# Effective theories of classical-quantum dynamics

**By**

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*A thesis submitted to*

University College London

*for the degree of*

Doctor of Philosophy

Department of Physics and Astronomy

University College London

December 2024

I, Isaac Layton, confirm that the work presented in this thesis is my own. Where information has been derived from other sources, I confirm that this has been indicated in the thesis.

Signed ..... Date .....

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**Abstract**

In this work, we study systems operating in a regime where a partially classical, partially quantum effective description is valid. Our central focus is provided by a recently characterised general form of classical-quantum dynamics, which allows for a consistent treatment of classical-quantum systems in terms of both stochastic unravellings and linear master equations. We first show that these dynamics provide a consistent version of the mean-field and reversible bracket approaches to backreaction, which we use to provide a precise regime of validity to standard semi-classical approaches. Utilising partial versions of the $W$, $Q$ and $P$ quasiprobability representations, we then show that these dynamics can be derived from quantum theory in the classical limit of a quantum subsystem strongly decohered by its environment. Finding the general necessary and sufficient conditions for classical-quantum detailed balance, we then construct a class of dynamics that allow the thermal state of the combined classical-quantum system to be preserved, which we use to prove the second law of thermodynamics for classical-quantum systems. Aside from the three fundamental classes of effective classical-quantum dynamics we introduce, we provide a number of technical tools important to their study, such as characterising when the quantum system remains pure conditioned on the classical trajectory. We illustrate our findings by introducing several models, including an analytically solvable model of a one-dimensional classical system coupled to a qubit, and a numerically solvable model of a classical-quantum oscillator system that exhibits thermalisation. This work provides the foundations for general studies of non-relativistic models of effective classical-quantum systems in a variety of contexts, from continuous quantum measurement to molecular dynamics.

# Impact Statement

Approximating complex quantum systems with simpler models is an essential part of studying a wide range of important problems in science, from drug discovery to the development of solar cells. In this work we provide the framework for a new class of approximation methods for quantum systems, which we refer to as effective classical-quantum dynamics. Here, part of the system is approximated classically to reduce the complexity of the problem, while the remainder retains a quantum description to capture important features of the original dynamics.

While effective classical-quantum dynamics have garnered some interest over time, many early attempts were not consistent, while consistent later attempts were only studied in specific models and otherwise unconnected from each other. The current work generalises and interrelates earlier approaches, providing both new tools for understanding how effective classical-quantum systems arise, as well as new classes of dynamics to study effective classical-quantum dynamics in practical settings.

The main achievement of the current work is showing how effective classical-quantum dynamics arise as a classical limit of a fully quantum system. Providing the first physical demonstration of how consistent classical-quantum dynamics can arise from quantum theory, we use partial versions of the $P$, $W$ and $Q$ quasiprobability distributions of quantum optics to demonstrate how a subsystem may appear effectively classical when decohered strongly by its environment.

An important check of the current work is showing how our approach relates to existing semi-classical methods. In particular, we show how our approach arises as a consistent version of two semi-classical methods, notably mean-field dynamics and reversible classical-quantum

brackets, and demonstrate how our current work may be used to precisely bound the timescales and states for which semi-classical methods are valid for.

Finally, we demonstrate how these methods can apply in thermal environments, which are important in the study of molecular dynamics. In doing so, we demonstrate that these dynamics can be explicitly shown to obey the second law of thermodynamics, providing the first steps towards a general theory of non-equilibrium thermodynamics for classical-quantum systems. The main technical result here is a general characterisation of sufficient and necessary conditions for classical-quantum detailed balance. We illustrate these findings with two models, one analytically solvable, the other numerically solvable, which we use to illustrate the applications of our work to both continuous measurement theory and transitions between adiabatic energy levels in molecules.

# List of Publications and Preprints

The work presented in this thesis contains material from the following publications and preprints:

1. Isaac Layton, Jonathan Oppenheim, and Zachary Weller-Davies. A healthier semi- classical dynamics. arXiv preprint arXiv:2208.11722, 2022. [1]

2. Isaac Layton and Jonathan Oppenheim. The classical-quantum limit. PRX Quantum, 5 (2):020331, 2024. [2]

3. Isaac Layton and Harry Miller. Restoring the second law to classical-quantum dynamics, (paper in preparation) [3]

Other publications and preprints by the author are:

4. Isaac Layton, Jonathan Oppenheim, Andrea Russo and Zachary Weller-Davies. The weak field limit of quantum matter back-reacting on classical spacetime. JHEP 08 (2023) 163 [4]

# Acknowledgments

Although the work presented in this thesis is my own, it is equally owned by all the amazing people that were around in my life while I worked on it.

Firstly, I would like to express a huge thanks to Jonathan. As funny as it would be to joke "the only thing I owe my supervisor is forty quid", the truth is that I owe him a lot more than £40. Aside from introducing me to a topic that I have since fallen in love with, Jonathan created a research environment that I only later came to realise was exceptional for its scope, openness, creativity and fun. He taught me the importance of a good idea, and the patience and time needed for it to bear fruit. Above all, I am incredibly grateful for Jonathan introducing me to Maite Arcos, Emanuele Panella, Andrea Russo, Andy Svesko and Zach Weller-Davies, who have all made my life much richer, and for creating an atmosphere at UCL that will provide a high water mark for anything else I do in my life.

Outside of this immediate group, I was lucky enough to interact with a number of great physicists over the course of the PhD. Of those at UCL, I would like to thank Sougato Bose, Toby Cubitt, Lluis Masanes, and all of the CS department crew for many great seminars and discussions. Further afield, I would like to thank Harry Miller, who was the perfect collaborator to work with on a seemingly long and tough problem. I am also grateful to Ryan Barouki and Nicola Pranzini for many discussions on (and sometimes extremely off) the current topics over many years. I would also like to thank my examiners Dan Browne and Jonathan Halliwell for a number of helpful and insightful suggestions on the current work.

Of my contemporaries at UCL, I am most indebted to Zach, who not only helped lay down the theoretical and conceptual basis of most of this work, but was kind enough to involve me

too. Working with Zach was the first time I saw how the seeds of a calculation become reality, often with awe-inspiring speed. He also introduced me to the basic rule of studying classical-quantum systems – understand the classical version, then the quantum version, then put them together – which works 100% of the time I remember to use it.

I also need to express a big thank you to Maite, who started the PhD at the same time as me. Any initial trepidation I felt quickly went away when I realised that I would be spending my PhD with someone who was relaxed, funny and extremely modest, and who has continuously been an inspiration from then on.

The work in this thesis would also not have been possible without Andrea. Providing the calming presence in otherwise stressful times, he was and is a perfect role model of how to balance physics and life.

I would also like to thank Emanuele, who despite being junior to me taught me much more about physics than I did him, and provided great company on long days spent both home and abroad.

A special thanks is reserved to Andy, who aside from marrying my wife and I in holy matrimony, was consistently more supportive, helpful and interested in the work that went into this thesis than could be expected, even of a great friend.

Finally, I would like to thank my wife, Emily. For every word of this thesis, there were at least two words expressing how close some calculation or section or paper was to completion (and two more explaining later why that estimate fell short). For your immense patience, love, and introducing the soon-to-be-common physics phrase “it takes two to tangle”, I will always be grateful.

*To my parents*

For teaching me creativity and craft.

# Contents

# Chapter 1

# Introduction

## 1.1 Classical *and* quantum

The central theme of this work is the study of systems with both classical and quantum degrees of freedom. We refer to these as classical-quantum* systems.

The idea of combining classical and quantum is as old as quantum theory itself. Indeed, the very first attempts at building models of quantum mechanical systems were those built by mixing classical ideas with newly developed notions of quanta [5]. While much of old quantum theory described systems in a no-man's land between our current established theories of classical and quantum mechanics, the work at this time also provided the first examples of systems where the classical and quantum degrees of freedom were identified separately and distinctly. In the earliest models of the atom, the nucleus was assumed to be given a fixed, classical position, in contrast to the quantised orbits of the electrons [6]. In the analysis of the Stern-Gerlach experiment, the quantisation of the magnetic field was investigated by studying the resulting effect on a beam of silver atoms treated classically, so as to relate the splitting of the two beams to the size of the magnetic moment [7–9]. More fundamentally, Bohr was famous for stressing, at length, the importance of treating the measurement apparatus of an experiment classically [10].

*Of course, one could equally say "quantum-classical", but this gets the order wrong, both historically and alphabetically.

In fact, once the Born rule was introduced [11], early quantum theory could be argued to provide a clear interpretation of how classical and quantum systems interact. This postulate tells us that the random outcomes of a measurement, i.e. the change in a classical apparatus, are determined by the wavefunction of the quantum system. As the classical apparatus randomly takes on a new configuration, so the wavefunction of the quantum system also collapses, in a way that is correlated with the change in the classical apparatus.

This sketch provides the blueprint for how all consistent models of classical-quantum systems behave. Understanding how physically motivated and mechanical versions of this evolution can arise is main goal of this work.

## 1.2 Standard classical-quantum dynamics

Despite the suggestive nature of the Born rule, when interpreted as describing a stochastic interaction between a quantum system and a classical measurement device, the two early approaches used to study classical-quantum dynamics were instead deterministic.

The first example of classical-quantum dynamics appears to have arisen in an entirely different context to quantum measurement – that of semi-classical gravity. Attempts to understand how quantum matter should affect a classical theory of gravity led to suggestions that classical spacetime would be affected by the quantum matter fields according to the expectation value of the stress energy tensor [12–14]. Written in a more basic form [15], for a classical system described by two conjugate degrees of freedom $q$ and $p$, and a quantum system described by the quantum state $|\psi\rangle$, this dynamics takes the form

$$d|\psi\rangle_t = -\frac{i}{\hbar}H|\psi\rangle_t dt \tag{1.1}$$

$$dq_t = \frac{p_t}{m}dt \tag{1.2}$$

$$dp_t = -\langle\psi|\frac{\partial H}{\partial q}|\psi\rangle_t dt, \tag{1.3}$$

where here $H = H(q,p)$ is a Hermitian operator valued function of phase space. Since this dynamics appears commonly in the context of semi-classical gravity, we shall refer to dynamics of this kind as standard semi-classical dynamics, or mean-field dynamics. This latter name

comes from the fact that the force on the classical system is given by the expectation value.

A second early type of classical-quantum approach began from the desire to treat both classical and quantum parts of the system on equal footing [16–18]. Defined for when the classical system is described by a phase space and for a Hermitian operator-valued function of phase space $H(q,p)$, this dynamics is a straightforward generalisation of classical and quantum Hamiltonian dynamics and takes the form

$$\frac{\partial \varrho}{\partial t} = -\frac{i}{\hbar}[H,\varrho] + \frac{1}{2}\big(\{H,\varrho\} - \{\varrho,H\}\big), \tag{1.4}$$

where here $\{\cdot,\cdot\}$ denotes the standard Poisson bracket, and $\varrho(q,p,t)$ is an operator-valued function of phase space describing the classical-quantum system. The first term describes the standard unitary evolution of quantum mechanics, while the second term, known as the Alexandrov bracket [17], provides a symmetrised version of the Poisson bracket describing both the pure classical evolution and the effect of the quantum system on the classical one. Despite being suggested earlier, we use the terminology of [19], and refer to this dynamics as the quantum-classical Liouville equation.

There are three important features illustrated in these dynamics that will be extremely relevant from this point on.

The first is that we see two equivalent descriptions of the classical-quantum system. The first one, provided in the mean-field dynamics, is that of individual classical and quantum trajectories in phase space and Hilbert space i.e. $q_t$, $p_t$ and $|\psi\rangle_t$. The second, given in the quantum-classical Liouville equation, is an ensemble picture, determined by the operator-valued function of phase-space $\varrho(q,p,t)$, which we refer to as the *classical-quantum state*. Understanding how these two descriptions and their respective dynamics relate in general is a central theme of this work.

The second important feature is that both dynamics attempt to describe the effect of the quantum system on the classical one. Known as *back-reaction*, this has historically provided the main barrier to describing non-trivial interactions between classical and quantum systems – indeed, consistent models of such interactions were thought for some time to be impossible [20–22]. Note that in contrast, having the classical system affect the quantum one is straightforward to achieve by taking any well-defined quantum dynamics which has time-dependent parameters determined by the configuration of a classical system.

The third important feature of both of these models is the appearance of the Hermitian operator-valued function of phase space, $H$. We shall refer to this object as the *classical-quantum Hamiltonian*. This object appears routinely throughout the study of classical-quantum systems, both for these early models and for the more advanced dynamics we study in this work, and should be understood as one of the central objects of any classical-quantum description.

## 1.3 Consistent classical-quantum dynamics

In the intervening years between the development of these two core models and today, a huge number of dynamics describing how classical and quantum systems can be coupled have been proposed [15, 23–38]. These range from models writing the entire system in Hilbert space [16, 28, 33], to models entirely in a classical phase space [32], to models using alternative formulations of mechanics [29, 30].

Unfortunately, the vast majority of these methods fail one of the two basic requirements needed for a sensible classical-quantum theory: positivity and linearity. Approaches based on reversible classical-quantum bracket evolution laws, such as the quantum-classical Liouville equation [16–19, 24, 29, 32], do not preserve the positivity of the classical-quantum state $\varrho(q, p, t)$ [15]. This means that these dynamics cannot be understood in terms of individual classical trajectories in phase space and quantum trajectories in Hilbert space. On the other hand, the approaches based on the mean-field dynamics or other expectation value laws [15, 35, 38] necessarily lead to non-linear evolution laws at the level of $\varrho(q, p, t)$, preventing such an object from having a valid statistical interpretation.

Ironically, the first consistent models of classical-quantum dynamics were those based on the first identified coupling between classical and quantum systems: measurement. This was first noted by Blanchard and Jadcyck, who provided jumping models of interacting classical and quantum systems following the Born rule [23, 39, 40]. These models were made more physical by Diosi and co-workers [25, 26, 41], who noted that the same process could be applied to continuous-variable classical systems, using ideas from the recently developed continuous measurement theory [42, 43].

The key features of these theories, and all consistent classical-quantum theories, is that the evolution laws are irreversible. Although known for some time [44, 23], this was recently re-established by an important theorem known as the CQ Pawula theorem, which characterised the general form of completely-positive, linear, trace-preserving, Markovian and continuous in phase space classical-quantum dynamics [45, 46]. This theorem generalises the Pawula theorem [47], characterising the evolution of positive real-valued functions, to the case where we consider positive semi-definite operator-valued functions (c.f. Appendix D). The necessary irreversibility of the theory appears in the form of a trade-off, requiring a minimal amount of decoherence in the quantum system for a given diffusion in the classical system, whenever the quantum system back-reacts on the classical one [48].

Providing the main technical basis of our current work, the form of dynamics characterised by the CQ Pawula theorem allows one to construct a wide range of consistent models of classical-quantum systems. We shall see that these models may be completely specified by a set of matrices and operators. The bulk of the dynamics, and the part governed by positivity constraints, is specified by three matrices $D_0$, $D_1$, $D_2$, which correspond to the decoherence, back-reaction, and diffusion with respect to a given set of coordinates in phase space and operators $L_\alpha$ in Hilbert space. The rest determines the purely classical or purely quantum parts of the dynamics: a vector $D_1^C$ which determines the drift in the classical system and a Hermitian operator, which we denote $\bar{H}$, that controls the unitary part of the quantum evolution.

## 1.4 Effective classical-quantum dynamics

Equipped with a general form of consistent classical-quantum dynamics, one may be content that the problem of constructing dynamics for classical-quantum systems is essentially solved.

However, the real world presents us with an unfortunate truth – if we want to model something and solve the equations of motion, we must pick a specific form of dynamics. This is most apparent when we note that in standard classical mechanics, we rarely model the motion of a projectile, or the speed of a block sliding down a slope, from the general form of dynamics that preserves the positivity of classical probability distributions! Instead, we understand that

the world is often well-described by specific forms of dynamics, such as Hamiltonian dynamics in conservative systems, or Langevin equations in situations where the environment is thermal, and so on.

One is thus faced with a basic problem: what are the general classes of the classical-quantum dynamics which are expected to apply to classical-quantum systems? Rephrased in more technical terms, which forms of operators $\bar{H}$ and $L_\alpha$, and which $D$ matrices, does one expect to use to provide a reasonable approximation at modelling a given classical-quantum system?

In this work, we attempt to answer this question by appealing to the principle of an *effective theory*. While this may be interpreted in a number of ways, we shall here take an effective theory to be one which does not claim to be a true description of a system, but rather captures the correct features. Indeed, such theories are understood to be useful exactly because they are *effective* at describing some observed phenomena in certain settings, even if they do not seem likely candidates as a fundamental theory. This is an extremely natural philosophy to use for classical-quantum systems, which by definition combine two distinct types of system into one description, and thus an odd candidate for a fundamental theory of nature.

In what follows we shall think of effective classical-quantum systems in two distinct ways. The first is independent of the underlying theory from which classical-quantum mechanics derives, and instead postulates that an effective classical-quantum description is valid. In this context, the classicality of a subsystem is guaranteed by being able to assign a well-defined classical-quantum state $\varrho$ to the system, which remains well-defined by the consistency (i.e. positivity and linearity) of the dynamics. Here classicality is guaranteed a priori – the challenge is thus to find dynamics that are physically motivated by requiring relationships with existing approaches and established principles.

The second way we shall think of effectively classical-quantum theories is as a certain regime of a fully quantum theory. While there are many notions of classicality within quantum theory [49–61], in this work we utilise the theory of partial quasiprobability distributions, which represent the state of a bipartite quantum system partly in phase space and partly in Hilbert space. Defining effective classical-quantum states as those for which the positivity of a partic-

ular distribution guarantees that there is no entanglement between the effectively classical and quantum degrees of freedom, and that all measurement statistics are equivalent to a fundamental classical-quantum theory, we identify effective classical-quantum dynamics in this context with evolution of a quantum system that preserves the positivity of this distribution in time.

These two viewpoints lead us to consider three different ways of motivating general forms of consistent classical-quantum dynamics:

1. How can consistent classical-quantum dynamics be related to standard classical-quantum approaches?

2. Can classical-quantum dynamics be derived as a classical limit of fully quantum models?

3. Which dynamics preserve the thermal state of the combined classical-quantum system?

We shall find that these define three distinct classes of effective classical-quantum dynamics, that all may be understood to generalise the standard semi-classical approaches in different ways.

## 1.5 Main results in miniature

To illustrate the three classes of dynamics which comprise the main results of this work, we will consider a simple model of a qubit coupled to a classical particle. In particular, let us assume that the interaction of the two systems is such that when the qubit is the $|0\rangle$ state, the classical system experiences a potential on the right, and when in the $|1\rangle$ state, a potential on the left. This gives the basic classical-quantum Hamiltonian as

$$H(q,p) = \frac{p^2}{2m}\mathbb{1} + \lambda(q - l\sigma_z)^2 \tag{1.5}$$

where here $\sigma_z$ denotes the $z$ Pauli operator with $\sigma_z|0\rangle = |0\rangle$ and $\sigma_z|1\rangle = -|1\rangle$, $\mathbb{1}$ denotes the identity operator, $l$ is the separation from the minimum of the potential to the origin, $\lambda$ controls the strength of the potential, and $m$, $q$ and $p$ are the mass, position and momentum of the classical particle.

### 1.5.1 A consistent semi-classical dynamics

In this model, the standard semi-classical approach based on the mean-field dynamics of (1.1) to (1.3) takes the form,

$$d|\psi\rangle_t = -\frac{i}{\hbar}H(q_t, p_t)|\psi\rangle_t dt \tag{1.6}$$

$$dq_t = \frac{p_t}{m}dt \tag{1.7}$$

$$dp_t = -2\lambda q_t dt + 2\lambda l\langle\sigma_z\rangle dt, \tag{1.8}$$

while the quantum-classical Liouville approach of Eq. (1.4) takes the form

$$\frac{\partial\varrho}{\partial t} = -\frac{i}{\hbar}[H(q,p),\varrho] - \frac{p}{m}\frac{\partial\varrho}{\partial q} + 2\lambda q\frac{\partial\varrho}{\partial p} - \lambda l\{\sigma_z, \frac{\partial\varrho}{\partial p}\}_+, \tag{1.9}$$

where here $\langle\sigma_z\rangle$ is shorthand for $\langle\psi|_t\sigma_z|\psi\rangle_t$ and $\{\cdot,\cdot\}_+$ denotes the anticommutator. These two inequivalent dynamics [62] each independently satisfy a single desirable property: the first dynamics maintains the positivity of the classical-quantum state, while the second ensures the evolution is linear.

However, one may instead postulate a single dynamics that resembles both of these two distinct dynamics, with the additional property that the classical-quantum state evolves both linearly *and* completely positively. A simple form of such dynamics takes the form in the trajectory picture

$$d|\psi\rangle_t = -\frac{i}{\hbar}H(q_t,p_t)|\psi\rangle_t dt + \frac{\lambda l}{\sigma}(\sigma_z - \langle\sigma_z\rangle)|\psi\rangle_t dW_t - \frac{\lambda^2 l^2}{2\sigma^2}(\sigma_z - \langle\sigma_z\rangle)^2|\psi\rangle_t dt \tag{1.10}$$

$$dq_t = \frac{p_t}{m}dt \tag{1.11}$$

$$dp_t = -2\lambda q_t dt + 2\lambda l\langle\sigma_z\rangle dt + \sigma dW_t, \tag{1.12}$$

and in the master equation picture

$$\frac{\partial\varrho}{\partial t} = -\frac{i}{\hbar}[H(q,p),\varrho] - \frac{p}{m}\frac{\partial\varrho}{\partial q} + 2\lambda q\frac{\partial\varrho}{\partial p} - \lambda l\{\sigma_z, \frac{\partial\varrho}{\partial p}\}_+ + \frac{\lambda^2 l^2}{\sigma^2}(\sigma_z\varrho\sigma_z - \varrho) + \frac{\sigma^2}{2}\frac{\partial^2\varrho}{\partial p^2} \tag{1.13}$$

where here $dW_t$ is the Wiener increment and $\sigma$ is a free parameter. It is straightforward to see that the trajectory picture resembles the standard mean-field semi-classical approach, but with additional terms related to the noise in the classical system. Similarly, we see that the master

equation takes the form of the quantum-classical Liouville approach, but with additional terms to ensure complete-positivity.

We may understand the dynamics of Eqs. (1.10) to (1.12) as follows. The classical system experiences diffusion, and a back-reaction force as if it were experiencing the force of the potential centred on either the left or the right. As it evolves, the initial randomness of its motion means that which potential it is evolving in is not deducible from the initial part of its trajectory. Only after sufficient time has passed will the motion be clearly deducible to be based in the potential on the left; in this time, the quantum system will have collapsed (whilst remaining pure conditioned on the classical trajectory) to the $|1\rangle$ state. An example of how a typical trajectory appears in a related qubit model is plotted in Figure 3.1. Averaging over the individual trajectories, and asking what the probability of finding the classical system at a given $q, p$, and what the corresponding ensemble average of quantum states arriving at this point in phase space is, provides the equivalent master equation description of Eq. (1.13).

### 1.5.2 Effective dynamics from the classical-quantum limit

Rather than postulating a form of consistent dynamics, we may also ask whether one can arrive at effective classical-quantum dynamics by taking the classical limit of one subsystem in a fully quantum model i.e. a classical-quantum limit. For the simple model above this corresponds to the bipartite quantum Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + \lambda(\hat{q} - l\sigma_z)^2, \tag{1.14}$$

where here the $C$ system, that we wish to take the classical limit of, is characterised by position and momentum operators $\hat{q}$ and $\hat{p}$ (with hats to distinguish that these are now treated as operators), while the $Q$ subsystem, which we wish to remain quantum, is described by the Pauli operator $\sigma_z$.

While many methods of taking a classical limit exist, we find that a basic method, in which the environment acts to project the $C$ system onto the coherent states on a timescale $\tau$, leads to a consistent classical-quantum dynamics in a double scaling limit of $\hbar \to 0$ and $\tau \to 0$ such

that $\hbar = E_f\tau$. The unravelling takes the form

$$\begin{aligned} d|\psi\rangle_t = &-\frac{i}{\hbar}\big[H(q_t,p_t) - \frac{\hbar\lambda l}{E_f}\frac{p_t}{m}\sigma_z\big]|\psi\rangle_t dt + \frac{\lambda l s}{\sqrt{E_f}}(\sigma_z - \langle\sigma_z\rangle)|\psi\rangle_t dW_t \\ &+ \frac{i\lambda l s}{\sqrt{E_f}}(\sigma_z - \langle\sigma_z\rangle)|\psi\rangle_t dV_t - \frac{s^2\lambda^2 l^2}{E_f}(\sigma_z - \langle\sigma_z\rangle)^2|\psi\rangle_t dt \end{aligned} \tag{1.15}$$

$$dq_t = \frac{p_t}{m}dt + \sqrt{E_f}s dV_t \tag{1.16}$$

$$dp_t = -2\lambda q_t dt + 2\lambda l\langle\sigma_z\rangle dt + \frac{\sqrt{E_f}}{s}dW_t, \tag{1.17}$$

while the corresponding master equation is of the form

$$\begin{aligned} \frac{\partial\varrho}{\partial t} = &-\frac{i}{\hbar}[H(q,p) - \frac{\hbar\lambda l}{E_f}\frac{p}{m}\sigma_z, \varrho] - \frac{p}{m}\frac{\partial\varrho}{\partial q} + 2\lambda q\frac{\partial\varrho}{\partial p} - \lambda l\{\sigma_z, \frac{\partial\varrho}{\partial p}\}_+ - is^2\lambda l[\sigma_z, \frac{\partial\varrho}{\partial q}] \\ &+ \frac{2s^2\lambda^2 l^2}{E_f}(\sigma_z\varrho\sigma_z - \varrho) + \frac{E_f s^2}{2}\frac{\partial^2\varrho}{\partial q^2} + \frac{E_f}{2s^2}\frac{\partial^2\varrho}{\partial p^2} \end{aligned} \tag{1.18}$$

Here $H$ is the classical-quantum Hamiltonian given in (1.5) and $dV_t$ denotes another Wiener process increment uncorrelated with $dW_t$, while $s$ is a positive parameter quantifying how tightly the environment collapses to coherent states peaked in position versus momentum.

We note immediately that this dynamics resembles the postulated form of dynamics given in Eqs. (1.10) to (1.12), with the addition of diffusion in the position of the effective classical system, an additional Hamiltonian term, an additional back-reaction term that acts like a white-noise Hamiltonian term, and a larger overall decoherence to ensure the additional back-reaction still leads to completely-positive evolution. That the back-reaction operators take the same form as in the postulated dynamics, i.e. given by derivatives of $H$, is in fact a feature of the particularly simple form of Hamiltonian, with a more complex form of back-reaction operator found in the general case.

### 1.5.3 Thermal state preserving classical-quantum dynamics

Alternatively, we may ask which dynamics preserves the combined classical-quantum thermal state of the system i.e. the classical-quantum state

$$\pi(q,p) = \frac{1}{\mathcal{Z}}\exp\bigg[-\beta\bigg(\frac{p^2}{2m}\mathbb{1} + \lambda(q - l\sigma_z)^2\bigg)\bigg], \tag{1.19}$$

where $\mathcal{Z}$ is the appropriate normalisation. While such a dynamics has no guarantee to arise from a fully quantum model, the fact that the thermal state is preserved in time guarantees the thermodynamic consistency of the model, allowing for heat and entropy to be defined in a manner consistent with the second law of thermodynamics. In this setting, the dynamics may be understood to be an effective description of a system described by classical and quantum variables that is in contact with a thermal environment.

In this work, we find a form of dynamics that preserves the thermal state, satisfies detailed balance, and reduces to standard underdamped dynamics in the appropriate classical limit. For the model given above this takes the form

$$d|\psi\rangle_t = -\frac{i}{\hbar}H(q_t,p_t)|\psi\rangle_t dt + \lambda l\sqrt{\frac{\beta}{2\gamma}}(\sigma_z - \langle\sigma_z\rangle)|\psi\rangle_t dW_t - \frac{\lambda^2 l^2\beta}{4\gamma}(\sigma_z - \langle\sigma_z\rangle)^2|\psi\rangle_t dt \tag{1.20}$$

$$dq_t = \frac{p_t}{m}dt \tag{1.21}$$

$$dp_t = -2\lambda q_t dt + 2\lambda l\langle\sigma_z\rangle dt - \frac{\gamma}{m}p_t dt + \sqrt{\frac{2\gamma}{\beta}}dW_t, \tag{1.22}$$

and in the master equation picture

$$\frac{\partial\varrho}{\partial t} = -\frac{i}{\hbar}[H(q,p),\varrho] - \frac{p}{m}\frac{\partial\varrho}{\partial q} + 2\lambda q\frac{\partial\varrho}{\partial p} - \lambda l\{\sigma_z,\frac{\partial\varrho}{\partial p}\}_+ + \gamma\frac{\partial}{\partial p}(p\varrho) + \frac{\beta\lambda^2 l^2}{2\gamma}(\sigma_z\varrho\sigma_z - \varrho) + \frac{\gamma}{\beta}\frac{\partial^2\varrho}{\partial p^2}. \tag{1.23}$$

As before, the dynamics is closely related to the postulated form of dynamics given in Eqs. (1.10) to (1.12). Here the additional term is a classical friction term with friction coefficient $\gamma$, which ensures that the system reaches the thermal state defined in Eq. (1.19). In general however, a more complex form of back-reaction operator is required to achieve this for classical-quantum Hamiltonians $H$ which do not commute with themselves at different points in phase space.

## 1.6 Applications of classical-quantum dynamics

Aside from foundational interest in their own right, the study of effective classical-quantum dynamics has some potential to provide practical insights into areas of physics and chemistry.

The most direct application is in the study of continuous quantum measurement and feedback [42, 43]. As we show in this work, classical-quantum dynamics can be understood as describing a continuous measurement of a quantum system, in which the signal obtained is used to apply a force to a classical system, which in turn controls the Hamiltonian and measurement strength on the classical system. The flip-side of this is that the tools of classical-quantum dynamics may in principle be used to study continuous measurement and feedback theory, thus providing a basic arena for applications of our current work and for in-principle experimental tests of the tools of classical-quantum theories.

In practice, the core aim of this work is to describe classical-quantum systems beyond the conventional regime of continuous measurement and feedback, and in particular to describe effective classical-quantum systems in which the interactions between the classical and quantum sectors are direct, rather than via a series of macroscopic signal processors and amplifiers as would be found in realisations based on continuous measurement theory. To understand which experimentally achievable systems may be used to do this is largely beyond the scope of the current work, but a promising application is in the study of chemical physics. Here, the high complexity of simulating the quantum many-body system of a molecule, as well as the clear difference in masses between the nuclei and electrons, means that an effective classical-quantum description is both necessary and natural in this setting [19, 63, 64]. The current work thus has the possibility of being both applied as a set of improved methods, and experimentally tested, by studying non-adiabatic problems in molecular dynamics [65] .

Aside from these applications, the appeal of the current theory is the comparative ease at constructing and simulating classical-quantum models. In a given setting, and a given choice of classical-quantum Hamiltonian, one may directly simulate one of the three main classes of dynamics that we provide, and (the statistics) of observables that result. In this sense, the current work may have application in a number of theoretical and experimental settings where a natural split into classical and quantum degrees of freedom has been made, such as in the study of systems at classical-quantum boundaries [66–68], or semi-classical regimes of optics [69–71].

Finally, in keeping with one of the earliest motivations of studying the backreaction of

quantum systems on classical ones, the study of effective classical-quantum dynamics has some potential to help clarify problems and provide new tools in the study of semi-classical theories of gravity [15, 25, 41, 72, 46]. While the current work may not be directly applied without a better understanding of how relativistic models of diffusion and decoherence may be constructed [73], the current work provides some idea of the features, and potential solutions, a consistent semi-classical framework based on effective classical-quantum dynamics could provide in these contexts.

## 1.7 Summary of the thesis

We first establish a number of important results helping to characterise the structure of classical-quantum dynamics, in both the trajectory and ensemble pictures. Following the same structure as the basic qubit-particle model described in Sec. 1.5, we then study effective classical-quantum dynamics in three distinct ways, which form the three main sections of this work. This leads to the following four main chapters of this thesis:

### Chapter 2: Classical-quantum mechanics

In the first section of this work, we establish the formalism we will use for the rest of the thesis i.e. the formalism of classical-quantum mechanics. First providing an overview of the key relations and results regarding the kinematics and dynamics of classical-quantum systems, we then describe a number of technical results for understanding classical-quantum dynamics: how to relate classical-quantum unravellings to their master equation forms (Sec. 2.3), how to understand whether a quantum state is pure conditioned on a classical degree of freedom (Secs. 2.4 and 2.5), demonstrating that one may always "purify" a classical-quantum dynamics by enlarging the phase space that the dynamics takes place in (Sec. 2.6), showing that classical-quantum dynamics is able to be constructed as a general form of continuous measurement and feedback loop (Sec. 2.7), as well as describing an alternative form of classical-quantum dynamics with simpler sufficient and necessary conditions for positivity (Sec. 2.8)

This chapter is based on the paper [1], which is joint work with Jonathan Oppenheim and

Zach Weller-Davies, and also includes a technical result appearing in [3], which is joint work with Harry Miller.

### Chapter 3: A consistent semi-classical dynamics

In the second chapter of this work we argue that consistent classical-quantum dynamics should in some sense reproduce or encompass other effective theory approaches to classical-quantum dynamics – namely the mean-field and quantum-classical Liouville approaches given in Eqs. (1.1) to (1.3) and Eq. (1.4). Motivating first the problem from the context of semi-classical gravity (Sec. 3.1), we begin by analysing the standard semi-classical (or mean-field) dynamics, which we show fails the basic assumption of linearity of the classical-quantum state (Sec. 3.2). We then demonstrate that by including additional stochastic terms that the dynamics may be put in a completely-positive and linear form, given in Eqs. (3.8) and (3.9), which we refer to as a "healed" semi-classical dynamics (Sec. 3.3). While these forms of dynamics were known in earlier work for basic Hamiltonians [26], we here are able to provide general forms of dynamics, with sufficient and necessary conditions for positivity. We show that this provides a tool to find conditions under which the mean-field approach is approximately valid as a theory (Sec. 3.4). We also show that the dynamics when written in master equation form also describe a consistent version of the quantum-classical Liouville equation (Sec. 3.5), which we write down in Eq. (3.15). Finally, we conclude with some possible lessons of this formalism in the context of semi-classical gravity (Sec. 3.6).

This chapter is based on the paper [1] , which is joint work with Jonathan Oppenheim and Zach Weller-Davies.

### Chapter 4: Effective dynamics from the classical-quantum limit

The second way we motivate classical-quantum dynamics as an effective theory is perhaps the most important – we investigate how classical-quantum systems can arise as a limit from a full quantum theory. Referring to such a limit as a "classical-quantum" limit, we first show why the standard $\hbar \to 0$ classical limit fails (Sec. 4.2), before defining a new notion involving decoherence into the coherent state basis (Sec. 4.3). The main technical result is finding the

general form of dynamics under this form of classical limit (Sec. 4.4), which we provide in Eq. (4.4.5). Defining a notion of an effectively classical subsystem using the technical tools of partial quasi-probability representations (Sec. 4.5), we show that this dynamics leads to completely-positive evolution in a particular partial quasi-probability distribution based on the $P$ representation of quantum optics, and thus correctly describes effective classical-quantum dynamics arising from a fully quantum theory (Sec. 4.6). Writing the same classical-quantum limit dynamics in unravelling form in Eqs. (4.7.1) and (4.7.2), we then illustrate how the limit we provide describes a notion of a stochastic classical limit (Sec. 4.8). Finally, we study limiting properties of this dynamics using the example of a classical-quantum oscillator system (Sec. 4.9).

This chapter is based on the paper [2], which is joint work with Jonathan Oppenheim.

### Chapter 5: Thermal state preserving classical-quantum dynamics

The third method of motivating classical-quantum dynamics as an effective theory is to assume that the combined thermal state of the classical-quantum system is preserved in time. A natural assumption for effective descriptions such as Langevin dynamics which trace out fast moving degrees of freedom of the thermal environment, this approach is interesting from an effective theory perspective because we here do not need to specify which theory the effective classical-quantum description arises from. We begin our investigation by demonstrating that classical-quantum dynamics which preserve the combined thermal state of the classical-quantum system necessarily obey the second law of thermodynamics (Sec. 5.2). We then show how a large class of such dynamics may be constructed with two operators, $L_z$ and $M_{xy}$ (Sec. 5.3), which we write down for an underdamped classical system in master equation and unravelling forms in Eq. (5.3.17) and Eqs. (5.3.18) to (5.3.20). We illustrate these forms of thermal-state preserving dynamics using an analytically solvable model of a single classical degree of freedom coupled to a qubit (Sec. 5.4), and a numerically solveable model of two coupled oscillators (Sec. 5.5). Finally we find the general form of classical-quantum dynamics that satisfy detailed balance, which we demonstrate holds for the previously introduced dynamics in terms of $L_z$ and $M_{xy}$ (Sec. 5.6).

This chapter is based on the upcoming paper [3], which is joint work with Harry Miller.

### Additional material:

Aside from the work that appears in the above four chapters, a number of supporting results are included in the appendices. Of general relevance is further information on linearity and complete positivity in classical-quantum theories (Appendix A), conditioning on the classical degrees of freedom (Appendix B), as well as basic classical-quantum models and their simulation (Appendix C). We also describe a number of technical steps needed for the main results of the paper, including how the Pawula and CQ Pawula theorems may be used to check the positivity of Liouville and quantum-classical Liouville dynamics (Appendix D), the derivation of a classical-quantum generator using a classical-quantum limit (Appendix E) and the derivation of the classical-quantum detailed balance conditions (Appendix M).

# Chapter 2

# Classical-quantum mechanics

We start by reviewing the framework of classical-quantum mechanics i.e. the kinematics and dynamics of classical-quantum systems. The key feature we emphasise is that there exist two equivalent and interchangeable pictures: one in which the combined system is described by a pair of points in a classical state space and a quantum Hilbert space, the other where the total state of the system is described by the classical-quantum state, a hybrid object that generalises both the classical probability distribution and the quantum density operator. We then introduce the general class of dynamics that allow both descriptions to be used consistently and interchangeably, taking the form of stochastic unravellings in the trajectory picture and classical-quantum master equations in the ensemble picture. We then go on to prove a number of technical results that help characterise these dynamics in both master equation and unravelling pictures, which provide the main technical basis of the work of [1] and also include a technical result important for [3].

## 2.1 Classical-quantum kinematics

We begin by recalling the formalism necessary to collectively describe the kinematics – i.e. states and observables – of a combined classical-quantum system [17, 18, 15, 23, 74, 46]. The classical degrees of freedom are characterised by points $z$ in a classical state space $\mathcal{M} \subseteq \mathbb{R}^n$ i.e. by $n$ real numbers $z = (z_1, \ldots, z_n)$. This may correspond to phase space, in the case

of underdamped evolution, or configuration space when the evolution is overdamped. On the other hand, the quantum system is characterised by a separable Hilbert space $\mathcal{H}$, which may correspond to single qubit or bosonic quantum systems, or many interacting quantum degrees of freedom.

The most intuitive picture of classical-quantum systems is that on the level of individual trajectories [15, 26, 42, 1]. Here, at any given time $t$, the classical system is described by a point in classical state space $z_t \in \mathcal{M}$, while the quantum system is described by a density operator $\rho_t$ i.e. a unit trace positive semi-definite operator acting on $\mathcal{H}$. Since the classical and quantum systems may be subject to noise, one must in general allow for $z_t$ and $\rho_t$ to be random variables. Considered as functions of time, the random variables $z_t$ and $\rho_t$ thus define stochastic processes, which we denote using a subscript $t$ and use $\mathbb{E}[\,\cdot\,]$ to denote their expectation value as random variables. For notational convenience, we will use $z_t^i$ to denote the $i$th element of the random variable $z_t$. In general, each realisation of $z_t$ and $\rho_t$ generate distinct individual trajectories in the classical and quantum state spaces, providing an intuitive picture of classical-quantum dynamics using the standard classical and quantum frameworks.

An equivalent description at the ensemble level is provided by the classical-quantum state [15, 74, 46]. Here, the entire information about the classical-quantum system is contained in an operator-valued function of phase space $\varrho(z,t)$, known as the classical-quantum state, which must be (1) positive semi-definite at all points $z$, and (2) normalised to one after integrating over the classical state space and tracing over Hilbert space i.e. $\int dz\ \mathrm{tr}\varrho(z,t) = 1$. This object is given physical meaning by identifying the classical probability distribution $P(z,t)$ with its trace

$$P(z,t) = \mathrm{tr}\varrho(z,t), \tag{2.1}$$

and identifying the quantum state conditioned on a given classical outcome $z$, which we denote $\rho(z,t)$, with its normalised value

$$\rho(z,t) = \frac{\varrho(z,t)}{\mathrm{tr}\varrho(z,t)}, \tag{2.2}$$

each of which are guaranteed to satisfy the required positivity and normalisation properties by virtue of the two conditions on $\varrho(z,t)$. Using these, the classical-quantum state may also be

written as

$$\varrho(z,t) = \rho(z,t)P(z,t), \tag{2.3}$$

which can be seen to be equivalent to the definition in terms of positivity and normalisation. From this, we see that the classical-quantum state provides a natural generalisation of the classical probability distribution or quantum density matrix to the combined classical-quantum case, and thus is important for characterising both the consistency and properties of classical-quantum dynamics.

A key feature of this framework is that the trajectory and ensemble descriptions can be directly related to each other [1]. In particular, the two representations are related by the fundamental expression

$$\varrho(z,t) = \mathbb{E}[\delta(z - z_t)\rho_t], \tag{2.4}$$

where here $\delta(z - z_t)$ denotes a delta function centred on the point $z_t$. To see how this relation arises, we first note that the probability distribution may be written in terms of the random variable $z_t$ as

$$P(z,t) = \mathbb{E}[\delta(z - z_t)], \tag{2.5}$$

which follows from the definition of the expectation value, while the quantum state conditioned on $(z,t)$ may be written as

$$\rho(z,t) = \mathbb{E}[\rho_t | z_t = z] \tag{2.6}$$

where here $\mathbb{E}[\,\cdot\,|z_t = z]$ denotes the expectation conditioned on the outcome $z_t = z$. Substituting these into the definition of $\varrho(z,t)$ given in (2.3), one sees that the two expectation values may be combined into one due to the presence of the delta function, thus recovering the expression (2.4).

A subtle but important conceptual feature of classical-quantum systems is that the state assigned to describe the quantum system depends on the degree of conditioning on the classical system [1]. Taking first the extreme case, where no information about the classical system is available, the quantum system is described by the unconditioned state $\rho(t)$, which is found by integrating over the classical degrees of freedom in the classical-quantum state

$$\rho(t) = \int dz\ \varrho(z,t). \tag{2.7}$$

Using (2.4), one can check that this may be written in the trajectory picture simply as $\rho(t) = \mathbb{E}[\rho_t]$. An intermediate case occurs when the only final state of the classical system $z$ is known, which gives the $z_t = z$ conditioned quantum state given in (2.2) and (2.6). Finally, one may consider the other extreme case, where the entirety of the classical trajectory $\{z_s\}_{s\leq t}$ is known and conditioned upon. Since any remaining ambiguity in $\rho_t$ at this point would not be physical (see Appendix B), we will always choose to represent dynamics such that $\rho_t$ corresponds to the state of the quantum system conditioned on the entire classical trajectory up to time $t$ i.e.

$$\rho_t = \mathbb{E}[\rho_t|\{z_s\}_{s\leq t}]. \tag{2.8}$$

This choice ensures that the state $\rho_t$ always has a physical meaning by virtue of the reality of the classical trajectories [75, 1]. In the special case that $\rho_t$ is pure, individual realisations of pure states are physically well-defined and unamibiguous, and we shall denote the quantum system here using the corresponding vector in Hilbert space $|\psi\rangle_t$. This may be understood as directly analogous to the case of perfectly efficient continuous quantum measurement, where the quantum system remains pure conditioned on the classical measurement signal (c.f. Section 2.7).

Finally, turning to observables, we note that we may define expectation values on both the level of trajectories [42] and on the level of the ensemble [17, 18, 15]. To start with, we define a classical-quantum observable to be a Hermitian operator-valued function of phase space, which we shall denote $A(z), B(z), \ldots$ etc. Since this defines a quantum observable, one may define a stochastic quantity simply by taking the standard quantum expectation value with respect to a given realisation of $z_t$ and $\rho_t$

$$\langle A(z)\rangle_t = \mathrm{tr}[A(z_t)\rho_t]. \tag{2.9}$$

Referring to this as the trajectory expectation value of $A(z)$, a given realisation of this random variable corresponds physically to averaging the outcomes of $A(z)$ measurements made on the quantum system when a specific classical trajectory occurs. On the other hand, we may also define the ensemble expectation value of a classical-quantum observable by as

$$\langle\langle A(z)\rangle\rangle = \int dz\ \mathrm{tr}[A(z)\varrho(z)], \tag{2.10}$$

where the double angled brackets indicate that here one must integrate over the classical state

space and trace over the quantum Hilbert space. To relate the trajectory and ensemble expectation values, we may substitute (2.4) into the definition of the ensemble expectation value to see that

$$\langle\langle A(z)\rangle\rangle(t) = \mathbb{E}[\langle A(z)\rangle_t], \tag{2.11}$$

i.e. the ensemble expectation value of a classical-quantum observable at time $t$ is equal to the mean value of the corresponding trajectory expectation value.

