{(2)}$		$\rho \perp \varrho$	
A_α	count rate	t_{int}	count rate	t_{int}	count rate	t_{int}
0.64	$1.25 \times 10^6/400\,\text{s}$	400 s	$1.13 \times 10^6/400\,\text{s}$	400 s	$1 \times 10^4/2\,\text{s}$	2 s
0.22	$1.3 \times 10^6/400\,\text{s}$	400 s	$1.18 \times 10^6/800\,\text{s}$	800 s	$1 \times 10^4/2\,\text{s}$	2 s
0.01	$1.3 \times 10^6/400\,\text{s}$	400 s	$1.18 \times 10^6/800\,\text{s}$	800 s	$1 \times 10^4/2\,\text{s}$	2 s

Table F.1 – The photon count rate and the integration time t_{int} used to measure the reference states as well as the orthogonal states for the three different values of the relative amplitude A_α. The integration time has been increased for the reference states to improve the accuracy of the experimentally determined degree of non-Markovianity.

	$\rho \in \partial U(\rho_0^{(1)})$			
A_α	count rate	t_{int}	$t_{\text{int}}(0\lambda)$	$t_{\text{int}}(\theta = \frac{\pi}{50} \cdot x)$
0.64	$1.4 \times 10^4/2\,\text{s}$	2 s	20 s	20 s, $x \in \{22, \ldots, 29\}$
0.22	$1.4 \times 10^4/2\,\text{s}$	2 s	20 s	20 s, $x \in \{19, \ldots, 32\}$
0.01	$1.5 \times 10^4/2\,\text{s}$	2 s	20 s	20 s, $x \in \{21, \ldots, 30\}$
	$\rho \in \partial U(\rho_0^{(2)})$			
0.64	$9.5 \times 10^3/2\,\text{s}$	2 s	20 s	20 s, $x \in \{6, \ldots, 14\}$
0.22	$9.7 \times 10^3/2\,\text{s}$	2 s	20 s	20 s, $x \in \{1, \ldots, 16\}$
0.01	$9.9 \times 10^3/2\,\text{s}$	2 s	20 s	20 s, $x \in \{1, \ldots, 12\}$

Table F.2 – The photon count rate and the integration time t_{int} used to measure the states on the enclosing surfaces, determined by $0.3 \cdot \rho_0^{(1,2)} + 0.7 \cdot \rho$ for pure states ρ that are parametrized by an equidistant grid with respect to the polar angles θ and ϕ, for the three different values of the relative amplitude A_α. The integration time for the initial states $t_{\text{int}}(0\lambda)$ is increased due to the significance of possible errors for these states. Moreover, the states located close to planes that are parallel to the equatorial plane are measured more precisely in order to increase the accuracy of the determined degree of non-Markovianity. The used integration times and the concerned θ-angles are specified in the last column.

Appendix G

Results on the trace norm

In this section, the representation (4.36) of the Helstrom matrix is proven and it is shown how one concludes that the upper bound in Eq. (4.35) is attained if and only if $\rho_1 \perp \rho_2$ holds. To derive the representation, one needs the so-called Jordan-Hahn decomposition (Bengtsson and Zyczkowski, 2007; Nielsen and Chuang, 2000), providing a decomposition of any Hermitian operator, which is, for example, also employed to show the orthogonality of optimal states (cf. Eq. (4.25) and theorem 4.3) and the local representation of the trace-distance-based measures of quantum non-Markovianity (cf. theorems 4.1 and 4.4).

Lemma G.1. *Let X be a Hermitian operator on a Hilbert space $\mathcal{H}$. Then, there exist positive operators $X_+ \geq 0$ and $X_- \geq 0$ satisfying $X_+X_- = X_-X_+ = 0$ and*

$$X = X_+ - X_- \ . \tag{G.1}$$

This result holds for finite and infinite systems and can be proven by means of the functional calculus for elements of C^*-algebras (Blackadar, 2006). It is also known from measure theory where signed measures are decomposed (Elstrodt, 2009).

Theorem G.1. *Let $\{p_j\}$ denote a binary probability distribution. For two quantum states ρ_1 and ρ_2, the trace norm of the associated Helstrom matrix $\Delta = p_1\rho_1 - p_2\rho_2$ satisfies*

$$\|\Delta\|_1 = 2 \max_{\Pi} \mathrm{Tr}\{\Pi\Delta\} + p_2 - p_1 \ . \tag{G.2}$$

Proof. Let Q, S denote the positive and orthogonal operators obtained from the Jordan-Hahn decomposition of the Helstrom matrix Δ, i.e., one has $\Delta = Q - S$ and, thus, $\mathrm{Tr}\{\Delta\} = p_1 - p_2 = \mathrm{Tr}\{Q\} - \mathrm{Tr}\{S\}$ due to the normalization of states. Moreover, by definition of the trace norm, it follows that $\|\Delta\|_1 = \mathrm{Tr}\{Q\} + \mathrm{Tr}\{S\}$ holds which can be rewritten as

$$\|\Delta\|_1 = 2\mathrm{Tr}\{Q\} - (p_1 - p_2) \ . \tag{G.3}$$

For a projection Π, one then finds

$$\mathrm{Tr}\{\Pi\Delta\} = \mathrm{Tr}\{\Pi(Q-S)\} \leq \mathrm{Tr}\{\Pi Q\} \leq \mathrm{Tr}\{Q\} = \tfrac{1}{2}\left(\|\Delta\|_1 + p_1 - p_2\right) \ , \tag{G.4}$$

where equality holds if and only if Π denotes the projection onto the support of the operator Q as $Q \perp S$. Thus, one concludes

$$\max_{\Pi} \mathrm{Tr}\{\Pi\Delta\} = \tfrac{1}{2}\big(\|\Delta\|_1 + p_1 - p_2\big) \ , \tag{G.5}$$

which is equivalent to Eq. (G.2). □

Based on this representation, one shows that $\|\Delta\|_1 = 1$ if and only if $\rho_1 \perp \rho_2$ (cf. Eq. (4.35)). In fact, if one has $\|\Delta\|_1 = 1$ for some states ρ_1 and ρ_2 along with a (nontrivial) probability distribution $\{p_j\}$, it directly follows from Eq. (G.2)

$$\max_{\Pi} \mathrm{Tr}\{\Pi\Delta\} = p_1 \ . \tag{G.6}$$

Hence, the maximizing projection Π satisfies

$$p_1 \mathrm{Tr}\{\Pi\rho_1\} - p_2 \mathrm{Tr}\{\Pi\rho_2\} = p_1 \ . \tag{G.7}$$

However, since one has $0 \leq \mathrm{Tr}\{\Pi\rho\} \leq 1$ for any state ρ and $p_{1,2} \neq 1$, it is clear that Eq. (G.7) can only be true if $\mathrm{Tr}\{\Pi\rho_1\} = 1$ and $\mathrm{Tr}\{\Pi\rho_2\} = 0$ hold. While the first equation implies that Π projects onto a subspace V which contains the support of ρ_1, the second equation shows that the support of ρ_2 must be orthogonal to V and, therefore, one needs to have $\rho_1 \perp \rho_2$.

The converse is readily obtained from the definition of the trace norm. For two orthogonal states $\rho_1 \perp \rho_2$, it follows that

$$\|\Delta\|_1 = p_1 \mathrm{Tr}\{\rho_1\} + p_2 \mathrm{Tr}\{\rho_2\} = p_1 + p_2 = 1 \ , \tag{G.8}$$

due to positivity and the normalization of the states.

Appendix H

Factorizing processes despite environmental correlations

Based on the interaction between the polarization and frequency degrees of freedom induced by a quartz plate, one may construct a dynamical process which factorizes despite of an initially correlated state of the environment. The state of a photon with fixed polarization $\lambda(= H, V)$ and frequency ω, traveling through a quartz plate, is transformed as

$$U_Q(t)|\lambda\rangle_S \otimes |\omega\rangle_E = e^{i\omega n_\lambda t}|\lambda\rangle_S \otimes |\omega\rangle_E \,, \tag{H.1}$$

where n_λ denotes the refraction index for a photon with polarization λ (Liu *et al.*, 2011). If the state of the frequency degrees of freedom is described by $|\chi\rangle_E = \int \mathrm{d}\omega\, f(\omega)|\omega\rangle_E$ with $\int \mathrm{d}\omega\, |f(\omega)|^2 = 1$, then the coherence factor $\kappa(t)$ given by (4.30) which describes the dephasing of the polarization state is found to obey

$$\kappa(t) = \int \mathrm{d}\omega\ |f(\omega)|^2 \cdot \exp[i\omega\Delta n \cdot t] \,, \tag{H.2}$$

where $\Delta n \equiv n_V - n_H$.

Now, extending to two photons traveling through quartz plates, one may derive a factorizing dynamical process for the polarization degrees in the presence of a correlated environmental state (Breuer, 2012b). More precisely, for a two-photon frequency state[1] $|\chi'\rangle_{E_1E_2} = \sum_{j,k=0}^{1} \alpha_{jk}|\omega'_j\rangle_{E_1} \otimes |\omega'_k\rangle_{E_2}$ with $\sum_{j,k} |\alpha_{jk}|^2 = 1$ (cf. Fig. H.1), the reduced dynamics of the joint polarization state obtained for the interaction $U_{SE}^{12}(t,0) = U_Q(t) \otimes U_Q(t)$ is characterized by

$$\kappa_1(t) = \sum_{j,k=0}^{1} |\alpha_{jk}|^2 e^{i\Delta n\omega'_j t} \,, \qquad \kappa_{12}(t) = \sum_{j,k=0}^{1} |\alpha_{jk}|^2 e^{i\Delta n(\omega'_j+\omega'_k)t} \,, \tag{H.3}$$

$$\kappa_2(t) = \sum_{j,k=0}^{1} |\alpha_{jk}|^2 e^{i\Delta n\omega'_k t} \,, \qquad \Lambda_{12}(t) = \sum_{j,k=0}^{1} |\alpha_{jk}|^2 e^{i\Delta n(\omega'_j-\omega'_k)t} \,. \tag{H.4}$$

[1] Note that the frequency degrees of freedom of photon pairs obtained from a spontaneous parametric downconversion process are well approximated by $|\chi\rangle_{E_1E_2} = \int \mathrm{d}\vec{\omega}\, f(\omega_1,\omega_2)|\omega_1\rangle_{E_1} \otimes |\omega_2\rangle_{E_2}$ for sufficiently weak laser pulses pumping the nonlinear crystal. For a strong pump pulse the state of the photons is, however, rather described by an EPR state (2.136) (Lund *et al.*, 2014). Clearly, choosing $f(\omega_1,\omega_2) = \sum_{j,k=0}^{1} \alpha_{jk}\delta(\omega_1-\omega'_j)\delta(\omega_2-\omega'_k)$ in the state $|\chi\rangle_{E_1E_2}$ one obtains $|\chi'\rangle_{E_1E_2}$.

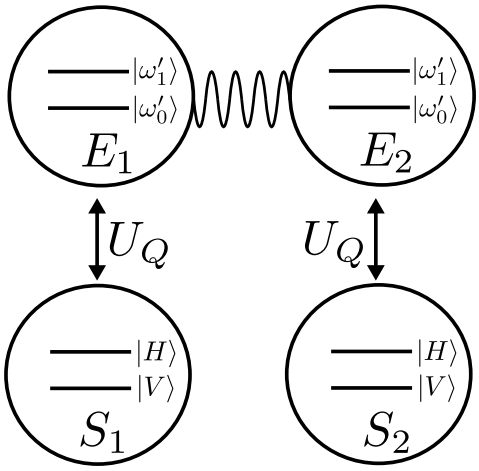

Figure H.1 – Schematic picture of a two-photon system where each polarization degree of freedom is coupled locally to the frequency spectrum according due the action of quartz plates which is described by the unitary U_Q (see Eq. (H.1)). As only two frequencies are supported, the environment effectively defines a two-level system.

That is, using the notation $\varrho_{\lambda_1\lambda_1',\lambda_2\lambda_2'} = \langle\lambda_1\lambda_1'|\rho_S^{12}(0)|\lambda_2\lambda_2'\rangle$, the polarization states evolve according to

$$\rho_S^{12}(t) = \begin{pmatrix} \varrho_{VV,VV} & \kappa_2(t)\,\varrho_{VV,VH} & \kappa_1(t)\,\varrho_{VV,HV} & \kappa_{12}(t)\,\varrho_{VV,HH} \\ & \varrho_{VH,VH} & \Lambda_{12}(t)\,\varrho_{VH,HV} & \kappa_1(t)\,\varrho_{VH,HH} \\ & & \varrho_{HV,HV} & \kappa_2(t)\,\varrho_{HV,HH} \\ \text{c.c.} & & & \varrho_{HH,HH} \end{pmatrix} . \tag{H.5}$$

Clearly, the dynamical map factorizes, i.e., one has $\Phi_{t,0}^{12} = \Phi_{t,0}^1 \otimes \Phi_{t,0}^2$ if and only if

$$\kappa_{12}(t) = \kappa_1(t) \cdot \kappa_2(t) \qquad \text{and} \qquad \Lambda_{12}(t) = \kappa_1(t) \cdot \kappa_2(t)^* \tag{H.6}$$

hold which amounts to a factorizing distribution $|\alpha_{jk}|$. That is, $\Phi_{t,0}^{12}$ factorizes if and only if $|\alpha_{jk}|$ satisfies

$$|\alpha_{jk}|^2 = p_j \cdot q_k \ , \tag{H.7}$$

where $p_j = \sum_k |\alpha_{jk}|^2$ and $q_k = \sum_j |\alpha_{jk}|^2$ for all $j,k \in \{0,1\}$ as one directly observes.

On the contrary, the environmental state $|\chi'\rangle_{E_1E_2}$ is separable (cf. Eq. (2.28)) if and only if its coefficient matrix $\alpha = (\alpha_{jk})$ is rank deficient which is equivalent to $\det\alpha = 0$. Choosing $\alpha_{11} = \alpha_{00} = 1/2$ and $\alpha_{10} = -\alpha_{01} = 1/2$, this constraint is clearly violated (one readily deduces that $\det\alpha = 1/2$) but the coefficient matrix still satisfies condition (H.7) as one has $|\alpha_{jk}|^2 = 1/4$ for all indices j and k. Hence, this choice provides an example for a factorizing dynamics in the presence of an entangled state of the environment. Note that the associated environmental state for this example is even maximally entangled.