## 2.2 Classical-quantum dynamics

Having defined the trajectory and ensemble descriptions, characterised either by $z_t$ and $\rho_t$ or by the classical-quantum state $\varrho(z,t)$, we now turn to studying dynamics in these two pictures, which correspond to stochastic unravellings and master equations respectively.

We start by discussing which properties of classical-quantum dynamics are necessary for the time evolution to be consistent with the trajectory and ensemble pictures of classical-quantum systems – see Appendix A for further details. Firstly, we note that if a trajectory level picture exists in terms of $z_t$ and $\rho_t$, then the corresponding ensemble level classical-quantum state $\varrho(z,t)$ is necessarily positive semi-definite everywhere in phase space. For the trajectory picture to remain valid over time, the dynamics must therefore preserve the positivity of the classical-quantum state. Moreover, for this to be valid when applied to just part of a quantum system, this dynamics must also be completely-positive. Finally, we note that since the classical-quantum state has a statistical interpretation, it is important to consider dynamics that is linear in $\varrho(z,t)$, just as one does when considering dynamics of either quantum density operators $\rho(t)$ or classical probability distributions $P(z,t)$.

Alongside the necessary assumptions of complete-positivity and linearity, we will make two additional assumptions on the class of dynamics we work with. Firstly, we will focus our attention on dynamics that are Markovian in the classical-quantum state, consistent with the vast majority of proposed classical-quantum dynamics [37]. Secondly, to consistently describe classical degrees of freedom such as position and momentum, we additionally assume that the dynamics generate trajectories that are continuous in the classical degrees of freedom.

To write down the general form of classical-quantum dynamics in the ensemble picture, we use the formalism of classical-quantum master equations. First developed in [17, 15, 25], one may write their generic form as

$$\frac{\partial \varrho}{\partial t} = \mathcal{L}\varrho, \tag{2.12}$$

where $\mathcal{L}$ is a classical-quantum superoperator that acts as the generator of dynamics. Under the assumptions made above, i.e. that the dynamics is completely-positive, linear, Markovian and continuous in phase space, the general form of this generator is characterised by the CQ Pawula theorem [45, 46]. Denoting by $L_\alpha$ a set of $p$ operators acting on the Hilbert space, and assuming summation over repeated Roman letters $i, j = 1, \ldots, n$ or Greek letters $\alpha, \beta = 1, \ldots, p$, we may write this generator in the form

$$\begin{aligned}\mathcal{L}\varrho = &- \frac{\partial}{\partial z_i}(D^C_{1,i}\varrho) + \frac{1}{2}\frac{\partial^2}{\partial z_i \partial z_j}(D_{2,ij}\varrho) \\ &- i[\bar{H}, \varrho] + D_0^{\alpha\beta}\big(L_\alpha \varrho L_\beta^\dagger - \frac{1}{2}\{L_\beta^\dagger L_\alpha, \varrho\}_+\big) \\ &- \frac{\partial}{\partial z_i}\left(D^{\alpha}_{1,i}{}^* L_\alpha \varrho + \varrho D^\alpha_{1,i} L_\alpha^\dagger\right).\end{aligned} \tag{2.13}$$

The first line describes purely classical dynamics, with the classical drift vector given by $D_1^C$, a real vector of length $n$, and the diffusion matrix denoted $D_2$, a real positive semi-definite $n \times n$ matrix. The purely quantum dynamics is determined by the Hermitian operator $\bar{H}$ describing the unitary evolution and the complex positive semi-definite $p \times p$ decoherence matrix $D_0$. Finally, the quantum back-reaction term appears on the final line, controlled by the $n \times p$ matrix $D_1$ with elements denoted $D^\alpha_{1,i}$. All of the $D$ matrices and operators $H$ and $L_\alpha$ may have dependence on $z$.

For this dynamics to be completely-positive, two positivity conditions must be satisfied. The first is known as the decoherence-diffusion trade-off

$$D_0 \succeq D_1^\dagger D_2^{-1} D_1, \tag{2.14}$$

which states that when the back-reaction on the classical system is non-zero, there must be a minimum amount of decoherence and diffusion in the system. Here $D_2^{-1}$ denotes the pseudoinverse of the diffusion matrix $D_2$, and $A \succeq B$ is shorthand notation for the statement that $A - B \succeq 0$ i.e. the matrix $A - B$ is positive semi-definite. The second positivity condition

controls the degrees of freedom in which diffusion is necessary, and is written as

$$(\mathbb{I} - D_2 D_2^{-1}) D_1 = 0. \tag{2.15}$$

where here $\mathbb{I}$ denotes the $n \times n$ identity matrix. When the operators $L_\alpha$ are orthogonal and traceless, positivity conditions (2.14) and (2.15) provide sufficient and necessary conditions for positivity, but are sufficient to establish positivity for arbitrary $L_\alpha$.

This dynamics may also be written in the trajectories picture using the formalism of classical-quantum unravellings. Built using techniques from continuous quantum measurement theory [42], and appearing as a special case in [26], the general form of classical-quantum unravellings was provided in [1] (see also [76] for a later discussion). Defining $W_t^i$ to be a component of an $n$ dimensional Wiener process with corresponding increments $dW_t^i$ satisfying $dW_t^i dW_t^j = \delta_{ij} dt$, we may write the general form of classical-quantum unravelling as the following set of stochastic differential equations

$$dz_t^i = D_{1,i}^C dt + \langle D_{1,i}^\alpha{}^* L_\alpha + D_{1,i}^\alpha L_\alpha^\dagger \rangle dt + \sigma_{ij} dW_t^j \tag{2.16}$$

and

$$\begin{aligned} d\rho_t = &- i[\bar{H}, \rho_t] dt \\ &+ D_0^{\alpha\beta} (L_\alpha \rho L_\beta^\dagger dt - \frac{1}{2} \{L_\beta^\dagger L_\alpha, \rho_t\}_+) dt \\ &+ D_{1,j}^\alpha{}^* \sigma_{ij}^{-1} (L_\alpha - \langle L_\alpha \rangle) \rho_t dW_t^i \\ &+ D_{1,j}^\alpha \sigma_{ij}^{-1} \rho_t (L_\alpha^\dagger - \langle L_\alpha^\dagger \rangle) dW_t^i \end{aligned} \tag{2.17}$$

where here in the above $\langle A \rangle$ denotes $\mathrm{tr}[A\rho_t]$ i.e. the trajectory expectation value given in (2.9). As before, the $D$ coefficients, $\bar{H}$ and $L$ may all depend on $z_t$, and this dynamics must satisfy both (2.14) and (2.15) to be well-defined. We show in Section 2.4 using properties of the pseudoinverse $\sigma^{-1}$ that one may replace all of the appearances of $dW_t^i$ in Eq. (2.17) with $dz_{t,i}$, verifying that $\rho_t$ satisfies Eq. (2.8).

A special limit of the dynamics occurs when the decoherence in the system is minimal. In particular, when the decoherence-diffusion trade-off is saturated

$$D_0 = D_1^\dagger D_2^{-1} D_1, \tag{2.18}$$

one can show that the dynamics maintains the purity of initial pure states, which we reproduce in Section 2.3. In this case, one may rewrite the quantum part of dynamics entirely in terms of a pure quantum state $|\psi\rangle_t$, which takes the form

$$\begin{aligned} d|\psi\rangle_t = &- iH|\psi\rangle_t dt \\ &+ D^{\alpha 0}_{1,j}\sigma^{-1}_{ij}(L_\alpha - \langle L_\alpha\rangle)|\psi\rangle_t dW_i \\ &- \frac{1}{2}D^{\alpha\beta}_0(L^\dagger_\beta - \langle L^\dagger_\beta\rangle)(L_\alpha - \langle L_\alpha\rangle)|\psi\rangle_t dt \\ &+ \frac{1}{2}D^{\alpha\beta}_0(\langle L^\dagger_\beta\rangle L_\alpha - \langle L_\alpha\rangle L^\dagger_\beta)|\psi\rangle_t dt. \end{aligned} \tag{2.19}$$

The condition (2.8) guarantees that $|\psi\rangle_t$ may indeed be understood to be the quantum state conditioned on $\{z_s\}_{s\leq t}$ i.e. that the state $|\psi\rangle_t$ is uniquely and unambiguously determined from the observations of the classical trajectory up to time $t$. The two representations for pure states (2.19) and (2.17) can be shown to be equivalent using the standard Ito rules [42].

Since classical-quantum dynamics may be equipped with a notion of purity, it is natural to ask whether they may be purified, in the same way that quantum mechanics is purified by the church of the larger Hilbert space [77]. In Section 2.6 we show this is possible for any classical-quantum dynamics i.e. a dynamics with $D_0 \neq D_1^\dagger D_2^{-1} D_1$ may be embedded in a larger Hilbert space or phase space such that $D_0' = D_1^\dagger D_2^{-1} D_1$ is satisfied and thus trajectories of pure quantum states remain pure condiitoned on the available classical degrees of freedom. We refer to this latter case as *the temple of the large phase space* and demonstrate its utility in Chapter 5.

Finally, we note an alternative characterisation of the form of classical-quantum dynamics. Letting $K_i$ denote phase-space dependent operators associated to each classical degree of freedom $z_i$, $\tilde{L}_\alpha$ denote traceless phase-space Lindblad operators, and $G$ denoting a generic phase-space dependent operator, we may write the general classical-quantum generator in the

form

$$\begin{aligned}\mathcal{L}(\varrho) = &-\frac{i}{\hbar}[G,\varrho] - \frac{\partial}{\partial z_i}\left(K_i\varrho + \varrho K_i^\dagger\right) \\ &+ \frac{1}{2}\frac{\partial^2}{\partial z_i \partial z_j}(D_{2,ij}\varrho) \\ &+ D_{2,ij}^{-1}\big(K_i\varrho K_j^\dagger - \frac{1}{2}\{K_j^\dagger K_i, \varrho\}_+\big) \\ &+ \tilde{L}_\alpha \varrho \tilde{L}_\alpha^\dagger - \frac{1}{2}\{\tilde{L}_\alpha^\dagger \tilde{L}_\alpha, \varrho\}_+\end{aligned} \tag{2.20}$$

which is completely positive *if and only if*

$$D_2 \succeq 0, \quad G = G^\dagger \tag{2.21}$$

and there exists a complex-valued phase space dependent vector $v$ of length $n$ such that if $K$ denotes the operator valued vector $K = (K_1, \ldots, K_n)^T$ then

$$(\mathbb{I} - D_2^{-1}D_2)K = v\mathbb{1}. \tag{2.22}$$

We show the equivalence of this generator and its positivity conditions to Eqs. (2.13) to (2.15) in Section 2.8. Aside from a somewhat simpler form than Eq. (2.13), this form proves useful when studying the positivity conditions for systems where the operators determining the back-reaction depend on phase space and may naturally include components proportional to the identity operator.

## 2.3 Equivalence of unravelling and master equation dynamics

In this section, we prove that equations (2.16) and (2.17) give rise to the continuous CQ master equation (2.13). To make this section clearer, we denote the stochastic classical variable using an upper-case $Z_t$. To start with, we note that by the definition $\varrho(z,t) = \mathbb{E}[\delta(Z_t - z)\rho_t]$, the dynamics of $Z_t$ and $\rho_t$ induce the following evolution on the CQ state

$$d\varrho(z,t) = \frac{\partial \varrho(z,t)}{\partial t}dt = \mathbb{E}[d(\delta(Z_t - z)\rho_t)]. \tag{2.23}$$

One must therefore calculate

$$\mathbb{E}[d(\delta(Z_t - z)\rho_t)] = \mathbb{E}[d\delta(Z_t - z)\rho_t + \delta(Z_t - z)d\rho_t + d\delta(Z_t - z)d\rho_t]. \tag{2.24}$$

For clarity we shall go through each term individually. Using Ito's lemma with Eq. (2.16) the first term in Equation (2.24) reads

$$\begin{aligned}\mathbb{E}[d\delta(Z_t - z)\rho_t] =&\mathbb{E}[\frac{\partial}{\partial Z_i}[\delta(Z_t - z)]\rho_t(D^C_{1,i}(Z_t,t) + \langle D^{\alpha*}_{1,i}(Z_t,t)L_\alpha + D^\alpha_{1,i}(Z_t,t)L^\dagger_\alpha\rangle)]dt \\ &+ \mathbb{E}[\frac{1}{2}\frac{\partial^2}{\partial Z_i \partial Z_j}[\delta(Z_t - z)]\rho_t\sigma_{ik}(Z_t,t)\sigma^T_{kj}(Z_t,t)]dt.\end{aligned} \tag{2.25}$$

To simplify Equation (2.25) we can use some well known facts about the delta functional. Using the two identities $\partial_{Z_i}\delta(Z-z) = -\partial_{z_i}\delta(Z-z)$ and $f(Z)\delta(Z-z) = f(z)\delta(Z-z)$ for any function $f$, the right hand side of Equation (2.25) becomes

$$-\frac{\partial}{\partial z_i}\mathbb{E}[\delta(Z_t - z)\rho_t(D^C_{1,i}(z) + \langle D^{\alpha*}_{1,i}(z)L_\alpha + D^\alpha_{1,i}(z)L^\dagger_\alpha\rangle)]dt + \frac{1}{2}\frac{\partial^2}{\partial z_i \partial z_j}\mathbb{E}[\delta(Z_t - z)\rho_t D_{2,ij}(z)]dt. \tag{2.26}$$

The second term in Equation (2.24) is simpler to calculate and gives the pure quantum evolution terms

$$\mathbb{E}[\delta(Z_t - z)d\rho_t] = -i[\bar{H}, \varrho] + D_0^{\alpha\beta}\big(L_\alpha \varrho L^\dagger_\beta - \frac{1}{2}\{L^\dagger_\beta L_\alpha, \varrho\}_+\big)dt. \tag{2.27}$$

For the final term in Equation (2.24), only the second order terms $dW^2 = dt$ are relevant. Using the second positivity condition (2.15), i.e. that $\sigma\sigma^{-1}D_1 = D_1$, then

$$\mathbb{E}[d\delta(Z_t - z)d\rho_t] = \mathbb{E}[\frac{\partial}{\partial z_i}[\delta(Z_t - z)]\rho_t D^{\alpha*}_{1,i}(Z_t,t)(L_\alpha - \langle L_\alpha\rangle) + D^\alpha_{1,i}(Z_t,t)(L^\dagger_\alpha - \langle L^\dagger_\alpha\rangle))]dt. \tag{2.28}$$

Using again the standard properties of the delta function to bring the derivative outside the expectation, we find that the final term takes the form

$$\begin{aligned}\mathbb{E}[d\delta(Z_t - z)d\rho_t] =& -\frac{\partial}{\partial z_i}(D^{\alpha*}_{1,i}(z)L_\alpha \varrho(z) + D^\alpha_{1,i}\varrho(z)L^\dagger_\alpha)dt \\ &+ \frac{\partial}{\partial z_i}\mathbb{E}[\delta(Z_t - z)\rho_t(\langle D^{\alpha*}_{1,i}(z)L_\alpha + D^\alpha_{1,i}(z)L^\dagger_\alpha)\rangle]dt,\end{aligned} \tag{2.29}$$

where here we have used the definition of the classical-quantum state $\varrho(z,t) = \mathbb{E}[\delta(Z_t - z)\rho_t]$. Summing the three contributions, we find that terms containing products of expectation values and $\rho_t$ cancel to give a linear equation of motion for $\varrho(z,t)$ given by that of the continuous master equation in Equation (2.13).

## 2.4 Proof of $\rho_t = \mathbb{E}[\rho_t|\{z_s\}_{s\leq t}]$

Having demonstrated the equivalence of the unravelling and master equations, it remains to show that the state of the quantum system is uniquely determined when conditioning on the

classical trajectory i.e. $\rho_t = \mathbb{E}[\rho_t|\{z_s\}_{s\leq t}]$. It is worth first noting that in the case when $\sigma$ is invertible this is particularly intuitive – observations of $dz_{t,i}$ here uniquely determine the noise processes $dW_t^i$, and thus Equation (2.17) may be integrated to uniquely determine the state at any later time.

To prove this for all real-valued $\sigma$ it is convenient to first rewrite the dynamics in a vectorised form. Defining the vectors $dz_t = (dz_t^1, \ldots, dz_t^n)^T$, $dW_t = (dW_t^1, \ldots, dW_t^n)^T$ for the classical stochastic processes and $L = (L_1, \ldots, L_p)^T$, $L^* = (L_1^\dagger, \ldots, L_p^\dagger)^T$ for the quantum Lindblad operators, the dynamics takes the form

$$dz_t = D_1^C dt + \langle D_1^* L + D_1 L^* \rangle dt + \sigma dW_t \tag{2.30}$$

$$\begin{aligned} d\rho_t = &-i[H, \rho_t]dt + L^T D_0 \rho_t L^* dt - \frac{1}{2}\{L^\dagger D_0^T L, \rho_t\}_+ dt \\ &+ dW_t^T \sigma^{-1} D_1^* (L - \langle L \rangle)\rho_t + dW_t^T \sigma^{-1} D_1 \rho_t (L^* - \langle L^* \rangle). \end{aligned} \tag{2.31}$$

To see that the dynamics indeed satisfies $\rho_t = \mathbb{E}[\rho_t|\{z_s\}_{s\leq t}\}$, we first take the transpose of (2.30) and multiply it by $(\sigma\sigma^T)^{-1}$ to find that

$$dz_t^T (\sigma\sigma^T)^{-1} = dW_t^T \sigma^T (\sigma\sigma^T)^{-1} + (D_1^C + \langle D_1^* L + D_1 L^* \rangle)^T dt \ (\sigma\sigma^T)^{-1} \tag{2.32}$$

However, by the properties of the generalised inverse, $\sigma^{-1} = \sigma^T(\sigma\sigma^T)^{-1}$ for real-valued $\sigma$. As a consequence, we find that

$$dW_t^T \sigma^{-1} = \big[dz_t^T - (D_1^C + \langle D_1^* L + D_1 L^* \rangle)^T dt\big](\sigma\sigma^T)^{-1} \tag{2.33}$$

which may be inserted into equation (2.31) to give

$$\begin{aligned} d\rho_t = &-i[H, \rho_t]dt + L^T D_0 \rho_t L^* dt - \frac{1}{2}\{L^\dagger D_0^T L, \rho_t\}_+ dt \\ &+ \big[dz_t^T - (D_1^C + \langle D_1^* L + D_1 L^* \rangle)^T dt\big](\sigma\sigma^T)^{-1} D_1^* (L - \langle L \rangle)\rho_t \\ &+ \big[dz_t^T - (D_1^C + \langle D_1^* L + D_1 L^* \rangle)^T dt\big](\sigma\sigma^T)^{-1} D_1 \rho_t (L^* - \langle L^* \rangle). \end{aligned} \tag{2.34}$$

Since the evolution of $\rho_t$ is determined completely by that of $z_t$, this demonstrates that indeed $\rho_t$ is unique conditioned on the classical trajectory and thus that $\rho_t = \mathbb{E}[\rho_t|\{z_s\}_{s\leq t}\}$.

## 2.5 Conditions for purity preservation

To determine the conditions for purity, we first must calculate $d\text{tr}\{\rho_t^2\}$ for an initially pure quantum state. The Ito rules imply that

$$d\text{tr}\{\rho_t^2\} = \text{tr}\{2\rho_t d\rho_t + d\rho_t d\rho_t\} \tag{2.35}$$

into which one may substitute (2.31). Since the Hamiltonian and stochastic terms first order in $d\rho_t$ vanish under the trace, and only the stochastic terms are relevant at second order, we find

$$\begin{aligned} d\text{tr}\{\rho_t^2\} =& 2\text{tr}\{\rho_t L^T D_0 \rho_t L^* dt - \frac{1}{2}\rho_t\{L^\dagger D_0^T L, \rho_t\}_+ dt\} \\ &+ \text{tr}\{dW_t^T \sigma^{-1} D_1^*(L - \langle L\rangle)\rho_t \; dW_t^T \sigma^{-1} D_1^*(L - \langle L\rangle)\rho_t\} \\ &+ \text{tr}\{dW_t^T \sigma^{-1} D_1^*(L - \langle L\rangle)\rho_t \; dW_t^T \sigma^{-1} D_1 \rho_t(L^* - \langle L^*\rangle)\} \\ &+ \text{tr}\{dW_t^T \sigma^{-1} D_1 \rho_t(L^* - \langle L^*\rangle) \; dW_t^T \sigma^{-1} D_1^*(L - \langle L\rangle)\rho_t\} \\ &+ \text{tr}\{dW_t^T \sigma^{-1} D_1 \rho_t(L^* - \langle L^*\rangle) \; dW_t^T \sigma^{-1} D_1 \rho_t(L^* - \langle L^*\rangle)\}. \end{aligned} \tag{2.36}$$

Since for pure states $\text{tr}\{A\rho_t B\rho_t\} = \text{tr}\{A\rho_t\}\text{tr}\{B\rho_t\}$, the terms containing $D_1$ twice or $D_1^*$ twice vanish, and the mixed terms may be rearranged into one term by taking the transpose on part of each expression and using the cyclic property of the trace. Doing so gives

$$\begin{aligned} d\text{tr}\{\rho_t^2\} =& 2\text{tr}\{\rho_t L^T D_0 \rho_t L^* dt - \frac{1}{2}\rho_t\{L^\dagger D_0^T L, \rho_t\}_+ dt\} \\ &+ 2\text{tr}\{\rho_t(L^\dagger - \langle L^\dagger\rangle) D_1^T \sigma^{T^{-1}} dW_t dW_t^T \sigma^{-1} D_1^*(L - \langle L\rangle)\rho_t\}. \end{aligned} \tag{2.37}$$

Using again the relation $\text{tr}\{A\rho_t B\rho_t\} = \text{tr}\{A\rho_t\}\text{tr}\{B\rho_t\}$ and the fact that the noise vectors satisfy $dW_t dW_t^T = \mathbb{I}dt$, the above expression reduces with some rearranging to

$$\begin{aligned} d\text{tr}\{\rho_t^2\} =& 2\langle L^\dagger\rangle D_0^T \langle L\rangle \; dt - 2\langle L^\dagger D_0^T L\rangle \; dt \\ &+ 2\langle L^\dagger D_1^T \sigma^{T^{-1}} \sigma^{-1} D_1^* L\rangle \; dt - 2\langle L^\dagger\rangle D_1^T \sigma^{T^{-1}} \sigma^{-1} D_1^* \langle L\rangle \; dt. \end{aligned} \tag{2.38}$$

To check the conditions for this to equal zero, we note that since $D_0 \succeq D_1^\dagger(\sigma\sigma^T)^{-1}D_1$ we can write $D_0^T - D_1^T \sigma^{T^{-1}} \sigma^{-1} D_1^* = B^\dagger B$ and so, defining a new vector of operators $\bar{L} = BL$ rewrite the above as

$$d\text{tr}\{\rho_t^2\} = 2\sum_{\alpha=1}^{p}(\langle\psi|\bar{L}_\alpha^\dagger|\psi\rangle\langle\psi|\bar{L}_\alpha|\psi\rangle - \langle\psi|\bar{L}_\alpha^\dagger\bar{L}_\alpha|\psi\rangle\langle\psi|\psi\rangle)dt. \tag{2.39}$$

Since each term in the above sum is less than or equal to zero by the Cauchy-Schwartz inequality, one can check that $d\text{tr}\{\rho_t^2\} \leq 0$ as expected. All terms are zero if and only if the $\bar{L}_\alpha|\psi\rangle \propto |\psi\rangle$, but since the $\bar{L}_\alpha$ are traceless and this must hold for all $|\psi\rangle$, it must be the case that $\bar{L} = BL = 0$. Thus $B$ is zero and hence we see that $d\text{tr}\{\rho_t^2\} = 0$ for an arbitrary pure state $\rho_t$ if and only if $D_0^T = D_1^T \sigma^{T^{-1}} \sigma^{-1} D_1^*$. Since $D_0$ is Hermitian and $\sigma^{T^{-1}}\sigma^{-1} = (\sigma\sigma^T)^{-1}$ is real, taking the complex conjugate shows that the dynamics keeps quantum states pure if and only if the decoherence-diffusion trade-off [78] is saturated such that $D_0 = D_1^\dagger (\sigma\sigma^T)^{-1} D_1$.

## 2.6 The church of the larger Hilbert space and the temple of the larger phase space

Recall the decoherence-diffusion trade-off of Equation (2.14),

$$D_0 \succeq D_1^\dagger (\sigma\sigma^T)^{-1} D_1 \tag{2.40}$$

We have thus far seen that any classical-quantum dynamics of equations (2.16) and (2.17) that saturate the trade-off such that $D_0 = D_1^\dagger (\sigma\sigma^T)^{-1} D_1$, has the property that when initially pure, both $\rho_t$ and the quantum state conditioned on the classical trajectory $\rho(t|\sigma\{z_s\}_{s\leq t})$ remain pure. We now demonstrate that any dynamics may be purified by a dynamics that saturates the trade-off in either an enlarged quantum Hilbert space or an enlarged classical phase space. Note that this is separate from the question of whether the dynamics may be considered within an entirely quantum theory, and thus purified in a Hilbert space alone – this is instead the content of Chapter 4.

Consider some general dynamics given by (2.16) and (2.17). Defining $\tilde{D}_0 = D_0 - D_1^\dagger (\sigma\sigma^T)^{-1} D_1$, then since the decoherence-diffusion trade-off is satisfied, this object must be positive semi-definite. As such, we are free to consider $D_1^\dagger (\sigma\sigma^T)^{-1} D_1$ and $\tilde{D}_0$ to be two distinct components of the decoherence for the classical-quantum dynamics. Since the first component explicitly saturates the trade-off, the $\tilde{D}_0$ component represents the additional decoherence that prevents the quantum state being pure at all times when conditioned on the classical degrees of freedom. The idea of purifying the system will be to find some additional degrees of freedom, quantum or classical, such that when they are traced out they give rise to this additional decoherence. The

evolution then saturates the trade-off in an enlarged state space, and thus has a description in terms of pure states $|\psi\rangle_t$.

To purify the dynamics using the conventional method of an enlarged Hilbert space, we first note that the positive semi-definite matrix $\tilde{D}_0(z_t)$ generates the following map on the quantum state at each time step $\delta t$ along a trajectory:

$$\rho_{t+\delta t} = \rho_t + \tilde{D}_0^{\alpha\beta}(z_t) L_\alpha \rho_t L_\beta^\dagger \delta t - \frac{1}{2}\tilde{D}_0^{\alpha\beta}(z_t)\{L_\beta^\dagger L_\alpha, \rho_t\}_+ \delta t. \tag{2.41}$$

Exploiting the singular value decomposition $\tilde{D}_0 = V\Sigma V^\dagger$ where $V$ is unitary and $\Sigma$ is a diagonal matrix with non-negative elements $d_\gamma$ for $\gamma = 1, \ldots, \text{rank } \tilde{D}_0$, we may define the operators

$$M_\gamma(z_t) = \begin{cases} \sqrt{d_\gamma}\sum_\alpha V_\gamma^\alpha L_\alpha \sqrt{\delta t} & \gamma = 1, \ldots, \text{rank } \tilde{D}_0 \\ I - \frac{1}{2}\tilde{D}_0^{\alpha\beta} L_\beta^\dagger L_\alpha \delta t & \gamma = \text{rank } \tilde{D}_0 + 1 \end{cases} \tag{2.42}$$

to write the map as

$$\rho_{t+\delta t} = \sum_{\gamma=1}^{\text{rank } \tilde{D}_0+1} M_\gamma(z_t)\rho_t M_\gamma^\dagger(z_t). \tag{2.43}$$

The map is therefore explicitly of the Kraus form and therefore CPTP. It therefore has a representation in terms of a unitary $U$ that acts on the quantum system in question and an additional environment Hilbert space $\mathcal{H}_E$ of dimension $d \geq \text{rank } \tilde{D}_0 + 1$. Specifically, if the unitary acts on the system and a reference state of the environment $|0\rangle$ as

$$U|\psi\rangle|0\rangle = \sum_{\gamma=1}^{\text{rank } \tilde{D}_0+1} M(z_t)_\gamma |\psi\rangle|\gamma\rangle, \tag{2.44}$$

then tracing out the environment gives back the map (2.41) (for more details, see for example [77]). Since this is true for every $\delta t$, it must be the case that we can fully describe the evolution due to $\tilde{D}_0$ by pure states in an enlarged Hilbert space. The remaining dynamics not generated by $\tilde{D}_0$ is pure conditioned on the classical degrees of freedom, and thus the whole dynamics saturates the decoherence-diffusion trade-off in this enlarged space. Note that a more realistic purification model generated by tracing out a bath would have a Hamiltonian and therefore be explicitly of the form of Equations (2.16) and (2.19). However, note that in this case one would also need to make a number of approximations to regain the Lindblad form of (2.41).

It is also possible to purify the dynamics by introducing additional classical degrees of freedom, and, in contrast to the quantum case, this leads to an explicit model of purification without need for approximation. Considering again $\tilde{D}_0 = D_0 - D_1^\dagger(\sigma\sigma^T)^{-1}D_1$ on the original Hilbert space (i.e. the elements $\tilde{D}_0^{\alpha\beta}$ refer to the same set of $L_\alpha$ as in (2.16) and (2.17)), we now consider an enlarged phase space $\mathcal{M} \times \tilde{\mathcal{M}}$ where $\tilde{\mathcal{M}}$ has phase space degrees of freedom $\tilde{z}_i$ for $i = 1, \ldots, \text{rank}\tilde{D}_0$. We then consider the following dynamics:

$$dz_t^i = (D_{1,i}^C(z_t) + \langle D_{1,i}^{\alpha *}(z_t)L_\alpha + D_{1,i}^\alpha(z_t)L_\alpha^\dagger\rangle)dt + \sigma_{ij}(z_t)dW_j \tag{2.45}$$

$$d\tilde{z}_t^i = \langle \tilde{D}_{1,i}^{\alpha 0}(z_t)L_\alpha + \tilde{D}_{1,i}^{0\alpha}(z_t)L_\alpha^\dagger\rangle dt + \tilde{\sigma}_{ij}(z_t)d\tilde{W}_j \tag{2.46}$$

and

$$\begin{aligned} d\rho_t = &-i[H(z_t), \rho_t]dt + D_0^{\alpha\beta}(z_t)L_\alpha\rho L_\beta^\dagger dt - \frac{1}{2}D_0^{\alpha\beta}(z_t)\{L_\beta^\dagger L_\alpha, \rho_t\}_+ dt \\ &+ D_{1,j}^{\alpha 0}\sigma_{ji}^{-1}(z_t)(L_\alpha - \langle L_\alpha\rangle)\rho_t dW_i + D_{1,j}^{0\alpha}\sigma_{ji}^{-1}(z_t)\rho_t(L_\alpha^\dagger - \langle L_\alpha^\dagger\rangle)dW_i \\ &+ \tilde{D}_{1,j}^{\alpha 0}\tilde{\sigma}_{ji}^{-1}(z_t)(L_\alpha - \langle L_\alpha\rangle)\rho_t d\tilde{W}_i + \tilde{D}_{1,j}^{0\alpha}\tilde{\sigma}_{ji}^{-1}(z_t)\rho_t(L_\alpha^\dagger - \langle L_\alpha^\dagger\rangle)d\tilde{W}_i, \end{aligned} \tag{2.47}$$

Here, $\tilde{z}_t^i$ denote the stochastic processes corresponding to degrees of freedom in $\tilde{\mathcal{M}}$, and have associated noise processes $d\tilde{W}_t^i$. $\tilde{D}_1$ and $\tilde{\sigma}$ can be seen in (2.46) to correspond to the drift and diffusion in the enlarged space, and satisfy the same requirements that $D_1$ and $\sigma$ do. Note that these are assumed to solely depend on the degrees of freedom in the original classical phase space $\mathcal{M}$. Packaging up the dynamics for $z_t^i$ and $\tilde{z}_t^i$ as a single classical vector over the whole phase space, these equations are of the form of Equations (2.16) and (2.17) and are thus Markovian and linear on the combined classical-quantum state.

We will then impose the condition that $\tilde{D}_1^\dagger(\tilde{\sigma}\tilde{\sigma}^T)^{-1}\tilde{D}_1 = \tilde{D}_0$. While there may be many ways of satisfying this in general, one simple and explicit construction is to consider $\tilde{D}_1 = \sqrt{\tilde{D}_0}$, the principle square root of $\tilde{D}_0$. This guarantees that rank $\tilde{D}_1$ = rank $\tilde{D}_0$, and is thus a valid $\tilde{D}_1$ by the earlier choice of dimension of $\tilde{\mathcal{M}}$. Since $\sqrt{\tilde{D}_0}^\dagger\sqrt{\tilde{D}_0} = \tilde{D}_0$, it suffices for $(\tilde{\sigma}\tilde{\sigma}^T)^{-1} = I$ and so we see that we can simply choose $\tilde{\sigma} = I$. It thus follows that we can always choose a suitable $\tilde{D}_1$ and $\tilde{\sigma}$ such that $\tilde{D}_1^\dagger(\tilde{\sigma}\tilde{\sigma}^T)^{-1}\tilde{D}_1 = \tilde{D}_0$.

With this condition satisfied, it is easy to check that the full decoherence-diffusion trade-off

is saturated for the constructed dynamics. In particular, one has that

$$D_0 = \begin{pmatrix} D_1 \\ \tilde{D}_1 \end{pmatrix}^{\dagger} \begin{pmatrix} (\sigma\sigma^T)^{-1} & 0 \\ 0 & (\tilde{\sigma}\tilde{\sigma}^T)^{-1} \end{pmatrix} \begin{pmatrix} D_1 \\ \tilde{D}_1 \end{pmatrix}, \tag{2.48}$$

which is satisfied by virtue of the definition of $\tilde{D}_0$ and the above constraints on $\tilde{D}_1$ and $\tilde{\sigma}$. Since the trade-off is saturated, it follows that the dynamics of (2.47) are purity preserving by the results of Appendix 2.3. Thus both $\rho_t$ and the quantum state conditioned on trajectories in the full phase space $\rho(t|\{z_s, \tilde{z}_s\}_{s\leq t})$ remain pure if they start pure.

To see that the above dynamics on $\mathcal{M} \times \tilde{\mathcal{M}}$ define a purification of the starting dynamics (2.16) and (2.17) on $\mathcal{M}$, consider an observer only with access to the degrees of freedom on $\mathcal{M}$. Denoting the conditioned quantum state as $\rho(t|\{z_s\}_{s\leq t})$, at each time step one must average $\rho_t$ over the possible realisations of $\tilde{z}_t$. Since the evolution of $\rho_t$ depends only on degrees of freedom in $\mathcal{M}$, the only information lost is the realization of the noise processes $d\tilde{W}_j$, and thus the evolution of the conditioned state $d\rho(t|\{z_s\}_{s\leq t}) = \mathbb{E}[d\rho_t|\{z_s\}_{s\leq t}]$ is computed by averaging over these noise processes. Mathematically equivalent to the formalism in continuous measurement theory of having multiple observers or inefficient detection [42], it follows from the rules of Ito calculus that $\mathbb{E}[\rho_t d\tilde{W}] = 0$, and thus we see that the dynamics of $\rho(t|\{z_s\}_{s\leq t})$ are exactly given by equation (2.17). It therefore follows that we recover the dynamics (2.16) and (2.17) when we trace out the portion of the phase space $\tilde{\mathcal{M}}$, as originally claimed.

## 2.7 Continuous classical-quantum dynamics as continuous measurement

Given the similarity of the formalism of the general classical-quantum unravellings appearing in (2.16) and (2.17) to the formalism of continuous quantum measurement theory [42], it is natural to ask whether the two may be related in general. In this section we demonstrate that this is indeed the case. The basic idea is that any continuous classical-quantum dynamics may be understood as a continuous measurement of a quantum system, where the measurement depends on the configuration of the classical system and the measurement signal is used to apply a force back on the classical system. This idea has its origins in [41], with proofs of the

general case appearing in [1] and [79].

To see this technically, we use the general formalism of continuous measurements given in [80]. Here the continuous measurement may be understood a series of POVMs given by the Kraus operators $\{\Omega_J\}$, where $J = (J^1, \ldots, J^n)$ is a vector of real numbers parametrising the outcomes of the POVM, which is performed in the interval $[t + dt)$. The outcome of the measurement at time $t$ will be labeled by the numbers $J_t^1 \ldots J_t^k$, and we shall assume that this determines the force on the classical system. After a time $dt$, this means that the change in the classical system is given $dz_t^i = D_{1,i}^C dt + J_t^i dt$, where here $D_1^C = D_1^C(z_t)$ is a real valued vector determining the independent dynamics of the classical system. The key assumption is that, in addition to this effect of the quantum system on the classical, we also allow the classical system to determine the quantum evolution by allowing the measurement $\{\Omega_{J_1 \ldots J_n}\}$ at time $t$ to depend on $z_t$, i.e, we allow for the measurement to depend on the current state of the classical system, which we write as $\{\Omega_J(z_t)\}$. Taking then the POVM given

$$\Omega_J(z_t) = \mathbb{1} - iH(z_t)dt - \frac{1}{2}D_0^{\alpha\beta}(z_t)L_\beta^\dagger L_\alpha dt + L_\alpha D_{1,i}^{\alpha *}(z_t)(D_2^{-1})_{ij}(z_t)J_t^j dt, \tag{2.49}$$

we see that this defines a valid POVM if and only the normalization conditions

$$\int d\mu_0(J)\Omega_J^\dagger \Omega_J = \mathbb{1}, \tag{2.50}$$

are satisfied. Picking the measure $d\mu_0(J)$ to be a multivariate Gaussian such that

$$\int d\mu_0(J)(J_t^i dt) = 0, \ \int d\mu_0(J)(J_t^i dt)(J_t^j dt) = (\sigma\sigma^T)_{ij} = D_{2,ij}dt, \tag{2.51}$$

the above condition is satisfied provided we take $D_0 = D_1^\dagger D_2^{-1} D_1$. Calculating the mean of $J_t^i$ we find that

$$\int d\mu_0(J)\mathrm{tr}[\rho\Omega_J^\dagger\Omega_J]J_t^i = \langle D_{1,i}^\alpha(z_t)L_\alpha^\dagger + D_{1,i}^{\alpha *}(z_t)L_\alpha\rangle + O(dt^2), \tag{2.52}$$

while the second moments give the variance as $(\sigma\sigma^T)_{ij}$. As such, the statistics of the measurement outcomes can be described by the stochastic differential equation

$$J_t^i dt = \langle D_{1,i}^\alpha(z_t)L_\alpha^\dagger + D_{1,i}^{\alpha *}(z_t)L_\alpha\rangle dt + \sigma_{ij}(z_t)dW_j, \tag{2.53}$$

and thus that the evolution of the classical system is given by

$$dz_t^i = D_1^C(z_t)dt + \langle D_{1,i}^\alpha(z_t)L_\alpha^\dagger + D_{1,i}^{\alpha *}(z_t)L_\alpha\rangle dt + \sigma_{ij}(z_t)dW_t^j, \tag{2.54}$$

as given in (2.16). To see how to arrive at the quantum evolution (2.17), we note that the quantum state conditioned on the measurement outcome $J = J^1 \dots J^n$ is given

$$\rho' = \frac{\Omega_J \rho \Omega_J^\dagger}{\mathrm{tr}[\Omega_J \rho \Omega_J^\dagger]}, \tag{2.55}$$

which upon substitution of $\Omega_J$ and $J_t^i dt$ one finds the change in the state given by the $d\rho$ given in the continuous classical-quantum unravelling which saturates the decoherence diffusion trade-off i.e. Eq. (2.17) with $D_0 = D_1^\dagger D_2^{-1} D_1$. To obtain the general form of master equation, as in (2.17), one can simply use the temple of the larger phase space i.e. take this proof to hold in an enlarged phase space, before tracing over the additional classical degrees of freedom. Any classical-quantum master equation which does not saturate the trade-off can thus be interpreted as a continuous measurement process where some measurement outcomes are not recorded i.e. an inefficient quantum measurement process [42].

Finally, we note that this interpretation of classical-quantum dynamics as a continuous measurement process provides a particularly simple interpretation of the decoherence-diffusion trade-off $D_0 \succeq D_1^\dagger D_2^{-1} D_1$. Here we see that the more weakly we measure the quantum system, the less decoherence we necessarily cause on the system – but the corresponding weaker measurement has greater uncertainty in its outcomes, and thus leads to greater diffusion in the classical system.

## 2.8 An equivalent general form of classical-quantum dynamics

For the study of general classical-quantum dynamics, it is useful to have a form of classical-quantum dynamics for which we know both the sufficient and necessary conditions for positivity. However, using the form of dynamics provided in Eq. (2.13), written in terms of a fixed basis of traceless and orthonormal operators $L_\alpha$, is not convenient for computing the form of dynamics satisfying generic properties. This is because any operator $L_\alpha$ that includes terms proportional to the identity will necessarily not be included in this form, even if this is a natural choice, such as for the $\{z_i, H\}$, $L_z^H$ and $L_z$ operators introduced in the following chapters.

Fortunately, one is able to characterise the completely positive sufficient and necessary

conditions by an alternative representation of the general form of dynamics, which is given

$$\begin{aligned}\frac{\partial \varrho}{\partial t} =& -i[S,\varrho] - \frac{\partial}{\partial z_i}\left(K_i\varrho + \varrho K_i^\dagger\right) \\ &+ \frac{1}{2}\frac{\partial^2}{\partial z_i \partial z_j}(D_{2,ij}\varrho) + D_{2,ij}^{-1}\big(K_i\varrho K_j^\dagger - \frac{1}{2}\{K_j^\dagger K_i,\varrho\}_+\big) \\ &+ \tilde{D}_0^{\alpha\beta}\big(L_\alpha \varrho L_\beta^\dagger - \frac{1}{2}\{L_\beta^\dagger L_\alpha,\varrho\}_+\big)\end{aligned} \tag{2.56}$$

and is completely positive *if and only if*

$$\tilde{D}_0 \succeq 0, \quad D_2 \succeq 0, \quad S = S^\dagger, \tag{2.57}$$

and there exists a phase space dependent vector $v$ of length $n$ such that if $K$ denotes the operator valued vector $K = (K_1,\ldots,K_n)^T$ then

$$(\mathbb{I} - D_2^{-1}D_2)K = v\mathbb{1}. \tag{2.58}$$

Here the $L_\alpha$ are an arbitrary set of traceless and orthogonal operators that may have phase space dependence.

To see that this dynamics is equivalent to the general form of dynamics above, we note that defining

$$K_i = \frac{1}{2}D_{1,i}^C\mathbb{1} + (D_{1,i}^\alpha)^* L_\alpha \tag{2.59}$$

brings the generator of Eq. (2.13) into the form of Eq. (2.56) when

$$S = \bar{H} - \frac{i}{4}D_{1,i}^C D_{2,ij}^{-1}(D_{1,j}^\alpha{}^* L_\alpha - D_{1,j}^\alpha L_\alpha^\dagger) \qquad \tilde{D}_0 = D_0 - D_1^\dagger D_2^{-1}D_1. \tag{2.60}$$

To see that the above conditions are necessary and sufficient for complete positivity, we note that $S$ is Hermitian iff $\bar{H}$ is Hermitian, and that $\tilde{D}_0$ by definition is positive semi definite iff $D_0 \succeq D_1^\dagger D_2^{-1}D_1$. Finally, when $(\mathbb{I} - D_2D_2^{-1})D_1 = 0$ then

$$(\mathbb{I} - D_2D_2^{-1})K = \frac{1}{2}(\mathbb{I} - D_2D_2^{-1})D_1^C\mathbb{1} + (\mathbb{I} - D_2D_2^{-1})D_1 L = \frac{1}{2}(\mathbb{I} - D_2D_2^{-1})D_1^C\mathbb{1} \tag{2.61}$$

i.e. $v = \frac{1}{2}(\mathbb{I} - D_2D_2^{-1})D_1^C$. Conversely, if $(\mathbb{I} - D_2D_2^{-1})K = v\mathbb{1}$, then we see that

$$\frac{1}{2}(\mathbb{I} - D_2D_2^{-1})D_1^C\mathbb{1} + (\mathbb{I} - D_2D_2^{-1})D_1 L = v\mathbb{1} \tag{2.62}$$

which since the $L_\alpha$ are linearly independent and traceless, implies that $(\mathbb{I} - D_2D_2^{-1})D_1 = 0$.

Finally, to find the form of the additional decoherence as given in Eq. (2.20), we note that when $\tilde{D}_0$ is positive semi-definite, one may diagonalise the dissipator to write it in terms of a set of traceless (but not necessarily orthonormal) operators $\tilde{L}_\alpha$. These two forms are equivalent, since when written in diagonal form, one may always rewrite in a non-diagonal form, with positive semi-definite $\tilde{D}_0$, by decomposing each $\tilde{L}_\alpha$ in terms of an orthonormal basis.

## 2.9 Discussion

The main technical results of this chapter can thus be summarised as follows: (1) proving the equivalence of general classical-quantum unravellings and master equations; (2) showing that $D_0 = D_1^\dagger D_2^{-1} D_1$ implies the preservation of purity of the quantum state; (3) demonstrating that the unravelling satisfies $\rho_t = \mathbb{E}[\rho_t|\{z_s\}_{s\leq t}]$; (4) proving that any classical-quantum dynamics may be purified using the church of the larger Hilbert space or the temple of the large phase space; (5) showing the equivalence of the classical-quantum dynamics with continuous measurement and feedback; and (6) providing an alternative characterisation of classical-quantum dynamics in terms of phase-space dependent, non-zero trace operators with known sufficient and necessary conditions for positivity.

Together, the results help to provide some basic intuition of the physics behind classical-quantum dynamics. Continuous, completely-positive and linear master equation pictures of classical-quantum dynamics may always be unravelled into continuous trajectories in terms of $z_t$ and $\rho_t$. When the decoherence is minimal in the quantum system, i.e. $D_0 = D_1^\dagger D_2^{-1} D_1$, the information gained from observing the classical trajectory is always sufficient to keep any initially pure quantum states pure. When the dynamics does not satisfy $D_0 = D_1^\dagger D_2^{-1} D_1$, the additional decoherence $\tilde{D}_0 = D_0 - D_1^\dagger D_2^{-1} D_1$ can be thought of excess decoherence due to either correlations with another quantum system or from tracing out additional classical degrees of freedom. Finally, since the dynamics can be thought of in terms of continuous measurement and feedback, we see that typical classical-quantum interactions can be heuristically thought of as a process by which the classical system measures the quantum one, causing some collapse of the quantum system in the process.

# Chapter 3

# A consistent semi-classical dynamics

In this short chapter, we discuss how the preceding formalism of general classical-quantum dynamics may be used to construct general models which improve upon standard approaches to semi-classical dynamics. Initially motivating these considerations from the perspective of semi-classical gravity, we first write down the standard semi-classical dynamics in a Hamiltonian form. We then use the unravelling to write down a more consistent version of this dynamics, before illustrating this dynamics with some numerical simulations. We then discuss how the mean-field dynamics is recovered in a certain limit, before concluding with a discussion of the potential applications of this framework in the context of gravity.

## 3.1 Motivation and background

Many of the difficulties in modern physics, such as the correct description of black holes, inflationary cosmology, or measurement, seem to occur in the semi-classical regime. There are several reasons for choosing a semi-classical description: there may exist no fully quantum description, such as in the case of gravity; a full quantum theory exists, but is computationally unattainable; or that some fundamental degree of freedom, such as the measurement record of the experimenter or spacetime geometry, is presupposed to be classical in nature. Regardless of whether semi-classicality is viewed as effective or fundamental, it is important to understand which dynamics of classical and quantum systems are consistent, and which cause the

semi-classical description to break down.

When the quantum system is controlled by the classical one without back-reaction, the dynamics is described by unitary quantum mechanics, with the quantum state $|\psi\rangle$ at time $t$ determined by a Hamiltonian $H$ that depends on classical degrees of freedom $z$

$$\frac{d|\psi\rangle}{dt} = -\frac{i}{\hbar}H(z)|\psi\rangle. \tag{3.1}$$

Such dynamics are consistent with a semi-classical description, in the sense that the standard rules of quantum and classical mechanics may be applied without modification to each system independently.

However, defining consistent dynamics where the classical system is affected by the quantum one, i.e. experiences back-reaction, has proved more difficult. In the case of gravity, the standard approach to include backreaction is via the semi-classical Einstein equations, which source the Einstein tensor $G_{\mu\nu}$ by the expectation value of the stress energy tensor $T_{\mu\nu}$ [12–14]

$$G_{\mu\nu} = 8\pi G\langle T_{\mu\nu}\rangle \tag{3.2}$$

(we use units where $c = 1$, and $G$ here is the gravitational constant). Assuming the quantum degrees of freedom evolve according to quantum field theory in curved spacetime, Equation (3.1) with $z = (g, \pi, N, \bar{N})$ (i.e. the gravitational degrees of freedom) and Equation (3.2), together provide the standard theory of semi-classical gravity [81, 82].

Although the equations of semi-classical gravity can be derived from effective low energy quantum gravity, they are commonly understood to fail when fluctuations of the stress-energy tensor are large in comparison to its mean value [83–90, 82, 91, 15]. However, the case where the fluctuations are significant are often precisely the regimes we most wish to understand, such as in considering the gravitational field associated to Schrodinger cat states of massive bodies [92, 93], or vacuum fluctuations during inflation [94–97]. In these cases, the equations of semiclassical gravity fail because they fail to allow for a build up of correlations between the classical and quantum degrees of freedom. For these regimes, background field methods are not appropriate, and an alternate effective theory of semi-classical gravity is required.

An early proposal in this direction was provided by [26], which noted the similarity of the dynamics of continuous measurement theory and that of semi-classical or mean-field approaches

at coupling classical and quantum degrees of freedom. More recently, other approaches based on continuous measurement theory [98, 74, 99] have been used to study semi-classical effects in the Newtonian regime.

The main aim of this chapter is to re-explore this idea, using the general formalism of classical-quantum dynamics presented in Chapter 2. This allows us to extend these earlier semi-classical proposals to the case of arbitrary classical-quantum Hamiltonians, complete with sufficient and necessary conditions on the diffusion in the classical system for the dynamics to be consistent. While motivated by gravity, the technical conclusions follow equally well for any systems based on mean-field methods, such as those used in molecular dynamics [63, 64], and indeed our results demonstrate a connection with another common approach in physical chemistry, known as the quantum-classical Liouville equation [19].

## 3.2 Standard semi-classical dynamics

In this section, we introduce the standard approach to constructing semi-classical dynamics, and study why it does not lead to a consistent treatment of semi-classical physics.

As pointed out in earlier work [15], the equations of semi-classical gravity, Equation (3.1) with $z$ representing the time local gravitational degrees of freedom and Equation (3.2), may be understood as a special case of a more general approach taken to describe back-reaction. In this chapter we shall refer to this as the *standard semi-classical approach*, though it is also known in other fields as mean field dynamics [100] or Ehrenfest dynamics [63].

To write down the standard semi-classical dynamics, we first assume the existence of a Hermitian operator-valued function of phase space $H(z)$, that we refer to as the classical-quantum Hamiltonian. This Hamiltonian describes both the standard classical and quantum Hamiltonians $H_C(z)$ and $H_Q$ respectively, as well as their interactions via a traceless Hermitian operator-valued function of phase space $H_I(z)$, which arise in the following canonical decomposition of the classical-quantum Hamiltonian

$$H(z) = H_C(z)\mathbb{1} + H_Q + H_I(z), \tag{3.3}$$

where $\mathbb{1}$ is the identity operator on the Hilbert space.

For a given classical-quantum Hamiltonian $H(z)$, we write down the standard semi-classical dynamics as follows. The classical evolution is deterministic and has back-reaction given by the expectation value of the quantum state,

$$dz_t^i = \langle \{z_i, H\} \rangle dt, \tag{3.4}$$

where here $\{\cdot, \cdot\}$ denotes the Poisson bracket of classical mechanics, the angled brackets denote the inner product with respect to $|\psi\rangle_t$ i.e. $\langle A \rangle = \langle \psi|_t A |\psi\rangle_t$, and we implicitly understand all the classical variables $z_i$ appearing on the right hand side to be the values evaluated at $t$ i.e. $z_t^i$. Meanwhile, the quantum evolution is given by Hamiltonian evolution that depends on the phase space degree of freedom

$$d|\psi\rangle_t = -\frac{i}{\hbar} H(z_t) |\psi\rangle_t dt. \tag{3.5}$$

Note that this dynamics allows initial correlations between the classical and quantum sectors, and we ignore more pathological versions e.g. in which the phase-space dependence in Equation (3.5) is an ensemble average over the classical degrees of freedom.

There are number of features of the standard semi-classical equations, (3.4) and (3.5), that make the dynamics at least at first glance desirable. Firstly, when the interaction Hamiltonian, $H_I(z)$, is zero, it is straightforward to check that that the dynamics reduces to the standard equations of classical and quantum Hamiltonian mechanics. Secondly, even when the interaction Hamiltonian is non-zero, the dynamics retains a number of expected features: the classical system evolves continuously in phase space, the quantum state $|\psi\rangle_t$ remains normalised, and the evolution laws are autonomous (i.e. only depend on $z_s$ and $|\psi\rangle_s$ at $s = t$, with the coefficients having no explicit dependence on $t$) as is the case for standard classical or quantum mechanics.

However, it is well-known that the standard semi-classical dynamics comprising Equations (3.4) and (3.5) lead to a number of violations of the standard principles of quantum theory, inducing a break-down of either operational no-signalling, the Born rule, or composition of quantum systems under the tensor product [22, 92, 99, 101]. These arguments appeal to the fact that the dependence of $Z_t$ on $|\psi\rangle_t$, generated by Equation (3.4), means that the evolution of (3.5) need not even be a linear map [102–104], and thus can be ruled due to the inconsistency of non-linear modifications to quantum mechanics [105–108].

Alternatively, one can directly rule out the standard semi-classical dynamics as a consistent theory by observing that the evolution law for $\varrho(z,t)$ is non-linear. To see this, we first note that by use of the chain rule,

$$d\varrho = \mathbb{E}[d\delta(z-z_t)\rho_t] + \mathbb{E}[\delta(z-z_t)d\rho_t], \tag{3.6}$$

where here $\rho_t = |\psi\rangle_t\langle\psi|_t$. Using the chain rule with equation (3.4) and (3.5) to compute both $d\delta(z-Z_t)$ and $d\rho_t$ to first order in $dt$, we find that

$$\frac{\partial\varrho}{\partial t} = -\frac{\partial}{\partial z_i}\mathbb{E}[\mathrm{tr}(\{z_i,H\}\rho_t)\delta(z-z_t)\rho_t] - i[H(z),\varrho], \tag{3.7}$$

where we assume summation over the repeated $i$ index. Since the first term contains two occurrences of $\rho_t$, it cannot be written as a linear equation in terms of $\varrho$, unless each $\{z_i,H\}$ were proportional to the identity i.e. unless the interaction Hamiltonian $H_I(z)$ were everywhere zero. We thus see that when there is quantum back-reaction on the classical system, the standard semi-classical dynamics induce an evolution on $\varrho$ that is necessarily non-linear, and therefore inconsistent, as discussed in Appendix A.

## 3.3 Healed semi-classical dynamics

The general dynamics for the classical degrees of freedom $z_t$ and the quantum state $|\psi\rangle_t$, given by (2.16) and (2.19), provide a general class of dynamics to describe semi-classical systems. Using the freedom in the $D$ matrices and $H$, one may attempt to construct sensible semi-classical dynamics phenomenologically by fitting predictions of these models to data. An alternative approach is to find a dynamics that explicitly resembles the standard semi-classical dynamics of (3.4) and (3.5), which we will now turn to in this section.

Starting with Equations (2.16) and (2.17), we take the pure classical part of the drift to be generated by a classical Hamiltonian $H_C(z)$. For the interaction terms, one can use the freedom in the choice of Lindblad operators to pick $L_\alpha = \{z_\alpha, H_I\}$, where $H_I(z)$ is an interaction Hamiltonian, and then set $D^{0\alpha}_{1,i} = \frac{1}{2}\delta^\alpha_i$. This fixes the decoherence term to be $D_0 = \frac{1}{4}(\sigma\sigma^T)^{-1}$, since by assumption we assume the decoherence-diffusion trade-off is saturated. Finally, we ensure that that the first term of (2.17) has a Hamiltonian picked that coincides with the

classical-quantum Hamiltonian i.e. $\bar{H} = H/\hbar$ for $H(z) = H_C(z)\mathbb{1} + H_Q + H_I(z)$. Using this definition of $H(z)$ to simplify the various terms, we arrive at a set of equations that we dub "the healed semi-classical equations", given as

$$dz_t^i = \langle\{z_i, H\}\rangle dt + \sigma_{ij} dW_t^j \tag{3.8}$$

$$\begin{aligned} d|\psi\rangle_t = &-\frac{i}{\hbar} H|\psi\rangle_t dt + \frac{1}{2}\sigma_{ij}^{-1}\{z_j, H - \langle H\rangle\}|\psi\rangle_t dW_t^i \\ &- \frac{1}{8}\sigma_{ij}^{-1}\sigma_{ik}^{-1}\{z_j, H - \langle H\rangle\}\{z_k, H - \langle H\rangle\}|\psi\rangle_t dt \end{aligned} \tag{3.9}$$

where in the above $\sigma$ may be any real matrix such that

$$(\mathbb{I} - \sigma\sigma^{-1})\{z, H\} = a(z)\mathbb{1}, \tag{3.10}$$

for a real vector $a(z) \in \mathbb{R}^n$; that this is a sufficient and necessary condition for complete positivity follows from the discussion of Section 2.8. As before, while $\sigma$ may have arbitrary dependence on $z$, it cannot have dependence on the quantum state itself. For a given initial quantum state $|\psi_{t_i}\rangle$ and classical state $z_{t_i}$, these coupled stochastic differential equations determine the probability of ending up in any final pair of states $z_{t_f}$ and $|\psi_{t_f}\rangle$. An early example of this dynamics for the special case of linear, constant force coupling between two particles, one classical and one quantum, was described in [26].

Written in the above form, the differences with the standard semi-classical equations are clear. The classical evolution of the healed semi-classical Equation (3.8) takes the form of the standard semi-classical Equation (3.4), i.e. backreaction given by an expectation value, but with an additional diffusive noise term. Similarly, the quantum evolution of the healed semi-classical Equation (3.9) takes the form of the standard semi-classical Equation (3.5) i.e. pure unitary evolution, but with an additional stochastic term that tends to drive the quantum state towards a joint eigenstate of the operators $\{z_i, H\}$ and $H$, where one exists, and an additional deterministic term than ensures that $|\psi\rangle_t$ remains normalised at all times [109]. Despite the appearance of an expectation value in the backreaction drift term, the joint dynamics of these coupled equations gives statistics for $Z_t$ as if the classical system were diffusing around a force given by a random eigenstate of the operators $\{z_i, H\}$. The free parameters of the model $\sigma_{ij}$ determine both the rate at which the quantum state evolves to an eigenstate and the rate of

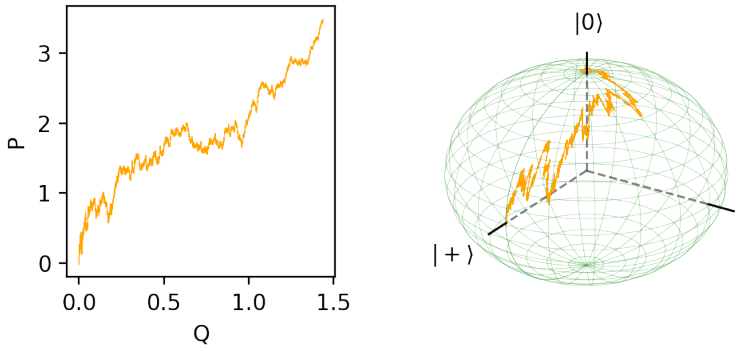


Figure 3.1: A numerically simulated classical-quantum trajectory for a classical particle interacting with a qubit, represented by a classical trajectory in phase space (left) and a quantum trajectory on the Bloch sphere (right). The classical-quantum Hamiltonian is such that the classical system experiences a force either up or down depending on whether the state is $|0\rangle$ or $|1\rangle$ – the quantum state is then chosen to evolve starting in the superposition state $|+\rangle$. Initially starting at the origin in phase space, the classical system follows a stochastic trajectory with positive drift, agreeing with the evolution of the quantum state, which follows a path on the surface of the Bloch sphere before reaching the fixed point $|0\rangle$. The classical trajectory serves as a measurement record of the value of the qubit, and conditioned upon it the quantum state remains pure at all times. Since the classical particle's motion is stochastic, it takes some time to resolve the value of the qubit. The trajectories shown here should be contrasted with the standard semi-classical prediction, which predicts zero drift in momentum, and quantum evolution corresponding to a rotation about the $z$ axis of the Bloch sphere. Further details, such as the specific Hamiltonian studied and the initial conditions, may be found in Appendix C.

diffusion of the classical system – that these two rates are explicitly inversely related is the expression of the decoherence-diffusion trade-off. The other positivity condition of (2.15) appears as the condition $(\mathbb{I} - \sigma\sigma^{-1})\{z, H\} = a(z)\mathbb{1}$ for some $a(z)$, which ensures that no combination of the classical degrees of freedom can be constructed such that a classical variable has a drift depending on a quantum expectation value without an associated noise term. When the back-reaction is zero, i.e. $H_I(z) = 0$, the positivity condition is satsified for all $\sigma$, and thus $\sigma$ may be taken to zero. In this limit, the equations reduce to uncoupled deterministic Hamiltonian classical and quantum mechanics.

To make the above discussion more concrete, consider the numerically simulated dynamics shown in Figures 3.1 and 3.2, of a qubit interacting with a 1D particle, and a toy model of a test particle moving in the Newtonian potential of a mass in superposition. Here the trajectories in phase space are shown on the left, while on the right the trajectory in Hilbert space is represented

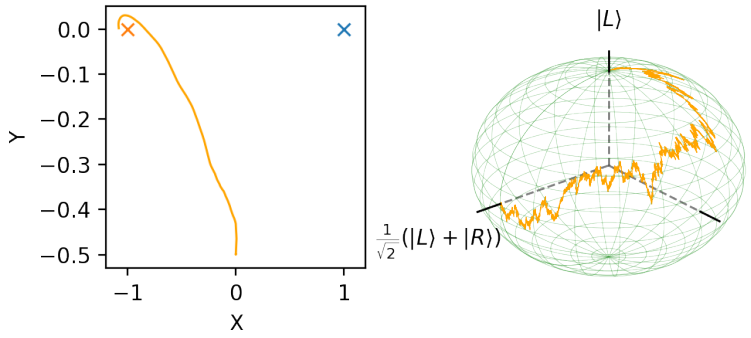


Figure 3.2: A numerically simulated classical-quantum trajectory for a toy model of a classical test particle moving in the Newtonian potential sourced by a mass in a spatial superposition of left $|L\rangle$ and right $|R\rangle$ states (positions marked in space by crosses). Initially starting at rest at $X = 0$ and $Y = -0.5$, the test particle is seen to eventually fall toward the mass being on the left, with the small initial motion toward the centre of the two possible locations accounted for by the diffusion in momentum. This should be contrasted with the prediction using the standard semi-classical equations, in which the test particle falls directly towards the middle of the two possible positions of the heavier mass. Since the classical trajectory here is plotted in configuration space, rather than phase space as in Fig. 3.1, the trajectory does not directly show the stochastic kicks in the momentum of the classical particle and thus appears comparatively smooth. See Appendix C for for more information.

by a path on the surface on the Bloch sphere. For both, we see that the classical trajectories correspond to the motion expected if the force on the classical system were determined by an eigenvalue of $\{p_i, H\}$, but with additional diffusion around this. The quantum trajectories are correlated with these classical trajectories, such that when the particle's momentum has increased significantly, or when the test mass has moved significantly towards the mass on the left, the corresponding quantum state is also in the corresponding eigenstate with high probability. A given change in the classical system is only significant if it is large compared to the background classical noise $\sigma$; this indicates why the changes in the quantum degree of freedom are inversely proportional to the noise strength in the classical system.

The full details of these models appear in Appendix *C*, where we simulate a number of simple toy models that arise as special cases of this general Hamiltonian dynamics, including a toy model for vacuum fluctuations sourcing the expansion rate in the early universe.

## 3.4 Regime of validity of the standard semi-classical equations

Having derived a general form of consistent semi-classical dynamics, we may test the regime of validity of the standard semi-classical equations (3.4) and (3.5) by studying when they can be approximately recovered from the consistent dynamics of (3.8) and (3.9).

The first important observation to make is that that the standard semi-classical equations cannot be derived as a limit of the healed ones. Specifically, while the free parameters contained in the matrix $\sigma$ of the healed semi-classical equations may be varied such that either (3.8) or (3.9) approximately takes the form of the respective standard semi-classical equation, the appearance of both $\sigma$ and $\sigma^{-1}$ prevent the recovery of both equations in any limit, with either the diffusion or decoherence necessarily becoming large as $\sigma \to \infty$ or $\sigma \to 0$. In the special case that $\sigma = 0$, the positivity condition reduces to $\{z, H\} = a(z)\mathbb{1}$ for some $a(z) \in \mathbb{R}^n$ i.e. that the classical-quantum Hamiltonian is of the form $H(z) = H_C(z)\mathbb{1} + H_Q$, meaning that the quantum backreaction on the classical system must also be zero. As should be expected, the failure to recover the standard semi-classical equations from their healthier versions unless the quantum backreaction is zero is consistent with the analysis in Sec. 3.2, where the dynamics induced on the classical-quantum state was found only to be linear provided $H_I(z)$ was zero.

The standard semi-classical equations are thus inconsistent if applied to all states. However, using Equations (3.8) and (3.9), we can find a regime in which the standard semi-classical equations are approximately valid for a given initial quantum state $|\phi\rangle$. Specifically, we will ask which initial states $|\phi\rangle$ and timescales $\tau$ the healed semi-classical equations can be approximated by the standard ones i.e. when the additional terms corresponding to diffusion and decoherence have a negligible impact on observations.

For the classical degrees of freedom to appear to evolve deterministically, one should consider timescales much larger than the noise to signal ratio of the system, such that any noise fluctuations are removed by coarse-graining in this time window [110]. Provided the classical system evolves slowly, and is only weakly affected by the quantum one, we may approximate the signal provided by the $i$th degree of freedom of the classical system as the square of the initial drift $\langle\phi|\{z_i, H\}|\phi\rangle$, and the noise in this degree of freedom as $(\sigma\sigma^T)_{ii}$, the initial value of this component of the diffusion matrix. For the dynamics of (3.8) to reduce to (3.4), one

must consider timescales $\tau$ large compared to the largest possible ratio of the diffusion and the square of the drifts of all the classical phase space degrees of freedom $i$ i.e.

$$\tau \gg \max_i \frac{(\sigma\sigma^T)_{ii}}{\langle\phi|\{z_i, H\}|\phi\rangle^2}. \tag{3.11}$$

On the other hand, for the quantum system to appear to evolve unitarily, one must consider timescales very short compared to the decoherence time of the quantum system. The decoherence rate may be computed for an initially pure quantum state via the sum of the variances of the diagonal Lindblad operators $\bar{L}_i$ acting on the system [111], which in our case take the form $\bar{L}_i = \sigma_{ij}^{-1}\{Z_j, H\}$. This means that (3.9) only reduces to (3.5) on timescales

$$\tau \ll \frac{1}{\sum_{ijk} \sigma_{ij}^{-1} \mathrm{cov}_{|\phi\rangle}(\{z_j, H\}, \{z_k, H\})\sigma_{ki}^{-T}} \tag{3.12}$$

where here $\mathrm{cov}_{|\phi\rangle}(A, B) = \langle AB\rangle - \langle A\rangle\langle B\rangle$ with expectation values taken with respect to $|\phi\rangle$. We thus see that simultaneously requiring the decoherence and diffusion to be negligible both upper and lower bounds the timescale $\tau$ for which the standard semi-classical equations approximate the consistent dynamics of the healed semi-classical equations, for a given initial quantum state $|\phi\rangle$.

The above conditions on initial quantum states $|\phi\rangle$ and timescales $\tau$ can be adapted to prove a concise necessary condition on the regime of validity of the standard semi-classical equations. Firstly, we note that (3.11) implies that $\tau$ must be much larger than each of the $i$ noise to signal ratios, and therefore that $\langle\phi|\{z_i, H\}|\phi\rangle^2$ must be much greater than the ratio of $(\sigma\sigma^T)_{ii}$ to $\tau$. Secondly, we note that the denominator of (3.12) may be rewritten as a trace of a positive semi-definite matrix $A = \sigma^{-1}C_{|\phi\rangle}\sigma^{-T}$, where $C_{|\phi\rangle}$ is the matrix of the covariances introduced previously. Using the inequality $\mathrm{tr}A \geq (v^T Av)/(v^T v)$, which holds for an arbitrary vector $v$, it follows from (3.12) that $\tau$ must be much smaller than $(v^T v)/(v^T Av)$ for all $v$. Taking $v$ to be given by each of the columns of $\sigma$, and using the positivity condition $(\mathbb{I} - \sigma\sigma^{-1})\{z, H\} = a(z)\mathbb{1}$ to replace $\sigma\sigma^{-1}C_{|\phi\rangle}\sigma^{-T}\sigma^T$ with $C_{|\phi\rangle}$, one finds that $\tau$ is much smaller that each of the ratios of $(\sigma\sigma^T)_{ii}$ to the $i$th diagonal of the covariance matrix $C_{|\phi\rangle}$ i.e. the variance, which we denote $\mathrm{var}_{|\phi\rangle}(\{z_i, H\}) = \langle\phi|\{z_i, H\}^2|\phi\rangle - \langle\phi|\{z_i, H\}|\phi\rangle^2$. Rearranging this final inequality and combining with the ones derived from (3.11), we arrive at the following set of inequalities

$$\langle\phi|\{z_i, H\}|\phi\rangle^2 \gg \frac{(\sigma\sigma^T)_{ii}}{\tau} \gg \mathrm{var}_{|\phi\rangle}(\{z_i, H\}), \tag{3.13}$$

which must hold for each $i$ in order for the standard semi-classical equations (3.4) and (3.5) to be a valid approximation to (3.8) and (3.9). We thus see that for there to exist any timescale $\tau$ for which the standard semi-classical equations are a good approximation to a consistent semi-classical dynamics, the force on the classical system, either from quantum backreaction or internal classical dynamics, must be much greater than its variance with respect to the quantum state. While this condition has been previously postulated [89], the analysis above provides a rigorous derivation, by requiring the standard semi-classical dynamics to be a valid approximation of a consistent semi-classical theory. Moreover, for a given quantum state $|\phi\rangle$ that satisfies $\langle\phi|\{z_i, H\}|\phi\rangle^2 \gg \mathrm{var}_{|\phi\rangle}(\{z_i, H\})$, the full set of inequalities (3.13) gives the timescale over which the dynamics will be valid, for a given diffusion/decoherence rate controlled by $\sigma$.

In the limiting case that the state $|\phi\rangle$ is an eigenstate of the operators $\{z_i, H\}$, the variance vanishes, and thus the standard semi-classical dynamics are valid approximation for all times provided the diffusion $\sigma\sigma^T$ is sufficiently small. In the Newtonian limit of gravity [4], the interaction is dominated by the mass density $\frac{\partial H}{\partial \Phi} = \hat{m}(x)$ and we see that the standard semi-classical equations are exactly valid only when the quantum state is in an approximate eigenstate of the mass density operator, which excludes macroscopic superpositions, as well as states which are spatially entangled: essentially the quantum state of matter must be approximately classical [88, 89, 94].

However, while the above analysis implies that there can exist certain states and timescales over which the standard semi-classical approach is a reasonable approximation to a consistent semi-classical dynamics, it must be emphasised that in practice the regime of validity may be very limited. The healed equations of (3.8) and (3.9) thus provide a semi-classical dynamics that extends the regime of validity of the standard semi-classical dynamics to arbitrary states and timescales.

An important example of where the healed semi-classical dynamics extends the regime of validity of the standard semi-classical equations, without considerable increased technical difficulty, is in the low noise, $\sigma \to 0$, limit of the theory. Here, one considers timescales long compared to the diffusion in the theory, such that the inequality of (3.11) holds, and the classical equations can be approximated by (3.4). However, rather than restricting to specific states and

timescales such that the decoherence is negligible, we instead keep the additional $\sigma^{-1}$ dependent terms in (3.9) that do not appear in (3.5). In the limit that $\sigma \to 0$, the quantum dynamics causes the quantum state to almost instantaneously evolve, with probabilities given by the Born rule, to an eigenstate of the operators $\{z_i, H\}$ [109, 42]. The classical evolution is thus well approximated by conditioning on eigenstates of the quantum state decohered in this basis, and then evolving according to classical equations of motion. This is in fact the way in which the semi-classical Einstein equations are often used in practice to deal with classical mixtures – here we see that this use of them is a limiting case of the healed semi-classical equations when the diffusive noise in the classical system is negligible. In this limit, the resulting classical system is still described by a probability distributions over final states, but this distribution is entirely due to the probability distribution over eigenstates of $\{z_i, H\}$ provided by the decohered quantum state.

While the low noise limit of the healed semi-classical dynamics may be a valid regime in which to study semi-classical physics, more generally one would like to understand what happens while the quantum state still has coherence. Here, the final probability distribution of the classical system is due to both the initial quantum state and diffusion in the classical system itself. In this case $\sigma$ is finite, and the full machinery presented thus far must be used.

## 3.5 Conditions for positivity and the quantum-classical Liouville equation

When we previously introduced our healthier version of semi-classical dynamics, we did not attempt to justify the appearance of the positivity condition (3.10). To see how this arises, we first write our dynamics in terms of the density operator, which can be written in vectorised notation (c.f. Section 2.4) as

$$\begin{aligned} d\rho_t = &-\frac{i}{\hbar}[H, \rho_t]dt + \{z_t, H\}^T D_0 \rho_t \{z_t, H\}dt - \frac{1}{2}\{\{z_t, H\}^T D_0^T \{z_t, H\}, \rho_t\}_+ dt \\ &+ \frac{1}{2} dW_t^T \sigma^{-1}(\{z_t, H\}\rho_t + \rho_t\{z_t, H\} - 2\langle\{z_t, H\}\rangle\rho_t), \end{aligned} \tag{3.14}$$

where here $D_0 = \frac{1}{4}(\sigma\sigma^T)^{-1}$. We may then write the dynamics in master equation form, using the steps outlined in Section 2.3. Doing so we arrive at the master equation representation of

the healed semi-classical dynamics

$$\begin{aligned}\frac{\partial \varrho}{\partial t} =& -\frac{i}{\hbar}[H,\varrho] + \frac{1}{2}\big(\{H,\varrho\} - \{\varrho,H\}\big) \\ &+ D_0^{ij}\big(\{z_i,H\}\varrho\{z_j,H\} - \frac{1}{2}\big\{\{z_j,H\}\{z_i,H\},\varrho\big\}_+\big) + \frac{1}{2}\frac{\partial^2}{\partial z_i \partial z_j}\big(D_{2,ij}\varrho\big)\end{aligned} \tag{3.15}$$

where again $D_0 = \frac{1}{4}(\sigma\sigma^T)^{-1}$ and $D_2 = \sigma\sigma^T$. To find the positivity conditions for this dynamics, we note that this takes the alternative form of dynamics given in Eq. (2.20) with $K_i = \frac{1}{2}\{z_i, H\}$, $G = H$, $D_2 = \sigma\sigma^T$ and no additional Lindbladian decoherence terms i.e. $\tilde{L}_\alpha = 0$. As such, we see that since $G = G^\dagger$ and $D_2$ is positive semi-definite, the sufficient and necessary condition for positivity provided by (2.58) is given

$$(\mathbb{I} - D_2^{-1}D_2)\frac{1}{2}\{z,H\} = v(z)\mathbb{1}, \tag{3.16}$$

for some vector $v(z)$, which upon using properties of the pseudoinverse and redefining $a(z) = 2v(z)$ gives the positivity condition (3.10) as claimed.

There is an interesting upshot of the above analysis. Namely, we see that the first two lines of the master equation picture take the form of the quantum-classical Liouville equation dynamics given in Eq. (1.4), with the backreaction term known as the Alexandrov-Gerasimenko bracket [17, 18, 15, 19]. The remaining terms can be understood to provide the necessary diffusion and decoherence on the classical and quantum systems required for complete-positivity [25, 74, 73]. We thus see that despite motivating this approach from the unravelling, mean-field perspective, we see that our dynamics also provides a consistent version of the other common form of classical-quantum dynamics, suggesting some importance to this form of Hamiltonian semi-classical dynamics.

Finally, we note that the conditions (3.11) to (3.13) also provide a regime of validity for the quantum-classical Liouville equation to hold as a description of an effectively classical-quantum system. Taking an initial classical-quantum state $\varrho(z) = \delta(z - z_0)|\phi\rangle\langle\phi|$, we see that we can apply the constraints (3.11) and (3.12), which here describe when the noise is small compared to average back-reaction on the classical system (i.e. the trace of Eq. (1.4)), and when the decoherence in the system is negligible. This being said, it is important to emphasise that outside of this regime of validity, the quantum-classical Liouville equation may in fact provide a better description of certain quantum dynamics than the healed dynamics we present here

(c.f. Chapter 4). However, when this is the case, the total system is necessarily no longer well described by an effective classical-quantum approximation, and thus cannot be unravelled in terms of individual classical and quantum trajectories.

## 3.6 Discussion

A consistent version of mean-field dynamics may shed light on some of the open problems in semi-classical physics. Of potential interest is understanding the role of vacuum fluctuations in cosmology and structure formation. Since we wish to investigate the role that vacuum fluctuations play in density inhomogeneity, this is a regime in which the semi-classical Einstein Equation (3.2) cannot be used. In practice, researchers consider situations in which the density perturbations have decohered [97, 96, 112–116], so that they can condition on their value and feed this into the Friedman-Robertson-Walker equation governing the expansion of the local space-time patch [117–119]. Such an approach is inconsistent with the semi-classical Einstein Equation [95]. As already discussed, this procedure can in fact be understood as the low noise, $\sigma \to 0$, limit of the healed semi-classical equations (3.8) and (3.9).

The semi-classical dynamics we have presented also provides a framework in which to ask what happens at earlier times when there are genuine quantum fluctuations. The toy model discussed in Appendix C and simulated in Figure 3.3 gives some indication of what we expect to happen. The total quantum state of the field can stay pure, even as the density of a local patch converges to a particular value. In the process, the quantum state of the field must become less entangled. The density, and thus the expansion factor at any particular point will be correlated with the density and expansion elsewhere, because the state of the field is initially highly entangled. In contrast to typical treatments, models in our framework exhibit additional fluctuations in the classical system due to diffusion, on top of the standard fluctuations due to the statistics of the decohered quantum state. Additionally, the semi-classical models presented here may be studied without a priori identifying sources of decoherence. Exploring features such as these in more realistic models would be of great interest, especially since here we can consistently evolve the system before the fluctuations have decohered.

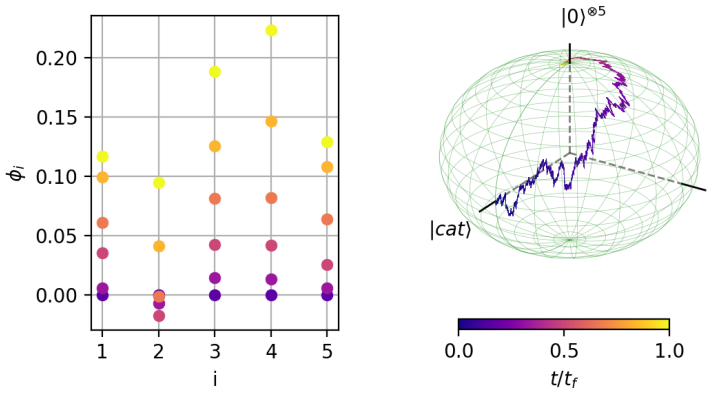


Figure 3.3: A numerically simulated classical-quantum system of five qubits each interacting locally with a classical degree of freedom, where the $|0\rangle$ ($|1\rangle$) state acts to increase (decrease) the local classical degree of freedom $\phi_i$. Initially in a cat state, the quantum system evolves to a local product state with no entanglement, while the local classical degrees of freedom shown at six equal time intervals from $t = 0$ to $t = t_f$ exhibit fluctuations around the expected increase due to diffusion. The Hamiltonian and initial conditions are provided in Appendix C.

A challenging, yet important, application of these consistent versions of mean-field dynamics would be in a consistent treatment of backreaction in the context of black hole evaporation [120]. While it is perhaps difficult to draw any conclusions, given the basic nature of our dynamics compared to the complexity of a fully relativistic treatment, we conclude by noting two relevant features of the dynamics we present to this problem.

Firstly, it is evident from equations (3.8) and (3.9) that a consistent treatment of semi-classical physics must take into account the fact that solutions to the dynamics should be described by ensembles of classical-quantum trajectories. This has an important consequence when it comes to ascertaining the purity of a quantum state – while the state of the quantum system conditioned on some partial classical information will be mixed, the dynamics of equation (3.9) preserves the purity of $\rho(t|\{z_s\}_{s\leq t})$, such that quantum state conditioned on the full classical trajectory remains pure. Put more compactly, although the entropy of the quantum state conditioned on the final classical state $z_f$ may be greater than zero, the quantum state conditioned on the classical trajectory has entropy $S(\rho(t|\{z_s\}_{s\leq t})) = 0$. Whether or not a

classical-quantum system appears to map pure quantum states to mixed states, thus depends on which classical degrees of freedom are available to be conditioned on.

Secondly, we note that the representation of classical-quantum dynamics as a continuous measurement presented in Section 2.7, provides some clue as to how the loss of predictability in the classical degrees of freedom in a semi-classical treatment may be reconciled with the complete predictability provided by a fully quantum treatment. Here, the classical trajectories are generated by the measurement signals of POVMs applied to the quantum state. In this case, since every POVM may be viewed as unitary evolution on a larger system containing a measurement device, and applying unitaries controlled by the measurement device state to a set of quantum states $|z\rangle$ that span the classical state space, we arrive at a fully quantum, albeit artificial, model of semi-classicality. Considering the problem in discrete time, with time step $\Delta t$, the action of the unitary at a given time step $k$ is given on an arbitrary quantum state $|\psi\rangle$, the $k$th initialised measurement apparatus state $|0\rangle_k$ and the classical system as

$$U_k(|\psi\rangle \otimes |0\rangle_k \otimes |z\rangle) = \int \Omega_J(z)|\psi\rangle \otimes |J\rangle_k \otimes |z + (D_1^C + J)\Delta t\rangle d\mu_0(J). \tag{3.17}$$

The preservation of the norm for all quantum states $|\psi\rangle$ follows from the definition of the POVM. While measuring the apparatus state at each time step leads to a discretized version of the classical-quantum evolution, leaving the system unmeasured leads to a highly entangled state encoding the full probability distribution of classical-quantum trajectories in the apparatus degrees of freedom. We can equally view this in the language of many worlds, where the apparatus states $|J\rangle_k$ keep track of the branch of the wavefunction. In the case of a unique final state $z_f$ for the classical evolution, the total state would necessarily factorise between the classical subsystem and the other two subsystems. In this case, any measurements on the final quantum state appear mixed by virtue of entanglement with an unmeasured reference system.

Ultimately, understanding whether the dynamics we introduce here may be of use in the study of semi-classical gravity relies upon a successful application of this formalism in this context, of which efforts are ongoing [46, 4, 121–125, 73]. However, the above considerations do suggest that if these efforts are successful, a consistent version of semi-classical dynamics has some potential to provide insight into the remaining deep questions in this field.

# Chapter 4

# Effective dynamics from the classical-quantum limit

In this chapter we consider what may be the most important problem in the topic of effective classical-quantum dynamics – how to derive classical-quantum dynamics from a fully quantum theory. The key idea will be to generalise the standard notion of a classical limit, such that one may take the classical limit of a subsystem. We shall see that we may understand effective classical-quantum dynamics as arising from quantum dynamics when a particular subsystem is strongly decohered by its environment.

## 4.1 Motivation and background

The classical limit describes the emergence of classical physics from quantum theory. Typically justified in a variety of ways, the most famous of these is to consider action large compared to the reduced Planck's constant, $\hbar$. This leads to the ubiquitous statement that the classical limit is taking $\hbar \to 0$. As well as explaining the success of classical mechanics for the description of macroscopic systems, the classical limit provides an important theoretical tool for simplifying the analysis of quantum systems that are too complex to study directly.

The classical limit allows one to replace a quantum system with an entirely classical descrip-

tion. However, many systems of interest operate in a regime where both classical and quantum features are important, and this leads to the following question:

> Can we take a limit of a quantum system such that one subsystem behaves classically, while the rest remains quantum?

A limit of this kind would have a wide variety of applications: from providing first principle derivations of quantum control and measurement set-ups [126, 127, 43]; to describing systems at the classical-quantum boundary [66–68]; formalising approaches in quantum chemistry where the nuclear degrees of freedom are treated as classical and the electronic degrees of freedom are treated quantum mechanically [63, 64, 19]; and more generally providing a framework to simplify complex many-body quantum dynamics while retaining essential quantum features. Beyond these more practical applications, it would be interesting if recently proposed models of classical-quantum theories of gravity [46, 48, 4, 128, 121, 124, 123] could arise as effective descriptions of quantum gravity.

In this chapter, we tackle the problem of taking such a classical limit. Since this involves mapping two quantum subsystems to a quantum subsystem and an effective classical subsystem, we call this a "quantum-quantum to classical-quantum" limit, or classical-quantum limit for short. Such a limit could also be referred to as a semi-classical limit, since the resulting effective theory contains both classical and quantum degrees of freedom, or as a classical limit for subsystems. We use this terminology in a more general sense than earlier work – this limit is taken to be able to include the effects of *back-reaction* on the effective classical system, and therefore should not be conflated with special cases in which the effective classical system is unaffected by the quantum one [129, 70].

Two important requirements to make on any classical-quantum limit of quantum theory is that it be physically motivated and consistent. Although the standard $\hbar \to 0$ classical limit is often well-motivated physically, we shall see that as a classical-quantum limit it fails to be consistent, in that it fails to describe an effective classical subsystem. In this case, the resulting dynamics is known as the quantum-classical Liouville equation [130, 18, 19], and does not lead to well-defined classical evolution on the subsystem in question [15]. The first example of a

limit procedure leading to consistent dynamics was provided in the pioneering work by Diósi [25] who considered two particles, each having a different Planck's constant. While this allowed for one of the first examples of consistent classical-quantum dynamics to be derived, it came at the expense of requiring a number of unphysical considerations, including modified quantum mechanical evolution laws and ad hoc sources of classical noise.

In the present chapter we demonstrate that a physically motivated and consistent limit procedure exists, starting from standard unitary quantum mechanics in a closed system. The key observation we make is the following: such closed system dynamics will always generate entanglement between subsystems, and thus always lead to a breakdown of classicality, independently of any parameter such as $\hbar$ that is usually used to quantify classicality. This means that the standard notions of a classical limit, such as $\hbar \to 0$, must be supplemented by an additional mechanism that removes the entanglement generated between subsystems.

In our framework, the classicality of a subsystem is guaranteed by decoherence due to its external environment. Already well understood to play an important role in the quantum-to-classical transition [131–136], the coupling to the environment in our framework leads to an associated decoherence timescale $\tau$ of the subsystem in question. By taking $\tau \to 0$, one can ensure that this subsystem is classical at all times. The key conceptual takeaway from this chapter is that a double scaling limit, in which $\hbar \to 0$ while $\tau \to 0$ such that the ratio $E_f = \hbar/\tau$ is fixed, provides a version of a classical limit that may be consistently applied to subsystems i.e. a classical-quantum limit.

The main technical result of this chapter is computing the explicit form of the dynamics in this double scaling limit, for arbitrary bipartite Hamiltonians for which a classical limit is possible, which is given in Equation 4.4.5. In order to prove the consistency of this dynamics, we show that the dynamics is a special case of the recently characterised completely-positive form [46, 45], which guarantees that the effective classical subsystem is well-defined. This distinguishes our dynamics from earlier attempts at deriving effective classical-quantum dynamics from quantum theory [137, 27], and provides a regime in which the general form of continuous dynamics introduced in [45] could arise as an effective theory. The resulting dynamics is generically an irreversible open-system dynamics, with decoherence and diffusion controlled by

the parameter $E_f$. The complete-positivity ensures the classical-quantum dynamics may be directly unravelled in terms of continuous classical trajectories in phase space and quantum trajectories in Hilbert space, which are given in Equations (4.7.1) and (4.7.2).

Alongside the main results, we find a number of related results:

- A partial version of the Glauber-Sudarshan quasiprobability distribution is introduced, and identified as the correct representation to require positivity of for effective classical-quantum dynamics in the Hilbert space.
- The dynamics of partial versions of the Glauber-Sudarshan and Husimi quasiprobability distribution are explicitly computed to $O(\hbar^0)$.
- The classical-quantum limit is shown to lead to dynamics independent on the choice of partial $Q$, $P$ or $W$ representation.
- The double scaling limit applied to a single system is shown to give a stochastic classical limit, of the kind described by [138].
- A simplified form of dynamics is found in Equation (4.8.3) for classical-quantum Hamiltonians that self-commute, which takes the form of $O(\hbar^0)$ partial Glauber-Sudarshan dynamics with the minimal additional decoherence and diffusion for complete-positivity.
- The explicit form of dynamics for the classical-quantum limit of two quantum harmonic oscillators is computed.
- The double scaling limit on a single system is shown to recover the standard $\hbar \to 0$ limit in the low diffusion limit $E_f \to 0$.
- Two distinct behaviours of the effective classical-quantum dynamics are found in the $E_f \to 0$ limit, namely a quantum Zeno type behaviour, and a coherent quantum control limit.