Appendix I

Coherence factors for nonlocal memory effects

In the following, the derivation of the coherence factors (5.17)–(5.20) is presented characterizing the dynamics of the model studied concerning nonlocal memory effects in Ch. 5. Assuming identical zero-mean two-mode Gaussian states with a covariance matrix

$$\boldsymbol{\sigma} = \begin{pmatrix} a_1 & 0 & c_1 & 0 \\ 0 & a_1 & 0 & c_2 \\ c_1 & 0 & a_2 & 0 \\ 0 & c_2 & 0 & a_2 \end{pmatrix} , \tag{I.1}$$

the characteristic function (5.11) reads

$$\begin{aligned} &\chi_{\rho_E}^{\sqrt{2}}\Big(([(-1)^r-(-1)^m]\vec{\beta}^{(1)}(t),[(-1)^s-(-1)^n]\vec{\beta}^{(2)}(t))\Big) \\ &= \prod_k \chi_{\rho_{\mathrm{G},k}}^{\sqrt{2}}\Big((\gamma_{k,rsmn}^{(1)}(t),\gamma_{k,rsmn}^{(2)}(t))\Big) \\ &= \exp\Big[-\sum_k\Big\{a_1|\gamma_{k,rsmn}^{(1)}(t)|^2 + a_2|\gamma_{k,rsmn}^{(2)}(t)|^2 \\ &\qquad + 2c_1\,\mathrm{Im}\big(\gamma_{k,rsmn}^{(1)}(t)\big)\cdot\mathrm{Im}\big(\gamma_{k,rsmn}^{(2)}(t)\big) \\ &\qquad + 2c_2\,\mathrm{Re}\big(\gamma_{k,rsmn}^{(1)}(t)\big)\cdot\mathrm{Re}\big(\gamma_{k,rsmn}^{(2)}(t)\big)\Big\}\Big] , \end{aligned} \tag{I.2}$$

where $\gamma_{k,r_1r_2m_1m_2}^{(j)}(t) \equiv [(-1)^{r_j}-(-1)^{m_j}]\beta_k^{(j)}(t)$. Starting from the definition of $\beta_k^{(j)}(t)$ (cf. Eq. (5.6)), one easily deduces that the following expressions

$$|\beta_k^{(j)}(t)|^2 = \left(\frac{g_k^{(j)}}{w_k^{(j)}}\right)^2 2\Big\{1-\cos\big(\omega_k^{(j)}t_j(t)\big)\Big\} , \tag{I.3}$$

$$\mathrm{Re}\big(\beta_k^{(j)}(t)\big) = \left(\frac{g_k^{(j)}}{w_k^{(j)}}\right)^2 \Big\{\cos\big(\omega_k^{(j)}t_j^s\big)-\cos\big(\omega_k^{(j)}(t_j(t)+t_j^s)\big)\Big\} , \tag{I.4}$$

$$\mathrm{Im}\big(\beta_k^{(j)}(t)\big) = \left(\frac{g_k^{(j)}}{w_k^{(j)}}\right)^2 \Big\{\sin\big(\omega_k^{(j)}t_j^s\big)-\sin\big(\omega_k^{(j)}(t_j(t)+t_j^s)\big)\Big\} . \tag{I.5}$$

It directly follows that $\kappa_1(t)$ and $\kappa_2(t)$ (cf. Eqs. (5.7) and (5.8) for their respective definitions) are determined by

$$\kappa_j(t) = e^{-2i\epsilon_j t}e^{-4a_j\sum_k|\beta_k^{(j)}(t)|^2} . \tag{I.6}$$

Performing the continuum limit for an ohmic spectral density $J_j(\omega) = \alpha_j \omega \cdot \exp[-\omega/\omega_c]$ with coupling strength α_j and cutoff frequency ω_c, one finds

$$\begin{aligned}\sum_k |\beta_k^{(j)}(t)|^2 &\to 2\alpha_j \int_0^\infty \mathrm{d}\omega\ e^{-\omega/\omega_c} \frac{1-\cos\big(\omega t_j(t)\big)}{\omega} \\ &= 2\alpha_j\, \mathcal{L}\left\{\frac{1-\cos\big(\omega t_j(t)\big)}{\omega}\right\}(1/\omega_c)\ , \end{aligned} \tag{I.7}$$

where $\mathcal{L}$ denotes the Laplace transform. By means of well-known fact that the Laplace transform of the function $f_y(t) = \big(1-\cos(yt)\big)/t$ evaluated at $s \neq 0$ is given by $\mathcal{L}\left\{f_y(t)\right\}(s) = \frac{1}{2}\ln(1+(y/s)^2)$ (cf. Eq. (5.15)) (Bronstein and Semendjajew, 1996), one finally obtains for the coherence factors $\kappa_1(t)$ and $\kappa_2(t)$ in the continuum limit

$$\kappa_j(t) = e^{-2i\epsilon_j t}\left\{1+\omega_c^2 t_j(t)^2\right\}^{-4a_j\alpha_j}\ . \tag{I.8}$$

To evaluate the characteristic function (I.2) for the two remaining coherence factors $\kappa_{12}(t)$ and $\Lambda_{12}(t)$ for a continuum of modes with an ohmic spectral density, one needs the relations for Laplace transforms of sinus-modulated functions,

$$\mathcal{L}\{\sin(xt)f(t)\}(s) = \frac{1}{2i}\{F(s-ix) - F(s+ix)\}\ , \tag{I.9}$$

as well as the following equation

$$\mathcal{L}\{f(t)/t\}(s) = \int_s^\infty \mathrm{dq}\ F(q)\ , \tag{I.10}$$

where F refers to the Laplace transform of the function f, i.e. one has $F(\cdot) = \mathcal{L}\{f(t)\}(\cdot)$. Employing that the Laplace transform of $\sin(yt)$ at s is known to be given by $y/(s^2+y^2)$, one deduces

$$\mathcal{L}\left\{\frac{\sin(yt)}{t}\right\}(s) = \int_s^\infty \mathrm{dq}\ \frac{y}{q^2+y^2} = \left[\arctan\Big(\frac{q}{y}\Big)\right]_s^\infty = \arctan\left(\frac{y}{s}\right)\ , \tag{I.11}$$

using Eq. (I.10) and the facts that $\frac{\pi}{2} - \arctan(s/y) = \operatorname{arccot}(s/y)$ holds and one has $\operatorname{arccot}(z) = \arctan(1/z)$ for any $z \neq 0$ (Bronstein and Semendjajew, 1996) which is satisfied here since $s = \omega_c^{-1} \neq 0$. By virtue of Eq. (I.9) and this result, it is thus found

$$\begin{aligned}\mathcal{L}\left\{\sin(xt)\frac{\sin(yt)}{t}\right\}(s) &= \frac{1}{2i}\left[\mathcal{L}\left\{\frac{\sin(yt)}{t}\right\}(s-ix) - \mathcal{L}\left\{\frac{\sin(yt)}{t}\right\}(s+ix)\right] \\ &= \frac{1}{2i}\left[\arctan\left(\frac{y}{s-ix}\right) - \arctan\left(\frac{y}{s+ix}\right)\right]\ . \end{aligned} \tag{I.12}$$

Clearly, $y/(s\pm ix)$ vanishes if and only if $y = 0$ and one has $\mathrm{Re}(y/(s\pm ix)) = ys/(s^2+x^2) \neq 0$ for any $y \neq 0$ because $s = \omega_c^{-1} \neq 0$. Therefore, the representation of arctan on $\mathbb{C}$ in terms of complex logarithms can be used. More precisely, one has

$$\arctan(z) = \frac{i}{2}\{\ln(1-iz) - \ln(1+iz)\}\ , \tag{I.13}$$

for any $z \in \mathbb{C} \setminus \{iy |\, y \in \mathbb{R}, |y| \geq 1\}$ where ln refers to some branch of the complex logarithm. It follows that Eq. (I.12) can be rewritten as

$$\begin{aligned}\mathcal{L}\left\{\sin(xt)\frac{\sin(yt)}{t}\right\}(s) &= \frac{1}{4}\ln\left(\frac{(s^2+x^2+xy)^2+(sy)^2}{(s^2+x^2-xy)^2+(sy)^2}\right)\\ &= \frac{1}{4}\ln\left(\frac{(x+y)^2+s^2}{(x-y)^2+s^2}\right)\,, \end{aligned} \tag{I.14}$$

Note that the logarithm in Eq. (I.14) refers to the usual real-valued logarithm obeying the well-known rules for multiplication and division. Choosing in Eq. (I.13) the principle branch of the logarithm which is defined by $\ln(z) = \ln|z| + i\arg(z) + 2\pi k i$ for $k = 0$, the purely imaginary contributions to Eq. (I.14) cancel out as one has $\arg(z^*) = -\arg(z)$.

Now, the coherence factors $\kappa_{12}(t)$ and $\Lambda_{12}(t)$, corresponding to $+$ and $-$ in the expression below, are determined by the characteristic function

$$\begin{aligned}&\chi_{\rho_E}^{\sqrt{2}}\Big((2\vec{\beta}^{\,(1)}(t), \pm 2\vec{\beta}^{\,(2)}(t))\Big)\\ &= \exp\Big[-4\sum_k\Big\{a_1|\beta_k^{(1)}(t)|^2 + a_2|\beta_k^{(2)}(t)|^2 \pm 2c_1\mathrm{Im}\big(\beta_k^{(1)}(t)\big)\cdot\mathrm{Im}\big(\beta_k^{(2)}(t)\big)\\ &\qquad\qquad \pm 2c_2\mathrm{Re}\big(\beta_k^{(1)}(t)\big)\cdot\mathrm{Re}\big(\beta_k^{(2)}(t)\big)\Big\}\Big]\,, \end{aligned} \tag{I.15}$$

which, upon inserting Eqs. (I.3)–(I.5) with $\omega_k^{(1)} = \omega_k^{(2)} = \omega_k$ and employing the identity $\cos(\alpha+\beta) = \cos(\alpha)\cos(\beta) - \sin(\alpha)\sin(\beta)$, reads

$$\begin{aligned}&\chi_{\rho_E}^{\sqrt{2}}\Big((2\vec{\beta}^{\,(1)}(t), \pm 2\vec{\beta}^{\,(2)}(t))\Big)\\ &= \exp\Big[-8\sum_k\Big\{\sum_{j=1}^{2}a_j\left(\frac{g_k^{(j)}}{\omega_k}\right)^2\big\{1-\cos\big(\omega_k t_1(t)\big)\big\}\\ &\qquad + \frac{g_k^{(1)}g_k^{(2)}}{\omega_k^2}\Big[\pm(c_+ - c_-)\prod_{j=1}^{2}\big\{\sin(w_k t_j^s) - \sin\big(\omega_k(t_j(t)+t_j^s)\big)\big\}\\ &\qquad\qquad \pm c_-\Big(\big\{\cos\big(w_k(t_1^s - t_2^s)\big) - 1\big\}\\ &\qquad\qquad\quad + \big\{1-\cos\big(\omega_k(t_1(t)+t_1^s-t_2^s)\big)\big\}\\ &\qquad\qquad\quad + \big\{1-\cos\big(\omega_k(t_2(t)+t_2^s-t_1^s)\big)\big\}\\ &\qquad\qquad\quad - \big\{1-\cos\big(\omega_k(t_1(t)-t_2(t)+t_1^s-t_2^s)\big)\big\}\Big)\Big]\\ &\qquad\Big\}\Big]\,. \end{aligned} \tag{I.16}$$

If the sum is replaced by the continuum of modes specified by an ohmic spectral densities $J(\omega)$, the exponent will consist of several Laplace transforms of the type of

$$\mathcal{L}\left\{\frac{1-\cos(yt)}{t}\right\}(s) \tag{I.17}$$

and

$$\mathcal{L}\left\{\sin(xt)\frac{\sin(yt)}{t}\right\}(s)\ , \tag{I.18}$$

which have been evaluated in Eqs. (I.7) and (I.14). By means of these results, one finally obtains the expressions for κ_{12} and Λ_{12} that are given in Eqs. (5.19) and (5.20) in the main text (see also Wißmann and Breuer (2014) for the expressions in case of $t_1^s = 0$).

Note that, choosing $\alpha_j = \alpha > 0$ and $a_j = -c_j = 1/2$ as well as $t_j^s = 0$ for either index j, one recovers the equations stated by Laine *et al.* (2012) for nonzero energy splitting ϵ_j. In fact, one deduces for the coherence factors in this case

$$\kappa_j(t) = \left\{1 + \omega_c^2 t_j(t)^2\right\}^{-2\alpha}\ , \tag{I.19}$$

$$\kappa_{12}(t) = e^{-2i(\epsilon_1+\epsilon_2)t}\left\{1 + \omega_c^2\big(t_1(t) - t_2(t)\big)^2\right\}^{-2\alpha}\ , \tag{I.20}$$

$$\Lambda_{12}(t) = e^{-4i\epsilon_2 t}\kappa_1(t)^2\kappa_2^*(t)^2\kappa_{12}(t)^{-1}\ . \tag{I.21}$$

It is, however, easily shown that the corresponding covariance matrix is unphysical[1] as it violates inequality (2.106). Moreover, the additional factors arising for consecutively applied interactions, implying that one has $t_2^s > 0$, have been ignored by Laine *et al.* (2013) leading to a significantly different dynamics.

It is worth stressing that the results are easily extended to complex-valued coupling strengths $g_k^{(j)}$ and covariance matrices that are not in standard form by means of the present techniques. In the general case, one encounters terms leading to the Laplace transform of cosine-modulated functions which are determined by

$$\mathcal{L}\{\cos(xt)f(t)\}(s) = \frac{1}{2}\{F(s - ix) + F(s + ix)\}\ . \tag{I.22}$$

Of course, the expression for the coherence factors comprise more and more terms making the derivation more involved.