The results in this chapter establish that the classical limit of a subsystem has a far richer structure than the classical limit of a single system, suggesting a new possible arena in which to apply methods developed to study the quantum-to-classical transition [133, 139, 140]. We

also provide a number of technical tools and definitions for the study of effective classical-quantum theories, which may be useful for categorising the large body of existing proposals for constructing hybrid theories [16, 28, 27, 29, 31, 33, 141, 34, 142]. Our findings also make clear that effectively classical systems are indeed consistent with quantum theory, and in fact may be derived from it, contrary to early arguments [20, 143, 22].

Aside from being of foundational interest, the form of dynamics we find in equation (4.4.5) or their approximated form (4.8.3) may be directly applied to study a wide range of quantum Hamiltonians in the classical-quantum limit. By using the stochastic unravellings of equations (4.7.1) and (4.7.2), one may numerically study the statistics of various observables of quantum systems in a regime where subsystems are effectively classical. This provides a general framework for studying the effects of backreaction from quantum systems on effectively classical ones, as well as a tool for reducing the complexity of simulations of many-body quantum dynamics in the presence of strongly decohering environments, which we anticipate could have a wide variety of applications.

The structure of this chapter is as follows: in Section 4.2 we introduce the Wigner and partial Wigner representations, and demonstrate using the latter how the $\hbar \to 0$ limit is insufficient in providing a classical limit of a subsystem. In Section 4.3 we introduce a discrete-time, decoherence channel model of an environment, and show how this leads to well-defined stochastic evolution in a double scaling limit. In Section 4.4 we present our main result, which is the derivation of the general form of classical-quantum dynamics under a bipartite Hamiltonian, under this double scaling limit. In Section 4.5 we introduce two other partial quasiprobability representations, the partial Glauber-Sudarshan and partial Husimi representations. These are used to illustrate two technical notions useful for characterising effective classical-quantum dynamics, which we use to determine that the positivity of the partial Glauber-Sudarshan distribution is a sufficient and necessary measure of the effective classicality of a subsystem. In Section 4.6 we study the main form of dynamics in the three different quasiprobability distributions introduced, and show the equivalence between them. In Section 4.7 the main results are unravelled in terms of stochastic trajectories in phase space and Hilbert space. Finally, in Sections 4.8 and 4.9, special cases of the general form of dynamics are given, in particular the self-commuting classical-quantum Hamiltonian case, and the low diffusion $E_f \to 0$ limit.

## 4.2 The standard $\hbar \to 0$ limit

To motivate the need for an alternate notion of a classical limit, we first begin by looking at where the standard classical limit succeeds and fails as a technique for deriving classical equations of motion. To do so, we will look at the simplest model of a quantum system with a classical limit, i.e. a single quantum system characterised by a canonical commutation relation with parameter $\hbar$. However, the results that follow may be reinterpreted in the standard way for general order parameters controlling the degree of classicality, such as coupling strength $g$ or number of systems $N$ [144].

### 4.2.1 $\hbar \to 0$ for a single system

Consider a single quantum system, that we denote $C$, with Hilbert space $\mathcal{H}^C$ and trace-one, positive semi-definite density operators $\hat{\rho}$ that form a set of states $S(\mathcal{H}^C)$. We will take this quantum system to be characterised by the canonical commutation relation $[\hat{q}, \hat{p}] = i\hbar$, and interpret the operators $\hat{q}$ and $\hat{p}$ as the position and momentum of the system. This system will have an associated Hamiltonian $\hat{H}$ which generates the free, unitary evolution of the $C$ system in the absence of any interactions with other systems.

A typical method of studying the classical limit of such a system is via the Wigner representation, which provides an alternate description of quantum mechanics in terms of functions of phase space [57, 57, 145–147]. Defining the operators $\hat{A}_{q,p} = \frac{1}{\pi\hbar} \int dy\ e^{-ipy/\hbar} |q - \frac{1}{2}y\rangle\langle q + \frac{1}{2}y|$, where $|q\rangle$ denotes the eigenstates of the position operator $\hat{q}$, one may map operators acting on $\mathcal{H}^C$ to functions of phase space $\mathcal{M}$ by taking the trace with respect to $\hat{A}_{q,p}$ i.e. $\hat{O} \mapsto \mathrm{tr}[\hat{A}_{q,p}\hat{O}]$. The most important example is the Wigner function $W(q,p)$, the phase space representation of the quantum state

$$W(q,p) = \mathrm{tr}[\hat{A}_{q,p}\hat{\rho}]. \tag{4.2.1}$$

By the properties of $\hat{A}_{q,p}$ and $\hat{\rho}$, it follows that $W(q,p)$ is real-valued and is normalised when integrated over phase space i.e. $\int W(q,p)\ dqdp = 1$. Unlike a probability distribution, it is not guaranteed to be non-negative for all $q, p$ in phase space, and hence is termed a *quasi*probability distribution. To study how unitary dynamics are represented in the Wigner representation, one

must also consider the Wigner representation of the Hamiltonian $\hat{H}$, given by the real-valued $H^W(q,p) = \mathrm{tr}[\hat{A}_{q,p}\hat{H}]$. The free unitary dynamics in the Wigner representation is then given by the Moyal bracket

$$\frac{\partial W}{\partial t} = -\frac{i}{\hbar}(H^W \star W - W \star H^W), \tag{4.2.2}$$

where here the star product of two phase space functions $f = f(q,p)$ and $g = g(q,p)$ is given

$$f \star g = f \; e^{\frac{i\hbar}{2}(\overleftarrow{\partial}_q \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_q)} \; g, \tag{4.2.3}$$

and to be interpreted in terms of the series expansion of the exponential, with the arrows denoting whether each derivative acts on the function on the left or the right. Expressions such as equation (4.2.2) may be found by using the standard result that products of operators on the Hilbert space are mapped to the star product of their Wigner representations i.e. $\hat{f}\hat{g} \mapsto f \star g$ [145, 147].

The Wigner representation is an entirely equivalent description of quantum mechanics, and does not *a priori* have anything to do with classical dynamics. However, by considering the dynamics to lowest order in $\hbar$, one arrives at an equation familiar from classical mechanics. Specifically, to lowest order in $\hbar$, the dynamics (4.2.2) takes the form

$$\frac{\partial W}{\partial t} = \{H, W\}, \tag{4.2.4}$$

where $\{\,\cdot\,,\,\cdot\,\}$ denotes the Poisson bracket, and $H$ denotes the classical Hamiltonian i.e. the $O(\hbar^0)$ part of $H^W$ [144]. This equation is the Liouville equation, and describes how classical probability distributions evolve under Hamiltonian flow. This leads to the statement that $\hbar \to 0$ gives the classical limit of a quantum system. Of course, it is not actually meaningful to send a dimensionful quantity like $\hbar$ to zero, although it is often a convenient shortcut in practice. The statement that classical equations of motion are recovered in the $\hbar \to 0$ limit is better understood as the statement that for a given $W(q,p)$, the higher order derivatives terms containing $\hbar$ in the expansion are negligible compared to the Liouville equation terms given above. This may be made more precise still by studying the evolution of quantum observables, and studying their commutation as a function of $\hbar$ [148, 50].

Even if one did not already know the form of the Liouville equation, one is still led to the $\hbar \to 0$ limit by considering when the dynamics preserves the *classicality* of initial states. A

full definition of effective classicality will be given in section 4.5, but for the time being we will simply state that for a quantum state $\hat{\rho}$ of a single system to be viewed as effectively classical, it is necessary for the corresponding Wigner function to be positive* i.e.

$$W(q,p) \geq 0 \quad \forall q,p \in \mathcal{M}. \tag{4.2.5}$$

Correspondingly, for the dynamics of the $C$ system to be effectively classical, it must also be positive i.e. preserve the positivity of all normalised functions of phase space. As should be expected, the general quantum dynamics of equation (4.2.2) is not positive, except in the cases that the Hamiltonian is at most quadratic in $q$ and $p$. To see this, one may appeal to the Pawula theorem, which characterises the general form of linear, trace-preserving and positive dynamics for real-valued functions of phase space [47]. The Pawula theorem states that unless the dynamics contains an infinite number of higher order derivatives with respect to $q$ and $p$, any positive dynamics must be of the Fokker-Planck form, with at most second order derivatives in $q$ and $p$ (see Appendix D for more details). Since the series expansion of (4.2.2) typically truncates at a finite number of terms (i.e. for Hamiltonians polynomial in position and momentum), the dynamics in such cases cannot be positive.

Considered in this way, the $\hbar \to 0$ limit may be understood as a method of enforcing positivity preservation on the quantum dynamics of a single system when represented in phase space. In particular, since the higher order derivative terms in equation (4.2.2) responsible for violating positivity also are higher order in $\hbar$, by truncating the expansion to lowest order in $\hbar$ the dynamics reduces to a dynamics that maps initial probability distributions to final probability distributions, and hence preserves the classicality of initial states.

### 4.2.2 $\hbar \to 0$ for a subsystem

However, let us now consider the same approach when the $C$ system is just a *subsystem* of a larger quantum system. Denoting the other subsystem $Q$, we again denote states of the joint

*When the quantum state is pure, this holds if and only if the Wigner function is Gaussian [149], while no such characterisation is available for mixed states. However, since any mixture of pure Gaussian states will have a positive Wigner distribution, and these pure Gaussian states will become well approximated by delta functions in the $\hbar \to 0$ limit, this necessary condition for effective classicality allows for any classical probability distribution to be obtained in the classical limit.

system as $\hat{\rho} \in S(\mathcal{H}^Q \otimes \mathcal{H}^C)$. Here again we take the closed system unitary evolution to be governed by an arbitrary Hamiltonian $\hat{H}$, which may include both self-Hamiltonians and an interaction Hamiltonian between the $C$ and $Q$ subsystems. We now wish to study whether the above procedure results in a well-defined *classical-quantum* limit – a limit in which the $C$ subsystem may be treated classically, while the generic $Q$ system is still described using standard quantum mechanics. For notational convenience in what follows, we will reserve the use of hats for operators with support on the C system Hilbert space $\mathcal{H}^C$; operators acting on $\mathcal{H}_Q$ alone will be left without.

To adapt the standard classical limit procedure to the case where $C$ is a subsystem, one may use a partial Wigner representation [15, 19]. This provides an equivalent representation of quantum mechanics in which one part of the system is described in terms of a phase space, while the other part remains described by operators in Hilbert space. Specifically, we map operators that act on $\mathcal{H}^Q \otimes \mathcal{H}^C$ to phase-space dependent operators on $\mathcal{H}^Q$ by taking the partial trace with respect to $\hat{A}_{q,p}$ i.e. $\hat{O} \mapsto \mathrm{tr}_C[\hat{A}_{q,p}\hat{O}]$. The only difference from the Wigner representation is that the trace is performed over the $C$ subsystem alone, leaving an operator-valued function of phase space. In this representation, the bipartite quantum state $\hat{\rho}$ is represented by the partial Wigner distribution $\varrho^W(q,p)$, which is an operator-valued function of the phase space associated to the $C$ system, given by

$$\varrho^W(q,p) = \mathrm{tr}_C[\hat{A}_{q,p}\hat{\rho}]. \tag{4.2.6}$$

By the properties of $\hat{A}_{q,p}$ and $\hat{\rho}$, it follows that $\varrho^W(q,p)$ is a Hermitian-valued operator and is normalised when integrated over phase space and traced over Hilbert space i.e. $\int \mathrm{tr}\varrho^W(q,p)\, dqdp = 1$. Analogously to how the real-valued Wigner function is not guaranteed to be positive, the Hermitian operator-valued function $\varrho^W(q,p)$ is not guaranteed to be positive semi-definite for all points in phase space. To study the unitary closed system dynamics of the bipartite quantum system in this representation, one may consider the partial Wigner representation of the Hamiltonian $\hat{H}$, given by the Hermitian operator-valued function of phase space $H^W(q,p) = \mathrm{tr}_C[\hat{A}_{q,p}\hat{H}]$. The closed system unitary dynamics then takes the form

$$\frac{\partial \varrho^W}{\partial t} = -\frac{i}{\hbar}(H^W \star \varrho^W - \varrho^W \star H^W), \tag{4.2.7}$$

which is analogous to (4.2.2) except for the fact that here the quantities are operators that act on $\mathcal{H}^Q$. This may be derived by noting that the relation $\hat{f}\hat{g} \mapsto f \star g$, mapping products of operators to star products of functions, still holds in the case of bipartite operators and their corresponding operator-valued partial Wigner transforms [19]. This dynamics will appear frequently in what follows, and it is thus convenient to define the associated generator $\mathcal{L}^W$ i.e. the generator of closed system evolution under the Hamiltonian $\hat{H}$ in the partial Wigner representation

$$\mathcal{L}^W = -\frac{i}{\hbar}(H^W \star \cdot \; - \; \cdot \star H^W), \tag{4.2.8}$$

where here we use $\cdot$ to denote the input to the generator.

If the argument was to follow as before, then taking $\hbar \to 0$ of the closed system unitary dynamics in the partial Wigner representation would lead to one system becoming effectively classical, while the other remaining quantum. Considering equation (4.2.8) to $O(1)$ in $\hbar$, the resulting equation

$$\frac{\partial \varrho^W}{\partial t} = -\frac{i}{\hbar}[H, \varrho^W] + \frac{1}{2}(\{H, \varrho^W\} - \{\varrho^W, H\}), \tag{4.2.9}$$

is known as the quantum-classical Liouville equation [19, 130, 18]. Here $H$ is the $O(\hbar^0)$ part of $H^W$ and we will refer to this as the classical-quantum Hamiltonian. The first term takes the form of a Liouville von-Neumann term, that describes unitary evolution of density operators. The second term, sometimes referred to as the Alexandrov-Gerasimenko bracket, is a version of the Poisson bracket that is symmetric in the ordering of the phase space dependent operators $H$ and $\varrho^W$. As before, this form of dynamics will appear repeatedly, and it will be useful to define the corresponding generator

$$\mathcal{L}^W\big|_{O(\hbar^0)} = -\frac{i}{\hbar}[H, \; \cdot \;] + \frac{1}{2}(\{H, \; \cdot \;\} - \{ \; \cdot \;, H\}), \tag{4.2.10}$$

which is simply the generator $\mathcal{L}^W$ of (4.2.8) truncated to $O(1)$ in $\hbar$.

However, there is a key difference between the Liouville and quantum-classical Liouville dynamics: while the Liouville equation preserves the classicality of the $C$ system, the quantum-classical Liouville equation does not. Although a full discussion of the effective classicality of subsystems will be provided in section 4.5, for the time being we will state that for a quantum

state $\hat{\rho}$ on the bipartite Hilbert space $\mathcal{H}^C \otimes \mathcal{H}^Q$ to be effectively classical on the $C$ subsystem, it is necessary for the corresponding operator-valued partial Wigner distibution to be positive semi-definite at all points in phase space i.e

$$\varrho^W(q,p) \succeq 0 \quad \forall q,p \in \mathcal{M}. \tag{4.2.11}$$

Taking (4.2.11) as a necessary condition for effective classicality of the $C$ subsystem guarantees that the state may be written as a positive probability distribution over phase space multiplied by a corresponding quantum state on $\mathcal{H}^Q$ at each point, and is the natural generalisation of (4.2.5) to operator-valued functions. For a dynamics to preserve the classicality of the $C$ subsystem, it therefore must be the completely-positive on all initial operator-valued functions of phase space. However, while the Liouville equation preserves the positivity of real-valued functions, the quantum-classical Liouville equation does not preserve the positivity of operator-valued functions of phase space [15]. This may be seen by appealing to the recently proved analogue of the Pawula theorem for operator-valued functions [45] (see also [76] for a later discussion of this result). Known as the CQ Pawula theorem, it showed that every trace-preserving, normalised and completely-positive Markovian dynamics on operator-valued functions of phase space is also separated into two classes, with one class truncating at second order in derivatives in phase space, and the other containing an infinite number of higher derivative terms (see Appendix D). Since the full dynamics of (4.2.8) typically truncates at a finite number of derivative terms, the $\hbar \to 0$ limit helps to bring the resulting form of equations closer to a completely-positive form, by removing all derivative terms second order and higher. However, as we show in Appendix D, even with these higher order derivatives removed, the resulting dynamics are still not of the required form for complete-positivity.

The problem ultimately lies in the fact that while $\hbar \to 0$ suppresses non-classicality arising from the higher order derivatives in $q$ and $p$, it has no effect on suppressing the entanglement that is generated between the $C$ and $Q$ quantum subsystems. Since entanglement may be generated for even linear coupling between subsystems, the quantum-classical Liouville equation (4.2.9) must also generically describe entanglement build up between the $C$ and $Q$ subsystems, and thus the generation of states that are not effectively classical on the $C$ subsystem.

Before moving on to see how one may resolve this, we should first address a technical de-

tail regarding the kinds of Hamiltonian that we consider. Up to this point, we have implicitly assumed that $H^W$, referring to either the Wigner or partial Wigner representation of the Hamiltonian $\hat{H}$, may be written as $H^W = H + O(\hbar^2)$. This assumption holds when $\hat{H}$ is a function of $\hat{q}$ and $\hat{p}$, and in such typical cases, the classical or classical-quantum Hamiltonian $H$ coincides with the function of phase space obtained by making the substitutions $\hat{q} \mapsto q$, $\hat{p} \mapsto p$. In general however, the Hamiltonian $\hat{H}$ may also depend explicitly on $\hbar$, and in these cases there is no guarantee that $H^W = H + O(\hbar^2)$. However, if $H^W$ contains any terms of $O(\hbar^{-1})$ or higher inverse powers of $\hbar$, there is no well-defined classical limit as $\hbar \to 0$ [144], and one may check that the dynamics truncated to $O(\hbar^0)$ in such cases are not positive. The only remaining case is thus where $H^W$ contains $O(\hbar)$ terms. We consider this in Appendix F, and find that it amounts to only a minor modification of the dynamics when $H^W = H + O(\hbar^2)$. For conceptual clarity we therefore present the following analysis under the assumption that $H^W = H + O(\hbar^2)$ – but this, up to a known modification, describes all possible Hamiltonians which permit a classical limit.

## 4.3 Decoherence timescale $\tau$ and a double scaling limit

The preceding section introduced the formalism of the Wigner and partial Wigner representations, and showed how the standard $\hbar \to 0$ limit is insufficient to describe a classical limit of a subsystem due to the presence of entanglement. In this section, we introduce a simple model of the effect of an environment on the $C$ subsystem, and show how this leads one to a double scaling limit involving the decoherence timescale $\tau$ of this subsystem.

We begin by noting that it is well-understood that $\hbar \to 0$ is not sufficient to ensure classicality, even in single systems. The key observation is that when $\hbar$ is small, but finite, the evolution generated by the Liouville equation will generally map an initial state $W(q, p, t_i)$ in which the higher order terms are negligible to a state at later times $W(q, p, t_f)$ in which they are not [133]. The resolution to this problem was to acknowledge that in practice, all quantum systems are open systems, and thus interact with their environments. In this case, the interaction with an environment leads to dispersion in the system, preventing any later states of the Wigner quasiprobability distribution $W(q, p, t_f)$ from becoming overly peaked in phase space and thus

preventing the higher order terms contributing, an analysis that has been put on more rigorous footing in recent work [150, 140]. More generally, acknowledging the role of the environment, which generically acts to decohere the system, has turned out to be an extremely successful way of explaining a number of features in the quantum-to-classical transition [131, 132, 134–136].

In what follows, we shall follow the above philosophy by modelling the effect of the environment on the subsystem that will be classicalised. The basic idea is that the interactions with an environment will lead to decoherence on the $C$ subsystem that can break the entanglement with the $Q$ subsystem. In other words, the decoherence induced by an environment will act to replace the quantum correlations between the $C$ and $Q$ subsystems with purely classical correlations, which will ensure that the resulting $\varrho^W$ is positive.

In order to include the effect of an environment, without overly increasing the complexity of the analysis, we will assume that the effective action of the environment is to collapse the $C$ subsystem into a classically definite state. The classically definite states will be taken to be *coherent states*, which are the states with minimum uncertainty in $q$ and $p$. Allowing them to have some squeezing, such that the ratio of the variances in position and momentum is given by $s^2 = \frac{\Delta q}{\Delta p}$, we will denote the coherent state with expectation values $\langle \hat{q} \rangle = q$ and $\langle \hat{p} \rangle = p$ as $|\alpha_s(q,p)\rangle$ [151, 152]. The environment is then modelled as performing a coherent state POVM with measurement operators $\hat{M}^s_{q,p} = (2\pi\hbar)^{-1/2} |\alpha_s(q,p)\rangle\langle\alpha_s(q,p)|$. Assuming for now that the observer has no access to the environmental degrees of freedom, the effect of the environment is a decoherence channel $\hat{\rho} \to \int dqdp \hat{M}^s_{q,p} \hat{\rho} \hat{M}^s_{q,p}$. In the partial Wigner representation this amounts to a convolution of $\varrho^W$ with a normalised Gaussian with variance $\hbar s^2$ in $q$ and $\hbar s^{-2}$ in $p$. Such a convolution is known as a Weierstrass transform [153], and has the following representation as a differential operator

$$\mathcal{D} = e^{\frac{\hbar s^2}{2}\frac{\partial^2}{\partial q^2} + \frac{\hbar}{2s^2}\frac{\partial^2}{\partial p^2}}. \tag{4.3.1}$$

This differential operator $\mathcal{D}$ provides a representation of the decoherence action of an environment, and will prove extremely useful.

Although we have specified the action of the environment as collapsing the states of the system to coherent states, we have not specified over which timescale. To do so, we will specify explicitly that the environment collapses the state of the system over a time $\tau$. This timescale $\tau$

is to be understood to be the decoherence timescale of the $C$ subsystem i.e. the time over which the interaction with the environment has decohered the $C$ subsystem to being in a classically definite state.

It is important to emphasise that, while providing a simplistic description of environmental decoherence, the basic features of this model can be identified in explicit physical examples. Decoherence into the coherent state basis has long been observed in models of decoherence [154], particularly in the context of quantum Brownian motion [155, 156], and indeed can be understood as arising under fairly general environmental conditions [157]. In these models, there are two standard timescales that arise. One is the decoherence timescale, given by $\tau_D \sim \hbar^2/\Delta x^2 D$ in the context of quantum Brownian motion, where $\Delta x$ is the spread in position quantum state, and $D$ is a model derived diffusion rate, and is extremely short for typical macroscopic objects [158, 156, 136]. The other is the typically longer localisation time [156, 136], which is a state-independent quantity given for quantum Brownian motion by $\tau_L \sim \sqrt{\hbar/Dm}$, where $m$ is the mass of the system, and has been shown to be associated with the timescale on which the system diagonalises in the coherent state basis [156]. We leave understanding in detail which of these two timescales may be most natural to future work, and instead generically refer to $\tau$ as a decoherence timescale without specific reference to either $\tau_D$ or $\tau_L$[†].

The joint specification of the map $\mathcal{D}$ and associated timescale $\tau$ leads to something akin to a Trotterised picture of dynamics, in which the effect of the environment is modelled by a decoherence channel that acts at discrete time intervals $\tau$. For now leaving aside the unitary dynamics generated by $\hat{H}$, this explicitly means that the total dynamics in the partial Wigner representation is given by the application of the differential operator $\mathcal{D}$ at times $0, \tau, 2\tau, \ldots$ and so on, with no evolution in between. Although different from the standard continuous time dynamics of typical open systems treatments [160], the advantage of this discrete-time approach is that after each action of the decoherence channel, the state is in a guaranteed classical state.

[†]At first glance, the state-independence and decoherence into the coherent basis is suggestive of using $\tau_L$. However, applying the double scaling limit of $\hbar$ and $\tau$ given below, it is straightforward to see that the resulting diffusion in momentum $E_f/s^2$ will not agree with the diffusion rate $D$, which must be taken to infinity to ensure a finite $E_f$. On the other hand, using $\tau_D$ with $\Delta x^2 = \Delta q^2 = \hbar s^2$ i.e. the spread in position of the coherent state [159], one finds that $\tau$ is in fact proportional to $\hbar$, with the correct constant of proportionality $E_f^{-1} = (Ds^2)^{-1}$ to ensure that the diffusion in momentum is indeed given by $D$.

In order to arrive at a well-defined continuum limit of this discrete-time model of decoherence, one would wish to take the decoherence timescale to zero i.e. $\tau \to 0$. Since the environment acts to select classical states on the $C$ subsystem, taking this limit ensures that the subsystem is in a classical state at all times. However, since each application of the decoherence map causes $\varrho^W$ to be convolved with a Gaussian with variances proportional to $\hbar$, taking $\tau \to 0$ while $\hbar$ remains finite would lead to the state of the system becoming infinitely spread in phase space in finite time. To prevent this from occurring, we observe that simultaneously taking the limit that $\hbar \to 0$ allows, in principle, for an infinite series of convolutions to still give a finite effect on the resulting distribution. To see which rates it may be sensible to take $\hbar$ and $\tau$ to zero, one may consider $t/\tau$ environmental decoherence steps, which gives the overall effect of the environment $\mathcal{G}_t$ after finite time $t$ as

$$\mathcal{G}_t = \lim_{\hbar,\tau\to 0} \mathcal{D}^{t/\tau} = \lim_{\hbar,\tau\to 0} e^{\frac{\hbar}{\tau}\left(\frac{s^2}{2}\frac{\partial^2}{\partial q^2}+\frac{1}{2s^2}\frac{\partial^2}{\partial p^2}\right)t}. \tag{4.3.2}$$

Remarkably, one can see that when the ratio $\hbar/\tau$ is fixed, the differential operator $\mathcal{G}_t$ corresponds exactly to the semi-group corresponding to a classical diffusion process, with the diffusion rate in $q$ given by $\hbar s^2/\tau$ and diffusion rate in $p$ given by $\hbar s^{-2}/\tau$. Despite starting from a strong measurement at each step in time, the resulting equations of motion describe continuous evolution in time and phase space. This motivates the following double-scaling limit as a candidate method of taking the classical-quantum limit:

$$\hbar \to 0,\ \tau \to 0, \quad s.t. \quad \frac{\hbar}{\tau} = E_f, \tag{4.3.3}$$

where we have chosen $E_f$ to denote the constant with dimensions of energy that describes the fixed ratio of the two. As before, the taking of dimensionful quantities to zero should be more carefully interpreted as statements about the relevant scales in the system. Here we may interpret the above double-scaling limit as the statement that the action associated to any observables of interest on the $C$ subsystem are large compared to the scale of $\hbar$, and change over much longer timescales than the decoherence time $\tau$ of the $C$ subsystem. The ratio of the reduced Planck's constant and the decoherence time give a measure of the size of the fluctuations in the system due to the environment, which is captured by the constant $E_f$.

Before we move on to study the dynamics that results from taking this limit, it is important to emphasise that the proposed limit should be understood as the application of the double

scaling limit to the discrete-time model of decoherence discussed so far. Indeed, it turns out that simply identifying a double scaling limit of the parameter controlling the decoherence timescale and $\hbar$ in a model describing environmental decoherence is not in general sufficient to derive a classical-quantum limit. A straightforward counterexample is provided in Appendix G, where we consider a continuous time Lindbladian dynamics with a parameter $\gamma$ controlling the overall decoherence rate in $\hat{q}$ and $\hat{p}$ on the $C$ subsystem. While a double scaling limit $\gamma \to \infty$, $\hbar \to 0$ s.t. $\gamma\hbar^2 = E_f$ leads to identical diffusive evolution in phase space to that described above, the resulting evolution for a bipartite quantum system is not completely-positive, and thus does not describe a well-defined classical-quantum limit. The failure of this approach appears to be related to the lack of equivalence between the two classes of dynamics considered in one of the earliest works on effective classical-quantum dynamics [137]. Although we will not consider this type of set-up any further, it turns out it was the first to appear in the discussion of double scaling classical limits, where the possibility of taking a double scaling limit of $\hbar$ and a measurement rate of a continuous measurement procedure to arrive at diffusive classical evolution on a single system was pointed out in the conclusion of [138]. A closer theoretical set-up to ours appears in the context of the quantum Zeno effect [161]. More recently, another related model with a different double scaling limit was considered in the context of holography [162].

## 4.4 Main results

In this section, we use the discrete-time model of decoherence and associated double scaling limit of the previous section to arrive at the general form of dynamics when one takes the classical-quantum limit we have introduced. This main result is given in equation (4.4.5). Since some of the technical steps are rather long, we reproduce here only the key conceptual points, and refer the reader to Appendix E for more details.

### 4.4.1 Derivation of the generator in the classical-quantum limit

In section 4.3, the effect of the environment was considered in isolation. However, the key question of interest is to consider how the environment and the free evolution of a generic quantum system interplay in the double-scaling limit we have arrived at. To study this, we must consider the total evolution after a time $\tau$, which should include both the environmental decoherence effects given by $\mathcal{D}$ and the free evolution generated in the partial Wigner representation by $\mathcal{L}^W$. The obvious question then arises of which ordering to choose of the two processes. This point will be made precise in section 4.6 when alternative partial quasiprobability representations are considered, but at this time we will simply postulate a reasonable choice, namely a symmetrised total evolution, in which the action of the environment is divided equally between one part before the free evolution generated by the Hamiltonian, and one part afterwards

$$\mathcal{E}_\tau^\hbar = \mathcal{D}^{\frac{1}{2}} e^{\mathcal{L}^W \tau} \mathcal{D}^{\frac{1}{2}}. \tag{4.4.1}$$

The total evolution operator $\mathcal{E}_\tau^\hbar$ describes the action of both the environment and the free evolution on the partial Wigner representation of the bipartite quantum system $CQ$, and we use the superscript and subscript to indicate the functional dependence on both $\tau$ and $\hbar$.

The evolution map $\mathcal{E}_\tau^\hbar$ describes the total change in the partial Wigner representation over a finite decoherence time $\tau$ with a finite value of $\hbar$. In order to take the classical-quantum limit described in (4.3.3) one must consider the infinitesimal evolution in $\tau$ generated when $\tau$ and $\hbar$ are taken to zero such that $\hbar = E_f \tau$. To do so, we first set $\hbar = E_f \tau$ in $\mathcal{E}_\tau^\hbar$, and consider the generator of the evolution map $\mathcal{E}_\tau := \mathcal{E}_\tau^{E_f \tau}$ in the $\tau \to 0$ limit, which takes the form

$$\mathcal{L} = \lim_{\tau \to 0} \big(\frac{\partial}{\partial \tau} \mathcal{E}_\tau\big) {\mathcal{E}_\tau}^{-1} + \frac{\partial}{\partial \tau} \big( \ln \mathcal{E}_0 \big|_{E_f = \frac{\hbar}{\tau}} \big). \tag{4.4.2}$$

The first term is the standard form of the generator often used to formally construct time-local dynamics [163, 164], and may be found by writing the state of the system at time $\tau$ as $\varrho(\tau) = \mathcal{E}_\tau \varrho(0)$, studying its rate of change in time, and then using the inverse of the evolution map $\mathcal{E}_\tau^{-1}$ to re-express this as a generator as acting on $\varrho(\tau)$. We shall see that this part of the generator captures a large proportion of the dynamics, and importantly the back-reaction of the quantum system on the classical one. However, by construction, this part of the generator only captures the $\tau$-dependent part of the dynamics. In fact, one can check that there is an

additional $\tau$-independent component $\mathcal{E}_0$, generated by $-\frac{i}{E_f}[H,\ \cdot\ ]$. As discussed in Appendix E, this term may be accounted for by reintroducing $\hbar = E_f\tau$, and computing the generator of this component, corresponding to the second term in (4.4.2). Since this term only effects the quantum system, the reappearance of $\hbar$ is to be expected: while $\hbar \to 0$ should be interpreted as the assumption that the relevant classical observables are much larger than $\hbar$, no assumption is made on the scale of relevant quantum observables. From this point on, any appearance of $\hbar$ should be interpreted as characterising the quantum features of the $Q$ subsystem.

To compute the above generator explicitly, one may substitute the evolution map into the form of the generator provided above. Explicitly, by substituting equation (4.4.1) into equation (4.4.2) with the $O(\hbar^0)$ expression for $\mathcal{L}^W$ and definition of $\mathcal{D}$ given in equations (4.2.10) and (4.3.1), we arrive at

$$\begin{aligned}\mathcal{L} = &-\frac{i}{\hbar}[H,\ \cdot\ ] \\ &+\frac{1}{2}(1+e^{\mathrm{ad}_{\frac{-i}{E_f}[H,\cdot]}})\left(\frac{E_f s^2}{2}\frac{\partial^2}{\partial q^2}+\frac{E_f}{2s^2}\frac{\partial^2}{\partial p^2}\right) \\ &+\frac{e^{\mathrm{ad}_{\frac{-i}{E_f}[H,\cdot]}}-1}{\mathrm{ad}_{\frac{-i}{E_f}[H,\cdot]}}\left(\frac{1}{2}\{H,\cdot\}-\frac{1}{2}\{\cdot,H\}\right),\end{aligned} \tag{4.4.3}$$

where here the $ad$ denotes the adjoint operation with respect to the generators of the classical-quantum dynamics i.e. $(ad_{\mathcal{A}}\mathcal{B})\varrho = (\mathcal{A}\mathcal{B}-\mathcal{B}\mathcal{A})\varrho$. Here the first line corresponds to the second term of equation (4.4.2), while the second and third lines arise from the first term. The complex structure of this part of the generator owes itself to the fact that the generators of the exponential maps that make up $\mathcal{E}_\tau$ do not commute with themselves for all $\tau$. This means that when the derivative in (4.4.2) is taken, one must be careful to use the derivative of the exponential map i.e. if $\mathcal{X}_\tau$ is a classical-quantum generator with dependence on $\tau$, then

$$\frac{\partial}{\partial\tau}e^{\mathcal{X}_\tau} = \frac{e^{\mathrm{ad}_{\mathcal{X}_\tau}}-1}{\mathrm{ad}_{\mathcal{X}_\tau}}\left(\frac{\partial\mathcal{X}_\tau}{\partial\tau}\right)e^{\mathcal{X}_\tau}, \tag{4.4.4}$$

which should be understood as a power series of $\mathrm{ad}_{\mathcal{X}}$ acting on the derivative of $\mathcal{X}_\tau$, which then acts on the exponential of $\mathcal{X}_\tau$, as is commonly considered in the derivation of the Baker-Campbell-Hausdorff formula [165].

To further simplify this expression for the generator of dynamics $\mathcal{L}$, one may explicitly compute how the adjoint acts on the phase space derivatives that appear in the various series

in (4.4.3). Amounting to computing part of the Lie algebra corresponding to classical-quantum generators, this allows allows one to map the expressions involving the adjoint action of classical-quantum generators (i.e. $\mathrm{ad}_{\frac{-i}{E_f}[H,\,\cdot\,]}$), to expressions involving the adjoints of quantum operators (i.e. $\mathrm{ad}_{\frac{-i}{E_f}H}$). Since the steps involved are rather long, we leave the details of this to Appendix E.

### 4.4.2 Classical-quantum limit master equation

Simplifying the dynamics in this way we arrive at our main result: the classical-quantum limit dynamics in master equation form, given by

$$\begin{aligned}\frac{\partial \varrho}{\partial t} =& -\frac{i}{\hbar}[H + H_{\text{eff}}, \varrho] \\ &- \frac{1}{2}\frac{\partial}{\partial q}\{L_p^H, \varrho\}_+ + \frac{1}{2}\frac{\partial}{\partial p}\{L_q^H, \varrho\}_+ \\ &+ \frac{is^2}{2}\frac{\partial}{\partial q}[L_q^H, \varrho] + \frac{i}{2s^2}\frac{\partial}{\partial p}[L_p^H, \varrho] \\ &+ \frac{1}{2E_f}(\bar{L}\varrho\bar{L}^\dagger - \frac{1}{2}\{\bar{L}^\dagger\bar{L}, \varrho\}_+) \\ &+ \frac{E_f s^2}{2}\frac{\partial^2 \varrho}{\partial q^2} + \frac{E_f}{2s^2}\frac{\partial^2 \varrho}{\partial p^2},\end{aligned} \tag{4.4.5}$$

where

$$\begin{aligned}L_q^H &= \frac{e^{\mathrm{ad}_{\frac{-i}{E_f}H}} - 1}{\mathrm{ad}_{\frac{-i}{E_f}H}}\left(\frac{\partial H}{\partial q}\right) \\ L_p^H &= \frac{e^{\mathrm{ad}_{\frac{-i}{E_f}H}} - 1}{\mathrm{ad}_{\frac{-i}{E_f}H}}\left(\frac{\partial H}{\partial p}\right) \\ \bar{L} &= sL_q^H + is^{-1}L_p^H,\end{aligned} \tag{4.4.6}$$

and

$$\begin{aligned}H_{\text{eff}} =& \frac{\hbar s^2}{4}\frac{\partial L_q^H}{\partial q} + \frac{\hbar}{4s^2}\frac{\partial L_p^H}{\partial p} \\ &+ \frac{\hbar}{4E_f}\sum_{n,m=0}^{\infty}\frac{C_{nm}}{(n+m+2)!} \\ &\times \{\mathrm{ad}^n_{\frac{-i}{E_f}H}\frac{\partial H}{\partial q}, \mathrm{ad}^m_{\frac{-i}{E_f}H}\frac{\partial H}{\partial p}\}_+.\end{aligned} \tag{4.4.7}$$

Here $C_{nm}$ denote numerical coefficients given by

$$C_{nm} = \sum_{r=0}^{m} \frac{(r+n)!}{r!n!} - \sum_{r=0}^{n} \frac{(r+m)!}{r!m!}, \tag{4.4.8}$$

which we show in Appendix E are antisymmetric coefficients that may be obtained from the Pascal triangle with integer boundary elements. The operators $L_q^H$ and $L_p^H$ are Hermitian, and have an alternative representation as

$$L_z^H = iE_f \frac{\partial}{\partial z}\big(e^{-\frac{i}{E_f}H}\big)e^{\frac{i}{E_f}H}, \tag{4.4.9}$$

for $z = q, p$. This can be seen to be equivalent to the definition in (4.4.6) with use of the derivative of the exponential map, as in (4.4.4).

To give some intuition about the dynamics, we sketch the role of each line as follows. The top line describes purely unitary evolution of the quantum system, governed by both the classical-quantum Hamiltonian $H$ and an effective Hamiltonian $H_{\text{eff}}$ that depends on $s$ and $E_f$. This additional Hamiltonian term arises due to the fluctuations induced by the environment [166], and is analogous to the Lamb and Stark shifts that renormalise the bare system Hamiltonian in standard open systems treatments [160]. The second line describes both the free classical evolution and the back-reaction of the quantum system upon it, and we shall see that in Section 4.8 that this reduces to the symmetrised Poisson bracket appearing in (4.2.9) for a special class of classical-quantum Hamiltonians. The third line describes how random fluctuations in the classical degrees of freedom are correlated with random fluctuations in the unitary dynamics of the quantum system i.e. noisy Hamiltonian quantum dynamics. The fourth line describes the Lindblad portion of the dynamics, which acts to decohere the quantum system into a basis determined by the Lindblad operators $L_q^H$ and $L_p^H$. Finally, the final line describes the previously described diffusion in the classical degrees of freedom, with overall strength proportional to $E_f$ and relative strengths in position and momentum determined by the parameter $s$.

To understand whether the evolution laws given by the above generator are consistent, it is important to check that the dynamics are linear, trace-preserving, and completely-positive on a suitable set of operator-valued functions of phase space. While this seems likely *a priori*, given that the generator above was derived from free evolution and environmental decoherence in a full quantum theory, it is often the case in the study of open quantum systems that approximations

lead to violations of one or more of these conditions [160]. In order to check this, we note that the simplified form of the dynamics given in (4.4.5) is of the canonical classical-quantum form of dynamics, first written in general form by [45] (see also [76] for a later discussion of this). Any dynamics of this form is linear and trace-preserving, and these properties are straightforward to directly check by hand. In order to check the positivity of a dynamics of this form, one must check a series of positivity conditions given by the CQ Pawula theorem [45]. The first step is to pick a basis of operators, and phase space degrees of freedom, in which to read off certain decoherence, back-reaction and diffusion matrices. Picking the basis $(q, p), (L_q^H, L_p^H)$ for convenience, one may refer to the general form given in Appendix E to see that that the decoherence $D_0$, back-reaction $D_1$ and diffusion $D_2$ are given by

$$D_0 = \begin{pmatrix} \frac{s^2}{2E_f} & -\frac{i}{2E_f} \\ \frac{i}{2E_f} & \frac{1}{2E_f s^2} \end{pmatrix} \tag{4.4.10}$$

$$D_1 = \begin{pmatrix} \frac{is^2}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{i}{2s^2} \end{pmatrix} \tag{4.4.11}$$

$$D_2 = \begin{pmatrix} E_f s^2 & 0 \\ 0 & \frac{E_f}{s^2} \end{pmatrix}. \tag{4.4.12}$$

The most basic requirements for positivity in the CQ Pawula theorem are the same as those of the Lindblad and Fokker-Planck equations. For the quantum degrees of freedom, these are the requirements that for all points in phase space the total Hamiltonian $H + H_{\text{eff}}$ is Hermitian and the decoherence matrix $D_0$ is positive semi-definite. For the classical degrees of freedom, it is that the real matrix $D_2$ is positive semi-definite for all points in phase space. One may check that these properties do indeed hold, with $H_{\text{eff}} = H_{\text{eff}}^\dagger$ following from $H = H^\dagger$. The key result of the classical-quantum Pawula theorem, is that the remaining conditions sufficient for complete-positivity of a classical-quantum dynamics are that $(\mathbb{I} - D_2 D_2^{-1}) D_1 = 0$ and that $D_0 \succeq D_1^\dagger D_2^{-1} D_1$, where $\mathbb{I}$ denotes the identity matrix of the dimension of the classical degrees of freedom, and $D_2^{-1}$ denotes the pseudoinverse of $D_2$. The first condition ensures that any classical degree of freedom that experiences quantum back-reaction has noise in it, and this holds

here since $D_2$ is full-rank. The second condition, known as the decoherence-diffusion trade-off [78], ensures that decoherence in the quantum system is sufficiently large to to be compatible with the rate of information gain about it by the classical system. One may explicitly check this condition with the above matrices and see that the decoherence-diffusion trade-off is satisfied, and in fact is saturated as $D_0 = D_1^\dagger D_2^{-1} D_1$. Thus, analogously to the standard classical limit of the Wigner distribution, the classical-quantum limit presented here arrives at a dynamics that is positive on all initial operator-valued functions of phase space.

As a final technical remark, it is worth noting that the above form of dynamics may be straightforwardly generalised from one describing a single pair of phase space coordinates $(q, p)$ to one describing many i.e. $(q_1, \ldots, q_n, p_1, \ldots, p_n)$. To see this, we note that generalising the $C$ subsystem to $[\hat{q}_i, \hat{p}_j] = i\hbar\delta_{ij}$ for $i, j = 1, \ldots, n$ and assuming decoherence into a tensor product of coherent states on each subsystem, each described by a parameter $s_i$, changes the decoherence map $\mathcal{D}$ and the partial Wigner evolution $\mathcal{L}^W$ in a particularly simple way. In particular, the only change in $\mathcal{D}$ is to include a sum from $i = 1$ to $i = n$ in the exponential, while $\mathcal{L}^W$ to $O(\hbar^0)$ has the inclusion of the same sum in the Poisson bracket term. Since these lead to the second and third lines in equation (4.4.3) respectively, it follows by linearity that the only change in the final result of equation (4.4.5) is the inclusion of a sum over the pairs of phase space degrees of freedom i.e. performing the substitution $s \mapsto s_i$, $q \mapsto q_i$, $p \mapsto p_i$ and summing from $i = 1, \ldots, n$ over any terms that these indices explicitly appear in. This form of dynamics leads to $D_0$, $D_1$ and $D_2$ matrices that are block diagonal, with each block taking the same form as those given in (4.4.10), (4.4.11) and (4.4.12), and thus the resulting dynamics is completely-positive as before.

## 4.5 Effective classical-quantum states and subset positivity

The analysis of both the insufficiency of the $\hbar \to 0$ limit and the apparent success of the double scaling limit have thus far been presented using the partial Wigner quasiprobability distribution $\varrho^W$. However, the positive semi-definiteness of $\varrho^W$ was stated to only be a *necessary* condition for the classicality of a subsystem. In this section, we introduce two other partial quasi-probability distributions, the partial Husimi and partial Glasuber-Sudarshan distribu-

tions, which we denote $\varrho^Q$ and $\varrho^P$, and show how the positivity of $\varrho^P$ is well motivated as a definition of the necessary *and sufficient* condition for the effective classicality of a subsystem. We then discuss how one may relax this definition, and how the notion of effective classicality used within this work may be compatible with other notions used in the literature. The considerations in this section and the next do not change the main result of equation (4.4.5), and those interested in understanding this general form of classical-quantum dynamics better may instead choose to go straight to section 4.7 or 4.8.

### 4.5.1 Effective classicality in a single system

We start by noting that a number of different proposals for defining the effective classicality of a quantum system exist in the literature, from decoherent histories [49–51], and correlations satisfying certain inequalities [52–54], to systems living in doubled Hilbert spaces [55, 56].

In this work, we shall use a particularly well-known type of effective classicality, based on the positivity of quasiprobability distributions [57–61]. To motivate this, it will be useful to introduce two common alternatives to the Wigner quasiprobability representation, the $Q$ and $P$ representations, well-known for their use in quantum optics [167–169]. In the $Q$ representation, states are represented by the Husimi distribution $Q$, which is defined explicitly as

$$Q(q,p) = \mathrm{tr}\left[\frac{|\alpha_s(q,p)\rangle\langle\alpha_s(q,p)|}{2\pi\hbar}\hat{\rho}\right], \tag{4.5.1}$$

while in the $P$ representation, states are represented by the Glauber-Sudarshan distribution $P$, which is defined implicitly by

$$\hat{\rho} = \int P(q,p)|\alpha_s(q,p)\rangle\langle\alpha_s(q,p)|dqdp. \tag{4.5.2}$$

While the $Q$ distribution is always a well-defined function of phase-space, the $P$ distribution in general must be understood as a generalised function [170, 152]. These expressions define the representation of states in each respective quasiprobability theory, and implicitly define the representation of measurements (see Appendix H).

One may identify the effective classicality of a single quantum system by studying the positivity of one of these representations. By construction, the Husimi $Q$ distribution is positive

for all quantum states. Therefore, the positivity of the $Q$ distribution cannot be useful as a measure of classicality, since under this definition all quantum states, even those in non-local superpositions, would be understood as effectively classical. On the other hand, one sees that the positivity of the $P$ distribution has a clear physical interpretation – that the quantum state can be written as a statistical mixture of coherent states i.e. a classical mixture of "the most classical states". For this reason, we take the positivity of the $P$ distribution to be a sufficient and necessary condition for the effective classicality of a single quantum system, as is common within quantum optics [58, 60]. Since the $W$ representation is related to the $P$ representation by a Weierstrass transform (see Appendix I), if the $P$ distribution is positive, the Wigner distribution will also be positive. This explains the original statement in section 4.2 that the positivity of the Wigner function is a necessary condition for the classicality of a single quantum system.

While this provides an intuitive notion of effective classicality, it turns out that it may be made more precise, and given an operational meaning, by considering the representation of both states *and* measurements in the $P$ representation. As we discuss in Appendix H, the representation of measurements in the $P$ representation is given by the $Q$ function of the corresponding POVM element. As such, all measurements in the $P$ representation have a positive representation, and thus when the $P$ function corresponding to the quantum state is also positive, the statistics of any measurement are equivalent to those obtained from a non-contextual probability theory [59, 61]. As we show in Appendix H, this provides an alternative operational definition of the effective classicality of a single quantum system, given by the states which cannot be distinguished from a fundamental classical system regardless of the measurement performed.

### 4.5.2 Effective classicality of a subsystem

To generalise the preceding discussion, and hence define a notion of the effective classicality of a subsystem, we will introduce two partial quasiprobability representations derived from the $Q$ and $P$ representations previously introduced. In particular, we may define the partial Husimi

distribution $\varrho^Q$ explicitly via

$$\varrho^Q(q,p) = \mathrm{tr}_C\left[\frac{|\alpha_s(q,p)\rangle\langle\alpha_s(q,p)|}{2\pi\hbar}\hat{\rho}\right], \tag{4.5.3}$$

and the partial Glauber-Sudarshan distribution $\varrho^P$ implicitly by

$$\hat{\rho} = \int \varrho^P(q,p) \otimes |\alpha_s(q,p)\rangle\langle\alpha_s(q,p)| dqdp. \tag{4.5.4}$$

Like $\varrho^W$, both $\varrho^Q$ and $\varrho^P$ are normalised to 1 when traced over Hilbert space and intergrated over phase space, and are useful for illustrating different properties of a given bipartite quantum state $\hat{\rho}$.

The partial Husimi $\varrho^Q$ is an operationally relevant quantity, giving the actual probabilities and corresponding quantum states on $Q$ of a coherent state POVM with measurement operators $\hat{M}_{q,p}$ on the $C$ subsystem, and is consequently positive semi-definite for all $q, p$. A consequence of the non-orthogonality of the coherent states is that the set of all operator-valued functions $\varrho^Q$ form a strict subset $\mathbf{H} \subset \mathbf{S}$ of positive operator-valued functions, in particular not including those with uncertainty in position and momentum less than the Heisenberg bound [151, 171, 27].

By contrast, the partial Glauber-Sudarshan $\varrho^P$ is not necessarily positive semi-definite at all points in phase space [152], but when it is, one may see from its definition that the bipartite quantum state is separable between the classical and quantum subsystems i.e. contains no entanglement [77]. When this is the case, the $C$ subsystem is in a mixture of coherent states that are classically correlated with the $Q$ subsystem. For this reason, by analogy with the $P$ distribution for a single system, we shall define the effective classicality of a subsystem by the positivity of the partial Glauber-Sudarshan distribution $\varrho^P$. In other words, we will state that a bipartite quantum state $\hat{\rho}$ is an effective classical-quantum state if and only if the corresponding distribution $\varrho^P$ is positive semi-definite. Since the partial Wigner $\varrho^W$ is related to $\varrho^P$ by a Weierstrass transform (see Appendix I), any positive semi-definite $\varrho^P$ necessarily implies that $\varrho^W$ is also positive, justifying the original claim that $\varrho^W \succeq 0$ is a neccessary condition for an effective classical subsystem.

As with the case of the Glauber-Sudarshan $P$ representation for a single system, this identification of the effective classicality of subsystems may be made more precise by also considering the representation of measurements in the partial Glauber-Sudarshan representation. As dis-

cussed in Appendix $H$, in the partial $P$ representation, POVM elements are represented by the partial $Q$ function found by replacing $\hat{\rho}$ with the POVM element in Equation (4.5.3). Since these are necessarily positive semi-definite, every measurement in the partial $P$ representation takes the same form as a measurement in a fundamental classical-quantum theory (c.f. Chapter 2). As such, when the partial Glauber-Sudarshan distribution $\varrho^P$ is also positive, the statistics of any measurement made on the bipartite quantum state are equivalent to those obtainable from a classical-quantum theory. As we show in Appendix H, this provides an alternative operational definition of effective classical-quantum states, as the states which are indistinguishable from classical-quantum states regardless of the measurement performed.

### 4.5.3 Relaxing the definition of effective classicality

The preceding discussion showed that the definition of effective classicality we use in this work is very strong, requiring that the statistics of measurements performed on the bipartite quantum system to be 'fakeable' by a fundamental classical-quantum system.

A basic way of relaxing this definition of effective classicality is to restrict the choices of measurements performed on the bipartite quantum system. For example, it is well known that by restricting to Gaussian states and measurements, which all have positive Wigner representations, dynamics that map positive Wigner functions to positive Wigner functions may also appear classical [61, 172]. Analogously, in the bipartite case, by restricting to measurements with positive partial Wigner functions, dynamics that preserves the positivity of the partial Wigner function alone would be sufficient to guarantee that the dynamics appears effectively classical. As discussed further in Appendix H, we thus may treat the states with positive partial quasiprobability distributions in other representations as effectively classical-quantum, provided the measurements are also understood to be suitably restricted.

Relaxing the requirement of positivity from the partial $P$ representation to other representations leads to a relaxation of the requirements of the dynamics. To see this, we first note that every positive semi-definite operator-valued function of phase space defines a valid positive partial $P$ distribution. This means that the corresponding dynamics in the partial $P$ representation must be positive on every initial state in order to define effective classical-quantum

dynamics. However, the same however does not hold for other partial quasi-probability distribitions: the set of states of $\varrho^W$ and $\varrho^Q$ form strict subsets of all positive operator-valued functions [151, 171, 27].

In these cases, while completely-positive dynamics defines a valid effective classical-quantum dynamics, another valid effective dynamics is provided by *subset-positive* dynamics. Recall that in Section 4.2, the notion of positivity of dynamics was used to argue for the validity of the Liouville equation as classical equation of motion, and against the quantum-classical Liouville equation as having describing a genuinely classical subsystem. The key property was that the positivity of the dynamics was considered on the set of all positive semi-definite operator-valued functions $\mathbf{S}$. However, there also exist dynamics which although do not preserve the positivity of all initial real or operator-valued functions of phase-space states, do preserve positivity of on a subset of initial conditions. For a given subset of all positive semi-definite functions $\mathbf{\Lambda} \subset \mathbf{S}$, we state that a dynamics is $\mathbf{\Lambda}$-*positive* if it is positive for all initial states belonging to that subset. Since subset-positive dynamics need not be positive on all initial states, it also need not be characterised by the Pawula [47] or CQ Pawula [45] theorems described in Appendix D.

An important example of such a subset-positive dynamics is provided by partial Husimi representation dynamics. Since the partial Husimi representation is always positive, the unitary dynamics in Hilbert space induces a positive dynamics on partial Husimi distributions [27]. However, this map is not positive on all initial states, but instead is $\mathbf{H}$-positive. While this subset-positive dynamics has many interesting features, the positivity should not be conflated with the interpretation as having an effectively classical subsystem, for the reason that all dynamics, even those that generate large amounts of entanglement, may be represented in this way. A single measurement of such a dynamics will only appear effectively classical-quantum when the measurements on the bipartite system are severely restricted, in this case to those with positive partial $P$ representations i.e. to coherent state POVMs on the $C$ subsystem and $Q$ system measurements conditioned on the POVM outcome.

### 4.5.4 Compatability with other notions of classicality

The definition of effective classicality in terms of the positivity of the partial Glauber-Sudarshan

representation was motivated by appealing to the formalism of positive representations of states and measurements. In this subsection, we discuss how our framework may also be adapted to fit with alternative notions of classicality.

Firstly, we note that a common notion of classicality is the non-disturbance of measurements, which is codified into tests of classicality such as Legget-Garg [53, 54]. To understand how measurement disturbance arises in our current framework, let us imagine we have the unitary bipartite evolution of two quantum systems, and perform a coherent state POVM on the $C$ subsystem at a time $t$. The probability distribution of outcomes, and the corresponding conditional measurement outcomes on the $Q$ subsystem are described by $\varrho^Q$. However, to describe the evolution correctly, the unconditioned post-measurement state must be updated, by a Weierstrass transform, to include the effect of the measurement. The description of measurement outcomes at a series of times $t_1, \ldots, t_n$ thus appears to depend explicitly on which times the system was measured, and thus appears inherently non-classical. In other words, to make accurate predictions for future observations, a record must be made of the times at which measurements were made on the $C$ subsystem, in clear contradiction with standard classical physics.

A strange, yet natural loophole, is to instead imagine that the $C$ system is *always* being measured. In this case, the system may be assigned definite values at every point in time, but no record is required to be made of which times the system was observed. By constantly measuring the system, the counterfactual of what would have happened if a measurement were made never needs to be considered. This exactly coincides with the idea of the environment playing the role of a witness [134, 135], and we see this explicitly in the discrete time model of environmental decoherence we introduce, with the POVM acting as a constant measurement of the system in the limit of $\tau \to 0$. In this model each measurement has a disturbing effect on the system, but in the double scaling limit, this appears as nothing other than a diffusion process on the classical degrees of freedom, and thus is compatible with a classical description.

Another notion of effective classicality is via the decoherent histories framework [49–51, 137]. In this framework, the probability of a certain classically definite history $z_1, \ldots, z_n$ at times

$t_1, \ldots, t_n$ is provided by considering the trace of projectors $\hat{P}(z_i, t_i) = e^{\frac{i}{\hbar}\hat{H}t_i}\hat{P}(z_i)e^{-\frac{i}{\hbar}\hat{H}t_i}$ i.e.

$$P(z_1, \ldots, z_n) = \mathrm{tr}[\hat{P}(z_n, t_n) \ldots \hat{P}(z_1, t_1)\hat{\rho}\hat{P}(z_1, t_1) \ldots \hat{P}(z_n, t_n)]. \tag{4.5.5}$$

Choosing projectors $P(z_i)$ given by the coherent states $|\alpha_i\rangle\langle\alpha_i|$ (where $|\alpha_i\rangle$ is shorthand for $|\alpha_s(q_i, p_i)\rangle\rangle$), and assuming a measurement is performed every time $\tau$, this takes the form

$$P(z_1, \ldots, z_n) = \mathrm{tr}\left[|\alpha_n\rangle\langle\alpha_n|e^{-\frac{i}{\hbar}\hat{H}\tau} \ldots |\alpha_1\rangle\langle\alpha_1|e^{-\frac{i}{\hbar}\hat{H}\tau}\hat{\rho}e^{+\frac{i}{\hbar}\hat{H}\tau}|\alpha_1\rangle\langle\alpha_1| \ldots e^{+\frac{i}{\hbar}\hat{H}\tau}|\alpha_n\rangle\langle\alpha_n|\right] \tag{4.5.6}$$

It is straightforward to see from the above that this exactly describes the discrete-time model of the environment provided previously, where the bipartite system evolves unitarily for time $\tau$ and then is projected onto the coherent states[‡].

To generalise this procedure to also include information about the $Q$ subsystem, we may instead take the *partial* trace. In doing so, we arrive at the probability of a classical history, multiplied by the quantum state conditioned on these measurement outcomes i.e. the classical-quantum state corresponding to a path in phase space, given by

$$\varrho(z_1, \ldots, z_n) = \mathrm{tr}_C\left[|\alpha_n\rangle\langle\alpha_n|e^{-\frac{i}{\hbar}\hat{H}\tau} \ldots |\alpha_1\rangle\langle\alpha_1|e^{-\frac{i}{\hbar}\hat{H}\tau}\hat{\rho}e^{+\frac{i}{\hbar}\hat{H}\tau}|\alpha_1\rangle\langle\alpha_1| \ldots e^{+\frac{i}{\hbar}\hat{H}\tau}|\alpha_n\rangle\langle\alpha_n|\right]. \tag{4.5.7}$$

While this provides some suggestion that the discrete time model and double scaling limit may be thought of in terms of decoherent histories, one must in practice check that there is negligible coherence between different classical histories, which is understood as the vanishing of the decoherence functional [51]. Whether this may be generalised in a similar way to (4.5.7) and be used to check that the $C$ subsystem has well-defined classical histories even when the $Q$ subsystem is observed is an interesting question which we leave to future work.

These two examples suggest that the basics of our framework i.e. the discrete time model of environmental decoherence, and the associated double scaling limit, may be understood in other frameworks of classicality beyond the positivity of the quasiprobability distributions considered previously.

We conclude this section by highlighting three subtleties of studying effectively classical

[‡]Indeed, as we demonstrate in the next section, this ordering of free evolution and projection is exactly the kind corresponding to the partial Glauber-Sudarshan distribution.

subsystems. Firstly, it is important to emphasise that a subsystem that is not effectively classical may become effectively classical when the $Q$ subsystem is traced out. In particular, it is possible to find examples of $\varrho^P$ that are not positive despite the fact that their trace $\mathrm{tr}\varrho^P$ is. As opposed to being a failure of the definitions we provide, this captures an important feature of classicality: namely that a given system is only classical with respect to a set of other systems that are accessible to measure. Indeed, the $C$ system will in general be expected to be entangled with another unobserved system such as an environment, or have entanglement amongst unobserved constituent parts (e.g. as in [162]). Secondly, it is worth highlighting that an ambiguity arises in the above definition of $\varrho^P$ – namely that the freedom in the squeezing parameter $s$ means that that one may in principle define different $P$ representations. In our model, we see that the environment provides a natural choice of $s$, namely that which is preserved by the dynamics. While seemingly strange that the dynamics enters this definition, this is also implicitly the case in standard discussions of $P$ function positivity in quantum optics, where the coherent states are defined as those displaced from the ground state of the Hamiltonian [169, 168]. Finally, once one goes beyond a single quantum subsystem that is being classicalised, it is not necessarily natural for the positivity of the partial Wigner function to even be a necessary condition for classicality. This is due to the possibility of entanglement amongst the subsystems that make up the $C$ subsystem, which nevertheless is not manifest at a macroscopic level. Although beyond the scope of the current work, in this case one expects that some entanglement should be permitted amongst the individual subsystems that make up the classical system, and thus the allowed set of measurements should be restricted to reflect that this entanglement is not detectable.

## 4.6 Equivalence between partial quasiprobability representations

In this section, we shed some light onto why the dynamics of equation (4.4.5) is completely-positive on all operator-valued functions of phase space, and on the original choice of operator ordering in the definition of $\mathcal{E}_\tau^\hbar$, by studying the dynamics of the partial Husimi $\varrho^Q$ and partial Glauber-Sudarshan $\varrho^P$ distributions introduced in the previous section. In doing so, we demon-

strate that the classical-quantum limit we have arrived at preserves the effective classicality of the $C$ subsystem.

To study the total dynamics of the partial Glauber-Sudarshan and partial Husimi distributions in the classical-quantum limit, we first note that the decoherence channel used to model the environment in these representations is identical to that of the partial Wigner distribution, and so may be modelled as before as $\mathcal{D}$. To study the unitary dynamics generated by the Hamiltonian in each representation, we show in Appendix I how one may find the generators of the partial Husimi $\mathcal{L}^Q$ and the partial Glauber-Sudarshan $\mathcal{L}^P$ by mapping first to the Wigner distribution by the differential operator $\mathcal{D}^{\mp\frac{1}{2}}$, using the free Wigner evolution, and then mapping back using the inverse $\mathcal{D}^{\pm\frac{1}{2}}$, for $\varrho^Q$ and $\varrho^P$ respectively. Considering the corresponding generators to $O(1)$ in $\hbar$, we find the following generator of partial Husimi evolution

$$\begin{aligned}\mathcal{L}^Q\big|_{O(\hbar^0)} =& -\frac{i}{\hbar}[H,\ \cdot\ ] + \frac{1}{2}(\{H,\ \cdot\ \} - \{\ \cdot\ , H\}) \\ & - \frac{is^2}{2}[\frac{\partial H}{\partial q}, \frac{\partial\ \cdot}{\partial q}] - \frac{i}{2s^2}[\frac{\partial H}{\partial p}, \frac{\partial\ \cdot}{\partial p}] \\ & - i[\frac{s^2}{4}\frac{\partial^2 H}{\partial q^2} + \frac{1}{4s^2}\frac{\partial^2 H}{\partial p^2},\ \cdot\ ],\end{aligned} \tag{4.6.1}$$

which was first written down in [27], though without the final term, and the following generator of partial Glauber-Sudarshan evolution

$$\begin{aligned}\mathcal{L}^P\big|_{O(\hbar^0)} =& -\frac{i}{\hbar}[H,\ \cdot\ ] + \frac{1}{2}(\{H,\ \cdot\ \} - \{\ \cdot\ , H\}) \\ & + \frac{is^2}{2}[\frac{\partial H}{\partial q}, \frac{\partial\ \cdot}{\partial q}] + \frac{i}{2s^2}[\frac{\partial H}{\partial p}, \frac{\partial\ \cdot}{\partial p}] \\ & + i[\frac{s^2}{4}\frac{\partial^2 H}{\partial q^2} + \frac{1}{4s^2}\frac{\partial^2 H}{\partial p^2},\ \cdot\ ].\end{aligned} \tag{4.6.2}$$

Using these, one may then construct the generator of evolution $\mathcal{E}^\hbar_\tau$ as in (4.4.1) and take the double-scaling limit as described previously to find the generator of the dynamics. However, in order to derive the same evolution map, and thus the same generator, one can check that one must choose different operator orderings depending on the representation! In particular, one can see from the above argument using $\mathcal{D}^{\pm\frac{1}{2}}$ to map between representations, that three distinct operator orderings of the free evolution and the environmental decoherence steps lead to the same evolution map:

$$\mathcal{E}^\hbar_\tau = \ e^{\mathcal{L}^Q\tau}\mathcal{D} = \mathcal{D}^{\frac{1}{2}}\ e^{\mathcal{L}^W\tau}\mathcal{D}^{\frac{1}{2}} = \mathcal{D}e^{\mathcal{L}^P\tau}. \tag{4.6.3}$$

The key observation to understand the difference in operator ordering in each case is to note that the environment plays a different role in each partial quasiprobability representation in order to maintain classicality. As discussed in section 4.5, the unitary dynamics in the partial Husimi representation are only positive on initial states with sufficient spread in phase space. Consequently, in this representation the decohering action of the environment must be taken *before* the unitary evolution, such that any arbitrarily peaked states in phase space are first convoluted before they are evolved. Conversely, in the partial Glauber-Sudarshan representation, the state $\varrho^P$ is only positive when all entanglement has been removed; in this case the environment acts *after* the unitary evolution to ensure any entanglement built up by the unitary evolution is destroyed at the end of each step. Since the partial Wigner representation $\varrho^W$ lies exactly half-way between $\varrho^Q$ and $\varrho^P$ by Weierstrass transform (see Appendix I for more details), the original symmetrised dynamics postulated in (4.4.1) turns out to be exactly that which performs both steps in half-measure. In all of these cases, the map that is defined is completely-positive on all positive semi-definite operator-valued functions.

The above analysis also guarantees that the dynamics of equation (4.4.5) preserves the effective classicality of the $C$ subsystem. As discussed in Section 4.5, the positivity of the partial Glauber-Sudarshan probability distribution provides sufficient and necessary conditions for the quantum state of the bipartite system to be an effective classical-quantum state. Thus, by here explicitly showing that the dynamics of $\varrho^P$ are also positive, we guarantee that the $C$ subsystem may be treated as effectively classical in the double scaling limit. This may be equivalently argued using the fact that the map between the different representations becomes the identity in the limit that $\hbar \to 0$, and thus that $\varrho^W$ coincides with $\varrho^P$ in the classical limit. For the same reason, ensuring that the dynamics in the three representations all agree, as it does above, provides an important consistency check on the validity of any classical-quantum dynamics arising from a classical limit.

## 4.7 Trajectories in the classical-quantum limit

We assumed up to this point that the observer has no access to the environmental degrees of freedom that store the information about the $C$ subsystem. However, one could assume that

the observer has sufficient information about the environment to reconstruct the outcome of the effective coherent state POVM that it induces at each time step [173, 174, 43]. In this case, the observer has access to the classical system's trajectory in phase space, and their best estimate of the quantum state deduced from the motion of the classical system leads to a quantum trajectory in Hilbert space.

The general form of dynamics describing classical-quantum trajectories allows us to unravel Equation (4.4.5) into coupled stochastic trajectories of the classical phase space degrees of freedom $z_t$ and mixed quantum states $\rho_t$ conditioned on these classical trajectories. A key result of Chapter 2 was that when the trade-off is saturated in the form $D_0 = D_1^\dagger D_2^{-1} D_1$, any initially pure state of the quantum system remains pure conditioned on the classical trajectory. Since this is the case here, this means that the general classical-limit dynamics of Equation (4.4.5) may be unravelled in terms of pure quantum states $|\psi\rangle_t$ which are unique for a given classical trajectory. Defining a column vector $z_t = (q_t, p_t)^T$ for the classical degrees of freedom, and the operator-valued column vector $L = (L_q^H, L_p^H)^T$, the stochastic dynamics takes the form

$$dz_t = (D_1^* + D_1)\langle L\rangle dt + \sigma dW_t, \tag{4.7.1}$$

$$\begin{aligned} d|\psi\rangle_t = &-\frac{i}{\hbar}(H + H_{\text{eff}})|\psi\rangle_t dt \\ &+ (L - \langle L\rangle)^T D_1^\dagger \sigma^{-T} |\psi\rangle_t dW_t \\ &- \frac{1}{2}(L - \langle L\rangle)^T (D_0^T L - D_0\langle L\rangle)|\psi\rangle_t dt. \end{aligned} \tag{4.7.2}$$

Here $\langle L\rangle = \langle\psi|_t L|\psi\rangle_t$, $\sigma$ denotes any $2\times 2$ matrix such that $\sigma\sigma^T = D_2$, and $dW_t = (dW_t^1, dW_t^2)^T$ denotes a column vector of two uncorrelated Wiener processes. The equations are formally identical to those used to describe continuous quantum measurement and the associated measurement signals, and we refer the reader to [42] for an excellent introduction to this formalism.

The unravelled form of dynamics makes clear that the semi-classical limit we present here does not lead to any loss of quantum information, provided an observer has access to the full classical trajectory (c.f. Secs. 2.4 and 2.5). Since this originates from a full quantum theory, we see that in principle the irreversibility introduced by tracing out an environment may be partially recovered in the classical limit.

The most important practical use of the stochastic unravelling equations we provide here

is for the simulation of dynamics in the classical-quantum limit. For the same reasons that unravellings of Lindbladian dynamics provide an important tool for studying open quantum systems [160], unravellings of classical-quantum master equations allow one to study both the mean values and statistics of various classical and quantum observables. As discussed for the master equation approach, these equations may also be generalised to the case where there are $n$ classical degrees of freedom $(q_1, \ldots, q_n, p_1, \ldots, p_n)$: in this case one must take $z_t = (q_t^1, \ldots, q_t^n, p_t^1, \ldots, p_t^n)^T$, $L = (L_{q_1}^H, L_{p_1}^H, \ldots, L_{q_n}^H, L_{p_n}^H)^T$, $dW_t = (dW_t^1, \ldots, dW_t^{2n})^T$, and take $D_0$, $D_1$ and $D_2$ to be block diagonal, with each block given by the form in equations (4.4.10)-(4.4.12), as discussed in section 4.4. With these modifications to the above equations, the dynamics of a wide variety of many body systems with bosonic subsystems may be studied numerically in the classical-quantum limit, and we refer the reader to Chapters 2 and 5 for examples of the simulation of classical-quantum unravellings.

## 4.8 Two special cases of dynamics

The general form of generator, given in equation 4.4.5 and their corresponding unravellings in (4.7.1) and (4.7.2) are the main results from this chapter, describing the general form of dynamics for a bipartite Hamiltonian $\hat{H}$ in the double-scaling classical limit on one subsystem. To gain some more insight into what this dynamics predicts, we will consider now two special cases.

The first case we will consider is the effect of the double-scaled classical limit on a single system. To study this, one can take a bipartite quantum Hamiltonian of the form $\hat{H} = (\hat{p}^2/2m + V(\hat{q})) \otimes \mathbb{1}$, where $\mathbb{1}$ is the identity operator on the $Q$ subsystem i.e. a Hamiltonian with trivial action on the $Q$ subsystem. The corresponding classical-quantum Hamiltonian may be computed to be $H = (p^2/2m + V(q))\mathbb{1}$, and defines the operators $L_p^H = (p/m)\mathbb{1}$, $L_q^H = \partial_q V(q)\mathbb{1}$, $H_{\text{eff}} = 0$. Using these definitions in the general dynamics (4.4.5) one finds that the unitary, Lindbladian, and mixed derivative-commutator terms all vanish, and the mixed derivative-anticommutator terms combine to give the Poisson bracket. This gives the following stochastic

dynamics on the classical system

$$\frac{\partial \varrho}{\partial t} = \{H, \varrho\} + \frac{E_f s^2}{2}\frac{\partial^2 \varrho}{\partial q^2} + \frac{E_f}{2s^2}\frac{\partial^2 \varrho}{\partial p^2}, \tag{4.8.1}$$

which describes diffusion around the classical Liouville equation given in (4.2.4). This example shows that the idea that that the limit is specific to subsystems is not neccesary – rather the double scaling limit we find provides a general notion of a "stochastic classical limit", that happens to also give consistent evolution when it is applied to subsystems alone. Although the existence of stochastic classical limits are somewhat of a folk wisdom in physics, the earliest concrete proposal we have found in the literature is a discussion in [138].

A second limiting case of the above dynamics is to consider the dynamics under the approximation

$$\mathrm{ad}^n_{\frac{-i}{E_f}H}\left(\frac{\partial H}{\partial z}\right) \approx 0, \tag{4.8.2}$$

for $z = (q, p)$ and $n > 0$. This is true exactly when $H(q, p)$ is self-commuting i.e. when $[H(z), H(z')] = 0$ for all $z, z'$ in phase space, and has an error of $O(\hbar^n)$ when the classical-quantum Hamiltonian takes the form $H = (p^2/2m_C)\mathbb{1} + P^2/2m_Q + V(q\mathbb{1} - Q)$, where $Q$ and $P$ are operators on the quantum subsystem satisfying $[Q, P] = i\hbar$. Making this approximation, we find that $L^H_q = \partial_q H$, $L^H_p = \partial_p H$ and $H_{\text{eff}} = (\hbar s^2/4)\partial_q^2 H + (\hbar/4s^2)\partial_p^2 H$. The dynamics in (4.4.5) then reduces in form to the following

$$\begin{aligned}
\frac{\partial \varrho}{\partial t} =& -\frac{i}{\hbar}[H, \varrho] + \frac{1}{2}\big(\{H, \varrho\} - \{\varrho, H\}\big) \\
&+ \frac{is^2}{2}[\frac{\partial H}{\partial q}, \frac{\partial \varrho}{\partial q}] + \frac{i}{2s^2}[\frac{\partial H}{\partial p}, \frac{\partial \varrho}{\partial p}] \\
&+ i[\frac{s^2}{4}\frac{\partial^2 H}{\partial q^2} + \frac{1}{4s^2}\frac{\partial^2 H}{\partial p^2}, \varrho] \\
&+ \frac{1}{2E_f}(\bar{L}\varrho\bar{L}^\dagger - \frac{1}{2}\{\bar{L}^\dagger\bar{L}, \varrho\}_+) \\
&+ \frac{E_f s^2}{2}\frac{\partial^2 \varrho}{\partial q^2} + \frac{E_f}{2s^2}\frac{\partial^2 \varrho}{\partial p^2},
\end{aligned} \tag{4.8.3}$$

where we have defined the Lindblad operator $\bar{L} = sL^H_q + is^{-1}L^H_p$ as in equation (4.4.6). The first line gives the unitary evolution and Alexandrov bracket from the quantum-classical Liouville equation (4.2.9). However, the second and third lines, formed from $H_{\text{eff}}$ and the mixed derivative-commutator terms, contain exactly the additional terms associated to the dynamics

of the partial Glauber-Sudarshan representation i.e. the first three lines give $\mathcal{L}^P|_{O(\hbar^0)}$, previously found in (4.6.2). We thus see that the total dynamics is exactly the dynamics of the partial Glauber-Sudarshan representation to lowest order in $\hbar$, with additional terms corresponding to noise in the classical and quantum systems. Since the approximation made above occurs at the level of the operators, the complete positivity of the dynamics is unchanged, and thus may still be unravelled by using the simplified forms of the operators $L_q^H$, $L_p^H$ and $H_{\text{eff}}$ in equations (2.16) and (2.17).

The majority of work in the literature on completely-positive classical-quantum dynamics, including the earlier Chapter 3, concluded that the natural form of dynamics would take the form of the quantum-classical Liouville equation with minimal additional noise terms to ensure positivity [25, 46, 1]. However, as the above example shows, when derived in a physical manner from a full quantum theory, a more natural model is instead the $O(\hbar^0)$ partial Glauber-Sudarshan dynamics of (4.6.2) supplemented with the minimal terms necessary for positivity. This result seems particularly reasonable when one considers that it is the positivity in the partial Glauber-Sudarshan distribution, and not the partial Wigner distribution, that guarantees the classicality of the $C$ subsystem, as discussed in Section 4.6. The biggest difference between these models lies in the additional back-reaction terms with first derivatives in position, which lead to a decoherence rate that is twice as large as that expected by including additional terms in the partial Wigner representation.

## 4.9 The $E_f \to 0$ limit

The double scaling limit we have presented leads generically to irreversible dynamics, with the parameter characterising the diffusion in the classical system given by $E_f$. A question we now turn to is whether one may recover a deterministic evolution, as in the standard classical limit, by tuning this free parameter.

### 4.9.1 $E_f \to 0$ for self-commuting Hamiltonians

The first example to look at is the result of the double scaling classical limit on a single system. The dynamics in this case was computed earlier in equation (4.8.1), taking the form of Hamiltonian dynamics with additional diffusion in both position and momentum proportional to $E_f$. In the limit $E_f \to 0$, one thus recovers the Liouville equation (4.2.4), i.e. deterministic evolution under the classical Hamiltonian. This additional $E_f \to 0$ limit may be physically interpreted as saying that if one considers large macroscopic scales, any noise due to the environment is negligible, and thus reversible Hamiltonian dynamics is recovered [158]. Indeed, this is the same kind of limit that permits us to disregard the miniscule effects of Brownian motion at the macroscopic scales of everyday objects i.e. that the amount of diffusion caused by the environment is vanishingly small compared to the other forces on macroscopic objects[§]. Since the Liouville equation (4.2.4) was previously obtained directly from the standard $\hbar \to 0$ limit, we see that when applied to single systems, the stochastic notion of a classical limit that we have presented reduces to the standard notion in the $E_f \to 0$ limit.

Given that the $E_f \to 0$ limit recovers a deterministic classical limit on a single system, it is interesting to consider whether the same may be true when one considers the classical limit of a subsystem. To explore this question, we will first consider the limiting case described in equation (4.8.3) for self-commuting classical-quantum Hamiltonians. In this case, the parameter appears in two places: proportional to the strength of classical diffusion, and inversely proportional to the strength of the decoherence on the quantum system. One thus sees that while taking $E_f$ to be small reduces the amount of classical diffusion, it leads to very large decoherence on the quantum degrees of freedom in a basis determined by the Lindblad operator $\bar{L}$. In the limit $E_f \to 0$, decoherence acts to instantaneously select an eigenstate of the operator $\bar{L}$, and then freeze the quantum system in this eigenstate, via the quantum zeno effect [175, 161, 39]. In doing so, the quantum system is essentially classicalised, with any superpositions being supressed by the strong decoherence. Since the back-reaction on the classical system is determined by the eigenvalues of the operator $\bar{L}$, the classical system then undergoes deterministic evolution with

[§]Indeed, using the definition of $\tau$ considered previously in terms of the decoherence time $\tau_D$, we see that $E_f \to 0$ corresponds in the physical model of quantum Brownian motion to taking the diffusion coefficient $D$ to zero, as would occur in e.g. a low temperature limit of the model.

drift given by the eigenstate that the quantum system is frozen in. Such a dynamics may be understood to be reversible on a subset of initial quantum states that are eigenstates of the Lindblad operator $\bar{L}$, but in general is highly non-deterministic, with a generic initial quantum state being rapidly decohered by the interaction.

The above example illustrates that in the $E_f \to 0$ limit, dynamics arising from classical-quantum Hamiltonians that are self-commuting exhibit rapid decoherence in the quantum system. It turns out however that this is not a generic feature of dynamics in the $E_f \to 0$ limit, which we may illustrate with the following example.

### 4.9.2 $E_f \to 0$ for non self-commuting Hamiltonians: a classical-quantum limit of two quantum harmonic oscillators

Consider a system of two interacting quantum particles in one dimension, with the $Q$ subsystem characterised by the canonical commutation relation $[Q, P] = i\hbar$ and the $C$ subsystem as usual by $[\hat{q}, \hat{p}] = i\hbar$. The system will be taken to have free evolution given by the bipartite quantum Hamiltonian $\hat{H} = \hat{p}^2/2m_C + P^2/2m_Q + \lambda(\hat{q} - Q)^2$. Taking the classical-quantum limit of the $C$ subsystem gives a classical-quantum Hamiltonian $H = (p^2/2m_C)\mathbb{1} + P^2/2m_Q + \lambda(q\mathbb{1} - Q)^2$. For this model, one may compute the Lindblad and effective Hamiltonian operators of equations (4.4.6) and (4.4.7) exactly, exploiting the fact that the adjoint action closes under the set of linear operators in $\mathbb{1}, Q, P$ to obtain

$$L_q^H = \frac{E_f}{\hbar}\left[\sqrt{2\lambda m_Q}\sin\left(\frac{\sqrt{2\lambda}\hbar}{E_f\sqrt{m_Q}}\right)(q\mathbb{1} - Q) + [1 - \cos\left(\frac{\sqrt{2\lambda}\hbar}{E_f\sqrt{m_Q}}\right)]P\right], \tag{4.9.1}$$

$$L_p^H = \frac{p}{m_C}\mathbb{1}, \tag{4.9.2}$$

$$\begin{aligned} H_{\text{eff}} =& \frac{p}{2m_C}\left[\frac{2E_f m_Q}{\hbar}[\cos\left(\frac{\sqrt{2\lambda}\hbar}{E_f\sqrt{m_Q}}\right) - 1] + \sqrt{2\lambda m_Q}\sin\left(\frac{\sqrt{2\lambda}\hbar}{E_f\sqrt{m_Q}}\right)\right]Q \\ &+ \frac{p}{2m_C}\left[1 + \cos\left(\frac{\sqrt{2\lambda}\hbar}{E_f\sqrt{m_Q}}\right) - \frac{\sqrt{2m_Q}E_f}{\sqrt{\lambda}\hbar}\sin\left(\frac{\sqrt{2\lambda}\hbar}{E_f\sqrt{m_Q}}\right)\right]P, \end{aligned} \tag{4.9.3}$$

where we have dropped terms proportional to the identity in $H_{\text{eff}}$. These explicit forms of Lindblad and effective Hamiltonian operators may be used in the master equation (4.4.5) or the unravelling equations (2.16) and (2.17) to study the classical-quantum oscillator dynamics for arbitrary $E_f$.

Let us now consider this dynamics in the low diffusion, $E_f \to 0$ limit. The key feature of interest is that as $E_f$ goes to zero, the non-trivial Lindblad operator $L_q^H$ responsible for quantum back-reaction on the classical system also vanishes. Moreover, one can check that the parts of $\bar{L}\varrho\bar{L}^\dagger - \frac{1}{2}\{\bar{L}^\dagger\bar{L}, \varrho\}_+$ responsible for decoherence also vanish, at a faster rate than the rate at which the decoherence strength increases. In other words, in the $E_f \to 0$ limit, both the back-reaction and decoherence of the quantum system are zero. To study the rest of the dynamics in the low diffusion limit, we first note that the remaining terms of $\bar{L}\varrho\bar{L}^\dagger - \frac{1}{2}\{\bar{L}^\dagger\bar{L}, \varrho\}_+$ lead to unitary evolution on the quantum system, with a Hamiltonian given by $(\hbar p/2m_C E_f)L_q^H$. Remarkably, although this Hamiltonian and $H_{\text{eff}}$ do not independently have well-defined $E_f \to 0$ limits, their sum does and has its limit given by $(p/m_C)P$. We thus find that in the $E_f \to 0$ limit, the classical-quantum oscillator dynamics reduces to unitary dynamics on the quantum system under the classical-quantum Hamiltonian $H$ and an additional term $(p/m_C)P$, and the classical system experiences no back-reaction:

$$dq_t = \frac{p_t}{m_C}dt, \qquad dp_t = 0, \tag{4.9.4}$$

$$d|\psi\rangle_t = -\frac{i}{\hbar}(H + \frac{p_t}{m_C}P)|\psi\rangle_t dt. \tag{4.9.5}$$

In this limit, the strong monitoring by an environment on the $C$ subsystem thus acts to effectively remove the back-reaction of the quantum system on the classical one, leaving simply coherent control of the quantum system by the classical one, despite the strength of interaction remaining fixed. Under the additional assumption that the $C$ subsystem is moving sufficiently slowly, one recovers coherent control under the classical-quantum Hamiltonian. This reproduces the results of earlier work on classical-quantum limits, which considered the special case in which the back-reaction is zero [129, 70]. In our setting, this effect is reminiscent of dynamical decoupling, where the application of unitary pulses on a quantum system may reduce the interaction with an external environment [176]. Incidentally, one can check that the $\hbar \to 0$ limit of the operators defined in equations (4.9.1) and (4.9.3) are still well-defined, and reduce the form of dynamics to that given in (4.8.3); the apparent difference in limiting behaviour as $E_f$ becomes small is due to the non-commutativity of the two limits $E_f \to 0$ and $\hbar \to 0$.

The two examples above show that in the low diffusion limit, $E_f \to 0$, the classical-quantum dynamics we find can exhibit two very different behaviours; one in which the quantum system

rapidly decoheres, and affects the classical system, the other in which it evolves with unitary evolution, and has no back-reaction on the classical system. In the regime that a classical system appears to evolve without diffusion, it thus appears to be the case that any quantum degrees of freedom that are affecting the evolution of the system must be rapidly decohered and effectively classical, or do not influence the dynamics of the classical system, and undergo unitary evolution depending on the classical state of the system. It would be interesting to study how generic the latter case is, and indeed whether there exist other behaviours aside from these two.

## 4.10 Discussion

The main results, given in master equation form in (4.4.5) or stochastic unravelling form in (2.16) and (2.17), provide a physically motivated and consistent effective classical-quantum dynamics derived from a full quantum theory. A special limiting case of this, given in equation (4.8.3), provides a form of dynamics close to the quantum-classical Liouville equation that may be directly unravelled in classical trajectories in phase space and quantum trajectories in Hilbert space. Beyond the coupled quantum harmonic oscillators example given, understanding the kinds of dynamics obtained via this classical-quantum limit in further models, from optics to condensed matter theory, would be of great interest. With the form of Lindblad and effective Hamiltonian operators computed, the average and statistical properties of such systems may be numerically simulated using the stochastic unravellings of (2.16) and (2.17).

An important research direction to understand in greater detail is the conditions under which the above dynamics are a good approximation to a full quantum dynamics. While the work in this chapter demonstrated that a classical-quantum limit gives a rich dynamical structure, the analysis was the classical-quantum analogue of the steps leading from the full Wigner dynamics of equation (4.2.2) to the Liouville equation in (4.2.4). Understanding whether the various approaches that characterise the conditions under which one may make this approximation [133, 139, 177, 150, 140] can be generalised to the more complex case of a classical-quantum limit is an important open question.

The methods presented here rely on the assumption that the environment may be modelled in a particularly simple way, as a series of discrete-time decoherence channels on the subsystem that is classicalised. It would be interesting to understand whether the results we obtain here may also be derived directly from continuous-time models of an environment (c.f. Appendix G). Moreover, the effect of the environment in this proposed classical-limit procedure is particularly simplistic, characterised only by the total strength of phase space diffusion $E_f$ and a parameter $s$ quantifying the relative strength of diffusion in position and momentum. In real systems, the environment may induce a large number of additional effects on the dynamics such as friction, and in such cases we expect the corresponding classical-quantum dynamics to be modified to reflect this.

Beyond this, it would be interesting to understand dynamics which relax the requirement of preserving effective classical-quantum states. In its most modest form, this could arise from restricting the set of measurements performed on a system undergoing Markovian evolution, using the formalism of section 4.5, such that even in the presence of entanglement the system appears classical. More generally, dynamics that do not preserve effective classical-quantum states could arise analogously to how relaxing complete-positivity in the study of open quantum systems can sometimes approximate full non-Markovian dynamics more accurately than when the dynamics is of Lindblad form [178]. In this regard, making precise the notions of *almost always classical-quantum*, or *approximately classical-quantum*, are likely to be important.

For these reasons, the classical-quantum limit introduced here is likely to be one of many, and we anticipate that considerable further work is required to understand the full landscape and applications of effective classical-quantum dynamics that arise from quantum theory.

# Chapter 5

# Thermal state preserving classical-quantum dynamics

In this chapter, we study dynamics of classical-quantum systems in thermal environments. This is made possible by identifying two operators, $L_z$ and $M_{xy}$, that allow general forms of dynamics to be constructed that preserve the thermal state of the combined classical-quantum system. We see that this will allow us to prove explicitly that this class of dynamics is consistent with the second law of thermodyanmics, which we illustrate in two models. The main technical result is finding necessary and sufficient conditions for completely-positive, linear, Markovian and continous in phase space classical-quantum dynamics to satisfy detailed balance.

## 5.1 Motivation and background

A basic test of any theory is that it is consistent with the laws of thermodynamics. First used to bound the efficiency of large engines, the principles of thermodynamics are now understood to apply to the smallest scales, and to systems far from equilibrium. The great utility of thermodynamics is its universality, with all systems, whether described by classical mechanics or quantum mechanics, expected to be in accordance with it.

It is thus natural to expect that the rules of thermodynamics must also apply in contexts where both classical *and* quantum degrees of freedom are present. However, despite a huge range of dynamics having been suggested to describe the interactions between classical and quantum systems [17, 18, 15, 24–37], the question of whether any can be constructed to be compatible with the laws of thermodynamics has been largely left unanswered*. Indeed, this is in part because the common approaches used to study classical-quantum hybrids, namely mean-field methods [64] and reversible quantum-classical evolution laws [17–19], manifestly fail to satisfy both of the basic consistency requirements of a probability theory, namely linearity and positivity, which necessarily lead to violations of the second law of thermodynamics [179, 180]. While a recent approach based on mean-field dynamics showed success for systems close to equilibrium using perturbation theory [38], a form of classical-quantum dynamics that demonstrates consistency with thermodynamics out of equilibrium and for arbitrary coupling strengths has remained unknown.

In this chapter, we demonstrate that constructing classical-quantum dynamics consistent with the laws of thermodynamics is indeed possible. The central idea of this chapter is to identify the inherent irreversibility in classical-quantum dynamics as arising due to a thermal environment. First suggested in one of the earliest works on the topic [26], this perspective is natural when considering classical-quantum systems as arising when a quantum subsystem is decohered strongly enough by its environment for it to become effectively classical, as shown in Chapter 4. The thermal nature of the environment naturally leads us the main focus of this chapter: *we shall study dynamics which preserve the thermal state of the combined classical-quantum system in time*. While the possibility of such thermal-state preserving dynamics has been considered for some time in the context of physical chemistry [181–184], the approaches taken to achieve this are arguably closer to numerical methods than true dynamics, with even approximate preservation of the thermal state coming at the expense of violating basic physical assumptions such as the continuity of classical trajectories [185–187].