[1] In fact, any 4×4-matrix of the form $\begin{pmatrix} \frac{1}{2}\mathbb{1}_2 & c\mathbb{1}_2 \\ c\mathbb{1}_2 & \frac{1}{2}\mathbb{1}_2 \end{pmatrix}$ is unphysical unless one has $c = 0$ for which the dynamics obviously factorizes.

Appendix J

Maximally correlating unitaries

In this part of the thesis, the unitary extension of the map (cf. Eq. (6.8))

$$U : |\phi_{jk}\rangle \otimes |\Phi\rangle \mapsto |\psi_{jk}\rangle \otimes |\Phi_j\rangle \ , \tag{J.1}$$

which characterizes the state transformation in a premeasurement of an observable A with spectral decomposition $A = \sum_{j=1}^{N_A} \sum_{k=1}^{n_j} a_j |\phi_{jk}\rangle\langle\phi_{jk}|$ using a pointer observable $B = \sum_{j=1}^{N_A} a_j |\Phi_j\rangle\langle\Phi_j|$ (cf. Sec. 6.1), is explicitly determined for a von Neumann-Lüders measurement, that is, where one has $|\psi_{jk}\rangle = |\phi_{jk}\rangle$ for any pair of indices (cf. Eq. (6.10)).

Note that the map (J.1) can be extended to a unitary operator on the joint Hilbert space $\mathcal{H}_{OP} = \mathcal{H}_O \otimes \mathcal{H}_P$ as $\{|\phi_{jk}\rangle \otimes |\Phi\rangle\}$ and $\{|\psi_{jk}\rangle \otimes |\Phi_j\rangle\}$ are orthonormal sets which may thus be extended to orthonormal bases of $\mathcal{H}_{OP}$. Any bijective map U between any two such bases satisfying Eq. (J.1) for all indices j and k can then be extended uniquely by linearity and continuity to a unitary operator on $\mathcal{H}_{OP}$. Note that one may similarly extend such a mapping via conjugate linearity leading to an antiunitary operator (Beltrametti *et al.*, 1990). Clearly, the unitary extension U' of U is only unique up to the choice of the orthonormal basis of $\mathcal{H}_{OP}$ comprising the sets $\{|\phi_{jk}\rangle \otimes |\Phi\rangle\}$ and $\{|\psi_{jk}\rangle \otimes |\Phi_j\rangle\}$.

The unitary may also be considered as resulting from two partial isometries. That is, the map U' on $\mathcal{H}_O \otimes \mathcal{H}_P$ is defined through

$$U'|_{\mathcal{W}} = U \ , \qquad U'|_{\mathcal{W}^\perp} = V \ , \tag{J.2}$$

where the closed subspace $\mathcal{W}$ of $\mathcal{H}_O \otimes \mathcal{H}_P$ is given by $\mathcal{W} = \mathcal{H}_O \otimes \mathrm{span}\{|\Phi\rangle\}$ and V defines a partial isometry with initial space $\mathcal{W}^\perp$ and final space $\mathrm{Im}(U)^\perp$. This means that $V^\dagger V$ defines a projection onto $\mathcal{W}$, whereas $VV^\dagger$ projects onto $\mathrm{Im}(U)^\perp$ (Conway, 2000). Similarly, U defines a partial isometry with initial space $\mathcal{W}$ and final space given by $\mathrm{Im}(U)$ which defines a closed subspace as one may easily show. Due to this, one has $\mathcal{H}_{OP} = \mathcal{W} \oplus \mathcal{W}^\perp = \mathrm{Im}(U) \oplus \mathrm{Im}(U)^\perp$ showing that U defined by Eq. (J.2) is surjective and satisfies $U^\dagger U = \mathbb{1}_{OP}$ which implies that it is indeed unitary. The nonuniqueness of the unitary extension U' can thus also be understood as arising from the partial isometry V which is arbitrary.

Despite the nonuniqueness, it is rather difficult, in general, to state an explicit expression for a partial isometry V and, thus, for the unitary extension of the map given by Eq. (J.1). However, for a von Neumann-Lüders measurement being characterized by the fact that $|\psi_{jk}\rangle = |\phi_{jk}\rangle$ holds for any pair of indices, this can

be done as is shown in the following: Let $g : \{1, \ldots, N_A\}^2 \to \{1, \ldots, N_A\}$ refer to a symmetric function for which $g(\cdot, k)$ is bijective for any index k and, moreover, it satisfies $g(j,k) \neq j$ and $g(j,k) \neq g(j,l)$ for all j and pairwise different indices k and l. Introducing the notation $\{|\tilde{\Phi}_k\rangle|\, k = 1 \ldots, N_A\}$ for the orthonormal basis $\{|\Phi\rangle\} \cup \{|\tilde{\Phi}_k\rangle|\, k = 2, \ldots, N_A\}$ of the probe Hilbert space $\mathcal{H}_P$, the linear operator

$$V = \sum_{k=2}^{N_A} \sum_{j=1}^{N_A} \Pi_{g(j,k)} \otimes |\Phi_j\rangle\langle\tilde{\Phi}_k| \;, \tag{J.3}$$

where $\Pi_{g(j,k)} \equiv \sum_{l=1}^{n_{g(j,k)}} |\phi_{g(j,k)l}\rangle\langle\phi_{g(j,k)l}|$ so that one has $U = \sum_{j=1}^{N_A} \Pi_j \otimes |\Phi_j\rangle\langle\tilde{\Phi}_1|$, defines a partial isometry with initial and final space given by $\mathrm{Im}(U)^\perp$ and $\mathcal{W}^\perp$, respectively. That is, it obeys $V^\dagger V = P_{\mathcal{W}^\perp}$ and $VV^\dagger = P_{\mathrm{Im}(U)^\perp}$ where P_X denotes to the projection onto the closed subspace X. Clearly, one has $V|_{\mathcal{W}} = 0$ and the projections onto $\mathcal{W}^\perp$ and $\mathrm{Im}(U)$ read

$$P_{\mathcal{W}^\perp} = \mathbb{1}_{\mathcal{H}_O} \otimes \sum_{j=2}^{N_A} |\tilde{\Phi}_j\rangle\langle\tilde{\Phi}_j| \;, \qquad P_{\mathrm{Im}(U)} = \sum_{j=1}^{N_A} \Pi_j \otimes |\Phi_j\rangle\langle\Phi_j| \;, \tag{J.4}$$

as one, e.g., finds

$$P_{\mathrm{Im}(U)} U = \sum_{j,k=1}^{N_A} \Pi_k \Pi_j \otimes |\Phi_k\rangle\langle\Phi_k|\Phi_j\rangle\langle\tilde{\Phi}_1| = U \tag{J.5}$$

due to the orthogonality of the elements $|\Phi_j\rangle$ and the fact that the operators Π_k define projections.

To show that $\mathrm{Im}(V) \perp \mathrm{Im}(U)$ holds, one first considers the scalar product for states $|\phi'\rangle \otimes |\varphi\rangle \in \mathcal{W}^\perp$ and $|\phi\rangle \otimes |\tilde{\Phi}_1\rangle \in \mathcal{W}$ where $|\phi\rangle$ and $|\phi'\rangle$ refer to states on $\mathcal{H}_O$ and one has $|\varphi\rangle = \sum_{k=2}^{N_A} t_k |\tilde{\Phi}_k\rangle$ with $\sum_k |t_k|^2 = 1$. In fact, one then obtains

$$\begin{aligned} \langle\phi'| \otimes \langle\varphi|V^\dagger U|\phi\rangle \otimes |\tilde{\Phi}_1\rangle &= \sum_{k=2}^{N_A} \sum_{j,l=1}^{N_A} t_k^* \langle\phi'|\Pi_{g(j,k)}\Pi_l|\phi\rangle\langle\tilde{\Phi}_j|\Phi_l\rangle \\ &= \sum_{k=2}^{N_A} \sum_{j=1}^{N_A} t_k^* \langle\phi'|\Pi_{g(j,k)}\Pi_j|\phi\rangle = 0 \;, \end{aligned} \tag{J.6}$$

as one has $g(j,k) \neq j$ for any index k by assumption. Due to linearity of the map V and the scalar product, this finally implies $\langle\tilde{\phi}'|V^\dagger U|\phi\rangle \otimes |\tilde{\Phi}_1\rangle = 0$ for all $|\phi\rangle \in \mathcal{H}_O$ and $|\tilde{\phi}'\rangle \in \mathcal{W}^\perp$ showing that $\mathrm{Im}(V) \perp \mathrm{Im}(U)$.

Moreover, since $g(\cdot, k)$ defines a bijection for any index k, too, and one has $g(j,k) \neq g(j,l)$ for any j and pairwise different indices k and l, one deduces

$$\begin{aligned} V^\dagger V &= \sum_{k,l=2}^{N_A} \sum_{i,j=1}^{N_A} \Pi_{g(j,k)}\Pi_{g(i,l)} \otimes |\tilde{\Phi}_k\rangle\langle\Phi_j|\Phi_i\rangle\langle\tilde{\Phi}_l| \\ &= \sum_{k=2}^{N_A} \sum_{j=1}^{N_A} \Pi_{g(j,k)} \otimes |\tilde{\Phi}_k\rangle\langle\tilde{\Phi}_k| \\ &= \mathbb{1}_{\mathcal{H}_O} \otimes \sum_{k=2}^{N_A} |\tilde{\Phi}_k\rangle\langle\tilde{\Phi}_k| = P_{\mathcal{W}^\perp} \;, \end{aligned} \tag{J.7}$$

and, similarly,

$$\begin{aligned} VV^\dagger &= \sum_{k,l=2}^{N_A} \sum_{i,j=1}^{N_A} \Pi_{g(i,l)} \Pi_{g(j,k)} \otimes |\Phi_i\rangle\langle\tilde{\Phi}_l|\tilde{\Phi}_k\rangle\langle\Phi_j| \\ &= \sum_{k=2}^{N_A} \sum_{j=1}^{N_A} \Pi_{g(j,k)} \otimes |\Phi_j\rangle\langle\Phi_j| \\ &= \sum_{j=1}^{N_A} (\mathbb{1}_{\mathcal{H}_O} - \Pi_j) \otimes |\Phi_j\rangle\langle\Phi_j| \\ &= \mathbb{1}_{\mathcal{H}_O \otimes \mathcal{H}_P} - \sum_{j=1}^{N_A} \Pi_j \otimes |\Phi_j\rangle\langle\Phi_j| = P_{\mathrm{Im}(U)^\perp} \ . \end{aligned} \tag{J.8}$$

Hence, one concludes that V defines a partial isometry with initial space $\mathcal{W}^\perp$ and final space $\mathrm{Im}(U)^\perp$. The unitary operator U' extending the partial isometry U is thus given by (cf. Eq. (6.10))

$$U' = U + V = \sum_{j,k=1}^{N_A} \Pi_{g(j,k)} \otimes |\Phi_j\rangle\langle\tilde{\Phi}_k| \ , \tag{J.9}$$

which is obviously unitary.

Note that the function g can, for example, be chosen as $g(j,k) = [j+k-2]_{N_A}$ where $[\cdot]_{N_A}$ defines the coset with respect to division by N_A. Clearly, $g(\cdot,k)$ represents a bijection for arbitrary k and one has $[j+k-2]_{N_A} \neq j$ as well as $[j+k-2]_{N_A} \neq [j+l-2]_{N_A}$ for any indices $j,k,l \in \{1,\ldots,N_A\}$ if k and l are pairwise different.

Appendix K

Heisenberg equations of motion

Here, the Heisenberg equations of motion for the representatives of the SU(N)-generators as well as the canonical operators for uncoupled and interacting quantum object and probe are proven (see Eqs. (6.58), (6.62), (6.64) and (6.65)) which are used in Sec. 6.3 to derive a dynamical probing scheme being characterized by the convergence of expectation values.

First, consider the evolution of the generators $\hat{\Sigma}$ with respect to the free evolution generated by $H_O = \vec{\alpha}_H^T \hat{\Sigma}$. As neither quantity depends explicitly on time, the dynamical equation of the jth component of $\hat{\Sigma}(t) = \exp[itH_O]\hat{\Sigma}\exp[-itH_O]$, which is understood component-by-component, reads

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\hat{\Sigma}_j(t) &= -i\,[\hat{\Sigma}_j(t), \vec{\alpha}_H^T\hat{\Sigma}] \\ &= -i\sum_{k=0}^{N^2-1} e^{itH_O}\,[\hat{\Sigma}_j, \alpha_{H,k}\hat{\Sigma}_k]\,e^{-itH_O} \\ &= 2\sum_{k,l=0}^{N^2-1} f_{jkl}\,\alpha_{H,k}\,\hat{\Sigma}_l(t) = -2\big(\Theta(\vec{\alpha}_H)\hat{\Sigma}(t)\big)_j\ , \end{aligned} \tag{K.1}$$

employing the commutation relation (6.60) for the representatives of SU(N)-generators along with the definition of the mapping Θ (see Eq. (6.61)). Note that due to the antisymmetric property of the structure constant f_{jkl} of the SU(N)-algebra, it follows that for any $\vec{\alpha}, \vec{\alpha}' \in \mathbb{R}^{N^2-1}$ one has

$$\big(\Theta(\vec{\alpha})\vec{\alpha}'\big)_j = \sum_{k,l=0}^{N^2-1} f_{jkl}\alpha_l\alpha'_k = -\sum_{k,l=0}^{N^2-1} f_{jlk}\alpha'_k\alpha_l = -\big(\Theta(\vec{\alpha}')\vec{\alpha}\big)_j\ , \tag{K.2}$$

which thus implies $\Theta(\vec{\alpha})\vec{\alpha} = 0$.