The main contribution of this chapter is to identify two classes of operators that allow

*A recent review [37] noted that most models do not demonstrate consistency with thermodynamics; those that were claimed to do so also fail the basic assumption of positivity, which means that the system cannot be interpreted as having an effectively classical subsystem, as discussed in Section 4.5.

for the construction of linear and completely-positive dynamics that preserve general classical-quantum thermal states. To illustrate this, we provide two general forms of dynamics, corresponding to overdamped and underdamped classical particles coupled to arbitrary quantum systems. Beyond simply reducing to the correct classical limits, we show that our dynamics generalise the standard approaches of classical-quantum coupling, notably mean-field dynamics [64] and quantum-classical Liouville dynamics [19], to the case where the dynamics is completely-positive, linear and preserves the thermal state of the combined classical-quantum system.

A major result of this chapter is to show that our dynamics, and indeed any thermal-state preserving, completely-positive and linear classical-quantum dynamics, necessarily satisfy the second law of thermodynamics for arbitrary initial states. Defining notions of entropy and heat for the combined classical-quantum system, the framework we provide allows one to study both entropy production and heat fluctuations in classical-quantum systems arbitrarily far from equilibrium. This chapter thus provides the first steps towards a general theory of non-equilibrium classical-quantum thermodynamics, combining the respective theories of classical and quantum non-equilibrium thermodynamics [188, 189] into one cohesive framework.

An important application of our framework is in the study of measurement and control of quantum systems. With Bohr's original conception of quantum theory as inherently describing the interactions between a quantum system and classical measuring device, we may understand the present framework as a physical and thermodynamically consistent description of this process. Since any interaction between classical and quantum systems is fundamentally irreversible [44, 23, 25, 45, 46], this chapter provides a framework for studying this using quantitative measures such as entropy production. Aside from any foundational interest, since classical-quantum theories are equivalent to measurement-based feedback [79] (c.f. Sec. 2.7), this chapter paves the way for a wide range of models that describe autonomous incoherent feedback systems embedded in thermal environments. This is expected to become increasingly relevant as quantum technologies are further developed into the regime in which fluctuating mesoscopic classical degrees of freedom are used to read out and control microscopic quantum degrees of freedom.

A second key application of this chapter is to provide a thermodynamically consistent frame-

work for improving upon existing semi-classical methods used in physics and chemistry. Notably, since the dynamics we provide reduces to a completely-positive and linear version of mean-field dynamics in the trajectory picture, we see that our dynamics provides a method of studying transitions between adiabatic energy levels due heat fluctuations, whilst ensuring that the classical and quantum degrees of freedom still evolve continuously.

To illustrate the framework in these two contexts, we introduce and solve two classical-quantum models. The first is a model of a mesoscopic overdamped classical degree of freedom coupled to a two-level quantum system. While this only provides a toy model, we show that the resulting dynamics admit an analytic solution for arbitrary initial states, which to our knowledge provides the first non-perturbative analytic solution of a classical-quantum master equation. We use this toy model to investigate entropy production during quantum measurement, and how the relaxation of a classical control system in a thermal environment can be used to perform a unitary transformation on a quantum system. The second model we introduce is a thermodynamically consistent model of a classical oscillator linearly coupled to a quantum oscillator. Using simulation methods developed originally in the context of continuous measurement theory [190–192], we numerically solve this model to show how our dynamics can exhibit thermalisation in the adiabatic basis, as well as showing how the second law bounds the statistics of heat fluctuations for thermalising systems.

Finally, we turn our attention to a particular class of thermal state-preserving dynamics satisfying a property known as detailed balance. Ensuring that there are no persistent currents flowing through the system in thermal equilibrium, detailed balance is known to give rise to many important results in non-equilibrium thermodynamics such as fluctuation theorems [193, 194], Onsager relations [195] and reaction kinetics [196].

The main technical result of this chapter is the full characterisation of classical-quantum detailed balance, for dynamics that are completely-positive, linear, Markovian and continuous in phase space. This is given in form of Equations (5.6.35) to (5.6.40), which provide constraints on the unitary, diffusion, back-reaction and decoherence parts of the classical-quantum dynamics in order to satisfy detailed balance with respect to a given fixed point. Generalising the work of [197–199] to the classical-quantum setting, we use these conditions to prove that the overdamped

and underdamped dynamics that we introduce satisfy detailed balance. Our findings provide an important tool for characterising a range of classical-quantum systems with fixed points, which we expect could provide insights into a number of recent applications of linear and completely-positive classical-quantum dynamics, from measurement and feeedback theory [200] to recent interest in fundamentally stochastic theories of gravity [46, 1, 201, 48, 4, 128, 121, 124, 123, 125].

The outline of the chapter is as follows. In Section 5.2 how the notions of entropy, energy and the second law can arise classical-quantum systems. In Section 5.3 we introduce two operators that allow us to construct overdamped and underdamped thermal state preserving dynamics, and demonstrate how our dynamics generalises the mean-field and quantum-classical Liouville approaches to dynamics that are completely-positive and linear. In Sections 5.4 and 5.5 we introduce and solve two models to illustrate the general features of our dynamics and its applications. Finally, in Section 5.6 we find the general conditions for classical-quantum detailed balance for Markovian classical-quantum with continuous classical trajectories, which we demonstrate are satisfied by the dynamics we introduce.

In the majority of the chapter, to streamline the notation without significant loss of clarity, we will opt to denote operators on Hilbert space simply using capital letters (e.g. $H$, $L_z$, $M_{xy}$) or Greek letters (e.g. $\rho$, $\varrho$) that are otherwise undistinguished from other scalar quantities (e.g. $S$, $E$, $\Sigma$). However, for pedagogical reasons, in Sections 5.4 and 5.5 we include hats to distinguish operator-valued quantities from real numbers, and these sections may be used as a reference for any other parts of the chapter where ambiguity arises.

## 5.2 Entropy production and the second law for classical-quantum dynamics

In this section we introduce the main concepts relating classical-quantum dynamics to thermodynamics. After introducing notions of classical-quantum thermal states and entropy, we show how if a classical-quantum dynamics preserves the thermal state, and satisfies the basic consistency requirements of complete-positivity and linearity, it necessarily obeys the second law of thermodynamics.

### 5.2.1 Classical-quantum entropy, energy and thermal states

We begin by defining the entropy of a classical-quantum system. The entropy associated to a classical-quantum state $\varrho(z,t)$ can be defined as a hybrid of both the Shannon and von-Neumann entropies [202], namely

$$S(\varrho(z)) = -\int dz\ \mathrm{tr}\varrho(z)\ \ln\ \varrho(z), \tag{5.2.1}$$

Just as with the standard Shannon or von-Neumann quantum entropy, one may use this to quantify the uncertainty of the classical-quantum state and similarly its information content. Since we deal with continuous variable classical systems, the entropy associated to the classical degrees of freedom is strictly speaking a differential entropy, and thus only well-defined for certain subsets of states [203]. In practice, we shall typically only use the classical-quantum *relative entropy*, which may be defined between two classical states as

$$S[\varrho(z)||\sigma(z)] = \int dz \mathrm{tr}\varrho(z)\big[\ln\ \varrho(z) - \ln\ \sigma(z)\big]. \tag{5.2.2}$$

This is a divergence measure that acts as a hybrid between the quantum relative entropy and classical Kullback-Liebler divergence, and is well-defined for arbitrary bounded classical-quantum states. An important property of the classical-quantum relative entropy is that it is monotonic under the action of a completely-positive and linear map $\Lambda$ i.e. that

$$S[\Lambda(\varrho)||\Lambda(\sigma)] \leq S[\varrho||\sigma]. \tag{5.2.3}$$

Known in information theory as the data processing inequality [203], the fact that this holds even for the classical-quantum states and maps that we have presented here follows from a straightforward embedding of the classical-quantum system into a fully quantum system – see e.g. [76].

Alongside entropy, the other key ingredient of a theory of thermodynamics is that of energy. To define a notion of energy in the combined classical-quantum system, we assume the existence of a Hermitian operator valued function of phase-space that we refer to as the classical-quantum Hamiltonian, and denote by $H(z)$. While assigning a Hamiltonian to open systems may be

subject to some ambiguity [204–206], we leave any subtleties arising from this for future study. The classical-quantum Hamiltonian determines the average energy $E$ in the classical-quantum system by the formula

$$E = \int dz \mathrm{tr}[H(z)\varrho(z)] \tag{5.2.4}$$

which we write in the notation of (2.10) as $E = \langle\langle H(z)\rangle\rangle$. Rather than taking the classical-quantum Hamiltonian to directly determine the form of dynamics in the system, as with the standard mean-field or quantum-classical Liouville approaches, $H(z)$ here simply determines the energetics of the combined classical-quantum system. Assigning energy to both the individual classical and quantum systems, as well as to their interactions, $H(z)$ can be generically decomposed as

$$H(z) = H^C(z)\mathbb{1} + H^Q + H^I(z) \tag{5.2.5}$$

where the classical Hamiltonian $H^C(z)$ is a real-valued function, $\mathbb{1}$ is the identity operator on the Hilbert space, the quantum Hamiltonian $H^Q$ is a Hermitian valued operator independent of phase space, and the interaction Hamiltonian $H^I(z)$ is traceless. The eigenbasis of the classical-quantum Hamiltonian as a function of phase space is commonly referred to as the adiabatic basis [63] and will be denoted as

$$H(z)|n(z)\rangle = \epsilon_n(z)|n(z)\rangle \tag{5.2.6}$$

where $\epsilon_n(z)$ are the corresponding eigenvalues, giving the energy for a given energy level and classical configuration.

The concepts of entropy and energy naturally lead to a notion of a classical-quantum thermal state. If a given classical-quantum system has a known average energy $E$, then applying the maximum entropy principle [202] with the constraint $\langle\langle H(z)\rangle\rangle = E$ one finds that the classical-quantum thermal state $\pi$ is given by

$$\pi(z) = \frac{e^{-\beta H(z)}}{\mathcal{Z}}. \tag{5.2.7}$$

Here $\mathcal{Z}$ is given by

$$\mathcal{Z} = \int dz \mathrm{tr}[e^{-\beta H(z)}]. \tag{5.2.8}$$

which together with $H(z) = H(z)^\dagger$ ensures that $\pi(z)$ defines a valid classical-quantum state, while $\beta$ defines the inverse temperature. It is straightforward to see that when $H(z)$ reduces to

$H^C(z)\mathbb{1}$ or $H^Q$, the above thermal state definition reduces to standard classical and quantum thermal states.

### 5.2.2 Heat exchange and entropy production

In thermodynamic systems, an important role is played by the environment, which allows the system to gain or dissipate heat and become more or less ordered. While we shall remain agnostic about the nature of the environment to the classical-quantum system, other than assuming that it can always be assigned a fixed temperature and that it is sufficiently large that the dynamics of the classical-quantum system are well-approximated as Markovian, we will need to define a number of quantities that implicitly rely on the ability of the system to exchange energy and information with its surroundings.

The first such quantity that we shall define is the heat exchanged with the environment. Taking the initial time to be $t_i$, we define the average heat exchanged between then and time $t$ on the level of the ensemble as

$$\mathcal{Q}(t) = \langle\langle H(z)\rangle\rangle(t) - \langle\langle H(z)\rangle\rangle(t_i). \tag{5.2.9}$$

At the same time, on the level of trajectories, we define the stochastic heat exchanged via the difference in trajectory expectation values of the classical-quantum Hamiltonian

$$Q_t = \langle H(z)\rangle_t - \langle H(z)\rangle_{t_i}. \tag{5.2.10}$$

When the quantum state is pure, this amounts to computing the change in $\langle\psi|H(z)|\psi\rangle$ along a trajectory. These ensemble and trajectory definitions of heat are related by taking the expectation value over trajectories

$$\mathcal{Q}(t) = \mathbb{E}[Q_t], \tag{5.2.11}$$

which follows from (2.11). We thus see that this framework allows one to study both the average transfer of heat with the environment, as well as study the stochastic fluctuations of this quantity.

The second quantity that we shall define is the entropy production in a classical-quantum system. A central quantity in non-equilibrium thermodynamics, entropy production provides

a measure of the irreversibility of a process, and is defined by balancing the rate of change of the system entropy with outgoing currents. Using the above definitions of entropy and heat for the classical-quantum system, we may define entropy production $\Sigma$ in the classical-quantum context as

$$\Sigma(t) = \Delta S(t) - \beta \mathcal{Q}(t) \tag{5.2.12}$$

where here $\Delta S(t)$ denotes the change in the system entropy from time $t_i$ to time $t$. The rate of change of this quantity is denoted $\dot{\Sigma}$ and is known as the entropy production rate, taking the form

$$\dot{\Sigma}(t) = \dot{S}(t) - \beta \dot{\mathcal{Q}}(t), \tag{5.2.13}$$

where here $\dot{\mathcal{Q}}$ and $\dot{S}$ to denote the rate of change in time of the heat exchange and entropy respectively.

### 5.2.3 Thermal state preservation and the second law

We first establish a basic requirement to make of any classical-quantum dynamics that is consistent with thermodynamics. If two systems at the same temperature are put into contact, one expects, on average, that no energy flows between the two. In our case, this means that the state of a classical-quantum system in contact with a thermal environment at inverse temperature $\beta$ should not change if the initial state of the classical-quantum system is a thermal state at the same inverse temperature. Written in terms of a generic classical-quantum generator $\mathcal{L}$ as introduced in (2.12), this leads us to the basic assumption that

$$\mathcal{L}(\pi) = 0, \tag{5.2.14}$$

i.e. that the thermal state is preserved in time by the dynamics. A typical assumption in both classical and quantum non-equilibrium thermodynamics [188, 160], and sometimes discussed in the classical-quantum context [183, 202, 185], dynamics satisfying Eq. (5.2.14) represent a subset of generic classical-quantum dynamics which have a well-defined fixed point.

The preservation of the thermal state has an important consequence for classical-quantum dynamics that also satisfy the basic properties of complete-positivity and linearity. We start by

noting that it is well known from open quantum system theory any linear, completely positive dynamics with a fixed point is sufficient to guarantee a non-negative entropy production rate consistent with the second law of thermodynamics [207–209, 189]. To see that the same holds in the classical-quantum case, we first rewrite the entropy production rate in terms of the classical-quantum relative entropy as

$$\dot{\Sigma}(t) = -\frac{\partial}{\partial t} S[\varrho(z,t)||\pi(z)], \tag{5.2.15}$$

which follows from the definitions of the classical-quantum thermal state $\pi$ and heat transfer $\mathcal{Q}$. As anticipated from both classical and quantum thermodynamics, we see that the classical-quantum entropy production rate quantifies how the distinguishability between the classical-quantum state $\varrho(z)$ and the thermal state $\pi$ changes over time. Using the fact that the dynamics satisfies $\mathcal{L}(\pi) = 0$, this may be rewritten as

$$\dot{\Sigma}(t) = \lim_{\delta t \to 0} \frac{S[\varrho(z,t)||\pi(z)] - S[e^{\delta t \mathcal{L}}\varrho(z,t)||e^{\delta t \mathcal{L}}\pi(z)]}{\delta t}. \tag{5.2.16}$$

The entropy production rate thus depends on the difference of two relative entropies, differing by the application of the exponential map of the classical-quantum generator $\mathcal{L}$. Provided the generator $\mathcal{L}$ is completely-positive and linear, the right hand side is therefore necessarily positive by the data-processing inequality (5.2.3), and thus we see that the classical-quantum entropy production rate is necessarily positive

$$\dot{\Sigma}(t) \geq 0. \tag{5.2.17}$$

This provides a general formulation of the second law in a classical-quantum system, with the entropy production rate $\dot{\Sigma}(t)$ quantifying the irreversibility of the dynamics. Integrating this over time, and comparing to Eq. (5.2.12), we can rewrite this as a Clausius inequality

$$\Delta S(t) \geq \beta \mathcal{Q}(t), \tag{5.2.18}$$

recovering the standard formulation of the second law as bounding the change in the system entropy by the heat transfers into an external environment.

We thus see that classical-quantum dynamics that are simultaneously linear, completely-positive and preserve the thermal state are necessarily consistent with the second law of thermodynamics – we shall refer to such dynamics as *thermodynamically consistent*. Although such

terminology may seem hasty, given that we have only shown agreement with one of the laws of thermodynamics, it turns out that in practice this is the most important one to achieve. To arrive at a first law of thermodynamics for our dynamics, one allows for a time-dependent classical-quantum Hamiltonian, which means that part of the change in the ensemble expectation value of classical-quantum Hamiltonian also is due to the deterministic changing of parameters in the system, which gives the change in energy two distinct components, identifiable as work and heat [188]. The remaining laws, i.e. the zeroth and third, are then understood as arising from particular applications of dynamics that are consistent with these two laws see e.g. [188] or [210].

Finally, is important to emphasise that the same argument of thermodynamic consistency cannot be made for dynamics failing the basic requirements of complete-positivity or linearity. In the case of the quantum-classical Liouville equation (4.2.9), since initially positive states can evolve to negative states, the relative entropy will not increase monotonically under the evolution, and indeed will generically not be well-defined. Similarly, for the mean-field dynamics of Eqs. (1.1) to (1.3), the failure of the evolution to generate a linear map on the initial classical-quantum state means that it fails a basic assumption needed to apply the data processing inequality. Furthermore, the non-linearity at the level of the unravelling leads to non-linear evolution of the quantum state, known to be in violation of the second law of thermodynamics [179]. We thus see that complete-positivity and linearity are natural assumptions to make on classical-quantum dynamics, purely on thermodynamic grounds.

## 5.3 Thermal state preserving classical-quantum dynamics

In this section we introduce two general classes of completely-positive and linear classical-quantum dynamics that preserve the classical-quantum thermal state. We show that these dynamics can be understood as generalisations of the standard overdamped and underdamped dynamics of a classical system to the case where it is interacting in the limit of a trivial quantum system. In the high temperature limit, the dynamics takes the form of a completely-positive completion of the standard forms of coupling between classical and quantum systems.

### 5.3.1 Overview of the problem

In the previous section, we saw that if a completely-positive and linear classical-quantum dynamics preserves the thermal state in time, the system has a well-defined second law of thermodynamics. Since the general form of classical-quantum dynamics that is Markovian and continuous is known to take the form of Eq. (2.13), the problem amounts to finding matrices $D$ and operators $L_\alpha$ and $\bar{H}$ such that $\mathcal{L}(\pi) = 0$. For such dynamics to be useful, it must be applicable to arbitrary $\pi(z)$ i.e. arbitrary classical-quantum Hamiltonians $H(z)$, rather than those satisfying special properties e.g. being simultaneously diagonaliseable everywhere in phase space in a fixed basis.

In contrast to the purely classical or quantum cases, there are a number of features that make even finding an example of such a dynamics extremely challenging. Firstly, the generator $\mathcal{L}$ includes both classical and quantum dissipative processes as well as coupling between the two systems via the unitary and back-reaction parts of the dynamics – each of these terms or combinations of them must vanish when applied to $\pi$ in order to preserve the thermal state. Secondly, the fact that the thermal state is an operator-valued function of phase space means that the diffusive and back-reaction parts of the dynamics involve derivatives of $\pi(z)$ that do not in general commute with $\pi(z)$ itself. This means that the operators $L_\alpha$ and $\bar{H}$ must necessarily be dependent on phase space and in general non-diagonaliseable in the same basis as $\pi(z)$. Finally, any dynamics must also simultaneously satisfy the two non-trivial positivity constraints (2.14) and (2.15).

Surprisingly, we demonstrate in this section that such a dynamics may indeed be found. Moreover, the dynamics satisfies a number of desirable properties, such as reducing to the correct classical limit, preserving the purity of quantum states conditioned on classical trajectories, and recovering a consistent form of standard approaches to classical-quantum coupling in the high temperature $\beta \to 0$ limit. The key feature that allows us to construct such dynamics is the identification of two kinds of operators defined in terms of the thermal state $\pi$, which ultimately will be seen in Sec. 5.6 to be related to the general conditions for a classical-quantum dynamics to satisfy detailed balance.

### 5.3.2 L and M operators

To construct classical-quantum dynamics that preserve the classical-quantum thermal state, i.e. $\mathcal{L}(\pi) = 0$, we first introduce two classes of operators. The first of these is a phase-space dependent operator, defined for each classical coordinate $z$ as

$$L_z = -\frac{2}{\beta}\frac{\partial \pi^{\frac{1}{2}}}{\partial z}\pi^{-\frac{1}{2}}. \tag{5.3.1}$$

These operators act to both determine the back-reaction and decoherence in the dynamics we consider. Although these operators are not in general Hermitian, they each satisfy the important property

$$L_z \pi^{1/2} = \pi^{1/2} L_z^\dagger, \tag{5.3.2}$$

which will be frequently used to verify thermodynamic properties of the resulting dynamics.

The second important class of operators to introduce are phase-space dependent operators defined for each ordered pair of classical coordinates (x,y) as

$$M_{xy} = \frac{i\hbar}{2}\int_0^\infty e^{-s\pi^{\frac{1}{2}}}[L_x^\dagger L_y, \pi^{\frac{1}{2}}]e^{-s\pi^{\frac{1}{2}}}\,ds. \tag{5.3.3}$$

This operator is Hermitian when $x = y$, and controls part of the unitary dynamics of the quantum system. Since $M_{xy}$ takes the form of a solution to a Lyapunov equation, it is equivalently defined by the equation

$$M_{xy}\pi^{\frac{1}{2}} + \pi^{\frac{1}{2}} M_{xy} = \frac{i\hbar}{2}[L_x^\dagger L_y, \pi^{\frac{1}{2}}]. \tag{5.3.4}$$

As with (5.3.2), this implicit definition of $M_{xy}$ will useful to prove properties of these dynamics.

While both $L_z$ and $M_{xy}$ are defined in terms of the square root of $\pi$, there are two useful relations that relate these operators to $\pi$ itself. The first of these is

$$L_z\pi + \pi L_z^\dagger = -\frac{2}{\beta}\frac{\partial \pi}{\partial z}, \tag{5.3.5}$$

follows directly from the definition (5.3.1) while the second

$$-\frac{i}{\hbar}[M_{xy}, \pi] = -L_x \pi L_y^\dagger + \frac{1}{2}\{L_x^\dagger L_y, \pi^{\frac{1}{2}}\}_+, \tag{5.3.6}$$

follows from (5.3.2) and (5.3.4). These two relations are important for proving that the dynamics that we construct satisfies $\mathcal{L}(\pi) = 0$.

Finally, it is important to recognise a particular limiting form of these operators. To see how these arise, we first note that we may use the definition of the derivative of the exponential map [165] to rewrite $L_z$ as

$$L_z = \frac{e^{\mathrm{ad}_{\frac{-\beta H}{2}}} - 1}{\mathrm{ad}_{\frac{-\beta H}{2}}} \left( \frac{\partial H}{\partial z} \right) \tag{5.3.7}$$

where $\mathrm{ad}_A B = [A, B]$ and the above fraction is interpreted as the series

$$\frac{e^{\mathrm{ad}_{\frac{-\beta H}{2}}} - 1}{\mathrm{ad}_{\frac{-\beta H}{2}}} = \sum_{n=0}^{\infty} \frac{1}{(n+1)!} \mathrm{ad}^n_{\frac{-\beta H}{2}}. \tag{5.3.8}$$

For sufficiently simple commutation relations, this series may be computed explicitly even when the series does not truncate. However, it is useful to note that in two cases, the series truncates to zeroth order. The first case occurs for a special class of Hamiltonians that satsify the property that $H(z)$ and $H(z')$ commute for all $z$, $z' \in \mathcal{M}$, which we refer to as *self-commuting*. The second case occurs in the high temperature $\beta \to 0$ limit of the dynamics for arbitrary $H(z)$. In both cases, all of the terms in the series with $n > 0$ vanish, with $L_z$ reducing to $\partial_z H$. For our other class of operators, $M_{xy}$, we note that (5.3.2) implies that the right-hand side of (5.3.4) vanishes when $L_x$ and $L_y$ are Hermitian. Since the above form of $L_z$ is Hermitian for any $z$, it must also be the case that $M_{xy} = 0$. In summary, we thus arrive at

$$L_z = \frac{\partial H}{\partial z} \qquad\qquad M_{xy} = 0 \tag{5.3.9}$$

$$\text{if } H \text{ is self-commuting or } \beta \to 0.$$

These limiting forms of the $L_z$ and $M_{xy}$ operators are useful for studying dynamics of simple models, such as that given in Section 5.4, as well as studying the classical and high-temperature limits of the dynamics we will present.

### 5.3.3 Overdamped dynamics

The first class of dynamics we introduce is an overdamped dynamics. Taking a single one-dimensional classical degree of freedom $x$, with mobility given by $\mu$, we describe its interactions

with a quantum system either via the following master equation

$$\begin{aligned}\frac{\partial \varrho}{\partial t} =& -\frac{i}{\hbar}[H + \frac{\mu\beta}{8}M_{xx}, \varrho] + \frac{\mu}{2}\frac{\partial}{\partial x}(L_x\varrho + \varrho L_x^\dagger) \\ &+ \frac{\mu}{\beta}\frac{\partial^2 \varrho}{\partial x^2} + \frac{\mu\beta}{8}(L_x\varrho L_x^\dagger - \frac{1}{2}\{L_x^\dagger L_x, \varrho\}_+),\end{aligned} \tag{5.3.10}$$

or via a stochastic unravelling as

$$dx_t = -\frac{\mu}{2}\langle L_x + L_x^\dagger\rangle dt + \sqrt{\frac{2\mu}{\beta}}dW_t \tag{5.3.11}$$

$$\begin{aligned}d\rho_t =& -\frac{i}{\hbar}[H + \frac{\mu\beta}{8}M_{xx}, \rho_t]dt \\ &+ \frac{\mu\beta}{8}(L_x\rho_t L_x^\dagger - \frac{1}{2}\{L_x^\dagger L_x, \rho_t\}_+)dt \\ &- \sqrt{\frac{\mu\beta}{8}}(L_x\rho_t + \rho_t L_x^\dagger - \langle L_x + L_x^\dagger\rangle\rho_t)dW_t,\end{aligned} \tag{5.3.12}$$

where here $dW_t$ defines the increment of a one dimensional Wiener process. This dynamics describes how an overdamped classical system subject to thermal noise is affected by the back-reaction from a quantum system, as well as how this interaction leads to noise in the otherwise unitary evolution of the quantum system.

While the above dynamics is ultimately postulated, it is straightforward to check that it satisfies a number of desirable properties. Firstly, the dynamics is completely-positive and linear at the level of the master equation. Secondly, the dynamics is thermodynamically consistent i.e. the thermal state is preserved in time. Additionally, the dynamics saturates the decoherence-diffusion trade-off, meaning that the quantum state of the system remains pure conditioned on the classical trajectory. Finally, the model correctly reproduces the standard overdamped classical dynamics in the classical limit.

To see how these properties arise, we first compare the form of (5.3.10) to the general form of completely-positive generator given in (2.13). Doing so, we see that it is of the same form, guaranteeing that the dynamics is norm-preserving and linear, with parameters given

$$\begin{aligned}\bar{H} = \frac{H}{\hbar} + \frac{\mu\beta}{8\hbar}M_{xx} \qquad & L = L_x \\ D_0 = \frac{\mu\beta}{8} \qquad D_1 = -\frac{\mu}{2} \qquad & D_2 = \frac{2\mu}{\beta}.\end{aligned} \tag{5.3.13}$$

In order for the dynamics to be completely-positive, the two positivity constraints (2.14) and (2.15) must also be satisfied. The second of these trivially holds since $D_2$ has an inverse, and

multiplying the scalar $D$ coefficients we see that (2.14) also holds. Since here $D_0 = D_1^2/D_2$, we see that the dynamics saturates the decoherence-diffusion trade-off, meaning that the dynamics has minimal decoherence and keeps intially pure quantum states pure, as shown in Section 2.5.

It is also straightforward to see that this dynamics preserves the thermal state i.e. satisfies $\mathcal{L}(\pi) = 0$. To do so, one must evaluate the right hand side of (5.3.10) with $\varrho = \pi$ and check that the result is zero. Doing so, one sees using (5.3.5) that the back-reaction and diffusion terms cancel, and using (5.3.6) that the $M_{xx}$ unitary term cancels with the decoherence term. Since the rest of the unitary term vanishes, due to $H$ commuting with $\pi$, we see that indeed $\mathcal{L}(\pi) = 0$ for this dynamics.

To see that this dynamics reduces to the standard dynamics in the classical limit, we consider the case where the classical-quantum Hamiltonian is proportional to the identity operator, $H(x) = H^C(x)\mathbb{1}$. Since $H(z)$ here is self-commuting, we may use the simplified forms of $L_x$ and $M_{xx}$ given in (5.3.9). Substituting these into the above dynamics, and using the fact that the operator $H$ is proportional to the identity operator, we find that the above dynamics reduces to

$$\frac{\partial \varrho}{\partial t} = \mu \frac{\partial}{\partial x}\left(\frac{\partial H}{\partial x}\varrho\right) + \frac{\mu}{\beta}\frac{\partial^2 \varrho}{\partial x^2} \tag{5.3.14}$$

in the master equation picture or

$$dx_t = -\mu \frac{\partial H}{\partial x} + \sqrt{\frac{2\mu}{\beta}} dW_t \tag{5.3.15}$$

in the unravelling picture. We thus see that our dynamics reduces to that of a single overdamped particle in a potential, with a diffusion coefficient that satisfies the Einstein relation.

As a final remark, we note that the above model may be generalised in a number of ways. Firstly, we show in Appendix J that one may straightforwardly use the $L_z$ and $M_{xy}$ operators to construct a dynamics that saturates the decoherence-diffusion trade-off for $n$ overdamped particles, as well as allowing for $x$-dependent correlations in the noise. Secondly, one may also add additional decoherence to the system, such that the decoherence-diffusion relation is not saturated. While a general method of doing so is discussed in 5.6, we may straightforwardly add additional decoherence in this model by adding in an additional dissipator term with Lindblad operators $\tilde{L} = L_x$ and decoherence coefficient $\tilde{D}_0$, which will also preserve the thermal

state provided an additional $\tilde{D}_0 M_{xx}$ term is added to the generator of the unitary part of the dynamics. We thus see that in general that the decoherence in the $L_x$ basis is given

$$D_0 \geq \frac{\mu\beta}{8}, \tag{5.3.16}$$

which provides a *lower bound* on the amount of decoherence in a quantum system interacting with an overdamped classical system, that arises by assuming that the dynamics is completely-positive and that the Einstein relation holds.

### 5.3.4 Underdamped dynamics

The second class of dynamics we will introduce is an underdamped dynamics. Taking the position of the classical degree of freedom to be $q$ and its conjugate momentum $p$, we make the standard assumption that the only dependence of the Hamiltonian on the classical momentum $p$ is a classical kinetic term $(p^2/2m)\mathbb{1}$. Choosing $\gamma$ to denote the friction coefficient, the dynamics takes the form

$$\begin{aligned}\frac{\partial\varrho}{\partial t} =& -\frac{i}{\hbar}[H + \frac{\beta}{8\gamma}M_{qq}, \varrho] \\ &+ \frac{1}{2}\frac{\partial}{\partial p}(L_q\varrho + \varrho L_q^\dagger) - \frac{p}{m}\frac{\partial\varrho}{\partial q} \\ &+ \gamma\frac{\partial}{\partial p}(\frac{p}{m}\varrho) + \frac{\gamma}{\beta}\frac{\partial^2\varrho}{\partial p^2} \\ &+ \frac{\beta}{8\gamma}(L_q\varrho L_q^\dagger - \frac{1}{2}\{L_q^\dagger L_q, \varrho\}_+),\end{aligned} \tag{5.3.17}$$

which for initially pure states may also be unravelled as

$$dq = \frac{p}{m}dt \tag{5.3.18}$$

$$dp = -\frac{1}{2}\langle L_q + L_q^\dagger\rangle dt - \frac{\gamma}{m}p dt + \sqrt{\frac{2\gamma}{\beta}}dW_t \tag{5.3.19}$$

$$\begin{aligned}d|\psi\rangle_t =& -\frac{i}{\hbar}(H + \frac{\beta}{8\gamma}M_{qq})|\psi\rangle dt \\ &- \frac{\beta}{16\gamma}(L_q^\dagger L_q - 2\langle L_q^\dagger\rangle L_q + \langle L_q^\dagger\rangle\langle L_q\rangle)|\psi\rangle dt \\ &- \sqrt{\frac{\beta}{8\gamma}}(L_q - \langle L_q\rangle)|\psi\rangle dW_t.\end{aligned} \tag{5.3.20}$$

The above describe in the ensemble and trajectory pictures how a classical particle subject to thermal noise and friction responds to a quantum potential, as well as how the quantum system sourcing this potential is affected by the decoherence that arises from this interaction.

As in the overdamped case, this underdamped dynamics satisfies a natural set of properties: (1) complete-positivity and linearity; (2) preserves the classical-quantum thermal state; (3) preserves pure quantum states when conditioned on the classical trajectory; and (4) recovers the correct classical limit.

Looking first at the properties of complete-positivity and pure-state preservation, we compare the master equation dynamics to (2.13) to find that the dynamics is characterised by

$$\begin{aligned} \bar{H} = \frac{H}{\hbar} + \frac{\beta}{8\gamma} M_{xx} \qquad L = L_q \qquad D_1^C = \frac{p}{m} \begin{pmatrix} 1 \\ -\gamma \end{pmatrix} \\ D_0 = \frac{\beta}{8\gamma} \qquad D_1 = \frac{1}{2} \begin{pmatrix} 0 \\ -1 \end{pmatrix} \qquad D_2 = \begin{pmatrix} 0 & 0 \\ 0 & 2\gamma/\beta \end{pmatrix}. \end{aligned} \tag{5.3.21}$$

Computing the pseudoinverse of $D_2$ and multiplying the $D$ matrices, we see that the dynamics satisfies (2.14), (2.15) and (2.18), ensuring that the dynamics both preserves the positivity of the classical-quantum state, and the purity of any initial state $\rho_t$ that starts off in a pure state. This latter property ensures that the unravelling given in Eqs. (5.3.18) to (5.3.20) indeed is equivalent to the master equation (5.3.10).

To see that the dynamics preserves the thermal state, we again replace $\varrho$ with $\pi$ on the right hand side of the master equation and check that all the terms cancel. In particular, we see here that the combination of the first and fourth lines of (5.3.17) vanish due to (5.3.6) and $[H, \pi] = 0$, while the second and third lines each vanish independently due to the inclusion of $(p^2/2m)\mathbb{1}$ in $H$ and the identity (5.3.5), ensuring that the dynamics preserve arbitrary thermal states $\pi$.

Finally, we check that the dynamics correctly reduces in the classical limit to the standard underdamped dynamics. Taking again the simplified forms appearing in (5.3.9) and taking $H$ proportional to the identity, we find the dynamics reduce in the master equation and unravelling

pictures to

$$\frac{\partial \varrho}{\partial t} = \{H, \varrho\} + \gamma \frac{\partial}{\partial p}(\frac{p}{m}\varrho) + \frac{\gamma}{\beta}\frac{\partial^2 \varrho}{\partial p^2} \tag{5.3.22}$$

and

$$dq = \frac{p}{m}dt \tag{5.3.23}$$

$$dp = -\frac{\partial H}{\partial q}dt - \frac{\gamma}{m}pdt + \sqrt{\frac{2\gamma}{\beta}}dW_t \tag{5.3.24}$$

as expected, describing the standard underdamped dynamics of a diffusing particle satisfying the Einstein relation.

As in the case of the overdamped dynamics, this dynamics may be generalised to include a range of additional phenomena not captured in the above model. Firstly, it straightforward to generalise the above dynamics to multiple particles and dimensions, by including an $L_q$ operator for each degree of freedom and direction and replacing each $q$ and $p$ with a sum over $q_i$ and $p_i$. Secondly, in the above, we assume that $H(q,p)$ contains no coupling between the momentum $p$ and the quantum degrees of freedom, which guarantees that the only necessary noise in the system is in $p$ directly. However, one may also write down models with noise in $q$ and $p$ such that arbitrary Hamiltonians $H(q,p)$ may be considered, and we provide such an example in Appendix J. Finally, we note that as in the overdamped case, one may include excess decoherence in the above model. Aside from using the general formalism given in Section 5.6, it is simple to see that one may include excess decoherence in the $L_q$ basis by replacing the $\beta/(8\gamma)$ coefficient of $M_{qq}$ and the quantum disspator with a generic $D_0$. In this case, we see that the decoherence rate in the $L_q$ basis must necessarily obey

$$D_0 \geq \frac{\beta}{8\gamma}, \tag{5.3.25}$$

which as in the overdamped case, provides a lower bound on the decoherence of a quantum system interacting with a classical system that obeys the Einstein relation.

### 5.3.5 The $\beta \to 0$ limit

Up to this point, the overdamped and underdamped dynamics we have provided have been written down as examples of completely-positive and thermal-state preserving dynamics, which

have minimal decoherence and are consistent with the classical limit. However, it turns out that our dynamics can also be understood as a completely-positive and linear version of the standard approaches to coupling classical and quantum systems, namely the mean-field dynamics and the quantum-classical Liouville equation, that preserves the classical-quantum thermal state even at low temperatures.

To see this, we first consider the high temperature, $\beta \to 0$, limit of the underdamped dynamics in the master equation representation. One may do so using the limiting forms of the operators $L_z$ and $M_{xy}$ provided in (5.3.9), which we can substitute into our dynamics to find our dynamics to lowest order in $\beta$ as

$$\begin{aligned}\frac{\partial \varrho}{\partial t} =& -\frac{i}{\hbar}[H,\varrho] + \frac{1}{2}\big(\{H,\varrho\} - \{\varrho,H\}\big) \\ &+ \gamma\frac{\partial}{\partial p}(\frac{p}{m}\varrho) + \frac{\gamma}{\beta}\frac{\partial^2 \varrho}{\partial p^2} \\ &+ \frac{\beta}{8\gamma}\left(\frac{\partial H}{\partial q}\hat{\varrho}\frac{\partial H}{\partial q} - \frac{1}{2}\{\frac{\partial H}{\partial q}^2, \hat{\varrho}\}_+\right),\end{aligned} \tag{5.3.26}$$

where we have rewritten two of the drift terms using the Poisson bracket. It is straightforward to see that the top line exactly coincides with the quantum-classical Liouville equation, given previously in (4.2.9). Since the completely-positivity of the dynamics is unchanged by the limit of the operators, we can understand the additional diffusion and decoherence terms as providing the minimal additional decoherence and diffusion required to supplement the quantum-classical Liouville equation to be completely-positive, as first noted was possible in [25]. However, while the dynamics of (5.3.26) satisfies complete-positivty and linearity, the thermal state $\pi$ will only be preserved approximately at high temperatures. The full underdamped dynamics given in (5.3.17) may therefore be understood as a completely-positive generalisation of the classical-quantum Liouville equation, that *additionally* satisfies the important requirement of preserving the classical-quantum thermal state $\pi$ for arbitrary inverse temperature $\beta$.

Moving now to the trajectory representation, we find that a similar conclusion may be found in the $\beta \to 0$ limit of the stochastic unravelling of the underdamped dynamics. Using again the limiting forms of operators given in (5.3.9), we find that the unravelling equations (5.3.18) to (5.3.20) take the form

$$dq = \frac{p}{m}dt \tag{5.3.27}$$

$$dp = -\langle\frac{\partial H}{\partial q}\rangle dt - \frac{\gamma}{m}pdt + \sqrt{\frac{2\gamma}{\beta}}dW_t \tag{5.3.28}$$

$$\begin{aligned} d|\psi\rangle_t = &-\frac{i}{\hbar}H|\psi\rangle dt \\ &-\frac{\beta}{16\gamma}\left(\frac{\partial H}{\partial q} - \langle\frac{\partial H}{\partial q}\rangle\right)^2|\psi\rangle dt \\ &-\sqrt{\frac{\beta}{8\gamma}}(\frac{\partial H}{\partial q} - \langle\frac{\partial H}{\partial q}\rangle)|\psi\rangle dW_t. \end{aligned} \tag{5.3.29}$$

Comparing to (1.1), we see that this dynamics takes the form of the mean field dynamics, with additional temperature and friction dependent terms in the classical momentum and quantum state evolution. Previously written down as a "healed version" of the mean field equations [26, 1], we note again that since the limit occurs at the level of the operators, this dynamics is necessarily still linear at the level of the classical-quantum state. However, as an unravelling of (5.3.26), it will only preserve the thermal state approximately at sufficiently high temperatures. We thus can understand the full unravelling dynamics (5.3.18) to (5.3.20) as a generalisation of the mean-field equations that satisfies both linearity and preserves the thermal state of the combined classical-quantum system.

## 5.4 Model I

In this section we introduce a simple toy model consisting of a classical particle that is over-damped (i.e. described by a single degree of freedom) that interacts with a quantum two-level system. We will use this analytically solvable model to illustrate both the entropy production during the measurement of a quantum two-level system, and how a quantum gate may be performed by allowing a classical control system to relax to equilibrium.

### 5.4.1 Set-up

In what follows, we consider a one-dimensional classical degree of freedom $x$, coupled to a quantum two-level system. In principle, this degree of freedom could be interpreted in a number of different ways, such as a classical signal arising from a continuous measurement of a two level system, or a current observed in a circuit coupled to a qubit – but we shall take the basic

picture and imagine that $x$ simply describes the position of an overdamped classical degree of freedom. Taking $\hat{Z}$ to be the standard Pauli spin-$Z$ operator, we will consider a classical-quantum Hamiltonian of the form

$$\hat{H}(x) = \lambda(x\hat{\mathbb{1}} - l\hat{Z})^2. \tag{5.4.1}$$

We may understand this Hamiltonian as a classical quadratic potential that depends on whether the quantum system is in the $|0\rangle$ or $|1\rangle$ state. The strength of the potential is controlled by the parameter $\lambda$, while the minimum of the potential is either $l$ or $-l$ depending on whether the quantum state is $|0\rangle$ or $|1\rangle$ respectively.

Assuming that this classical-quantum system is in contact with a thermal environment, the thermal state corresponding to this system is given

$$\hat{\pi}(x) = \frac{1}{\mathcal{Z}} e^{-\beta \hat{H}(x)}, \tag{5.4.2}$$

where here $\mathcal{Z}$ is given by

$$\mathcal{Z} = 2\sqrt{\frac{\pi}{\beta\lambda}}, \tag{5.4.3}$$

which ensures that $\hat{\pi}(x)$ is normalised.

### 5.4.2 Analytic solution

Since the Hamiltonian we study in this case takes a simple form, it turns out that the dynamics may be analytically solved in the master equation representation. Our first step is to compute the $\hat{L}_x$ and $\hat{M}_{xx}$ operators for this model. Since the classical-quantum Hamiltonian $\hat{H}(x)$ is self-commuting, i.e. $[\hat{H}(x), \hat{H}(x')] = 0$ for all $x, x'$, we may use the limiting forms provided in (5.3.9). Here, the $\hat{L}_x$ operator may be computed by simply taking the derivative of $\hat{H}(x)$ with respect to $x$, while the $\hat{M}_{xx}$ vanishes. The dynamics of this model is thus summarised by

$$\hat{L}_x = 2\lambda(x\hat{\mathbb{1}} - l\hat{Z}), \qquad \hat{M}_{xx} = 0. \tag{5.4.4}$$

Plugging these operator definitions into (5.3.10) and expanding the classical-quantum state in the eigenbasis of $\hat{Z}$ we obtain three independent equations,

$$\begin{aligned}
\frac{\partial \varrho_{00}}{\partial t} &= \mu \frac{\partial}{\partial x}(2\lambda(x-l)\varrho_{00}) + \frac{\mu}{\beta}\frac{\partial^2 \varrho_{00}}{\partial x^2} \\
\frac{\partial \varrho_{01}}{\partial t} &= \mu \frac{\partial}{\partial x}(2\lambda x \varrho_{01}) + \frac{\mu}{\beta}\frac{\partial^2 \varrho_{01}}{\partial x^2} + (\frac{i}{\hbar}4\lambda x l - \mu\lambda^2 l^2 \beta)\varrho_{01} \\
\frac{\partial \varrho_{11}}{\partial t} &= \mu \frac{\partial}{\partial x}(2\lambda(x+l)\varrho_{11}) + \frac{\mu}{\beta}\frac{\partial^2 \varrho_{11}}{\partial x^2}
\end{aligned} \tag{5.4.5}$$

where we leave out the dynamics of $\varrho_{10}$ since the solution is given by $\varrho_{10}(z,t) = \varrho_{01}^*(z,t)$. From the above dynamics, we can see explicitly that each component of the classical-quantum state evolves under different dynamics. The $\varrho_{00}$ component, corresponding to the positive eigenvalue of $\hat{Z}$, experiences diffusion with a restoring force to the point $x = l$, while the $\varrho_{11}$ component experiences diffusion instead with a restoring force to the point $x = -l$. The component corresponding to coherence, given by $\varrho_{01}$, experiences diffusion with a restoring force given by the average value of the two i.e. to the point $z = 0$. At the same time, the coherence simultaneously picks up a complex phase and is damped by a term corresponding to the decoherence in the system, with larger damping as any of $\mu$, $\beta$, $\lambda$ or $l$ increase.

Assuming that initial state of the quantum system is known to be in the state $\hat{\rho}_0$ with components $\rho_{00}, \rho_{01}, \rho_{10}$ and $\rho_{11}$, and that the classical system starts at the point $x_0$, the combined classical-quantum state at $t = 0$ is given $\hat{\varrho}(x,0) = \hat{\rho}_0 \delta(x - x_0)$. It is straightforward to check that with this initial condition, the above set of equations have an analytic solution of the form

$$\varrho_{00}(x,t) = \rho_{00}\sqrt{\frac{\beta\lambda}{\pi(1-e^{-4\mu\lambda t})}}\exp\big[-\frac{\beta\lambda(x - l(1-e^{-2\mu\lambda t}) - x_0 e^{-2\mu\lambda t})^2}{1-e^{-4\mu\lambda t}}\big] \tag{5.4.6}$$

$$\begin{aligned}
\varrho_{01}(x,t) =& \rho_{01}\sqrt{\frac{\beta\lambda}{\pi(1-e^{-4\mu\lambda t})}} \\
&\times \exp\big[-\frac{\beta\lambda(x - x_0 e^{-2\mu\lambda t})^2}{1-e^{-4\mu\lambda t}} + \frac{i}{\hbar}\frac{2l(x+x_0)}{\mu}\tanh\mu\lambda t - \mu\lambda^2 l^2 \beta t - \frac{4l^2(\mu\lambda t - \tanh\mu\lambda t)}{\mu^2\lambda\beta\hbar^2}\big]
\end{aligned} \tag{5.4.7}$$

$$\varrho_{11}(x,t) = \rho_{11}\sqrt{\frac{\beta\lambda}{\pi(1-e^{-4\mu\lambda t})}}\exp\big[-\frac{\beta\lambda(x + l(1-e^{-2\mu\lambda t}) - x_0 e^{-2\mu\lambda t})^2}{1-e^{-4\mu\lambda t}}\big] \tag{5.4.8}$$

Since the initial quantum state $\hat{\rho}$ can be taken to depend on $x_0$, this solution also provides a Green's function for the dynamics with arbitrary initial conditions.

The $\rho_{00}$ and $\rho_{11}$ components describe classical probability distributions relaxing to a probability distribution peaked around $z = \pm l$. The first term of the off-diagonal components to appears to show relaxation around the origin, with the second component giving the average cumulative phase due the unitary dynamics for a particle at $z$ in phase space at time $t$. However, there is also simultaneously decoherence of this part of the classical-quantum state, given by the third and fourth terms. The first of these is primary decoherence, due to the action of the operators $\hat{L}_x$, while the other is secondary decoherence, which arises from destructive interference of the different phases picked up by the various classical paths that end up at $(x, t)$.

### 5.4.3 Measurement and entropy production

We first consider a regime in which the classical degree of freedom acts as to measure the quantum system in the $z$-basis. In doing so, we can study the total entropy production of the measuring apparatus and quantum system during a quantum measurement.

We start by reviewing the concept of a quantum measurement in a classical-quantum formalism. Here, a quantum system in an initial state $\hat{\rho}_0$ is allowed to interact with a classical system that acts as a measurement device. The interaction with the classical system causes the quantum system to decohere in a particular basis, while the quantum back-reaction on the classical system causes the final classical configuration to be correlated with the quantum state. Conditioning on the final classical state, the observer deduces information about the final state of the quantum system, which may correspond to a projective measurement if the set of final states are orthogonal pure states.

To see that this arises in this model, we note that at long times, the above analytic solution tends to a stationary distribution $\hat{\varrho}^{st}(x)$, which we may normalise locally in phase space $\hat{\varrho}^{st}(x)/\mathrm{tr}\hat{\varrho}^{st}(x)$ to find the quantum state conditioned on the final classical position $x$, denoted $\hat{\rho}^{st}(x)$. This takes the form

$$\hat{\rho}^{st}(x) = \begin{pmatrix} \rho_{00}(\rho_{00} + \rho_{11}e^{-4\beta\lambda xl})^{-1} & 0 \\ 0 & \rho_{11}(\rho_{11} + \rho_{00}e^{4\beta\lambda xl})^{-1} \end{pmatrix}. \tag{5.4.9}$$

In the limit that $l \to 0$, the final quantum state contains no dependence on the final classical position, and simply corresponds to the intial quantum state $\hat{\rho}_0$ decohered in the $\hat{Z}$ eigenbasis. However, in general, the dependence on $x$ indicates that observing the classical configuration provides information about the quantum state. In the limit of large $l$, the conditioned quantum state reduces to being either the pure state $|0\rangle$ or $|1\rangle$, depending on whether $x > 0$ or $x < 0$. This provides the projective measurement regime of this model, in which the observations $x > 0$ or $x < 0$ of the final classical position $x$ correspond to the measurement outcomes $\pm 1$ of the operator $\hat{Z}$ in the standard quantum observables formalism. In general, the parameter $l$ here provides a measure of how successful a given measurement is at distinguishing the $|0\rangle$ and $|1\rangle$ states.

Having established that the dynamics of this model resemble that of a (possibly imperfect) measurement of the operator $\hat{Z}$, we now may turn to understand the entropy production in such a model. To do so, we initialise the classical state in a Gaussian probability distribution around the origin with variance $\sigma^2$, and take the initial quantum state to be $\hat{\rho}_0$. Using the analytic solution as a Green's function, we may integrate over the $x_0$ variable for this initial condition to find the subsequent evolution of the classical-quantum state. Numerically evaluating the integrals needed to compute the change in entropy and heat at each time $t$, we may plot the entropy production over time to find $\Sigma(t)=\Delta S(t) - \beta \mathcal{Q}(t)$, for different initial conditions and parameters of the model. In Figure 5.1 we plot the entropy production and change in entropy over time for two different initial states, $\hat{\rho}_0 = |+\rangle\langle+|$ and $\hat{\rho}_0 = \frac{1}{2}\hat{\mathbb{1}}$. We see here that the maximally mixed state configuration has decreasing entropy, due to the classical configuration becoming more ordered as the system relaxes. By contrast, the initially pure state configuration has an overall gain of entropy, with the entropy gain due to a loss of coherence outweighing the entropy loss due to the changes in the classical degrees of freedom. In both cases, the combined classical-quantum system experiences the same loss of heat into its surroundings over time, leading to an overall positive entropy production, that tends to a steady value as the system relaxes.

The above model demonstrates explicitly that measurements of quantum states with coherence lead to greater entropy production than those without. While intuitively reasonable, given the clear difference in entropy changes in the two cases, the current framework provides a real

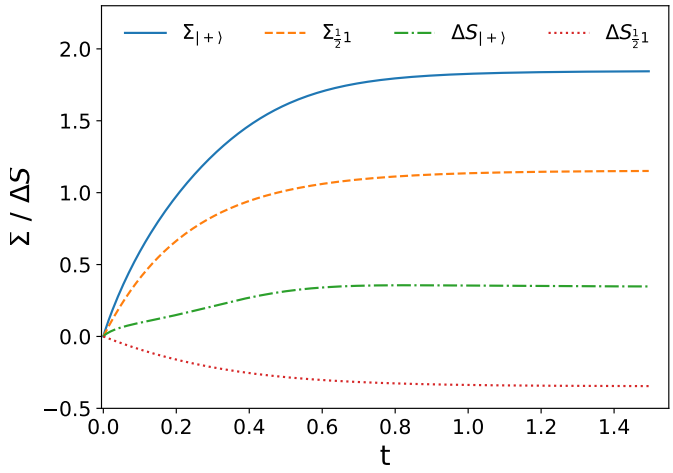


Figure 5.1: The entropy production $\Sigma$ and change in entropy $\Delta S$ over time for a classical-quantum system with the quantum state either in a pure state $|+\rangle$ or a maximally mixed state $\frac{1}{2}\hat{\mathbb{1}}$, over the course of a $\hat{Z}$ measurement. Here the classical system starts in a Gaussian state centered on the origin with variance $\sigma$. We here plot this with free parameters $\beta, \lambda, l, \mu, \hbar$ and $\sigma$ all equal to 1.

time description of this process. Understanding the consequences of this in general settings, or in more physically motivated models, is likely to be an interesting area of future study.

### 5.4.4 Coherent control via relaxation

The previous example showed how this toy model may be used to study the non-equilibrium thermodynamics of quantum measurements. We now turn to illustrate how one may also use this model to understand quantum control in a thermodynamic setting in which both thermal fluctuations and quantum back-reaction affect a classical control system.

As with the previous example, we first review the concept of quantum control in the classical-quantum setting. Here, a quantum system evolves with a Hamiltonian that depends on the state of a classical system. Since the state of the classical system can change with time, it may act as a controller of the quantum dynamics, allowing the quantum system's Hamiltonian to be switched on or off such that a specific unitary operation is performed after a desired time.

In addition to this unitary part of the dynamics, the quantum system will experience some additional decoherence, either due to its environment or due to noise in the classical control system. To correctly describe this latter type of decoherence, one must average over all possible realisations of the noise in the classical controller, i.e. study the unconditioned quantum state.

To see how the overdamped particle controls the implementation of a unitary on the qubit in our toy model, we first revisit the analytic solution. Integrating over the classical degree of freedom in the solution for the classical-quantum state $\hat{\varrho}(x,t)$ given in equations (5.4.6) to (5.4.8), we find the unconditioned quantum state $\hat{\rho}(t)$ takes the form

$$\hat{\rho}(t) = \begin{pmatrix} \rho_{00} & \rho_{01}\exp\left[i\theta(t)+\Gamma(t)\right] \\ \rho_{10}\exp\left[-i\theta(t)+\Gamma(t)\right] & \rho_{11}, \end{pmatrix} \tag{5.4.10}$$

where the phase $\theta$ and damping factor $\Gamma$ are given as the following functions of time

$$\theta(t) = \frac{2lx_0}{\mu\hbar}(1-e^{-2\mu\lambda t}), \tag{5.4.11}$$

$$\Gamma(t) = -l^2\left(\mu\lambda^2\beta + \frac{4}{\mu\beta\hbar^2}\right)t + \frac{l^2(3+e^{-4\mu\lambda t}-4e^{-2\mu\lambda t})}{\mu^2\lambda\beta\hbar^2}. \tag{5.4.12}$$

Considering first the phase $\theta(t)$, we see that the quantum state undergoes a unitary transformation corresponding to a rotation about the $z$ axis of the Bloch sphere. Moreover, since at long times $\theta(t)$ tends to fixed value, the evolution of the phase corresponds to applying the following unitary on the initial state

$$\hat{U} = e^{i\phi\hat{Z}} \qquad \phi = \frac{x_0 l}{\mu\hbar}, \tag{5.4.13}$$

provided $t \gg (\mu\lambda)^{-1}$. The "switching off" of the Hamiltonian evolution that enables this specific unitary to be implemented at long times is due to the time evolution of the classical system, which turns off the interaction as it relaxes towards the origin. Since the total unitary applied is dependent on the $x_0$, we see that the toy model provides a model of quantum control where choosing an initial non-equilibrium classical state, and allowing the system to relax towards a fixed point, allows for a specific unitary gate to be performed on a quantum system.

The success of performing this unitary transformation is determined by the loss of coherence. In this toy model the decoherence is in the $\hat{Z}$ eigenbasis and is entirely determined by $\Gamma(t)$, which must remain small over a timescale $t \gg (\mu\lambda)^{-1}$ in order for the unitary to be performed with

low noise. Immediately, we see that a key parameter to achieve this is the spacing $l$ between the two potential sites, which must remain small in order for the unitary to be performed accurately. Since the spacing of the potentials does not affect the timescale after which the unitary has been implemented, we see that provided $l$ can be made arbitrarily small, and that $x_0$ may be made sufficiently large to compensate this to achieve a given choice of unitary, the model describes a unitary control operation with arbitrary accuracy.

Although this toy model provides a proof-of-principle of how quantum control may be implemented via an relaxation process, it fails a number of requirements needed for a realistic description of an experimental platform. For starters, the Hamiltonian of the model we consider is decomposeable in terms of $\hat{\mathbb{1}}$ and $\hat{Z}$, meaning that it is limited to performing rotations around the $z$-axis. Moreover, since $l$ must be small, a high degree of control of the parameters $l$ and $x_0$ would be needed here to achieve a high precision unitary. However, the above method, where the dynamics are solved to find the unconditioned quantum state $\hat{\rho}(t)$, which may have its phase and decoherence compared to find optimal parameters of performance, provides a blueprint for future studies in more complex realistic models.

## 5.5 Model II

In this section we numerically study a model of a classical oscillator interacting with a quantum oscillator via a linear coupling. As we shall see, this model features a classical-quantum Hamiltonian that is not self-commuting in phase space, and illustrates a number of interesting features, including thermalisation. As with the previous example, in the entirety of this section we denote operators with hats.

### 5.5.1 Set-up

We consider here a one-dimensional model of an underdamped classical oscillator coupled to a quantum oscillator. The position and momentum of the classical system are denoted $q, p$, while the corresponding operators for the quantum system will be denoted $\hat{q}, \hat{p}$ and satisfy the canonical commutation relation. The classical-quantum Hamiltonian that governs the dynamics

of this system is given

$$\hat{H}(q,p) = \frac{\hat{p}^2}{2m_q} + \frac{1}{2}m_q\omega^2(q\hat{\mathbb{1}} - \hat{q})^2 + \big(\frac{p^2}{2m_c} + \frac{1}{2}m_c\Omega^2 q^2\big)\hat{\mathbb{1}}. \tag{5.5.1}$$

Here the first two terms describe the quantum oscillator and its coupling to the classical system, while the last two terms proportional to the identity describe the classical harmonic oscillator. As such, $m_q$ and $m_c$ are the quantum and classical particle masses, while $\omega$ represents the angular frequency of the coupling between the classical and quantum systems in terms of the quantum mass, and $\Omega$ denotes the classical oscillator's angular frequency. In this system, the classical oscillator will experience friction, with a corresponding friction coefficient $\gamma$. The whole classical-quantum system is also assumed to be in an environment with inverse temperature $\beta$.

To find the adiabatic basis for this model, we must solve the eigenvalue problem for the operator $\hat{H}(q,p)$. Since the non-trivial part of this Hamiltonian corresponds to a quantum harmonic oscillator Hamiltonian displaced from the origin by $q$, it is intuitive that the adiabatic basis is given by displaced eigenstates of the quantum harmonic oscillator Hamiltonian. Letting $|n\rangle$ denote the number states, the adiabatic basis takes the form

$$|n(q,p)\rangle = e^{-\frac{i}{\hbar}q\hat{p}}|n\rangle \tag{5.5.2}$$

i.e. the standard number eigenstates of the quantum harmonic oscillator $|n\rangle$ displaced by distance $q$. The corresponding eigenvalues of $\hat{H}(q,p)$ are

$$\epsilon_n(q,p) = \hbar\omega(n + \frac{1}{2}) + \frac{p^2}{2m_c} + \frac{1}{2}m_c\Omega^2 q^2. \tag{5.5.3}$$

which can easily be seen to be the sum of the quantum oscillator energy for a given energy eigenstate $|n\rangle$ and the classical oscillator energy for a given $q$, $p$.

The thermal state corresponding to this system is given

$$\hat{\pi}(q,p) = \frac{1}{\mathcal{Z}}e^{-\beta\hat{H}(q,p)} \tag{5.5.4}$$

where here

$$\mathcal{Z} = \mathcal{Z}_C\mathcal{Z}_Q \tag{5.5.5}$$

for the classical and quantum thermal partition functions

$$\mathcal{Z}_C = \frac{2\pi}{\beta\Omega}, \qquad \mathcal{Z}_Q = \frac{1}{2\sinh\frac{\beta\omega\hbar}{2}}. \tag{5.5.6}$$

These may be found by representing the thermal state in the adiabatic basis, and taking the trace and integrating over phase space to ensure normalisation.

### 5.5.2 Computing $\hat{L}_q$ and $\hat{M}_{qq}$

Before studying properties of this dynamics, the first step is to explicitly compute the operators $\hat{L}_q$ and $\hat{M}_{qq}$ for the classical-quantum Hamiltonian $\hat{H}$ of this model. To do so, we shall need to exploit a number of relations describing power series of $\mathrm{ad}_{\frac{-\beta\hat{H}}{2}} = -(\beta/2)[\hat{H}, \cdot]$ .

To begin, we first note that the commutator of $\hat{H}$ with operators linear in $q\hat{\mathbb{1}} - \hat{q}$ and $\hat{p}$ takes a particularly simple form. In particular, the commutator of $\hat{H}$ with $q\hat{\mathbb{1}} - \hat{q}$ gives $-i\omega^2\hat{p}/m_q$, while when applied to $\hat{p}$ gives $im_q\omega^2\hbar(q\hat{\mathbb{1}} - \hat{q})$. We thus see that representing the operators as vectors

$$q\hat{\mathbb{1}} - \hat{q} \;\mapsto \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \hat{p} \;\mapsto \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{5.5.7}$$

we can represent the adjoint $\mathrm{ad}_{\frac{-\beta\hat{H}}{2}}$ as the following $2 \times 2$ matrix

$$\mathrm{ad}_{\frac{-\beta\hat{H}}{2}} \;\mapsto \begin{pmatrix} 0 & \frac{im_q\omega^2\beta\hbar}{2} \\ -\frac{i\beta\hbar}{2m_q} & 0 \end{pmatrix}. \tag{5.5.8}$$

Moreover, since the adjoint action acting on an operator linear in $q\hat{\mathbb{1}} - \hat{q}$ and $\hat{p}$ produces another operator linear in these operators, $\mathrm{ad}_{\frac{-\beta\hat{H}}{2}}$ closes on these operators, and thus the action of arbitrary series of $\mathrm{ad}_{\frac{-\beta\hat{H}}{2}}$ on linear combinations of $\hat{q}$ and $\hat{p}$ may be computed by finding the corresponding series for the $2 \times 2$ matrix (5.5.8).

Having established this, we first consider $\hat{L}_q$. Using the series form of $\hat{L}_z$ given in (5.3.7), we may compute $\hat{L}_q$ as a series of $\mathrm{ad}_{\frac{-\beta\hat{H}}{2}}$ acting on the derivative of the classical-quantum Hamiltonian

$$\frac{\partial\hat{H}}{\partial q} = m_c\Omega^2 q\hat{\mathbb{1}} + m_q\omega^2(q\hat{\mathbb{1}} - \hat{q}). \tag{5.5.9}$$

While the first term commutes with $\hat{H}$, and thus appears unmodified in $\hat{L}_q$, the rest of $\hat{L}_q$ must be computed by acting with the series of $\mathrm{ad}_{\frac{-\beta\hat{H}}{2}}$ given in Eq. (5.3.8) on the second term in Eq. (5.5.9). To find a closed form expression for this, we simply compute the corresponding series

for the $2 \times 2$ matrix (5.5.8), which gives

$$\frac{e^{\mathrm{ad}_{\frac{-\beta\hat{H}}{2}}} - 1}{\mathrm{ad}_{\frac{-\beta\hat{H}}{2}}} \mapsto \begin{pmatrix} \frac{2\sinh\frac{\hbar\omega\beta}{2}}{\beta\omega\hbar} & \frac{-2im_q(1-\cosh\frac{\hbar\omega\beta}{2})}{\beta\hbar} \\ \frac{2i(1-\cosh\frac{\hbar\omega\beta}{2})}{m_q\beta\hbar\omega^2} & \frac{2\sinh\frac{\hbar\omega\beta}{2}}{\beta\omega\hbar} \end{pmatrix}. \tag{5.5.10}$$

Applying this matrix to $(m_q\omega^2\ 0)^T$, the vector representing the second term of Eq. (5.5.9), one finally arrives at the form of $\hat{L}_q$ as

$$\hat{L}_q = \frac{2m_q\omega}{\hbar\beta}\sinh\frac{\hbar\omega\beta}{2}(q\hat{\mathbb{1}} - \hat{q}) + \frac{2i}{\hbar\beta}(1-\cosh\frac{\hbar\omega\beta}{2})\hat{p} + m_c\Omega^2 q\hat{\mathbb{1}}. \tag{5.5.11}$$

Taking the $\beta \to 0$ limit of this operator, one finds that $\hat{L}_q$ indeed reduces to the expression in Eq. (5.5.9), in agreement with the general result of Eqs. (5.3.9).

To compute $\hat{M}_{qq}$, we will exploit two identities that allow one to swap the position of $\hat{q}$ and $\hat{p}$ with the square root of the thermal state $\hat{\pi}^{\frac{1}{2}}$. These are given

$$\hat{\pi}^{\frac{1}{2}}(q\hat{\mathbb{1}} - \hat{q}) = \big[\cosh\frac{\hbar\omega\beta}{2}(q\mathbb{1} - \hat{q}) - \frac{i}{m_q\omega}\sinh\frac{\hbar\omega\beta}{2}\hat{p}\big]\hat{\pi}^{\frac{1}{2}}, \tag{5.5.12}$$

and

$$\hat{\pi}^{\frac{1}{2}}\hat{p} = \big[im_q\omega\sinh\frac{\hbar\omega\beta}{2}(q\hat{\mathbb{1}} - \hat{q}) + \cosh\frac{\hbar\omega\beta}{2}\hat{p}\big]\hat{\pi}^{\frac{1}{2}}. \tag{5.5.13}$$

To prove these, we note that

$$e^{-\frac{\beta}{2}\hat{H}}Ae^{\frac{\beta}{2}\hat{H}} = e^{\mathrm{ad}_{\frac{-\beta\hat{H}}{2}}}A \tag{5.5.14}$$

for any operator $\hat{A}$, and that for operators linear in $q\hat{\mathbb{1}} - \hat{q}$ and $\hat{p}$ we may represent the exponential of the adjoint as

$$e^{\mathrm{ad}_{\frac{-\beta\hat{H}}{2}}} \mapsto \begin{pmatrix} \cosh\frac{\hbar\omega\beta}{2} & im_q\omega\sinh\frac{\hbar\omega\beta}{2} \\ -\frac{i}{m_q\omega}\sinh\frac{\hbar\omega\beta}{2} & \cosh\frac{\hbar\omega\beta}{2} \end{pmatrix}. \tag{5.5.15}$$

Applying this matrix to the two vectors in (5.5.7) to compute the right hand side of (5.5.19), and then acting both sides on $\hat{\pi}^{\frac{1}{2}}$, we recover the two identities (5.5.12) and (5.5.13).

To compute $\hat{M}_{qq}$ using these identities, we assume that $\hat{M}_{qq}$ takes the form of a Hermitian operator that is at most quadratic in $q\hat{\mathbb{1}} - \hat{q}$ and $\hat{p}$. Plugging this form of $\hat{M}_{qq}$ into the left hand side of (5.3.4), and the previously computed $\hat{L}_q$ into the right hand side, we may use the commutation relations (5.5.12) to rearrange both sides of (5.3.4) to have $\hat{\pi}^{\frac{1}{2}}$ on the right most side. Acting with $\hat{\pi}^{\frac{1}{2}}$ on both sides, and comparing terms, we find the solution as

$$\hat{M}_{qq} = \frac{2m_q\omega}{\hbar\beta^2}(\sinh\frac{\hbar\omega\beta}{2} - \tanh\frac{\hbar\omega\beta}{2})\{\hat{q} - q\hat{\mathbb{1}}, \hat{p}\}_+ + \frac{2m_c\Omega^2}{\beta}(1-\cosh\frac{\hbar\omega\beta}{2})\hat{p}. \tag{5.5.16}$$

Since the solutions to Eq. (5.3.4) are unique, we see that the original assumption that $\hat{M}_{qq}$ was at most quadratic in $q\hat{\mathbb{1}} - \hat{q}$ and $\hat{p}$ was correct. It is straightforward to check that in the high temperature limit, $\beta \to 0$, $\hat{M}_{qq}$ correctly reduces to zero, consistent with the previously derived expression in Eqs. (5.3.9).

### 5.5.3 Relative position representation

Having found the operators $\hat{L}_q$ and $\hat{M}_{qq}$, one may in principle directly study the dynamics of Eqs. (5.3.18) to (5.3.20) to understand properties of the system. However, we will first introduce an alternate representation for describing the quantum system, which makes the dynamics simpler to both solve and interpret.

In the unravelling picture of classical-quantum dynamics, $|\psi\rangle$ represents the state of the quantum system in absolute space. However, given that the interactions between the two systems depend on their relative positions, it is convenient to describe the quantum system using a state vector that represents the quantum system relative to the classical position $q$. We refer to this as the *relative position representation*, and denote the quantum state in this representation $|\psi^{\mathfrak{r}}\rangle$. The absolute and relative position descriptions are related by the standard unitary transformation

$$|\psi^{\mathfrak{r}}\rangle = e^{\frac{i}{\hbar}q\hat{p}}|\psi\rangle. \tag{5.5.17}$$

In order for expectation values to be correctly computed in this representation, observables must also be transformed by a unitary transformation

$$\hat{A}^{\mathfrak{r}}(q,p) = e^{\frac{i}{\hbar}q\hat{p}}\hat{A}(q,p)e^{-\frac{i}{\hbar}q\hat{p}}, \tag{5.5.18}$$

which ensures that $\langle\psi^{\mathfrak{r}}|\hat{A}^{\mathfrak{r}}|\psi^{\mathfrak{r}}\rangle = \langle\psi|A|\psi\rangle$. To compute this in practice, we will make use of a version of the identity (5.5.19), namely that

$$e^{\frac{i}{\hbar}q\hat{p}}\hat{A}e^{-\frac{i}{\hbar}q\hat{p}} = e^{\mathrm{ad}_{\frac{i}{\hbar}q\hat{p}}}\hat{A}. \tag{5.5.19}$$

It is straightforward to check using this that the map $\hat{A} \mapsto \hat{A}^{\mathfrak{r}}$ amounts to replacing every appearance of $\hat{q} - q\mathbb{1}$ with $\hat{q}$.

The utility of this representation is apparent when we consider the relative position representation of the states and operators specific to our current model. Taking first the adiabatic

basis, we see that

$$|n^{\mathfrak{r}}(q,p)\rangle = |n\rangle \tag{5.5.20}$$

i.e. that the adiabatic basis in the relative position representation is simply the number basis of the quantum harmonic oscillator. Representing dynamics in terms of $|\psi^{\mathfrak{r}}\rangle$ thus allows us decompose the dynamics in a fixed basis, independent of the current state of the classical system, that nevertheless describes the adiabatic basis of the system.

This representation also simplifies the form of operators. Making the substitution $\hat{q} - q\mathbb{1}$ with $\hat{q}$ it is straightforward to see that the classical-quantum Hamiltonian in this representation takes the form

$$\hat{H}^{\mathfrak{r}}(q,p) = H_C^{\mathfrak{r}}(q,p)\hat{\mathbb{1}} + \hat{H}_Q^{\mathfrak{r}} \tag{5.5.21}$$

where

$$H_C^{\mathfrak{r}}(q,p) = \frac{p^2}{2m_c} + \frac{1}{2}m_c\Omega^2 q^2 \tag{5.5.22}$$

is the Hamiltonian of a classical harmonic oscillator and

$$\hat{H}_Q^{\mathfrak{r}} = \frac{\hat{p}^2}{2m_q} + \frac{1}{2}m_q\omega^2\hat{q}^2 \tag{5.5.23}$$

is the Hamiltonian of a quantum harmonic oscillator. Solving the eigenvalue problem in this representation, it is therefore straightforward to see both why the adiabatic basis is given by (5.5.2), and why the energy eigenvalues $\epsilon_n(q,p)$ are those written in (5.5.3).

Finally, we note an intuitive relation that connects unravellings to classical-quantum states in the relative position representation. If one takes $\hat{\varrho}(q,p)$, and maps this using (5.5.18), we find the classical-quantum state in the relative position representation $\hat{\varrho}^{\mathfrak{r}}(q,p)$. Using the fact that $\mathbb{E}[f(z_t)\delta(z-z_t)] = f(z)\mathbb{E}[\delta(z-z_t)]$, it is simple to see that this may equivalently be found using

$$\hat{\varrho^{\mathfrak{r}}}(q,p,t) = \mathbb{E}[|\psi^{\mathfrak{r}}\rangle_t\langle\psi^{\mathfrak{r}}|_t\delta(q-q_t)\delta(p-p_t)], \tag{5.5.24}$$

i.e. using the relation (2.4) and replacing $|\psi\rangle_t$ with $|\psi^{\mathfrak{r}}\rangle_t$. This identity is useful since it means that we may compute the classical-quantum state in the relative position representation directly from the distribution of trajectories in terms of $|\psi^{\mathfrak{r}}\rangle_t$, $q_t$ and $p_t$.

### 5.5.4 Numerical solution

To study the dynamics of this model, we shall use the unravelling approach introduced in Chapter 2, studying solutions to equations (5.3.18) to (5.3.20). To study these numerically in an efficient manner, we will use a simplified set of dynamics, employing both the relative position representation introduced in the previous section, and a particular invariance property of the dynamics under changes to the classical part of the Hamiltonian.

We begin by finding the equations of motion in the relative state representation. Since the expectation values remain the same provided both the states and operators are transformed as in (5.5.17) and (5.5.18), the classical equations for $q$ and $p$ remain unchanged. To find the equation of motion for $|\psi^{\mathfrak{r}}\rangle_t$, we take the derivative of (5.5.17) with respect to time. Doing so is straightforward to see two changes in the dynamics of the relative quantum state $|\psi^{\mathfrak{r}}\rangle_t$ versus the absolute quantum state $|\psi^{\mathfrak{r}}\rangle_t$. The first is that the time dependence of $q_t$ leads to an additional unitary term in the dynamics, with Hamiltonian $-p_t\hat{p}/m_c$. The second is that, in order to put write the dynamics in terms of $|\psi^{\mathfrak{r}}\rangle_t$, the operators $\hat{L}_q$, $\hat{M}_{qq}$ and $\hat{H}$ must all be replaced with their transformed versions $\hat{L}^{\mathfrak{r}}_q$, $\hat{M}^{\mathfrak{r}}_{qq}$ and $\hat{H}^{\mathfrak{r}}$.

To further simplify the form of the dynamics, we first use a particular invariance property of the general dynamics presented in Section 5.3. Namely, as we show in Appendix K, one may always remove the part of $\hat{L}_z$ proportional to the identity and corresponding term in $\hat{M}_{zz}$, and instead include it as an additional drift term in the dynamics. Guaranteeing that the form of decoherence and back-reaction is independent of any additional purely classical dynamics, in this case it allows us to remove the dependence of $\hat{L}^{\mathfrak{r}}_q$ and $\hat{M}^{\mathfrak{r}}_{qq}$ on the classical angular frequency $\Omega$ and replace it with an additional classical drift term $-m_c\Omega^2 q dt$ in equation (5.3.19). Finally, we drop from $\hat{H}^{\mathfrak{r}}(q,p)$ the term proportional to the identity, $H^{\mathfrak{r}}_C(q,p)\mathbb{1}$.

Taken together, the two steps lead to the following form of equations for $q_t, p_t$ and $|\psi^{\mathfrak{r}}\rangle_t$

$$dq_t = \frac{p_t}{m_C}dt \tag{5.5.25}$$

$$dp_t = -\frac{1}{2}\langle \hat{L}^{\mathfrak{r}}_q + \hat{L}^{\mathfrak{r}\dagger}_q\rangle dt - m_c\Omega^2 q_t dt - \frac{\gamma p_t}{m_c}dt + \sqrt{\frac{2\gamma}{\beta}}dW \tag{5.5.26}$$

$$
\begin{aligned}
d|\psi^{\mathfrak{r}}\rangle_t = &-\frac{i}{\hbar}(\hat{H}_Q^{\mathfrak{r}} + \frac{\beta}{8\gamma}\hat{M}_{qq}^{\mathfrak{r}} - \frac{p_t}{m_c}\hat{p})|\psi^{\mathfrak{r}}\rangle_t dt \\
&-\frac{1}{2}\frac{\beta}{8\gamma}(\hat{L}_q^{\mathfrak{r}\dagger}\hat{L}_q^{\mathfrak{r}} - 2\langle\hat{L}_q^{\mathfrak{r}\dagger}\rangle\hat{L}_q^{\mathfrak{r}} + \langle\hat{L}_q^{\mathfrak{r}\dagger}\rangle\langle\hat{L}_q^{\mathfrak{r}}\rangle)|\psi^{\mathfrak{r}}\rangle_t dt \\
&-\sqrt{\frac{\beta}{8\gamma}}(\hat{L}_q^{\mathfrak{r}} - \langle\hat{L}_q^{\mathfrak{r}}\rangle)|\psi^{\mathfrak{r}}\rangle_t dW_t
\end{aligned}
\tag{5.5.27}
$$

where here the expectation values are all taken with respect to $|\psi^{\mathfrak{r}}\rangle_t$, and the operators $\hat{L}_q^{\mathfrak{r}}$ and $\hat{M}_{qq}^{\mathfrak{r}}$ are defined as

$$
\hat{L}_q^{\mathfrak{r}} = -\frac{2m_q\omega}{\hbar\beta}\sinh\frac{\hbar\omega\beta}{2}\hat{q} + \frac{2i}{\hbar\beta}(1-\cosh\frac{\hbar\omega\beta}{2})\hat{p}, \tag{5.5.28}
$$

$$
\hat{M}_{qq}^{\mathfrak{r}} = \frac{2m_q\omega}{\hbar\beta^2}(\sinh\frac{\hbar\omega\beta}{2} - \tanh\frac{\hbar\omega\beta}{2})\{\hat{q},\hat{p}\}_+. \tag{5.5.29}
$$

To simulate these equations efficiently, we employ a numerical method introduced in the context of continuous measurement theory, known as Rouchon's method [190–192]. In this case, it allows one to simulate the coupled set of stochastic differential equations (5.5.25) to (5.5.27) in discrete time. Taking $t_i = 0$ and $t_f = N_{steps}\Delta t$, where $N_{steps}$ is the number of timesteps and $\Delta t$ is the time increment, we define $\Delta W^{(n)}$ as the $n$th sample of a Gaussian random variable with mean zero and variance $\Delta t$. We then compute the values of $q$, $p$ and $|\psi^{\mathfrak{r}}\rangle$ at time $t = (n+1)\Delta t$ by iterating the following set of equations

$$
q^{(n+1)} = q^{(n)} + \frac{p^{(n)}}{m_c}\Delta t \tag{5.5.30}
$$

$$
\begin{aligned}
p^{(n+1)} = &-\frac{1}{2}\langle\psi_{(n)}^{\mathfrak{r}}|\hat{L}_q^{\mathfrak{r}} + \hat{L}_q^{\mathfrak{r}\dagger}|\psi_{(n)}^{\mathfrak{r}}\rangle\Delta t - m_c\Omega^2 q^{(n)}\Delta t \\
&-\frac{\gamma p^{(n)}}{m_c}\Delta t + \sqrt{\frac{2\gamma}{\beta}}\Delta W^{(n)}
\end{aligned}
\tag{5.5.31}
$$

$$
\begin{aligned}
R_{(n)} = &\mathbb{1} - \frac{i}{\hbar}(\hat{H}_Q^{\mathfrak{r}} + \frac{\beta}{8\gamma}\hat{M}_{qq}^{\mathfrak{r}} - \frac{p^{(n)}}{m_c}\hat{p})\Delta t \\
&-\frac{\beta}{16\gamma}\hat{L}_q^{\mathfrak{r}\dagger}\hat{L}_q^{\mathfrak{r}}\Delta t \\
&+\frac{\beta}{8\gamma}\langle\psi_{(n)}^{\mathfrak{r}}|\hat{L}_q^{\mathfrak{r}} + \hat{L}_q^{\mathfrak{r}\dagger}|\psi_{(n)}^{\mathfrak{r}}\rangle\hat{L}_q^{\mathfrak{r}}\Delta t \\
&-\sqrt{\frac{\beta}{8\gamma}}\hat{L}_q^{\mathfrak{r}}\Delta W^{(n)} \\
&+\frac{\beta}{16\gamma}(\hat{L}_q^{\mathfrak{r}})^2((\Delta W^{(n)})^2 - \Delta t)
\end{aligned}
\tag{5.5.32}
$$

$$
|\psi_{(n+1)}^{\mathfrak{r}}\rangle = \frac{R_{(n)}|\psi_{(n)}^{\mathfrak{r}}\rangle}{\sqrt{\langle\psi_{(n)}^{\mathfrak{r}}|R_{(n)}^\dagger R_{(n)}|\psi_{(n)}^{\mathfrak{r}}\rangle}}. \tag{5.5.33}
$$

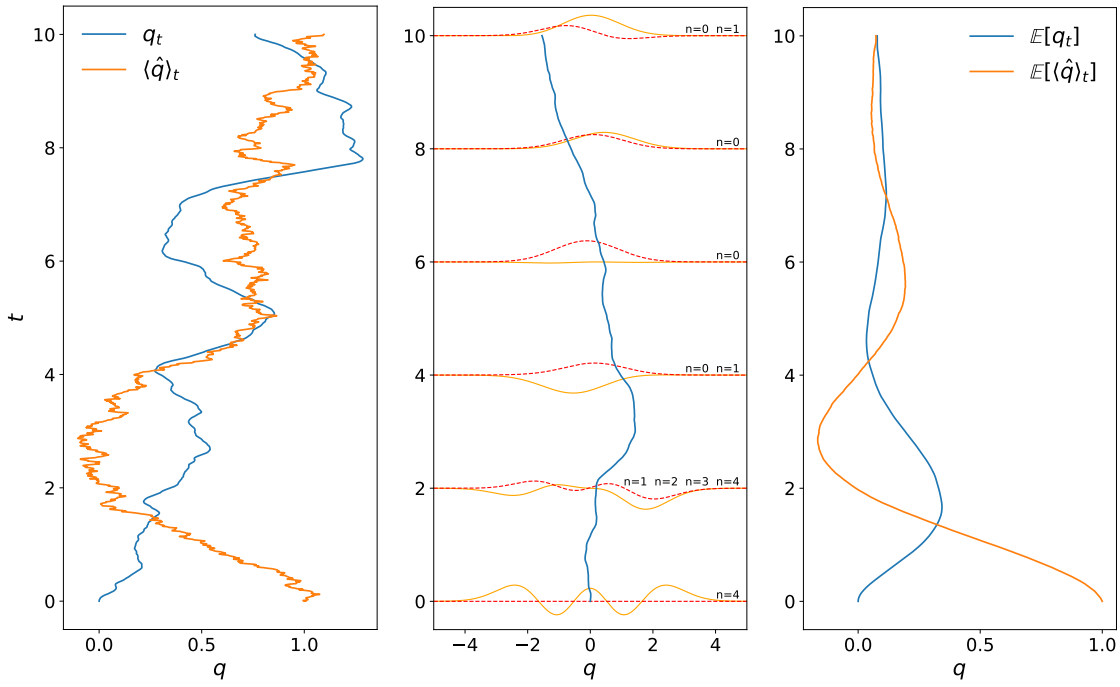


Figure 5.2: Simulations of trajectories for two coupled oscillators, one classical and one quantum, for parameters $\omega = m_C = m_Q = \hbar = 1$, $\beta = \gamma = 3$ and $\Omega = 10^{-5}$ between $t = 0$ and $t = 10$. *(left)* The classical position $q_t$ and expected position of the quantum state $\langle q\rangle_t$ is simulated and plotted for a single realisation, with $N_{max} = 20$ and $N_{steps} = 2 \times 10^4$. Here the classical system starts at the origin of phase space, while the quantum system starts in a coherent state with $\langle\hat{q}\rangle_0 = 1$ and $\langle\hat{p}\rangle_0 = 0$. *(middle)* The classical position $q_t$ is plotted with 6 distinct snapshots of the real (solid line) and imaginary (dashed line) parts of the wavefunction for a pair of trajectories starting at the origin in phase space and the 3rd excited adiabatic state, with $N_{max} = 50$ and $N_{steps} = 10^5$. On the right of each wavefunction, we denote the main components of the wavefunction in the adiabatic basis. *(right)* The expected values of the classical position $q_t$ and the trajectory expectation value $\langle q\rangle_t$ are plotted, performed by averaging over 2000 individual trajectories with the same initial conditions, $N_{max}$ and $N_{step}$ as in the left hand panel.

To represent the quantum state and operators for numerical simulation, we use the adiabatic basis in this representation i.e. the standard harmonic oscillator number states $|n\rangle$. Truncating these at a finite maximum energy level $N_{max}$, we may thus represent $|\psi^{\mathfrak{r}}_{(n)}\rangle$ as a complex vector of length $N_{max}$, and the operators $\hat{q}$ and $\hat{p}$ as $N_{max} \times N_{max}$ restrictions of their standard infinite dimensional number state representations. [211].

### 5.5.5 Individual and average trajectories

Having established a numerical method for studying the dynamics of this system, we begin to gain some insights into these dynamics by considering both individual and average trajectories of the joint classical-quantum system.

We begin by considering a typical trajectory, for which we plot both $q_t$ and $\langle \hat{q} \rangle_t$ in the left panel of Figure 5.2. Here we start the classical system at the origin, and the quantum system in a coherent state with $\langle \hat{p} \rangle = 0$ and $\langle \hat{q} \rangle = 1$. The mean position of the quantum system is noticeably less continuous than that of the classical system, which is due to the fact that the quantum state is conditioned on the classical momentum, which itself is experiencing fluctuations due to the environment.

It is also insightful to see how the wavefunction evolves along an individual trajectory, and how the quantum state is decomposed in the adiabatic basis. In the middle panel of Figure 5.2 we plot $q_t$, and additionally plot the real and complex parts of the wavefunction $\psi(x,t) = \langle q|\psi\rangle_t$ at equal instances in time, for an initially excited state beginning in $|\psi^{\mathfrak{r}}\rangle_0 = |4\rangle$ i.e. the third excited adiabatic state. The number of components for which the probability of occupation $|\langle n|\psi^{\mathfrak{r}}\rangle|^2$ is higher than 0.1 is indicated on the right hand side. We see here that the dynamics damps the excited components of the wavefunction, with the state after $t = 4$ being predominantly made up of the adiabatic ground state $|\psi^{\mathfrak{r}}\rangle = |0\rangle$.

Finally, while each individual classical trajectory will differ due to fluctuations, it is possible to see the effect of quantum backreaction on the classical system by averaging the trajectories over many realisations. In the right hand panel of Figure 5.2 we plot both $\mathbb{E}[q_t]$ and $\mathbb{E}[\langle\psi|\hat{q}|\psi\rangle_t]$ i.e. the ensemble averages over trajectories. Choosing the parameter $\Omega$ to be small as in the previous simulations such that the purely classical potential is negligible, we see from this plot that the quantum backreaction has a non-trivial effect on the mean classical evolution, with the two systems appearing to accelerate back and forth towards each other. The damping of the oscillations occurs due to the friction in the classical system, which dissipates the original energy stored in the interaction with the quantum oscillator.

### 5.5.6 Thermalisation

The dynamics describes a quantum system that remains pure conditioned on the classical trajectory. It is perhaps surprising therefore, that the joint classical-quantum system simultaneously appears to demonstrate thermalisation at the level of the classical-quantum state.

To begin, we first compute the form of the thermal state in the relative position representation. In particular, one may check that it takes the particularly simple form

$$\hat{\pi}^{\mathfrak{r}}(q,p) = \frac{1}{\mathcal{Z}} e^{-\beta \hat{H}_Q} e^{-\beta H_C(q,p)}, \tag{5.5.34}$$

where here $\mathcal{Z}$ is the same as in Eq. (5.5.5). Since this expression factorises, we see by comparison to (5.5.24) that we may check that the classical-quantum state $\hat{\varrho}(q,p)$ approaches the thermal state $\hat{\pi}(q,p)$ by checking in the relative position representation that

$$\lim_{t\to\infty} \mathbb{E}[|\psi^{\mathfrak{r}}\rangle_t\langle\psi^{\mathfrak{r}}|_t] = \frac{1}{\mathcal{Z}_Q} e^{-\beta \hat{H}_Q^{\mathfrak{r}}} \tag{5.5.35}$$

$$\lim_{t\to\infty} \mathbb{E}[\delta(q-q_t)\delta(p-p_t)] = \frac{e^{-\beta H_C(q,p)}}{\mathcal{Z}_C} \tag{5.5.36}$$

$$\lim_{t\to\infty} \hat{\varrho}^{\mathfrak{r}}(q,p) = \mathbb{E}[|\psi^{\mathfrak{r}}\rangle_t\langle\psi^{\mathfrak{r}}|_t]\ \mathbb{E}[\delta(q-q_t)\delta(p-p_t)] \tag{5.5.37}$$

i.e. that the reduced quantum and classical distributions approach the standard thermal states of the corresponding classical and quantum oscillators, and that the correlations between the classical and quantum degrees of freedom vanish.