Moreover, for the time evolution of the canonical operators $\hat{X}$ with respect to $H_P = \hat{X}^T R\hat{X}$ where R refers to a symmetric 2×2-matrix over the reals, one

deduces

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\hat{X}_j(t) &= -i[\hat{X}_j(t), H_P] \\ &= -i\sum_{k,l=1}^{2} R_{kl}\, e^{itH_P}\left\{\hat{X}_j\hat{X}_k\hat{X}_l - \hat{X}_k\hat{X}_l\hat{X}_j\right\} e^{-itH_P} \\ &= -i\sum_{k,l=1}^{2} R_{kl}\left\{i(\Omega_2)_{jk}\hat{X}_l(t) - i(\Omega_2)_{lj}\hat{X}_k(t)\right\} \\ &= 2\big(\Omega_2 R\hat{X}(t)\big)_j\ , \end{aligned} \tag{K.3}$$

by virtue of the canonical commutation relations $[\hat{X}_j, \hat{X}_k] = i(\Omega_2)_{jk}$ (see also Sec. 2.5.1).

To show Eqs. (6.64) and (6.65), i.e., the evolution equations for the generators $\hat{\Sigma}$ and the canonical operators $\hat{X}$ when the quantum object and the probe interact, which is described by the Hamiltonian $H_I = \vec{\alpha}_I^T\hat{\Sigma}\otimes\vec{\beta}_I^T\hat{X}$ for $\vec{\alpha}_I \in \mathbb{R}^{N^2-1}$ and $\vec{\beta}_I \in \mathbb{R}^2$, one proceeds as before after having separated the free part and the interaction of the Hamiltonian. More precisely, one finds

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\hat{\Sigma}_j(t) &= -i\big\{[\hat{\Sigma}_j(t), H_O\otimes\mathbb{1}_P] + [\hat{\Sigma}_j(t), H_I]\big\} \\ &= -2\big(\Theta(\vec{\alpha}_H)\hat{\Sigma}(t)\big)_j - i\sum_{k=0}^{N^2-1}\sum_{l=1}^{2} e^{itH}[\hat{\Sigma}_j, \alpha_{I,k}\hat{\Sigma}_k]\otimes\beta_{I,l}\hat{X}_l e^{-itH} \\ &= -2\big\{\big(\Theta(\vec{\alpha}_H)\hat{\Sigma}(t)\big)_j + \big(\Theta(\vec{\alpha}_I)\hat{\Sigma}(t)\big)_j\,\big(\vec{\beta}_I^T\hat{X}(t)\big)\big\}\ , \end{aligned} \tag{K.4}$$

and, similarly,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\hat{X}_j(t) &= -i\big\{[\hat{X}_j(t), \mathbb{1}_O\otimes H_P] + [\hat{X}_j(t), H_I]\big\} \\ &= 2\big(\Omega_2 R\hat{X}(t)\big)_j - i\sum_{k=0}^{N^2-1}\sum_{l=1}^{2} e^{itH}\alpha_{I,k}\hat{\Sigma}_k\otimes[\hat{X}_j, \beta_{I,l}\hat{X}_l]e^{-itH} \\ &= 2\big(\Omega_2 R\hat{X}(t)\big)_j + \big(\vec{\alpha}_I^T\hat{\Sigma}(t)\big)\big(\Omega_2\vec{\beta}_I\big)_j\ , \end{aligned} \tag{K.5}$$

which exactly is Eq. (6.64) and (6.65), respectively.

Appendix L

Contact potential for Bogoliubov modes

In this section the interaction Hamiltonian is derived for the coupling of an impurity atom that is immersed at a specific site of a lattice of cold atoms describing a Bose-Hubbard model in the superfluid phase. More specifically, the interaction Hamiltonian (cf. Eq. (6.124))

$$H_I = g \sum_{\vec{m}\neq\vec{n}\in\mathbb{N}_0^3} \phi_{\vec{m}\vec{n}} |\vec{m}\rangle\langle\vec{n}| \otimes \Big[n_0 + \sum_{k\neq 0} \beta_k (\hat{b}_k^\dagger + \hat{b}_k) \Big] \,, \tag{L.1}$$

where

$$\beta_k = \sqrt{\frac{n_0}{N_S}} \{ |u_k| - |v_k| \} \,, \tag{L.2}$$

$$|v_k|^2 = |u_k|^2 - 1 = \frac{1}{2} \{ (\epsilon_k + U n_0)/\omega_k - 1 \} \,, \tag{L.3}$$

is deduced, starting from the interaction

$$\tilde{H}_I = g \sum_{\vec{m}\neq\vec{n}\in\mathbb{N}_0^3} \sum_{j,k=1}^{N_S} \int_{\mathbb{R}^3} \mathrm{d}\vec{x}\; \psi_{\vec{n}}^*(\vec{x}) \psi_{\vec{m}}(\vec{x})\, W_j^*(x_1) W_k(x_1) |\vec{m}\rangle\langle\vec{n}| \otimes \hat{a}_j^\dagger \hat{a}_k \,, \tag{L.4}$$

that represents a density-density coupling of an impurity atom, described by a three-dimensional harmonic oscillator with eigenstates $|\vec{m} = (m_1, m_2, m_2)\rangle$ and the lattice of cold atoms with the assumption of a contact potential and a localized immersed atom at site j_0 as considered by Cosco *et al.* (2015). Here, $\psi_{\vec{m}}(\vec{x} = (x_1, x_2, x_3)) = \langle \vec{x}\,|\vec{m}\rangle$ denotes the wave function of the impurity's energy eigenstate $|\vec{m}\rangle$ and $W_j(x_1)$ refers to the Wannier function at the jth site of the lattice which extends along the x_1-axis.

Due to the assumption that the impurity is localized at site j_0, the immersed atom does not couple to sites different from that labeled by j_0. As a consequence, Eq. (L.4) reads

$$\tilde{H}_I = g \sum_{\vec{m}\neq\vec{n}\in\mathbb{N}_0^3} \phi_{\vec{m}\vec{n}} |\vec{m}\rangle\langle\vec{n}| \otimes \hat{a}_{j_0}^\dagger \hat{a}_{j_0} \,, \tag{L.5}$$

where one defines $\phi_{\vec{m}\vec{n}} \equiv \int_{\mathbb{R}^3} \mathrm{d}\vec{x}\; \psi_{\vec{n}}^*(\vec{x}) \psi_{\vec{m}}(\vec{x})\, |W_{j_0}^*(x_1)|^2$. By comparison with Eq. (L.1), one thus needs to determine the on-site number operator $\hat{a}_{j_0}^\dagger \hat{a}_{j_0}$ in terms

of the Bogoliubov modes characterizing the superfluid phase in order to deduce the interaction Hamiltonian H_I given in Eq. (L.1).

Following van Oosten *et al.* (2001), one first transforms the on-site creation and annihilation operators into momentum space. That is, one introduces creation and annihilation operators $\hat{c}_k^\dagger$ and $\hat{c}_k$, respectively, satisfying

$$\hat{a}_j = \frac{1}{\sqrt{N_S}} \sum_k \hat{c}_k e^{-ikr_j} \ , \tag{L.6}$$

$$\hat{a}_j^\dagger = \frac{1}{\sqrt{N_S}} \sum_k \hat{c}_k^\dagger e^{ikr_j} \ , \tag{L.7}$$

where N_S refers to the number of lattice sites (cf. Eq. (L.4)) and r_j defines the coordinate of site j. For a one-dimensional lattice with lattice constant a, one may thus set $r_j = j \cdot a$ so that the k-vectors, running over the first Brillouin zone of the lattice, are given by

$$k = \frac{2\pi}{aN_S} \cdot j \ , \tag{L.8}$$

where the index j obeys

$$j = \begin{cases} 0, \pm 1, \ldots, \pm(N_S - 1)/2 \ , & \text{if } N_S \text{ is odd} \ , \\ 0, \pm 1, \ldots, \pm(N_S/2 - 1), N_S/2 \ , & \text{if } N_S \text{ is even} \ . \end{cases} \tag{L.9}$$

Due to this one has $\sum_j \exp[-i(k - k')r_j] = N_S \delta_{k,k'}$. Employing the definitions (L.6) and (L.7), an on-site number operator may be equivalently written as

$$\hat{a}_j^\dagger \hat{a}_j = \frac{1}{N_S} \sum_{k,k'} \hat{c}_k^\dagger \hat{c}_{k'} e^{ir_j(k-k')} \ . \tag{L.10}$$

According to Bogoliubov's treatment originating from the theory of superfluidity, the Bose-Einstein condensation, which occurs in the mode $k = 0$ for a perfect Bose gas, is expected to persist also for sufficiently weak interactions and, therefore, the most relevant terms in Eq. (L.10) are those containing creation and annihilation operators associated with the zero mode (see Adams and Bru (2004) and references therein). This thus leads to

$$\hat{a}_j^\dagger \hat{a}_j \simeq \frac{1}{N_S} \Big[\hat{c}_0^\dagger \hat{c}_0 + \sum_{k \neq 0} \{ \hat{c}_k^\dagger \hat{c}_0 e^{ir_j k} + \hat{c}_0^\dagger \hat{c}_k e^{-ir_j k} \} \Big] \ , \tag{L.11}$$

where the sum extends over all nonzero k-vectors. For a large number of atoms in the condensate, i.e. $N_0 = \langle \hat{c}_0^\dagger \hat{c}_0 \rangle \gg 1$, one may furthermore employ the so-called Bogoliubov approximation, replacing the zero-mode operators by complex numbers (Adams and Bru, 2004). More specifically, substituting $\hat{c}_0^\dagger = \hat{c}_0 = \sqrt{N_S}$ in Eq. (L.11), the on-site number operator reads

$$\hat{a}_j^\dagger \hat{a}_j \simeq \frac{1}{N_S} \Big[N_0 + \sqrt{N_0} \sum_{k \neq 0} \{ \hat{c}_k^\dagger e^{ir_j k} + \hat{c}_k e^{-ir_j k} \} \Big] \ . \tag{L.12}$$

It remains to apply the Bogoliubov transformation which yields creation and annihilation operators $\hat{b}_k^\dagger$ and $\hat{b}_k$, respectively, with respect to which the Bose-Hubbard Hamiltonian is diagonal. According to van Oosten *et al.* (2001), these new bosonic operators are defined by

$$\begin{pmatrix} \hat{b}_k \\ \hat{b}_{-k}^\dagger \end{pmatrix} = \begin{pmatrix} u_k & v_k \\ v_k^* & u_k^* \end{pmatrix} \begin{pmatrix} \hat{c}_k \\ \hat{c}_{-k}^\dagger \end{pmatrix} \equiv B \begin{pmatrix} \hat{c}_k \\ \hat{c}_{-k}^\dagger \end{pmatrix} \ , \tag{L.13}$$

where the Bogoliubov coefficients must obey $|u_k|^2 - |v_k|^2 = 1$ in order to preserve the canonical commutation relations (cf. Eq. (2.91)) (see also Landau and Lifschitz (1992)). The inverse transformation is then clearly given by

$$\begin{pmatrix} \hat{c}_k \\ \hat{c}_{-k}^\dagger \end{pmatrix} = B^{-1} \begin{pmatrix} \hat{b}_k \\ \hat{b}_{-k}^\dagger \end{pmatrix} = \begin{pmatrix} u_k^* \hat{b}_k - v_k \hat{b}_{-k}^\dagger \\ u_k \hat{b}_{-k}^\dagger - v_k^* \hat{b}_k \end{pmatrix} \ , \tag{L.14}$$

as one has $B^{-1} = \left(\begin{smallmatrix} u_k^* & -v_k \\ -v_k^* & u_k \end{smallmatrix} \right)$. Upon inserting this into Eq. (L.12) and using the definition $n_0 \equiv N_0/N_S$, one obtains

$$\hat{a}_j^\dagger \hat{a}_j \simeq n_0 + \sqrt{\frac{n_0}{N_S}} \sum_{k \neq 0} (\hat{b}_k^\dagger e^{i r_j k} \{u_k - v_{-k}\} + \hat{b}_k e^{-i r_j k} \{u_k^* - v_{-k}^*\}) \ . \tag{L.15}$$

Note that the Bogoliubov coefficients are independent of the sign of the k-vector, i.e., they satisfy $u_k = u_{-k}$ and $v_k = v_{-k}$, which is easily found by taking the adjoint of the expression for $\hat{c}_k$ and $\hat{c}_{-k}^\dagger$ and changing the index from k to $-k$. Moreover, the coefficients are the solution to the equations ($\hbar = 1$)

$$\Big[(u_k)^2 + (v_k)^2 \Big] U n_0 - 2 u_k v_k (\epsilon_k + U n_0) = 0 \ , \tag{L.16}$$

$$\Big[|u_k|^2 + |v_k|^2 \Big] (\epsilon_k + U n_0) - U n_0 (u_k^* v_k + u_k v_k^*) = \omega_k \ , \tag{L.17}$$

which originate from the diagonalization of the Bose-Hubbard Hamiltonian that amounts to the relation

$$(B^{-1})^\dagger \begin{pmatrix} \epsilon_k + U n_0 & U n_0 \\ U n_0 & \epsilon_k + U n_0 \end{pmatrix} B^{-1} = \begin{pmatrix} \omega_k & 0 \\ 0 & \omega_{-k} \end{pmatrix} \ , \tag{L.18}$$

where $\epsilon_k \equiv 2J[1 - \cos(ka)]$. As, e.g., shown by van Oosten *et al.* (2001), a solution to Eqs. (L.16) and (L.17) is given by

$$\omega_k = \sqrt{\epsilon_k (\epsilon_k + 2 U n_0)} \ , \tag{L.19}$$

$$|v_k|^2 = |u_k|^2 - 1 = \frac{1}{2} \Big\{ \frac{\epsilon_k + U n_0}{\omega_k} - 1 \Big\} \ , \tag{L.20}$$

where one easily deduces for the phases of the Bogoliubov coefficients

$$\arg(u_k) = \arg(v_k) \tag{L.21}$$

upon inserting Eqs. (L.19) and (L.20) into Eq. (L.17). Because this constraint is also consistent with Eq. (L.16), one concludes that the coefficients may have arbitrary but equal phases.

Thus, choosing $\arg(u_k) = -r_{j_0}k$ and employing that $v_{-k} = v_k$ holds, Eq. (L.15) is ultimately written as

$$\hat{a}_{j_0}^\dagger \hat{a}_{j_0} \simeq n_0 + \sqrt{\frac{n_0}{N_S}} \sum_{k\neq 0} \{|u_k| - |v_k|\}(\hat{b}_k^\dagger + \hat{b}_k) \ , \tag{L.22}$$

which finally leads to the Hamiltonian (L.1) when inserted into the Hamiltonian (L.5). Note that Cosco *et al.* (2015) deduced and used the incorrect expression for $\beta_k = \sqrt{n_0/N_S}\{|u_k| - |v_k|\}$ where the minus sign has been replaced by a plus sign.

List of Figures

Bibliography

Accardi, L., Frigerio, A. and Lewis, J. T. *Quantum stochastic processes.* Publ. RIMS, Kyoto Univ. **18**, 97–133 (1982).

Adams, S. and Bru, J.-B. *Critical analysis of the Bogoliubov theory of superfluidity.* Physica A **332**, 60–78 (2004).

Addis, C., Haikka, P., McEndoo, S., Macchiavello, C. and Maniscalco, S. *Two-qubit non-Markovianity induced by a common environment.* Phys. Rev. A **87**, 052109 (2013).

Addis, C., Bylicka, B., Chruściński, D. and Maniscalco, S. *Comparative study of non-Markovianity measures in exactly solvable one- and two-qubit models.* Phys. Rev. A **90**, 052103 (2014).

Adesso, G. *Entanglement of Gaussian states.* Ph.D. thesis, Università degli Studi di Salerno (2006).

Adesso, G. and Datta, A. *Quantum versus classical correlations in Gaussian states.* Phys. Rev. Lett. **105**, 030501 (2010).

Albeverio, S. and Fei, S.-M. *A note on invariants and entanglements.* J. Opt. B: Quantum Semiclass. Opt. **3**, 223 (2001).

Ali, M. M., Lo, P.-Y., Tu, M. W.-Y. and Zhang, W.-M. *Non-Markovianity measure using two-time correlation functions.* Phys. Rev. A **92**, 062306 (2015).

Alicki, R. *Comment on "Reduced dynamics need not be completely positive".* Phys. Rev. Lett. **75**, 3020–3020 (1995).

Ando, T. and Choi, M.-D. *Non-linear completely positive maps.* In U. S. R. Nagel and M. Wolff (eds.), *Aspects of Positivity in Functional AnalysisProceedings of the Conference held on the Occasion of H.H. Schaefer's 60th Birthday*, vol. 122 of *North-Holland Mathematics Studies*, pp. 3–13. North-Holland (1986).

Apollaro, T. J. G., Di Franco, C., Plastina, F. and Paternostro, M. *Memory-keeping effects and forgetfulness in the dynamics of a qubit coupled to a spin chain.* Phys. Rev. A **83**, 032103 (2011).

Arnold, V. I. *Mathematical Methods of Classical Mechanics*, vol. 60 of *Graduate Texts in Mathematics.* Springer-Verlag New York, 2nd ed. (1997). Translated by K. Vogtmann and A. Weinstein.

Arveson, W. B. *Subalgebras of C^*-algebras.* Acta Math. **123**, 141–224 (1969).

Arvind, Dutta, B., Mukunda, N. and Simon, R. *The real symplectic groups in quantum mechanics and optics.* Pramana **45**, 471–497 (1995).

Ban, M., Kitajima, S. and Shibata, F. *Reduced dynamics and the master equation of open quantum systems.* Phys. Lett. A **374**, 2324–2330 (2010).

Bell, J. *Speakable and Unspeakable in Quantum Mechanics.* Collected Papers on Quantum Philosophy. Cambridge University Press, 2nd ed. (1987).

Beltrametti, E. G., Cassinelli, G. and Lahti, P. J. *Unitary measurements of discrete quantities in quantum mechanics.* J. Math. Phys. **31**, 91–98 (1990).

Bengtsson, I. and Zyczkowski, K. *Geometry of Quantum States.* Cambridge University Press (2007).

Bennett, C. H., DiVincenzo, D. P., Smolin, J. A. and Wootters, W. K. *Mixed-state entanglement and quantum error correction.* Phys. Rev. A **54**, 3824–3851 (1996).

Berry, M. V. *Quantal phase factors accompanying adiabatic changes.* Proc. R. Soc. Lond. A **392**, 45–57 (1984).

Blackadar, B. *Operator Algebras: Theory of C^*–Algebras and von Neumann Algebras*, vol. 122 of *Encyclopaedia of Mathematical Sciences.* Springer-Verlag Berlin Heidelberg, 1st ed. (2006).

Borrelli, M., Haikka, P., De Chiara, G. and Maniscalco, S. *Non-markovian qubit dynamics induced by coulomb crystals.* Phys. Rev. A **88**, 010101 (2013).

Bosch, S. *Algebra.* Springer-Lehrbuch. Springer-Verlag Berlin Heidelberg, 7th ed. (2009).

Botero, A. and Reznik, B. *Modewise entanglement of Gaussian states.* Phys. Rev. A **67**, 052311 (2003).

Braginsky, V. B., Khalili, F. Y. and Thorne, K. S. *Quantum Measurement.* Cambridge University Press (1992).

Braunstein, S. L. and Caves, C. M. *Statistical distance and the geometry of quantum states.* Phys. Rev. Lett. **72**, 3439–3443 (1994).

Breuer, H.-P. *Foundations and measures of quantum non-Markovianity.* J. Phys. B: At. Mol. Opt. Phys. **45**, 154001 (2012a).

Breuer, H.-P. *Counterexample* (2012b). Private communication.

Breuer, H.-P. and Petruccione, F. *The Theory of Open Quantum Systems.* Oxford University Press (2002). Reprint: 2010.

Breuer, H.-P., Kappler, B. and Petruccione, F. *Stochastic wave-function method for non-Markovian quantum master equations.* Phys. Rev. A **59**, 1633–1643 (1999).

Breuer, H.-P., Burgarth, D. and Petruccione, F. *Non-Markovian dynamics in a spin star system: Exact solution and approximation techniques.* Phys. Rev. B **70**, 045323 (2004).

Breuer, H.-P., Laine, E.-M. and Piilo, J. *Measure for the degree of non-Markovian behavior of quantum processes in open systems.* Phys. Rev. Lett. **103**, 210401 (2009).

Breuer, H.-P., Laine, E.-M., Piilo, J. and Vacchini, B. *Colloquium : Non-Markovian dynamics in open quantum systems.* Rev. Mod. Phys. **88**, 021002 (2016).

Briet, J. and Harremoës, P. *Properties of classical and quantum Jensen-Shannon divergence.* Phys. Rev. A **79**, 052311 (2009).

Brodutch, A., Datta, A., Modi, K., Rivas, A. and Rodríguez-Rosario, C. A. *Vanishing quantum discord is not necessary for completely positive maps.* Phys. Rev. A **87**, 042301 (2013).

Bronstein, I. and Semendjajew, K. *Teubner-Taschenbuch der Mathematik.* B.G. Teubner Verlagsgesellschaft Leipzig (1996).

Bures, D. J. C. *An extension of Kakutani's theorem on infinite product measures to the tensor product of semifinite w*-algebras.* Trans. Amer. Math. Soc. **135**, 199–212 (1969).

Burkard, R., Dell'Amico, M. and Martello, S. *Assignment Problems.* SIAM Philadelphia (2009).

Buscemi, F. *Channel correction via quantum erasure.* Phys. Rev. Lett. **99**, 180501 (2007).

Buscemi, F., Hayashi, M. and Horodecki, M. *Global information balance in quantum measurements.* Phys. Rev. Lett. **100**, 210504 (2008).

Buscemi, F., Hall, M. J. W., Ozawa, M. and Wilde, M. M. *Noise and disturbance in quantum measurements: An information-theoretic approach.* Phys. Rev. Lett. **112**, 050401 (2014).

Busch, P., Lahti, P. and Mittelstaedt, P. *The Quantum Theory of Measurement.* Lecture Notes in Physics. Springer-Verlag Berlin Heidelberg, 2nd ed. (1996).

Busch, P., Lahti, P. and Werner, R. F. *Proof of Heisenberg's error-disturbance relation.* Phys. Rev. Lett. **111**, 160405 (2013).

Busch, P., Lahti, P. and Werner, R. F. *Measurement uncertainty relations.* J. Math. Phys. **55**, 042111 (2014a).

Busch, P., Lahti, P. and Werner, R. F. *Colloquium : Quantum root-mean-square error and measurement uncertainty relations.* Rev. Mod. Phys. **86**, 1261–1281 (2014b).

Bylicka, B., Chruściński, D. and Maniscalco, S. *Non-Markovianity and reservoir memory of quantum channels: a quantum information theory perspective.* Sci. Rep. **4**, 5720 (2014).

Byrd, M. S. and Khaneja, N. *Characterization of the positivity of the density matrix in terms of the coherence vector representation.* Phys. Rev. A **68**, 062322 (2003).

Cahill, K. E. and Glauber, R. J. *Ordered expansions in boson amplitude operators.* Phys. Rev. **177**, 1857–1881 (1969).

Mendonça, P. E. M. F., Napolitano, R. d. J., Marchiolli, M. A., Foster, C. J. and Liang, Y.-C. *Alternative fidelity measure between quantum states.* Phys. Rev. A **78**, 052330 (2008).

Chaturvedi, S. and Shibata, F. *Time-convolutionless projection operator formalism for elimination of fast variables. Applications to Brownian motion.* Z. Phys. B **35**, 297–308 (1979).

Chen, K., Albeverio, S. and Fei, S.-M. *Concurrence of arbitrary dimensional bipartite quantum states.* Phys. Rev. Lett. **95**, 040504 (2005).

Choi, M. *Completely positive linear maps on complex matrices.* Linear Algebra Appl. **10**, 285–290 (1975).

Choi, M. D. *Positive linear maps on C^*-algebras.* Canad. J. Math. **24**, 520–529 (1972).

Chruściński, D. and Kossakowski, A. *Non-Markovian quantum dynamics: Local versus nonlocal.* Phys. Rev. Lett. **104**, 070406 (2010).

Chruściński, D. and Kossakowski, A. *Markovianity criteria for quantum evolution.* J. Phys. B: At. Mol. Opt. Phys. **45**, 154002 (2012).

Chruściński, D. and Maniscalco, S. *Degree of non-Markovianity of quantum evolution.* Phys. Rev. Lett. **112**, 120404 (2014).

Chruściński, D. and Wudarski, F. A. *Non-Markovian random unitary qubit dynamics.* Phys. Lett. A **377**, 1425–1429 (2013).

Chruściński, D. and Wudarski, F. A. *Non-Markovianity degree for random unitary evolution.* Phys. Rev. A **91**, 012104 (2015).

Chruściński, D., Kossakowski, A. and Rivas, A. *Measures of non-Markovianity: Divisibility versus backflow of information.* Phys. Rev. A **83**, 052128 (2011).

Coffman, V., Kundu, J. and Wootters, W. K. *Distributed entanglement.* Phys. Rev. A **61**, 052306 (2000).

Conway, J. B. *A Course in Operator Theory.* American Mathematical Society, Providence, RI, 1st ed. (2000).

Cosco, F. *Detection of superfluid excitations via local quantum probing* (2016). Private communication.

Cosco, F., Borelli, M., Plastina, F. and S. Maniscalco, S. *Detection of superfluid excitations via local quantum probing.* arXiv: 1511.00833(v1) [quant-ph] (2015).

Dajka, J., Łuczka, J. and Hänggi, P. *Distance between quantum states in the presence of initial qubit-environment correlations: A comparative study.* Phys. Rev. A **84**, 032120 (2011).

Davies, E. B. *Markovian master equations.* Commun. math. Phys. **39**, 91–110 (1974).

Davies, E. B. *Markovian master equations. II.* Math. Ann. **219**, 147–158 (1976).

Dhar, H. S., Bera, M. N. and Adesso, G. *Characterizing non-Markovianity via quantum interferometric power.* Phys. Rev. A **91**, 032115 (2015).

Dickson, L. E. *Elementary Theory of Equations.* John Wiley & Sons, Inc. (1914).

DiVincenzo, D. P. *Two-bit gates are universal for quantum computation.* Phys. Rev. A **51**, 1015–1022 (1995).

Dobrushin, L. *Prescribing a system of random variables by conditional distributions.* Theory Probab. Appl. **15**, 458–486 (1970).

Doll, R., Zueco, D., Wubs, M., Kohler, S. and Hänggi, P. *On the conundrum of deriving exact solutions from approximate master equations.* Chem. Phys. **347**, 243–249 (2008).

Dominy, J. M. and Lidar, D. A. *Beyond complete positivity.* Quantum Inf. Process. **15**, 1349–1360 (2016).

Dominy, J. M., Shabani, A. and Lidar, D. A. *A general framework for complete positivity.* Quantum Inf. Process. **15**, 465–494 (2016).

Dragt, A. J. *The symplectic group and classical mechanics.* Annals of the New York Academy of Sciences **1045**, 291–307 (2005).

Einstein, A., Podolsky, B. and Rosen, N. *Can quantum-mechanical description of physical reality be considered complete?* Phys. Rev. **47**, 777–780 (1935).

Elstrodt, J. *Maß- und Integrationstheorie.* Springer-Lehrbuch. Springer -Verlag Berlin Heidelberg (2009).

Endres, D. M. and Schindelin, J. E. *A new metric for probability distributions.* IEEE Trans. Inf. Theory **49**, 1858–1860 (2003).

Esposito, M., Harbola, U. and Mukamel, S. *Nonequilibrium fluctuations, fluctuation theorems, and counting statistics in quantum systems.* Rev. Mod. Phys. **81**, 1665–1702 (2009).

Fanchini, F. F., Karpat, G., Castelano, L. K. and Rossatto, D. Z. *Probing the degree of non-Markovianity for independent and common environments.* Phys. Rev. A **88**, 012105 (2013).

Fanchini, F. F., Karpat, G., Çakmak, B., Castelano, L. K., Aguilar, G. H., Farías, O. J., Walborn, S. P., Ribeiro, P. H. S. and de Oliveira, M. C. *Non-Markovianity through accessible information.* Phys. Rev. Lett. **112**, 210402 (2014).

Fannes, M. *Introduction to Many-Body Systems.* https://www.frias.uni-freiburg.de/downloads/veranstaltungen/physic-school-feb-2015 (2015). Lecture held at *Physics School: New trends in many-particle quantum transport*, FRIAS, University of Freiburg (Feb 23, 2015–Mar 06, 2015), (Link checked: 6/10/2016).

Ferraro, A., Olivares, S. and Paris, M. G. A. *Gaussian states in continuous variable quantum information.* Napoli Series on Physics and Astrophysics (2005).

Fuchs, C. and van de Graaf, J. *Cryptographic distinguishability measures for quantum-mechanical states.* IEEE Trans. Inform. Theory **45**, 1216–1227 (1999).

van Gaans, O. *Gradient flows in measure spaces.* https://www.math.leidenuniv.nl/ vangaans/TA2011-gradient-mei11.pdf (2011). Lecture notes of the course *Topics in Analysis* given at Leiden University in spring 2011 (Link checked: 5/6/2016).

Gardiner, C. W. *Handbook of Stochastic Methods for Physics, Chemistry and the Natural Sciences.* Springer Series in Synergetics. Springer-Verlag Berlin Heidelberg, 3rd ed. (2004).

Gessner, M. and Breuer, H.-P. *Detecting nonclassical system-environment correlations by local operations.* Phys. Rev. Lett. **107**, 180402 (2011).

Gessner, M., Laine, E.-M., Breuer, H.-P. and Piilo, J. *Correlations in quantum states and the local creation of quantum discord.* Phys. Rev. A **85**, 052122 (2012).

Gessner, M., Ramm, M., Häffner, H., Buchleitner, A. and Breuer, H.-P. *Observing a quantum phase transition by measuring a single spin.* EPL **107**, 40005 (2014a).

Gessner, M., Ramm, M., Pruttivarasin, T., Buchleitner, A., Breuer, H.-P. and Häffner, H. *Local detection of quantum correlations with a single trapped ion.* Nature Phys. **10**, 105–109 (2014b).

Gibbs, A. L. and Su, F. E. *On choosing and bounding probability metrics.* International Statistical Review **70**, 419–435 (2002).

Giedke, G., Kraus, B., Lewenstein, M. and Cirac, J. I. *Entanglement criteria for all bipartite Gaussian states.* Phys. Rev. Lett. **87**, 167904 (2001).

Giedke, G., Eisert, J., Cirac, J. I. and Plenio, M. B. *Entanglement transformations of pure Gaussian states.* Quant. Inf. Comp. **3**, 211 (2003a).

Giedke, G., Wolf, M. M., Krüger, O., Werner, R. F. and Cirac, J. I. *Entanglement of formation for symmetric Gaussian states.* Phys. Rev. Lett. **91**, 107901 (2003b).

Gilchrist, A., Langford, N. K. and Nielsen, M. A. *Distance measures to compare real and ideal quantum processes.* Phys. Rev. A **71**, 062310 (2005).

Giorda, P. and Paris, M. G. A. *Gaussian quantum discord.* Phys. Rev. Lett. **105**, 020503 (2010).

Gisin, N. *Hidden quantum nonlocality revealed by local filters.* Phys. Lett. A **210**, 151–156 (1996).

Glauber, R. J. *Coherent and incoherent states of the radiation field.* Phys. Rev. **131**, 2766–2788 (1963).

Gorini, V., Kossakowski, A. and Sudarshan, E. C. G. *Completely positive dynamical semigroups of N-level systems.* J. Math. Phys. **17**, 821–825 (1976).

Goussev, A., Jalabert, R. A., Pastawski, H. M. and Wisniacki, D. A. *Loschmidt echo.* Scholarpedia **7**, 11687 (2012). revision 127578.

Grabert, H., Schramm, P. and Ingold, G.-L. *Quantum Brownian motion: The functional integral approach.* Phys. Rep. **168**, 115–207 (1988).

Griffiths, D. J. *Introduction to Quantum Mechanics.* Pearson Prentice Hall, 2nd ed. (2004).

Grosse, I., Bernaola-Galván, P., Carpena, P., Román-Roldán, R., Oliver, J. and Stanley, H. E. *Analysis of symbolic sequences using the Jensen-Shannon divergence.* Phys. Rev. E **65**, 041905 (2002).

Guarnieri, G., Uchiyama, C. and Vacchini, B. *Energy backflow and non-Markovian dynamics.* Phys. Rev. A **93**, 012118 (2016).

Haikka, P., McEndoo, S., De Chiara, G., Palma, G. M. and Maniscalco, S. *Quantifying, characterizing, and controlling information flow in ultracold atomic gases.* Phys. Rev. A **84**, 031602 (2011).

Haikka, P., Goold, J., McEndoo, S., Plastina, F. and Maniscalco, S. *Non-Markovianity, Loschmidt echo, and criticality: A unified picture.* Phys. Rev. A **85**, 060101 (2012a).

Haikka, P., McEndoo, S., Chiara, G. D., Palma, G. M. and Maniscalco, S. *Robust non-Markovianity in ultracold gases.* Phys. Scr. **2012**, 014060 (2012b).

Haikka, P., McEndoo, S. and Maniscalco, S. *Non-Markovian probes in ultracold gases.* Phys. Rev. A **87**, 012127 (2013).

Hall, M. J. W., Cresser, J. D., Li, L. and Andersson, E. *Canonical form of master equations and characterization of non-Markovianity.* Phys. Rev. A **89**, 042120 (2014).

Harriman, J. E. *Geometry of density matrices. I. Definitions, N matrices and 1 matrices.* Phys. Rev. A **17**, 1249–1256 (1978).

Haseli, S., Karpat, G., Salimi, S., Khorashad, A. S., Fanchini, F. F., Çakmak, B., Aguilar, G. H., Walborn, S. P. and Ribeiro, P. H. S. *Non-Markovianity through flow of information between a system and an environment.* Phys. Rev. A **90**, 052118 (2014).

Hashitsumae, N., Shibata, F. and Shingu, M. *Quantal master equation valid for any time scale.* J. Stat. Phys. **17**, 155–169 (1977).

Hayashi, M. *Quantum Information – An introduction.* Springer-Verlag Berlin Heidelberg, 1st ed. (2006).

Heisenberg, W. *Über den anschaulichen Inhalt der quantentheoretischen Kinematik und Mechanik.* Z. Phys. **43**, 172–198 (1927).

Heisenberg, W. *The Physical Principles of the Quantum Theory.* University of Chicago Press, Dover Publications (1930).

Hellinger, E. *Neue Begründung der Theorie quadratischer Formen von unendlichvielen Veränderlichen.* J. Reine Angew. Math. **136**, 210–271 (1909).

Helstrom, C. W. *Quantum Detection and Estimation Theory.* Academic Press, New York (1976).

Henderson, L. and Vedral, V. *Classical, quantum and total correlations.* J. Phys. A: Math. Gen. **34**, 6899 (2001).

Hill, S. and Wootters, W. K. *Entanglement of a pair of quantum bits.* Phys. Rev. Lett. **78**, 5022–5025 (1997).

Hioe, F. T. and Eberly, J. H. *N-level coherence vector and higher conservation laws in quantum optics and quantum mechanics.* Phys. Rev. Lett. **47**, 838–841 (1981).

Holevo, A. S. *An analogue of the theory of statistical decisions in noncommutative probability theory.* Trans. Moscow Math. Soc. **26**, 133–149 (1972).

Holevo, A. S. *Bounds for the quantity of information transmitted by a quantum communication channel.* Probl. Inf. Trans. **9**, 177–183 (1973).

Holevo, A. S. *Problems in the mathematical theory of quantum communications.* Rep. Math. Phys. **15**, 273–278 (1977).

Holevo, A. S. *Probabilistic and Statistical Aspects of Quantum Theory.* North-Holland, Amsterdam (1982).

Horn, R. A. and Johnson, C. R. *Matrix Analysis.* Cambridge University Press (1990). Ch. 5 "Norms for Vectors and Matrices.".

Horodecki, M., Horodecki, P. and Horodecki, R. *Separability of mixed states: Necessary and sufficient conditions.* Phys. Lett. A **223**, 1–8 (1996).

Horodecki, P. *Separability criterion and inseparable mixed states with positive partial transposition.* Phys. Lett. A **232**, 333–339 (1997).

Hou, S. C., Yi, X. X., Yu, S. X. and Oh, C. H. *Alternative non-Markovianity measure by divisibility of dynamical maps.* Phys. Rev. A **83**, 062115 (2011).

Hou, S. C., Liang, S. L. and Yi, X. X. *Non-Markovianity and memory effects in quantum open systems.* Phys. Rev. A **91**, 012109 (2015).

Hübner, M. *Explicit computation of the Bures distance for density matrices.* Phys. Lett. A **163**, 239–242 (1992).

Hübner, M. *Computation of Uhlmann's parallel transport for density matrices and the Bures metric on three-dimensional Hilbert space.* Phys. Lett. A **179**, 226–230 (1993).

Husimi, K. *Some formal properties of the density matrix.* Proc. Phys.-Math. Soc. Jpn. **23**, 264 (1940).

Imamoglu, A., Awschalom, D. D., Burkard, G., DiVincenzo, D. P., Loss, D., Sherwin, M. and Small, A. *Quantum information processing using quantum dot spins and cavity qed.* Phys. Rev. Lett. **83**, 4204–4207 (1999).

Ingarden, R. and Kossakowski, A. *On the connection of nonequilibrium information thermodynamics with non-Hamiltonian quantum mechanics of open systems.* Ann. Physics **89**, 451–485 (1975).

Jaksch, D., Bruder, C., Cirac, J. I., Gardiner, C. W. and Zoller, P. *Cold bosonic atoms in optical lattices.* Phys. Rev. Lett. **81**, 3108–3111 (1998).

James, D. F. V., Kwiat, P. G., Munro, W. J. and White, A. G. *Measurement of qubits.* Phys. Rev. A **64**, 052312 (2001).

Jordan, T. F., Shaji, A. and Sudarshan, E. C. G. *Dynamics of initially entangled open quantum systems.* Phys. Rev. A **70**, 052110 (2004).

van Kampen, N. G. *Stochastic Processes in Physics and Chemistry.* North Holland, 3rd ed. (2007).

Kim, M. S., de Oliveira, F. A. M. and Knight, P. L. *Properties of squeezed number states and squeezed thermal states.* Phys. Rev. A **40**, 2494–2503 (1989).

Kim, Y.-H. *Quantum interference with beamlike type-II spontaneous parametric down-conversion.* Phys. Rev. A **68**, 013804 (2003).

Kimura, G. *The Bloch vector for N-level systems.* Phys. Lett. A **314**, 339–349 (2003).

Kimura, G. and Kossakowski, A. *The Bloch-vector space for N-level systems: The spherical-coordinate point of view.* Open Syst. Inf. Dyn. **12**, 207–229 (2005).

Kok, P. and Braunstein, S. L. *Event-ready entanglement.* In H.-P. Breuer and F. Petruccione (eds.), *Relativistic Quantum Measurement and Decoherence: Lectures of a Workshop Held at the Istituto Italiano per gli Studi Filosofici Naples, April 9-10, 1999*, vol. 559 of *Lecture Notes in Physics.* Springer-Verlag Berlin Heidelberg (2000).

Kolmogorov, A. N. *Foundations of the Theory of Probability.* Chelsea Publishing Company, New York (1956).

Kossakowski, A. *On necessary and sufficient conditions for a generator of a quantum dynamical semi-group.* Bull. Acad. Pol. Sci., Série Math. Astr. Phys. **20**, 1021–1025 (1972a).

Kossakowski, A. *On quantum statistical mechanics of non-Hamiltonian systems.* Rep. Math. Phys. **3**, 247–274 (1972b).

Kraus, K. *States, Effects, and Operations*, vol. 190 of *Lecture Notes in Physics.* Springer-Verlag Berlin Heidelberg (1983).

Kuang, L.-M., Zeng, A.-H. and Kuang, Z.-H. *Generation of entangled squeezed states in atomic Bose–Einstein condensates.* Phys. Lett. A **319**, 24–31 (2003).

Kullback, S. and Leibler, R. A. *On information and sufficiency.* Ann. Math. Statist. **22**, 79–86 (1951).

Kurtsiefer, C., Oberparleiter, M. and Weinfurter, H. *Generation of correlated photon pairs in type-II parametric down conversion – revisited.* J. Mod. Opt. **48**, 1997–2007 (2001).

Kwiat, P. G., Waks, E., White, A. G., Appelbaum, I. and Eberhard, P. H. *Ultra-bright source of polarization-entangled photons.* Phys. Rev. A **60**, R773–R776 (1999).

Laine, E.-M., Piilo, J. and Breuer, H.-P. *Witness for initial system-environment correlations in open-system dynamics.* EPL **92**, 60010 (2010a).

Laine, E.-M., Piilo, J. and Breuer, H.-P. *Measure for the non-Markovianity of quantum processes.* Phys. Rev. A **81**, 062115 (2010b).

Laine, E.-M., Breuer, H.-P., Piilo, J., Li, C.-F. and Guo, G.-C. *Nonlocal memory effects in the dynamics of open quantum systems.* Phys. Rev. Lett. **108**, 210402 (2012).

Laine, E.-M., Breuer, H.-P., Piilo, J., Li, C.-F. and Guo, G.-C. *Erratum: Nonlocal memory effects in the dynamics of open quantum systems [Phys. Rev. Lett. 108, 210402 (2012)].* Phys. Rev. Lett. **111**, 229901 (2013).

Laine, E.-M., Breuer, H.-P. and Piilo, J. *Nonlocal memory effects allow perfect teleportation with mixed states.* Sci. Rep. **4** (2014).

Lamberti, P. W., Majtey, A. P., Borras, A., Casas, M. and Plastino, A. *Metric character of the quantum Jensen-Shannon divergence.* Phys. Rev. A **77**, 052311 (2008).

Landau, L. D. and Lifschitz, E. M. *Statistische Physik, Teil 2: Theorie des kondensierten Zustandes.* No. 9 in Lehrbuch der Theoretischen Physik. Akademie Verlag, Berlin, 4th ed. (1992).

Langerholc, J. *Trace formalism for quantum mechanical expectation values.* J. Math. Phys. **6**, 1210–1218 (1965).

Lüders, G. *Über die Zustandsänderung durch den Meßprozeß.* Ann. Phys. **443**, 322–328 (1950).

Lewin, M. *On the coefficients of the characteristic polynomial of a matrix.* Discrete Math. **125**, 225–262 (1994).

Lin, J. *Divergence measures based on the Shannon entropy.* IEEE Trans. Inform. Theory **37**, 145–151 (1991).

Lin, J. and Wong, S. K. M. *A new directed divergence measure and its characterization.* Int. J. Gen. Syst. **17**, 73–81 (1990).

Lindblad, G. *On the generators of quantum dynamical semigroups.* Commun. math. Phys. **48**, 119–130 (1976).

Lindblad, G. *Non-Markovian quantum stochastic processes and their entropy.* Commun. math. Phys. **65**, 281–294 (1979).

Lindblad, G. *On the existence of quantum subdynamics.* J. Phys. A **29**, 4197–4207 (1996).

Liu, B.-H. *Experimental setup and details* (2014). Private communication.

Liu, B.-H., Li, L., Huang, Y.-F., Li, C.-F., Guo, G.-C., Laine, E.-M., Breuer, H.-P. and Piilo, J. *Experimental control of the transition from Markovian to non-Markovian dynamics of open quantum systems.* Nature Phys. **7**, 931–934 (2011).

Liu, B.-H., Cao, D.-Y., Huang, Y.-F., Li, C.-F., Guo, G.-C., Laine, E.-M., Breuer, H.-P. and Piilo, J. *Photonic realization of nonlocal memory effects and non-Markovian quantum probes.* Sci. Rep. **3**, 1781 (2013a).

Liu, B.-H., Wißmann, S., Hu, X.-M., Zhang, C., Huang, Y.-F., Li, C.-F., Guo, G.-C., Karlsson, A., Piilo, J. and Breuer, H.-P. *Locality and universality of quantum memory effects.* Sci. Rep. **4**, 6327 (2014).

Liu, J., Lu, X.-M. and Wang, X. *Nonunital non-Markovianity of quantum dynamics.* Phys. Rev. A **87**, 042103 (2013b).

Liu, L. and Tong, D. M. *Completely positive maps within the framework of direct-sum decomposition of state space.* Phys. Rev. A **90**, 012305 (2014).

Lorenzo, S., Plastina, F. and Paternostro, M. *Geometrical characterization of non-Markovianity.* Phys. Rev. A **88**, 020102 (2013).

Lu, X.-M. *Structure of correlated initial states that guarantee completely positive reduced dynamics.* Phys. Rev. A **93**, 042332 (2016).

Lu, X.-M., Wang, X. and Sun, C. P. *Quantum Fisher information flow and non-Markovian processes of open systems.* Phys. Rev. A **82**, 042103 (2010).

Lund, A. P., Laing, A., Rahimi-Keshari, S., Rudolph, T., O'Brien, J. L. and Ralph, T. C. *Boson sampling from a Gaussian state.* Phys. Rev. Lett. **113**, 100502 (2014).

Luo, S. and Zhang, Q. *Informational distance on quantum-state space.* Phys. Rev. A **69**, 032106 (2004).

Luo, S., Fu, S. and Song, H. *Quantifying non-Markovianity via correlations.* Phys. Rev. A **86**, 044101 (2012).

Ma, X. and Rhodes, W. *Multimode squeeze operators and squeezed states.* Phys. Rev. A **41**, 4625–4631 (1990).

Maassen, H. and Uffink, J. B. M. *Generalized entropic uncertainty relations.* Phys. Rev. Lett. **60**, 1103–1106 (1988).

Maccone, L. *Information-disturbance tradeoff in quantum measurements.* Phys. Rev. A **73**, 042307 (2006).

Maccone, L. *Entropic information-disturbance tradeoff.* EPL **77**, 40002 (2007).

Majtey, A. P., Lamberti, P. W. and Prato, D. P. *Jensen-Shannon divergence as a measure of distinguishability between mixed quantum states.* Phys. Rev. A **72**, 052310 (2005).

Marian, P., Marian, T. A. and Scutaru, H. *Bures distance as a measure of entanglement for two-mode squeezed thermal states.* Phys. Rev. A **68**, 062309 (2003).

Martinazzo, R., Vacchini, B., Hughes, K. H. and Burghardt, I. *Communication: Universal Markovian reduction of Brownian particle dynamics.* J. Chem. Phys. **134**, 011101 (2011).

Masillo, F., Scolarici, G. and Solombrino, L. *Some remarks on assignment maps.* J. Math. Phys. **52**, 012101 (2011).

Mazzola, L., Laine, E.-M., Breuer, H.-P., Maniscalco, S. and Piilo, J. *Phenomenological memory-kernel master equations and time-dependent Markovian processes.* Phys. Rev. A **81**, 062120 (2010).

Mazzola, L., Rodríguez-Rosario, C. A., Modi, K. and Paternostro, M. *Dynamical role of system-environment correlations in non-Markovian dynamics.* Phys. Rev. A **86**, 010102 (2012).

Misra, B. and Sudarshan, E. C. G. *The Zeno's paradox in quantum theory.* J. Math. Phys. **18**, 756–763 (1977).

Monras, A., Chęcińska, A. and Ekert, A. *Witnessing quantum coherence in the presence of noise.* New J. Phys. **16**, 063041 (2014).

Moshinsky, M. and Quesne, C. *Linear canonical transformations and their unitary representations.* J. Math. Phys. **12**, 1772–1780 (1971).

Moshinsky, M. and Winternitz, P. *Quadratic Hamiltonians in phase space and their eigenstates.* J. Math. Phys. **21**, 1667–1682 (1980).

Moyal, J. E. *Quantum mechanics as a statistical theory.* Mathematical Proceedings of the Cambridge Philosophical Society **45**, 99–124 (1949).

Nakajima, S. *On quantum theory of transport phenomena.* Prog. Theor. Phys. **20**, 948–959 (1958).

von Neumann, J. *Die Eindeutigkeit der Schrödingerschen Operatoren.* Math. Ann. **104**, 570–578 (1931).

von Neumann, J. *Über einen Satz von Herrn M. H. Stone.* Ann. of Math. (2) **33**, 567–573 (1932a).

von Neumann, J. *Mathematische Grundlagen der Quantenmechanik*, vol. 38 of *Grundlehren der mathematischen Wissenschaften in Einzeldarstellungen mit besonderer Berücksichtigung der Anwendungsgebiete.* Springer-Verlag Berlin Heidelberg, 1st ed. (1932b).

Nielsen, M. A. and Chuang, I. L. *Quantum Computation and Quantum Information.* Cambridge University Press (2000).

Niu, X.-L., Huang, Y.-F., Xiang, G.-Y., Guo, G.-C. and Ou, Z. Y. *Beamlike high-brightness source of polarization-entangled photon pairs.* Opt. Lett. **33**, 968–970 (2008).

Olivares, S. *Quantum optics in the phase space - A tutorial on Gaussain states.* Eur. Phys. J. Special Topics **203**, 3–24 (2012).

Ollivier, H. and Zurek, W. H. *Quantum discord: A measure of the quantumness of correlations.* Phys. Rev. Lett. **88**, 017901 (2001).

van Oosten, D., van der Straten, P. and Stoof, H. T. C. *Quantum phases in an optical lattice.* Phys. Rev. A **63**, 053601 (2001).

Österreicher, F. and Vajda, I. *A new class of metric divergences on probability spaces and its applicability in statistics.* Ann. Inst. Statist. Math. **55**, 639–653 (2003).

Ozawa, M. *Quantum measuring processes of continuous observables.* J. Math. Phys. **25**, 79–87 (1984).

Ozawa, M. *Entanglement measures and the Hilbert–Schmidt distance.* Phys. Lett. A **268**, 158–160 (2000).

Ozawa, M. *Uncertainty relations for noise and disturbance in generalized quantum measurements.* Ann. Phys. (N.Y.) **311**, 350–416 (2004).

Palma, G., Suominen, K.-A. and Ekert, A. *Quantum computation and dissipation.* Proc. R. Soc. Lond. A **452**, 567–584 (1996).

Parthasarathy, K. R. *What is a Gaussian state?* Commun. Stoch. Anal. **4**, 143–160 (2010).

Pechukas, P. *Reduced dynamics need not be completely positive.* Phys. Rev. Lett. **73**, 1060–1062 (1994).

Pechukas, P. *Pechukas replies:.* Phys. Rev. Lett. **75**, 3021–3021 (1995).

Peleg, S., Werman, M. and Rom, H. *A unified approach to the change of resolution: space and gray-level.* IEEE Trans. Pattern Anal. Mach. Intell. **11**, 739–742 (1989).

Peres, A. *Separability criterion for density matrices.* Phys. Rev. Lett. **77**, 1413–1415 (1996).

Peskin, M. and Schroeder, D. *An Introduction To Quantum Field Theory.* Westview Press (1995).

Petersen, I. R. *A direct coupling coherent quantum observer.* arXiv: 1408.0399(v2) [quant-ph] (2014a).

Petersen, I. R. *A direct coupling coherent quantum observer for a single qubit finite level quantum system.* arXiv: 1409.2594(v1) [quant-ph] (2014b).

Piilo, J., Maniscalco, S., Härkönen, K. and Suominen, K.-A. *Non-Markovian quantum jumps.* Phys. Rev. Lett. **100**, 180402 (2008).

Piovella, N., Cola, M. and Bonifacio, R. *Quantum fluctuations and entanglement in the collective atomic recoil laser using a Bose-Einstein condensate.* Phys. Rev. A **67**, 013817 (2003).

Pollock, F. A., Chęcińska, A., Pascazio, S. and Modi, K. *Using a biased qubit to probe complex systems.* arXiv:1507.05051(v1) [quant-ph] (2015).

Prigogine, I. *Non-Equilibrium Statistical Mechanics.* Interscience Publishers, New York (1962).

Prokof'ev, N. V. and Stamp, P. C. E. *Theory of the spin bath.* Rep. Progr. Phys. **63**, 669 (2000).

Rabin, J., Peyré, G., Delon, J. and Bernot, M. *Wasserstein barycenter and its application to texture mixing.* In A. M. Bruckstein, B. M. ter Haar Romeny, A. M. Bronstein and M. M. Bronstein (eds.), *Scale Space and Variational Method in Computer Vision, Third International Conference, SSVM 2011 Ein-Gedi, Israel, May 29–June 2, 2011 Revised Selected Papers*, no. 6667 in Lecture Notes in Computer Science (LNCS), pp. 435–446. Springer-Verlag Berlin Heidelberg (2012).

Rajagopal, A. K., Usha Devi, A. R. and Rendell, R. W. *Kraus representation of quantum evolution and fidelity as manifestations of Markovian and non-Markovian forms.* Phys. Rev. A **82**, 042107 (2010).

Riesz, M. *Sur les maxima des formes bilinéaire et sur les fonctionelles linéaires.* Acta Math. **49**, 465–497 (1927).

Rivas, A., Huelga, S. F. and Plenio, M. B. *Entanglement and non-Markovianity of quantum evolutions.* Phys. Rev. Lett. **105**, 050403 (2010).

Rivas, A., Huelga, S. F. and Plenio, M. B. *Quantum non-Markovianity: characterization, quantification and detection.* Rep. Prog. Phys. **77**, 094001 (2014).

Rockafellar, R. T. *Convex Analysis.* Princeton University Press (1972). 2nd printing.

Rodríguez-Rosario, C. A., Modi, K., Kuah, A., Shaji, A. and Sudarshan, E. C. G. *Completely positive maps and classical correlations.* J. Phys. A **41**, 205301 (2008).

Rodríguez-Rosario, C. A., Modi, K. and Aspuru-Guzik, A. *Linear assignment maps for correlated system-environment states.* Phys. Rev. A **81**, 012313 (2010).

Rodríguez-Rosario, C. A., Modi, K., Mazzola, L. and Aspuru-Guzik, A. *Unification of witnessing initial system-environment correlations and witnessing non-Markovianity.* EPL **99**, 20010 (2012).

Romero, K. M. F., Talkner, P. and Hänggi, P. *Is the dynamics of open quantum systems always linear?* Phys. Rev. A **69**, 052109 (2004).

Royer, A. *Reduced dynamics with initial correlations, and time-dependent environment and Hamiltonians.* Phys. Rev. Lett. **77**, 3272–3275 (1996).

Rubner, Y., Tomasi, C. and Guibas, L. J. *The earth mover's distance as a metric for image retrieval.* Int. J. Comput. Vis. **40**, 99–121 (2000).

Rudin, W. *Functional Analysis.* McGraw-Hill (1991).

Rungta, P., Bužek, V., Caves, C. M., Hillery, M. and Milburn, G. J. *Universal state inversion and concurrence in arbitrary dimensions.* Phys. Rev. A **64**, 042315 (2001).

Rüschendorf, L. *Monge–Kantorovich transportation problem and optimal couplings* (2005).

Ruskai, M. B. *Beyond strong subadditivity? Improved bounds on the contraction of generalized relative entropy.* Rev. Math. Phys. **06**, 1147–1161 (1994).

Sachdev, S. *Quantum Phase Transitions.* Cambridge University Press, 2nd ed. (2011).

Schatten, R. and von Neumann, J. *The cross-space of linear transformations II.* Ann. of Math. (2) **47**, 608–630 (1946).

Schleich, W. P. *Quantum Optics in Phase Space.* Wiley-VCH (2001).

Schoenberg, I. J. *Metric spaces and positive definite functions.* Trans. Amer. Math. Soc. **44**, 522–536 (1938).

Schrödinger, E. *Über das Verhältnis der Heisenberg-Born-Jordanschen Quantenmechanik zu der meinen.* Ann. Phys. **79**, 734–756 (1926).

Schrödinger, E. *Zum Heisenbergschen Unschärfeprinzip.* Sitzungsberichte der Preussischen Akademie der Wissenschaften, Physikalisch-Mathematische Klasse **14**, 296–303 (1930).

Schumacher, B. *Sending entanglement through noisy quantum channels.* Phys. Rev. A **54**, 2614–2628 (1996).

Schumacher, B. and Nielsen, M. A. *Quantum data processing and error correction.* Phys. Rev. A **54**, 2629–2635 (1996).

Scully, M. O. *Quantum Optics.* Cambridge University Press (1997).

Serafini, A., Illuminati, F. and Siena, S. D. *Symplectic invariants, entropic measures and correlations of Gaussian states.* J. Phys. B **37**, L21 (2004).

Serafini, A., Adesso, G. and Illuminati, F. *Unitarily localizable entanglement of Gaussian states.* Phys. Rev. A **71**, 032349 (2005).

Shabani, A. and Lidar, D. A. *Vanishing quantum discord is necessary and sufficient for completely positive maps.* Phys. Rev. Lett. **102**, 100402 (2009).

Shaji, A. and Sudarshan, E. *Who's afraid of not completely positive maps?* Phys. Lett. A **341**, 48–54 (2005).

Shibata, F. and Arimitsu, T. *Expansion formulas in nonequilibrium statistical mechanics.* J. Phys. Soc. Jap. **49**, 891–897 (1980).

Shibata, F., Takahashi, Y. and Hashitsume, N. *A generalized stochastic Liouville equation. Non-Markovian versus memoryless master equations.* J. Stat. Phys. **17**, 171–187 (1977).

Simon, B. *Holonomy, the Quantum Adiabatic Theorem, and Berry's Phase.* Phys. Rev. Lett. **51**, 2167–2170 (1983).

Simon, B. *Trace Ideals and Their Applications.* American Mathematical Society, Providence, RI, (2005).

Simon, R. *Peres-Horodecki separability criterion for continuous variable systems.* Phys. Rev. Lett. **84**, 2726–2729 (2000).

Simon, R., Mukunda, N. and Dutta, B. *Quantum-noise matrix for multimode systems: $U(n)$ invariance, squeezing, and normal forms.* Phys. Rev. A **49**, 1567–1583 (1994).

Smirne, A., Breuer, H.-P., Piilo, J. and Vacchini, B. *Initial correlations in open-systems dynamics: The Jaynes-Cummings model.* Phys. Rev. A **82**, 062114 (2010).

Smirne, A., Cialdi, S., Anelli, G., Paris, M. G. A. and Vacchini, B. *Quantum probes to experimentally assess correlations in a composite system.* Phys. Rev. A **88**, 012108 (2013a).

Smirne, A., Mazzola, L., Paternostro, M. and Vacchini, B. *Interaction-induced correlations and non-Markovianity of quantum dynamics.* Phys. Rev. A **87**, 052129 (2013b).

Smirne, A., Stabile, A. and Vacchini, B. *Signatures of non-Markovianity in classical single-time probability distributions.* Phys. Scr. **2013**, 014057 (2013c).

Song, H., Luo, S. and Hong, Y. *Quantum non-Markovianity based on the Fisher-information matrix.* Phys. Rev. A **91**, 042110 (2015).

Souza, L. A. M., Dhar, H. S., Bera, M. N., Liuzzo-Scorpo, P. and Adesso, G. *Gaussian interferometric power as a measure of continuous-variable non-Markovianity.* Phys. Rev. A **92**, 052122 (2015).

Stinespring, W. F. *Positive functions on C^*-algebras.* Proc. Amer. Math. Soc. **6**, 211–216 (1955).

Stone, M. H. *Linear transformations in Hilbert space. III. Operational methods and group theory.* Proc. Natl. Acad. Sci. USA **16**, 172–175 (1930).

Stone, M. H. *On one-parameter unitary groups in Hilbert space.* Ann. of Math. (2) **33**, 643–648 (1932).

Strømer, E. *Positive linear maps of operator algebras.* Acta Math. **110**, 223–278 (1963).

Sudarshan, E. C. G. *Equivalence of semiclassical and quantum mechanical descriptions of statistical light beams.* Phys. Rev. Lett. **10**, 277–279 (1963).

Sylvester, J. J. *Thoughts on inverse orthogonal matrices, simultaneous sign successions, and tessellated pavements in two or more colours, with applications to Newton's rule, ornamental tile-work, and the theory of numbers.* Phil. Mag. **34**, 461–475 (1867).

Takeuchi, S. *Beamlike twin-photon generation by use of type II parametric down-conversion.* Opt. Lett. **26**, 843–845 (2001).

Uhlmann, A. *The "transition probability" in the state space of a *-algebra.* Rep. Math. Phys. **9**, 273–279 (1976).

Vacchini, B. *A classical appraisal of quantum definitions of non-Markovian dynamics.* J. Phys. B: At. Mol. Opt. Phys. **45**, 154007 (2012).

Vacchini, B., Smirne, A., Laine, E.-M., Piilo, J. and Breuer, H.-P. *Markovianity and non-Markovianity in quantum and classical systems.* New J. Phys. **13**, 093004 (2011).

Vallender, S. S. *Calculation of the Wasserstein distance between probability distributions on the line.* Theory Probab. Appl. **18**, 784–786 (1974).

Vasershtein, L. N. *Markov processes over denumerable products of spaces describing large system of automata.* Probl. Inf. Trans. **5**, 47–52 (1969).

Vasile, R., Maniscalco, S., Paris, M. G. A., Breuer, H.-P. and Piilo, J. *Quantifying non-Markovianity of continuous-variable Gaussian dynamical maps.* Phys. Rev. A **84**, 052118 (2011).

Vedral, V. and Plenio, M. B. *Entanglement measures and purification procedures.* Phys. Rev. A **57**, 1619–1633 (1998).

Vedral, V., Plenio, M. B., Rippin, M. A. and Knight, P. L. *Quantifying entanglement.* Phys. Rev. Lett. **78**, 2275–2279 (1997).

Vidal, G. and Werner, R. F. *Computable measure of entanglement.* Phys. Rev. A **65**, 032314 (2002).

Villani, C. *Topics in Optimal Transportation.* American Mathematical Society, Providence, RI, (2003).

Villani, C. *Optimal Transport: Old and New*, vol. 338 of *Grundlagen der mathematischen Wissenschaften*. Springer-Verlag Berlin Heidelberg (2009).

Štelmachovič, P. and Bužek, V. *Dynamics of open quantum systems initially entangled with environment: Beyond the Kraus representation*. Phys. Rev. A **64**, 062106 (2001).

Štelmachovič, P. and Bužek, V. *Erratum: Dynamics of open quantum systems initially entangled with environment: Beyond the Kraus representation [Phys. Rev. A **64** , 062106 (2001)]*. Phys. Rev. A **67**, 029902 (2003).

Weedbrook, C., Pirandola, S., García-Patrón, R., Cerf, N. J., Ralph, T. C., Shapiro, J. H. and Lloyd, S. *Gaussian quantum information*. Rev. Mod. Phys. **84**, 621–669 (2012).

Werner, R. F. *Quantum states with Einstein-Podolsky-Rosen correlations admitting a hidden-variable model*. Phys. Rev. A **40**, 4277–4281 (1989).

Werner, R. F. and Wolf, M. M. *Bound entangled Gaussian states*. Phys. Rev. Lett. **86**, 3658–3661 (2001).

Weyl, H. *Quantenmechanik und Gruppentheorie*. Z. Phys. **46**, 1–46 (1927).

Wigner, E. *On the quantum correction for thermodynamic equilibrium*. Phys. Rev. **40**, 749–759 (1932).

Williamson, J. *On the algebraic problem concerning the normal forms of linear dynamical systems*. Amer. J. Math. **58**, 141–163 (1936).

Wiseman, H. M. *Extending Heisenberg's measurement-disturbance relation to the twin-slit case*. Found. Phys. **28**, 1619–1631 (1998).

Wißmann, S. *Characterization of optimal quantum states with maximal memory effects*. Master's thesis, Albert-Ludwigs-Universität Freiburg im Breisgau (2012). Http://nbn-resolving.de/urn:nbn:de:bsz:25-opus-91639.

Wißmann, S. and Breuer, H.-P. *Role of entanglement for nonlocal memory effects*. Phys. Rev. A **90**, 032117 (2014).

Wißmann, S., Karlsson, A., Laine, E.-M., Piilo, J. and Breuer, H.-P. *Optimal state pairs for non-Markovian quantum dynamics*. Phys. Rev. A **86**, 062108 (2012).

Wißmann, S., Leggio, B. and Breuer, H.-P. *Detecting initial system-environment correlations: Performance of various distance measures for quantum states*. Phys. Rev. A **88**, 022108 (2013).

Wißmann, S., Breuer, H.-P. and Vacchini, B. *Generalized trace-distance measure connecting quantum and classical non-Markovianity*. Phys. Rev. A **92**, 042108 (2015).

Wolf, M. M. and Cirac, J. *Dividing quantum channels*. Commun. math. Phys. **279**, 147–168 (2008).

Wolf, M. M., Eisert, J., Cubitt, T. S. and Cirac, J. I. *Assessing non-Markovian quantum dynamics.* Phys. Rev. Lett. **101**, 150402 (2008).

Wong, A. K. C. and You, M. *Entropy and distance of random graphs with application to structural pattern recognition.* IEEE Trans. Pattern Anal. Mach. Intell. **7**, 599–609 (1985).

Wootters, W. K. *Entanglement of formation of an arbitrary state of two qubits.* Phys. Rev. Lett. **80**, 2245–2248 (1998).

Wudarski, F. and Chruściński, D. *Markovian semigroup from non-Markovian evolutions.* Phys. Rev. A **93**, 042120 (2016).

Xiang, G.-Y., Hou, Z.-B., Li, C.-F., Guo, G.-C., Breuer, H.-P., Laine, E.-M. and Piilo, J. *Entanglement distribution in optical fibers assisted by nonlocal memory effects.* EPL **107**, 54006 (2014).

Zheng, S.-B. and Guo, G.-C. *Efficient scheme for two-atom entanglement and quantum information processing in cavity qed.* Phys. Rev. Lett. **85**, 2392–2395 (2000).

Zhong, L., Menzel, E. P., Candia, R. D., Eder, P., Ihmig, M., Baust, A., Haeberlein, M., Hoffmann, E., Inomata, K., Yamamoto, T., Nakamura, Y., Solano, E., Deppe, F., Marx, A. and Gross, R. *Squeezing with a flux-driven Josephson parametric amplifier.* New J. Phys. **15**, 125013 (2013).

Zwanzig, R. *Ensemble method in the theory of irreversibility.* J. Chem. Phys. **33**, 1338–1341 (1960).

Danksagung

Es ist vollbracht, mein *Opus Magnum* ist nun also fertig! Vollkommen auf mich alleine gestellt, wäre die Arbeit für die und an der Dissertation sehr viel schwieriger gewesen, denn neue Ideen oder Impulse, fachlicher Natur oder darüber hinaus, entspringen doch so häufig dem (wissenschaftlichen) Austausch mit anderen. Neben der Studienstiftung des deutschen Volkes, deren Förderung meines Dissertationprojektes eine große Bereicherung für mich dargestellt hat, möchte ich mich an dieser Stelle daher bei einigen Personen, die mich die letzten Jahre hindurch auf dem Weg zur Promotion begleitet haben, bedanken.

Mein großer Dank gilt Heinz-Peter Breuer, der mit viel Interesse und in zahllosen Gesprächen das Fortschreiten der Arbeit begleitet hat. Die Zusammenarbeit mit ihm war Quell vieler neuer Impulse und wichtiger Ideen. Für seine Offenheit, seine Rückendeckung und das mir entgegengebrachte Vertrauen danke ich ihm herzlich.

Bedanken möchte ich mich auch bei Bassano Vacchini für die bereichernde Kooperation und seine Wertschätzung meiner Arbeit. Außerdem will ich gerne meinen (ehemaligen) Kollegen, insbesondere Bruno Leggio und Sophie Beck sowie meinem Büronachbarn Nikolaj Kulvelis für ihre Hilfsbereitschaft und die angenehme Atmosphäre meinen Dank aussprechen. Die Unterstützung und das Wohlwollen Hermann Graberts, der immer Zeit und Muße für meine Fragen hatte, soll hier ebenfalls nicht unerwähnt bleiben.

Den „Bewohnern“ des neunten Stockes des Hochhauses des hiesigen Instituts danke ich für die häufige Gastfreundschaft bei Seminaren, auf Konferenzen oder für eine Tasse Kaffee. Allen voran seien Stefan Fischer und Andreas Buchleitner genannt, denen mein Dank für anregende und lehrreiche Gespräche sowie offene Ohren für vielerlei Belange gebührt.

Wenn die Zweifel an den eigenen Fähigkeiten oder dem Sinn der eigenen Tätigkeit wieder überhandzunehmen drohten, war es ein großes Glück euch, Laura, Hennie, Marc, Olaf und Christian zu kennen, die ihr doch stets für Ablenkung, Aufmunterung und Unterstützung in diesen Zeiten gesorgt habt – vielen Dank!

Zu guter Letzt möchte ich mich noch bei meinen Eltern und Großeltern bedanken, die mich Zeit meines Lebens bedingungslos unterstützt haben und die mir immerzu Vorbild waren und sind.

Publikationsliste

Aus dieser Dissertation sind nachfolgende Publikationen hervorgegangen:

[1] Wißmann, S., Leggio, B. and Breuer, H.-P. *Detecting initial system-environment correlations: Performance of various distance measures for quantum states*, Phys. Rev. A **88**, 022108 (2013).

[2] Liu, B.-H., Wißmann, S., Hu, X.-M., Zhang, C., Huang, Y.-F., Li, C.-F., Guo, G.-C., Karlsson, A., Piilo, J. and Breuer, H.-P. *Locality and universality of quantum memory effects*, Sci. Rep. **4**, 6327 (2014).

[3] Wißmann, S. and Breuer, H.-P. *Role of entanglement for nonlocal memory effects*, Phys. Rev. A **90**, 032117 (2014).

[4] Wißmann, S., Vacchini, B. and Breuer, H.-P. *Generalized trace distance measure connecting quantum and classical non-Markovianity*, Phys. Rev. A **92**, 042108 (2015).