Considering first the quantum dynamics, we first plot in the top of Figure 5.3 the numerically simulated ensemble average of the populations in the adiabatic basis i.e. $\mathbb{E}[|\langle n|\psi^{\mathfrak{r}}\rangle|^2]$. Starting in the state $|\psi^{\mathfrak{r}}\rangle_0 = |1\rangle$, we find that these approach the corresponding populations of the thermal state of the quantum harmonic oscillator. Despite the quantum state along any trajectory remaining pure, the diagonal part of the density matrix $\hat{\rho}^{\mathfrak{r}}(t) = \mathbb{E}[|\psi^{\mathfrak{r}}\rangle\langle_t\psi^{\mathfrak{r}}|_t]$ thus appears to thermalise in the adiabatic basis. Turning to the classical dynamics, we verify that the marginals of the classical thermal state are reached by plotting histograms of the position and momentum against the theoretical prediction, as shown in the middle and bottom of Figure 5.3.

While the above provides a strong indication of thermalisation, it is necessary to also check the remaining properties: (1) that the coherences of the quantum state in the adiabatic basis are

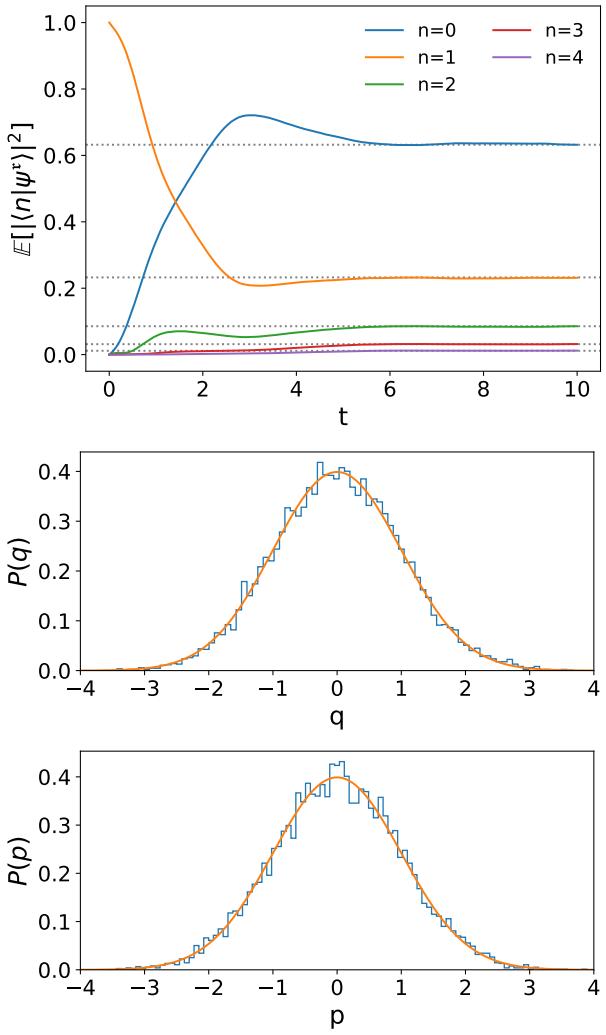


Figure 5.3: Three plots demonstrating the thermalisation of the classical-quantum state over $10^4$ numerically simulated trajectories. Here the initial quantum state is in the first excited state $|\psi^{\mathrm{r}}\rangle_0 = |1\rangle$, while the classical system is in a Gaussian probability distribution centered at the origin with standard deviations $\sigma_q = \sigma_p = 10^{-3}$. The model parameters are given $\omega = m_C = m_Q = \hbar = \beta = \gamma = \Omega = 1$, while the numerical simulation has $N_{max} = 10$ and $N_{steps} = 5000$, and is run from from $t = 0$ to $t = 10$. *(top)* The average populations in the adiabatic basis of the density operator in the relative position representation are shown up to the 4th excited state, which appear to converge to the corresponding values predicted from Eq. (5.5.35). *(middle and bottom)* The marginal distributions (solid orange line) of the classical thermal state appearing in Eq. (5.5.36) are plotted against a histogram of the numerically simulated final position and momentum of the classical system.

also damped in time (2) that the correlations between position and momentum vanish (3) that correlations between the classical and quantum degrees of freedom vanish. We explore these in Appendix L, and find evidence that the dynamics also causes coherences in the adiabatic basis to relax to zero, as well as the correlations (in the relative position representation) between the various degrees of freedom.

While the above numerical evidence does not rule out the existence of particular initial states which do not thermalise, it does suggest strongly that typical initial configurations relax to the thermal state given in Eq. (5.5.4). Proving this rigorously, such as using techniques from the theory of stochastic differential equations to demonstrate that Eqs. (5.5.35) to (5.5.37) indeed hold, is an interesting question that we leave to future work.

### 5.5.7 Heat fluctuations and the second law

Having developed both a numerical framework for simulating trajectories, and establishing that the model we describe appears to demonstrate thermalisation, we finally turn to combine these to demonstrate how the model illustrates fluctuations in the heat it exchanges with the environment, and how the average value of these fluctuations are bounded by the second law of thermodynamics.

We begin by computing the entropy of a particular initial classical-quantum configuration. We first note that since the classical-quantum entropy in (5.2.1) is invariant under phase-space dependent unitary transformations, we may compute the entropy directly in the relative position basis. Assuming the quantum system is in a pure quantum state in the relative position representation $|\psi^{\mathrm{r}}\rangle_0$ and the classical probability distribution is normally distributed around the origin in phase space with variances $\sigma_q^2$ and $\sigma_p^2$, the combined system is uncorrelated between the classical and quantum degrees of freedom, and thus the entropy is simply a sum of the entropies of the classical and quantum degrees of considered separately. Since the quantum state is initially pure, the quantum entropy is zero. Computing the classical part of the entropy is here well-defined since the classical probability distribution is Gaussian [203]. This gives the initial entropy of the classical-quantum system as

$$S(\hat{\varrho}_0) = 1 + \ln 2\pi\sigma_q\sigma_p. \tag{5.5.38}$$

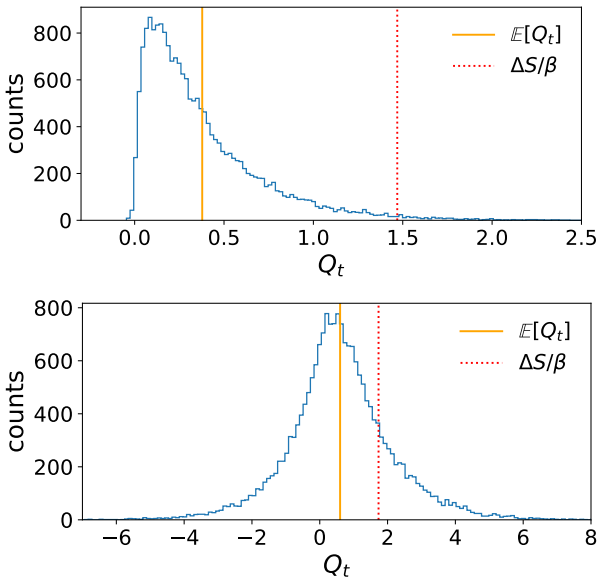


Figure 5.4: Distributions of the heat exchanged into the classical-quantum system as the system thermalises, with model parameters $\omega = m_C = m_Q = \hbar = \beta/\gamma = \Omega = 1$. *(top)* Heat distribution with $\beta = \gamma = 3$, $\sigma_q = \sigma_p = 0.1$, $N_{max} = 10$, $N_{steps} = 5000$ over $2 \times 10^4$ trajectories simulated from $t = 0$ to $t = 10$. *(bottom)* Heat distribution with $\beta = \gamma = 1$, $\sigma_q = \sigma_p = 1$, $N_{max} = 10$, $N_{steps} = 10^4$ over $2 \times 10^4$ trajectories simulated from $t = 0$ to $t = 20$.

For an arbitrary final state, one may compute the entropy to find $\Delta S$. Here we shall assume we are considering timescales long enough that the system has relaxed to the thermal state given in Eq. (5.5.4). Again utilising the fact that the entropy $S$ is invariant under unitary transformations, we may compute the entropy of $\hat{\pi}^{\mathfrak{r}}$, the thermal state in the relative position representation, which takes the simple uncorrelated form given in Eq. (5.5.34). As before, it is straightforward to compute the entropy here as the sum of the classical and quantum contributions

$$S(\hat{\pi}) = 1 + \ln \frac{4\pi}{\beta\Omega} + \frac{\beta\omega\hbar}{2} \coth \frac{\beta\omega\hbar}{2} - \ln \left[2 \sinh \frac{\beta\omega\hbar}{2}\right], \tag{5.5.39}$$

which gives the total change in entropy as

$$\Delta S = \ln 2 - \ln \beta\Omega\sigma_q\sigma_p + \frac{\beta\omega\hbar}{2} \coth \frac{\beta\omega\hbar}{2} - \ln \left[2 \sinh \frac{\beta\omega\hbar}{2}\right]. \tag{5.5.40}$$

From Eq. (5.2.18) and Eq. (5.2.11), we see that this provides a bound on the ensemble average of the heat exchanged into the system on along trajectory, given these initial conditions.

We may now compare the bound on heat exchange derived from the second law to the statistics of the heat exchange along individual trajectories. In the top of Figure 5.4 we plot the distribution of heat $Q_t$, for an initial state in which $|\psi^{\mathfrak{r}}\rangle_0 = |0\rangle$ i.e. in which the quantum system starts in the adiabatic ground state, and where the classical system is close to its ground state i.e. the origin in phase space. As expected, the vast majority of realisations lead to the system gaining energy, with the mean energy increase given by the vertical solid line. This can be seen to lower than the maximum upper limit of $\mathbb{E}[Q_t]$ allowed by the second law, which is marked by the dotted line. While the average satisfies the second law, individual realisations may gain more heat than their mean value, as evidenced by the small but non-zero set of counts to the right of the dashed line, which appear to fall off exponentially. In the bottom half of Figure 5.4 we plot the heat distribution at a higher temperature and lower friction, in the same quantum state but with a classical state with greater variance in phase space. Here we see more pronounced fluctuations of energy increase above the entropy bound, though a greater number of realisations dissipating heat into the environment ensure than the average satisfies the second law.

## 5.6 Detailed balance

While an equilibrium state is a minimal requirement for thermodynamic stability, a wide range of open systems in both classical and quantum regimes satisfy a stronger notion of *detailed balance*. In this section we extend the concept of detailed balance to hybrid classical-quantum systems, deriving the general sufficient and necessary conditions under which a classical-quantum system satisfies detailed balance. Using these conditions, we show that the two classes of dynamics introduced in 5.3 both satisfy classical-quantum detailed balance.

### 5.6.1 Alternative representation of the classical-quantum generator and the classical-quantum adjoint

Before starting our discussion of detailed balance in classical-quantum systems, we first remind the reader of two important forms of classical-quantum generators that will be needed in the

following sections.

The first is the alternative representation of the generator of completely-positive classical quantum dynamics introduced in Chapter 2. This is given by the generator (2.20), with associated positivity conditions (2.21) and (2.22). In this representation, the Hermitian operator $G$ determines the purely unitary quantum evolution. To avoid confusion with the classical-quantum Hamiltonian, which $G$ does not necessarily coincide with, we refer to this operator as the generator of unitary dynamics, or unitary generator for short. The back-reaction on each classical degree of freedom $z_i$ is determined by phase-space dependent operators $K_i$, which we shall refer to as the "backreaction operators". Rather than assuming these operators are traceless, and describing purely classical evolution by a separate drift term, the component of $K_i$ proportional to the identity operator describes the purely classical drift on the $i$th classical degree of freedom. The necessary decoherence corresponding to this backreaction is encoded in the decoherence term involving $K_i$ and the pseudoinverse of the diffusion matrix $D_2$. Finally, the Lindblad operators $\tilde{L}_\alpha$ determine any additional decoherence on top of the minimum required by the coupling to the classical system. These are thus necessarily zero if the decoherence-diffusion trade-off is saturated i.e. when the unravelling preserves the purity of initially pure quantum states.

The advantage of this representation is that sufficient and necessary conditions for complete-positivity may be checked without relying on a decomposition of the back-reaction operators in an orthonormal basis of operators. It turns out that this is extremely useful for checking detailed balance, as it allows operators such as the $L_z$ to be studied without needing to compute their explicit forms (such as was done for the classical-quantum oscillators model in 5.5.2). Aside from this, this form of dynamics provides some conceptual simplicity, such as explicitly separating out the decoherence necessary for positivity from additional kinds, and making it explicit which operator back-reacts on each classical degree of freedom.

The second generator we shall define is the adjoint generator of classical-quantum dynamics. As with the adjoint of the Fokker-Planck equation [198] or the GKLS equation [195], one may define the adjoint in the classical-quantum setting by studying the evolution of classical-quantum observables. Considering the definition of the expectation value given in (2.10), we

define the adjoint of the generator $\mathcal{L}$ as the classical-quantum superoperator $\mathcal{L}^\dagger$ that satisfies

$$\int dz \mathrm{tr} \mathcal{L}(\varrho) A = \int dz \mathrm{tr} \varrho \mathcal{L}^\dagger(A), \tag{5.6.1}$$

i.e. that governs the evolution of classical-quantum observables in the Heisenberg representation. Assuming that the classical-quantum state $\varrho$ satisfies vanishing boundary conditions at infinity, it is straightforward using integration by parts and properties of the trace to show that this can be written in the general form

$$\begin{aligned} \mathcal{L}^\dagger(A) = &\frac{i}{\hbar}[G, A] + K_i^\dagger \frac{\partial A}{\partial z_i} + \frac{\partial A}{\partial z_i} K_i \\ &+ \frac{1}{2} D_{2,ij} \frac{\partial^2 A}{\partial z_i \partial z_j} \\ &+ D_{2,ij}^{-1} \big( K_i^\dagger A K_j - \frac{1}{2} \{ K_j^\dagger K_i, A \}_+ \big) \\ &+ \tilde{L}_\alpha^\dagger A \tilde{L}_\alpha - \frac{1}{2} \{ \tilde{L}_\alpha^\dagger \tilde{L}_\alpha, A \}_+ . \end{aligned} \tag{5.6.2}$$

As should be expected, this dynamics takes the form of a generalisation of the standard classical and quantum adjoint dynamics, and as such satisfies many of the same properties. A particular property that is useful to note is that this map is unital i.e. that $\mathcal{L}^\dagger(\mathbb{1}) = 0$, since in this case the derivative, dissipator and commutator terms all vanish.

### 5.6.2 Defining detailed balance in classical-quantum systems

In this section we begin our discussion of classical-quantum detailed balance, providing a general definition of detailed balance in hybrid systems. This definition arises as a natural generalisation of the definitions of detailed balance of classical and quantum systems when characterised in terms of their generators, and we refer the reader to [197–199] for further details on this topic.

To define detailed balance in the classical-quantum setting, we must first introduce the concept of time-reversal. Taking a video of a particle in flight, and playing it in reverse, one sees that while the position $q$ of the particle remains unchanged, the momentum $p$ reverses sign. In a similar manner, for any set of classical variables $z = (z_1, \ldots, z_n)$, a subset known as the even variables will remain constant under time-reversal i.e. $z_i \mapsto z_i$, while the odd variables will each be multiplied by minus one i.e. $z_i \mapsto -z_i$. To capture this, we follow [198] and use

the notation

$$\epsilon z = (\epsilon_1 z_1, \ldots \epsilon_n z_n) \tag{5.6.3}$$

where here $\epsilon_i = \pm 1$ depending on whether the $i$th classical variable is even or odd. Using this notation, a function $f(z)$ of the classical variables is thus transformed under time-reversal to $f(\epsilon z)$. To denote the time-reversal of differential operators, such as the generator of dynamics $\mathcal{L}$, we use the shorthand notation $\mathcal{L}_\epsilon$, which implies changing all occurrences of $z_i$ to $\epsilon_i z_i$, including in derivatives.

An important feature of detailed balance is that it is always defined with respect to a given state. Although up to now we have focused on classical-quantum fixed points $\pi$ that are of the standard thermal form $\pi \propto \exp(-\beta H)$, for the remainder of our discussion of detailed balance we allow $\pi$ to be a generic fixed point. Aside from generalising the discussion, this is also a natural choice given the earlier form of our dynamics, where the key operators $L_z$ and $M_{xy}$ depended explicitly on $\pi$ rather than the $H$. For this section, we therefore allow $\pi$ to be a generic fixed point, that may be written generally in the form

$$\pi(z) = \frac{1}{\mathcal{Z}} e^{-\Phi(z)}, \tag{5.6.4}$$

where $\Phi(z)$ is a Hermitian operator that we refer to as the potential. In order to define detailed balance with respect to this state, we shall need to make three assumptions that are standard in the classical and quantum cases [197–199]. Firstly, we will assume that $\pi$ has boundary conditions such that it vanishes at infinity in the classical configuration/phase space; this ensures that the state can be normalised, and that the representation of the adjoint generator introduced in (5.6.2) may be used. Secondly, we assume that the state $\pi$ is invertible at every point in phase space i.e. the quantum degrees of freedom must always have a non-zero probability of being in an arbitrarily excited state. Finally will assume that $\pi$ is invariant under time-reversal i.e. $\pi(\epsilon z) = \pi(z)$, as is the case for the thermal state for time-reversal invariant Hamiltonians.

Having defined the notion of time-reversal and the requirements of the fixed point $\pi$, we may define detailed balance in the hybrid setting. A classical-quantum dynamics described by the generator $\mathcal{L}$ will be said to satisfy detailed balance with respect to $\pi$ if and only if there exists a Hermitian, time-reversal invariant operator $X$ that commutes with $\pi$ such that

$$\pi^{-1/2} \mathcal{L}(\pi^{1/2} A \pi^{1/2}) \pi^{-1/2} = \mathcal{L}_\epsilon^\dagger(A) - 2i[X, A] \tag{5.6.5}$$

for all operator-valued functions of phase space $A$.

To motivate this definition as the correct definition of detailed balance in the classical-quantum setting, we consider two limiting cases. Firstly, taking $\pi$ and $A$ to be proportional to the identity operator, one may check that this definition reduces to the requirement that

$$\pi^{-1}(z)\mathcal{L}(\pi(z)f(z)) = \mathcal{L}_{\epsilon}^{\dagger}(f(z)) \tag{5.6.6}$$

holds for all functions $f(z)$, where here $\mathcal{L}$ denotes a general generator of Fokker-Planck dynamics. This equation, alongside the assumption that $\pi$ is invariant under time-reversal, exactly coincides with the definition of detailed balance in the classical setting, when using the characterisation of detailed balance in terms of generators developed by Risken [198]. Secondly, taking $\pi$ and $A$ to have no dependence on $z$, we find that the detailed balance condition reduces to

$$\pi^{-\frac{1}{2}}\mathcal{L}(\pi^{\frac{1}{2}}A\pi^{\frac{1}{2}})\pi^{-\frac{1}{2}} = \mathcal{L}^{\dagger}(A) - 2i[X, A] \tag{5.6.7}$$

for all operators $A$, where here $X$ is any Hermitian operator such that $[X, \pi] = 0$. This provides a definition of detailed balance in the quantum setting [199]. Although other definitions of detailed balance are available in the quantum setting due to alternative operator orderings of $\hat{\pi}$, this "symmetric" definition is the weakest possible, and thus encompasses the broadest class of dynamics.

From the above, it is straightforward to see that the definition of classical-quantum detailed balance we provide is a straightforward generalisation of these two definitions, generated by combining the uniquely classical and quantum structures associated to each. Namely, by using the left-hand and right-hand sides of definition (5.6.7) which respect operator ordering, while including the time-reversal operation arising in definition (5.6.6) we arrive at the definition of detailed balance provided in (5.6.5). The only ambiguity that arises is whether $X$ is chosen to be invariant under time-reversal or not, since $X$ and time-reversal only simultaneously appear in the full classical-quantum case. In our definition we opt for the former, which ultimately is supported by the identification of $X$ with the classical-quantum Hamiltonian $H$ when we come to study detailed balance for the main dynamics introduced in Sec. 5.3.

Finally, we note an important feature of classical-quantum detailed balance that connects this concept to the earlier sections of this chapter. Taking $A$ to be the identity operator, and

independent of $z$, we see that the left hand side of (5.6.5) reduces to $\pi^{-\frac{1}{2}}\mathcal{L}(\pi)\pi^{-\frac{1}{2}}$. Doing the same for the right hand side, we see that the commutator with $X$ vanishes, leaving simply $\mathcal{L}_\epsilon^\dagger(\mathbb{1})$. Since the adjoint map under time-reversal remains unital, we see that the entirety of the right hand side vanishes. Acting with $\pi^{1/2}$ on either side of the lefthand side, we thus see that that $\mathcal{L}(\pi) = 0$. It therefore follows that classical-quantum detailed balance implies thermal state preservation i.e.

$$\begin{matrix}\mathcal{L} \text{ satisfies DB} \\ \text{w.r.t. } \pi\end{matrix} \implies \mathcal{L}(\pi) = 0. \tag{5.6.8}$$

Understanding how in practice to relate this condition to the thermal state preserving dynamics we have already provided in terms of $L_z$ and $M_{xy}$ will be the main aim of the rest of this section.

### 5.6.3 Detailed balance conditions for purity-preserving dynamics

In this section we derive conditions on the basic components of the classical-quantum master equation, such as the diffusion matrix and back-reaction operators, that are satisfied if and only if a dynamics satisfies classical-quantum detailed balance. To derive this general set of conditions, we first restrict ourselves to the subset of dynamics that preserve the decoherence-diffusion trade-off – this is later generalised in Section 5.6.4 to cases where the quantum state does not remain pure conditioned on the classical trajectory.

In order to derive a set of sufficient and necessary conditions, we first define a set of operators that are characterised by how they transform under time-reversal. In particular, we may define the symmetric and anti-symmetric parts of the Hamiltonian as

$$G^S(z) = \frac{G(z) + G(\epsilon z)}{2} \tag{5.6.9}$$

$$G^A(z) = \frac{G(z) - G(\epsilon z)}{2} \tag{5.6.10}$$

and the reversible and irreversible parts of the classical drift and backreaction operators $K_i$ as

$$K_i^{rev}(z) = \frac{K_i(z) - \epsilon_i K_i(\epsilon z)}{2} \tag{5.6.11}$$

$$K_i^{irr}(z) = \frac{K_i(z) + \epsilon_i K_i(\epsilon z)}{2}. \tag{5.6.12}$$

These operators satisfy the following relations

$$G^S(\epsilon z) = G^S(z) \tag{5.6.13}$$

$$G^A(\epsilon z) = -G^A(z) \tag{5.6.14}$$

$$K_i^{rev}(\epsilon z) = -\epsilon_i K_i^{rev}(z) \tag{5.6.15}$$

$$K_i^{irr}(\epsilon z) = \epsilon_i K_i^{irr}(z), \tag{5.6.16}$$

and hence allow the dynamics under time-reversal to be written in terms of quantities dependent on $z$ rather than $\epsilon z$.

Having defined this alternate set of operators, we are now able to derive necessary and sufficient conditions on these in order for classical-quantum detailed balance to hold. Since we are initially considering dynamics that saturates the trade-off i.e. that preserves the purity of quantum states in the unravelling, we first assume that all of the Lindblad operators responsible for additional decoherence vanish i.e. $\tilde{L}_\alpha = 0$ for all $\alpha$. Rewriting this simplified form of the generator $\mathcal{L}$ given in (2.20) in terms of $K_i^{rev}$,$K_i^{irr}$,$G^S$ and $G^A$, it is straightforward to compute the form of $\mathcal{L}_\epsilon^\dagger$ by performing the time-reversal operation on the $\mathcal{L}^\dagger$ and using the relations given in (5.6.13) to (5.6.16). Substituting in the forms of $\mathcal{L}$ and $\mathcal{L}_\epsilon$ into the definition of detailed balance (5.6.5), we find a sum of terms containing $A$, $\partial_i A$ and $\partial_i \partial_j A$ that must equal zero. Since these must hold for all $A$, the Hermitian and anti-Hermitian parts of each expression containing different derivatives of $A$ lead to independent conditions on the dynamics for detailed balance. Using the positivity conditions (2.21) and (2.22), in Appendix M we show that this leads to the following sufficient and necessary conditions for classical-quantum dynamics that saturate the decoherence-diffusion trade-off to also satisfy detailed balance

$$D_{2,ij}(\epsilon z) = \epsilon_i \epsilon_j D_{2,ij}(z) \tag{5.6.17}$$

$$K_i^{rev}\pi^{1/2} - \pi^{1/2}K_i^{rev\dagger} = ia_i\pi^{1/2}, \tag{5.6.18}$$

$$K_i^{irr}\pi^{1/2} + \pi^{1/2}K_i^{irr\dagger} = \frac{1}{2}\frac{\partial D_{2,ij}}{\partial z_j}\pi^{1/2} + D_{2,ij}\frac{\partial \pi^{1/2}}{\partial z_j} \tag{5.6.19}$$

$$-\frac{i}{\hbar}\{G^S, \pi^{1/2}\}_+ = O^S - i\{X, \pi^{1/2}\}_+ \tag{5.6.20}$$

$$-\frac{i}{\hbar}[G^A, \pi^{1/2}] = O^A, \tag{5.6.21}$$

where here $a_i$ are the elements of a real vector $a(z)$ that satisfy $a_i(\epsilon z) = -\epsilon_i a_i(z)$, $X$ is a Hermitian operator that is symmetric under time-reversal and commutes with $\pi$, and the operators $O^S$ and $O^A$ are defined as

$$\begin{aligned} O^S = &\frac{1}{2}\frac{\partial}{\partial z_i}(K_i^{irr}\pi^{1/2} - \pi^{1/2}K_i^{irr\dagger}) \\ &- \frac{1}{2}(\mathbb{I} - D_2 D_2^{-1})_{ij}(K_i^{irr}\frac{\partial \pi^{\frac{1}{2}}}{\partial z_j} - \frac{\partial \pi^{\frac{1}{2}}}{\partial z_j}K_i^{irr\dagger}) \\ &- \frac{1}{4}D_{2,ij}^{-1}\frac{\partial D_{2,ik}}{\partial z_k}(K_j^{irr}\pi^{1/2} - \pi^{1/2}K_j^{irr\dagger}) \\ &+ \frac{i}{2}D_{2,ij}^{-1}a_i(K_i^{rev}\pi^{1/2} + \pi^{1/2}K_i^{rev\dagger}) \\ &+ \frac{1}{2}D_{2,ij}^{-1}[K_i^{rev\dagger}K_j^{rev} + K_i^{irr\dagger}K_j^{irr}, \pi^{1/2}], \end{aligned} \tag{5.6.22}$$

and

$$\begin{aligned} O^A = &\frac{1}{2}\frac{\partial}{\partial z_i}(K_i^{rev}\pi^{1/2} + \pi^{1/2}K_i^{rev\dagger}) \\ &+ \frac{1}{2}(\mathbb{I} - D_2 D_2^{-1})_{ij}(K_i^{rev}\frac{\partial \pi^{\frac{1}{2}}}{\partial z_j} + \frac{\partial \pi^{\frac{1}{2}}}{\partial z_j}K_i^{rev\dagger}) \\ &- \frac{1}{4}D_{2,ij}^{-1}\frac{\partial D_{2,ik}}{\partial z_k}(K_j^{rev}\pi^{1/2} + \pi^{1/2}K_j^{rev\dagger}) \\ &+ \frac{i}{2}D_{2,ij}^{-1}a_i(K_i^{irr}\pi^{1/2} - \pi^{1/2}K_i^{irr\dagger}) \\ &+ \frac{1}{2}D_{2,ij}^{-1}\{K_i^{rev\dagger}K_j^{irr} + K_i^{irr\dagger}K_j^{rev}, \pi^{1/2}\}_+. \end{aligned} \tag{5.6.23}$$

We refer to these five conditions as the diffusion constraint, reversible back-reaction constraint, irreversible back-reaction constraint, symmetric unitary generator constraint and anti-symmetric unitary generator constraint respectively. These are extended to the case where classical-quantum dynamics does not necessarily saturate the decoherence-diffusion trade-off in the next section.

Before moving on, we observe some basic consequences of these conditions. Firstly, we see that the diffusion constraint is identical to the known classical condition on the diffusion matrix for detailed balance [197, 198] – we shall further investigate how these conditions reduce to the classical case in 5.6.5. Secondly, we see that the reversible and irreversible back-reaction constraints, which state that the back-reaction operators must be related to both $\pi^{1/2}$ and its first derivatives, are reminiscent of those for $L_z$ given in (5.3.2) and (5.3.1) respectively. Similarly, we see that as with the definition of the Hermitian $M_{xy}$ operators of (5.3.4), the

equation for $G^S$ takes the form of a Lyapunov equation, and thus can be directly solved to give

$$G^S = i\hbar \int_0^\infty e^{-s\pi^{1/2}} O^S e^{-s\pi^{1/2}} ds + X. \tag{5.6.24}$$

Turning now to the antisymmetric unitary generator constraint, it is important to note that while the constraint for $G^S$ purely constraints the quantum unitary evolution, the equation for $G^A$ includes a constraint on the form of $K^{irr}$, $K^{rev}$ and $D_2$ independent of $G^A$, namely that

$$\langle n(z)|O^A|n(z)\rangle = 0 \quad \forall n \tag{5.6.25}$$

where $|n(z)\rangle$ is the adiabatic basis defined for the generic fixed point $\pi$ i.e. the eigenstates of the potential operator $\Phi(z)$. Although the solution for $G^A$ is not unique, since any time-reversal anti-symmetric Hermitian operator that commutes with $\pi^{1/2}$ may be added to it, the part of the operator that does not commute with $\pi^{1/2}$ may be uniquely solved in terms of the adiabatic basis, giving the off-diagonal elements of $G^A$ in this basis as

$$G^A_{nm} = i\hbar \frac{\langle n(z)|O^A|m(z)\rangle}{\sqrt{p_m} - \sqrt{p_n}} \quad n \neq m \tag{5.6.26}$$

where here $p_n$ is the eigenvalue of $\pi$ corresponding to the adiabatic state $|n(z)\rangle$. Finally, we note that the time-reversal property of the vector $a$ ensures that each of the detailed balance conditions is consistent under time-reversal.

### 5.6.4 Detailed balance conditions for general dynamics

To extend the derivation from the case where the decoherence diffusion trade-off is saturated, to the case where it is not, we exploit the result in Section 2.6 that states that a generic classical-quantum dynamics may always be embedded in a larger classical phase space where the trade-off is saturated. This so called "temple of the larger phase space" is useful, because it allows us to leverage the expressions previously derived in the comparatively simpler setting where the trade-off is saturated.

To begin with, we take $\mathcal{L}$ to be an arbitrary completely-positive continuous CQ generator i.e. of the form of (2.20) with $\tilde{L}_\alpha$ non-zero, and fix a given fixed point $\pi$ to consider detailed balance with respect to. We then introduce an auxiliary classical degree of freedom $y_\alpha$ for each independent traceless Lindblad operator $\tilde{L}_\alpha$. These classical degrees of freedom may be taken

to be even under time reversal symmetry without loss of generality. In this enlarged phase space, we then define a new classical-quantum generator $\tilde{\mathcal{L}}$, which takes the form

$$\tilde{\mathcal{L}}(A) = \mathcal{L}(A) + \frac{1}{2}\frac{\partial^2 A}{\partial y_\alpha \partial y_\alpha} - \frac{\partial}{\partial y_\alpha}(\tilde{K}_\alpha A + A\tilde{K}_\alpha^\dagger), \tag{5.6.27}$$

where the traceless auxiliary back-reaction operators $\tilde{K}_\alpha$ have no dependence on the auxiliary degrees of freedom $y_\alpha$, and satisfy

$$\mathcal{D}(\tilde{K}_\alpha) = \mathcal{D}(\tilde{L}_\alpha), \tag{5.6.28}$$

and

$$\tilde{K}_\alpha(z)\pi^{\frac{1}{2}} + \pi^{\frac{1}{2}}\tilde{K}_\alpha^\dagger(\epsilon z) = 0. \tag{5.6.29}$$

The first of these conditions, (5.6.27) guarantees that the generator $\tilde{\mathcal{L}}$ recovers $\mathcal{L}$ upon tracing over the auxiliary degrees of freedom. The second condition (5.6.28) ensures that the $\tilde{\mathcal{L}}$ is both completely-positive and saturates the decoherence-diffusion trade-off. Finally, (5.6.29) amounts to stating that the purification we have chosen is not arbitrary, but is adapted to the choice of fixed state $\pi$ that we wish to prove the detailed balance of $\mathcal{L}$ with respect to.

Turning now to detailed balance, it is straightforward to prove using (5.6.27) and (5.6.29) that

$$\pi^{-\frac{1}{2}}\tilde{\mathcal{L}}(\pi^{\frac{1}{2}}A\pi^{\frac{1}{2}})\pi^{-\frac{1}{2}} - \tilde{\mathcal{L}}_\epsilon^\dagger(A) = \pi^{-\frac{1}{2}}\mathcal{L}(\pi^{\frac{1}{2}}A\pi^{\frac{1}{2}})\pi^{-\frac{1}{2}} - \mathcal{L}_\epsilon^\dagger(A). \tag{5.6.30}$$

An immediate consequence of this is that

$$\begin{array}{c}\mathcal{L} \text{ satisfies DB} \\ \text{w.r.t. } \pi\end{array} \iff \begin{array}{c}\tilde{\mathcal{L}} \text{ satisfies DB} \\ \text{w.r.t. } \pi\end{array} \tag{5.6.31}$$

i.e. that checking detailed balance for $\tilde{\mathcal{L}}$ with respect to $\pi$ is sufficient and necessary to conclude the same for $\mathcal{L}$.

Since $\tilde{\mathcal{L}}$ saturates the decoherence-diffusion trade-off, we can apply each of the detailed balance conditions already proven in equations (5.6.17) to (5.6.21), this time including the additional diffusion, decoherence and back-reaction associated to the auxiliary classical degrees of freedom $y_\alpha$, to find iff constraints for $\mathcal{L}$ to satisfy detailed balance. In the enlarged space, one can check from (5.6.27) that condition (5.6.17) is trivially satisfied on the auxiliary degrees of freedom, and thus provides no additional constraint. Similarly, computing the reversible and

irreversible parts of the auxiliary back-reaction operators $\tilde{K}_\alpha$ and substituting into (5.6.18) and (5.6.19), one finds that since $\pi$ is independent of $y_\alpha$ and the $\tilde{K}_\alpha$ are traceless, the constraints on the auxiliary backreaction operators $\tilde{K}_\alpha$ are equivalent to that of (5.6.29) and that the vector of real numbers $a_\alpha$ is zero. The only additional constraints come from considering the symmetric and anti-symmetric effective Hamiltonians, which in this case take the form

$$-\frac{i}{\hbar}\{G^S,\pi^{1/2}\}_+ = O^S - i\{X,\pi^{1/2}\}_+ + \frac{1}{4}[\tilde{K}_\beta^\dagger\tilde{K}_\beta + \tilde{K}_\beta^\dagger(\epsilon z)\tilde{K}_\beta(\epsilon z),\pi^{\frac{1}{2}}] \tag{5.6.32}$$

$$-\frac{i}{\hbar}[G^A,\pi^{1/2}] = O^A + \frac{1}{4}\{\tilde{K}_\alpha^\dagger\tilde{K}_\alpha - \tilde{K}_\alpha^\dagger(\epsilon z)\tilde{K}_\alpha(\epsilon z),\pi^{\frac{1}{2}}\}_+, \tag{5.6.33}$$

i.e. are modified by an additional term in terms of $\tilde{K}_\alpha$.

To relate the conditions (5.6.29), (5.6.32) and (5.6.33) on $\tilde{K}_\alpha$ to conditions on $\tilde{L}_\alpha$, we utilise (5.6.28). In particular, since the two GKLS disspators will be equal iff the Lindblad operators are related via unitary matrix [212, 213, 199], we can always rewrite the auxiliary back-reaction operators $\tilde{K}_\alpha$ as

$$\tilde{K}_\alpha = u_{\alpha\beta}\tilde{L}_\beta \tag{5.6.34}$$

where $u_{\alpha\beta}$ are the coefficients of some unitary matrix $u$ that may depend on phase space. Plugging this relation into the modified constraints (5.6.29), (5.6.32) and (5.6.33), we finally arrive at the final set of necessary and sufficient conditions for detailed balance with respect to $\pi$ as

$$D_{2,ij}(\epsilon z) = \epsilon_i\epsilon_j D_{2,ij}(z) \tag{5.6.35}$$

$$K_i^{rev}\pi^{1/2} - \pi^{1/2}K_i^{rev\dagger} = ia_i\pi^{1/2}, \tag{5.6.36}$$

$$K_i^{irr}\pi^{1/2} + \pi^{1/2}K_i^{irr\dagger} = \frac{1}{2}\frac{\partial D_{2,ij}}{\partial z_j}\pi^{1/2} + D_{2,ij}\frac{\partial\pi^{1/2}}{\partial z_j} \tag{5.6.37}$$

$$-\frac{i}{\hbar}\{G^S,\pi^{1/2}\}_+ = O^S - i\{X,\pi^{1/2}\}_+ + \frac{1}{2}[\tilde{N}^S,\pi^{\frac{1}{2}}] \tag{5.6.38}$$

$$-\frac{i}{\hbar}[G^A,\pi^{1/2}] = O^A + \frac{1}{2}\{\tilde{N}^A,\pi^{\frac{1}{2}}\}_+ \tag{5.6.39}$$

$$\tilde{L}_\alpha(z)\pi^{1/2} = -(u^\dagger(z)u^*(\epsilon z))_{\alpha\beta}\pi^{1/2}\tilde{L}_\beta^\dagger(\epsilon z), \tag{5.6.40}$$

where here we have defined $\tilde{N}^S$ and $\tilde{N}^A$ as the symmetric and anti-symmetric parts under time-reversal of the operator

$$\tilde{N} = \tilde{L}_\alpha^\dagger\tilde{L}_\alpha. \tag{5.6.41}$$

We thus see that when the decoherence-diffusion trade-off is not saturated, the symmetric and anti-symmetric unitary generator constraints found previously are modified to depend on the excess decoherence, while a sixth constraint (5.6.40), that we refer to as the decoherence constraint, provides conditions on the Lindblad operators of the excess decoherence that must be satisfied in order for the dynamics to satisfy detailed balance. This new set of conditions satisfies similar properties to before, in particular with analogous relations to (5.6.24), (5.6.25) and (5.6.26) that are straightforward to find using the same arguments.

### 5.6.5 Classical and quantum detailed balance

Having found the general form of conditions for a classical-quantum dynamics to satsify detailed balance, we now turn to check that these indeed correctly reproduce the known conditions in the purely classical and quantum cases.

We first turn to the purely classical limit. To do so, we first set $\tilde{L}_\alpha = 0$, allowing us to use the characterisation of detailed balance for dynamics that saturates the trade-off given in Eqs. (5.6.17) to (5.6.21). Setting $G = 0$, $K_i = \frac{1}{2} D_i^C \mathbb{1}$, where $D^C$ is a real-valued vector representing the classical drift, and letting $\pi$ be proportional to the identity, the constraints simplify considerably. We first note that in this case the reversible back-reaction constraint (5.6.18) is trivially satisfied and implies that $a_i$ is zero for all $z$. Since this means that $O^S$ also vanishes, we see that the symmetric unitary generator constraint is also necessarily satisfied. Turning now to the anti-symmetric unitary constraint, we note while $G^A$ vanishes, the additional condition (5.6.25) nevertheless provides a non-trivial condition on the classical dynamics. In particular, we see that since $\pi$ is proportional to the identity, every vector is a valid adiabatic state, and thus that the entire expression for $O^A$ must vanish for detailed balance to hold. Writing this final constraint alongside the diffusion and irreversible back-reaction constraints, and making the appropriate simplifications given the form of $K_i$ and properties of the pseudoinverse, we find the following three constraints in the classical limit

$$D_{2,ij}(\epsilon z) = \epsilon_i \epsilon_j D_{2,ij}(z) \tag{5.6.42}$$

$$D_{1,i}^{C,irr} = \frac{1}{2} \frac{\partial D_{2,ij}}{\partial z_j} + D_{2,ij} \frac{\partial \pi^{1/2}}{\partial z_j} \pi^{-1/2} \tag{5.6.43}$$

$$\frac{\partial}{\partial z_i}(D_{1,i}^{C,rev}\pi) = 0. \tag{5.6.44}$$

Additionally assuming that $D_2$ is full rank, such that its inverse is well-defined, and using the explicit form of $\pi$ provided in (5.6.4), it is straightforward to check that these conditions coincide with the necessary and sufficient conditions for classical detailed balance found in [197, 198].

To study the purely quantum dynamics, we take $K = 0$ and $D_2 = 0$, and assume that $\tilde{L}$, $S$ and $\pi$ have no dependence on phase space. In this case the only non-trivial constraints are

$$\tilde{L}_\alpha \pi^{1/2} = -(u^\dagger u^*)_{\alpha\beta}\pi^{1/2}\tilde{L}_\beta^\dagger, \tag{5.6.45}$$

and

$$-\frac{i}{\hbar}\{G, \pi^{1/2}\}_+ = -\frac{i}{\hbar}\{X, \pi^{1/2}\}_+ + \frac{1}{2}[\tilde{L}_\beta^\dagger \tilde{L}_\beta, \pi^{\frac{1}{2}}]. \tag{5.6.46}$$

Defining the additional unitary matrix $v = u^\dagger u^*$, this exactly reproduces the known conditions of [199]. In fact, the form that we derive makes it explicit that the unitary matrix $v$ must also be symmetric, which follows by taking the complex conjugate of Eq. (5.6.45).

### 5.6.6 Proving detailed balance for $L_z$, $M_{xy}$ dynamics

Having derived the form of sufficient and necessary conditions for detailed balance in classical-quantum systems and checked it agrees with the known conditions for classical and quantum detailed balance, we finally turn to show that the dynamics presented in Section 5.3 satisfies classical-quantum detailed balance.

Considering first the overdamped dynamics, we begin by finding the form of the symmetric and antisymmetric parts of the generator of the unitary dynamics, as well as the reversible and irreversible parts of the back-reaction operators. Comparing the form of (5.3.10) to (2.20) to read off $G$ and $K_x$, and using the definitions (5.6.9) to (5.6.12), we find the dynamics to be entirely characterised by the following operators

$$\begin{gathered} G^S = H + \frac{\mu\beta}{8}M_{xx} \qquad G^A = 0 \\ K_x^{rev} = 0 \qquad K_x^{irr} = -\frac{\mu}{2}L_x \qquad D_2 = \frac{2\mu}{\beta} \end{gathered} \tag{5.6.47}$$

Here we see that both $H$ and $M_{xx}$ are time-reversal invariant, while the anti-symmetric part of the unitary generator $G^A$ vanishes. As expected for an overdamped particle dynamics, the reversible part of the dynamics also vanishes.

To check detailed balance in the overdamped dynamics, we use the sufficient and necessary conditions derived in Sections 5.6.3 and 5.6.4. Since this dynamics saturates the trade-off, in this case we may use the simpler conditions given in (5.6.17) to (5.6.21) to check whether detailed balance is satisfied. Since the diffusion coefficient is constant and $x$ is an even variable under time-reversal, it is immediate to see that the diffusion constraint (5.6.17) is satisfied. Substituting in the definition of $L_x$ given in (5.3.1) it is straightforward to verify the the irreversible back-reaction constraint (5.6.19) holds, while $K^{rev} = 0$ implies that the reversible back-reaction constraint also holds with $a(x) = 0$. To see that the symmetric unitary generator constraint (5.6.20) holds, we first compute $O^S$. Since here $D_2$ is full rank, $a$ is zero, and $L_x$ satisfies (5.3.2), we see that $O^S$ simplifies to simply $(\mu\beta/16)[L_x^\dagger L_x, \pi^{1/2}]$. Comparing the resulting symmetric unitary generator constraint with the definition of $M_{xx}$ provided in (5.3.4), we see that Equation (5.6.20) holds, with the time-reversal invariant Hermitian operator $X$ being identified with the classical-quantum Hamiltonian $H$ divided by $\hbar$. Finally, one may use the same relations to see that $O^A = 0$, which since the antisymmetric part of the unitary generator $G^S$ is zero implies that the antisymmetric unitary generator constraint (5.6.21) is also satisfied. The overdamped dynamics thus satisfies classical-quantum detailed balance with respect to $\pi$ as claimed.

Turning now to the underdamped dynamics, we again first find the explicit forms of the symmetric and anti-symmetric parts of $G$ and the reversible and irreversible parts of $K$. Comparing (5.3.17) to (2.20) and using the defintions as before we find

$$\begin{aligned} G^S &= H + \frac{\beta}{8\gamma} M_{qq} \qquad & G^A &= \frac{i\hbar}{16}\beta\frac{p}{m}(L_q^\dagger - L_q) \\ K^{rev} &= \frac{1}{2}\begin{pmatrix} -p/m\mathbb{1} \\ -L_q \end{pmatrix} \qquad & K^{irr} &= \frac{1}{2}\begin{pmatrix} 0 \\ -\gamma p/m\mathbb{1} \end{pmatrix} \\ & & D_2 &= \begin{pmatrix} 0 & 0 \\ 0 & 2\gamma/\beta \end{pmatrix} \end{aligned} \tag{5.6.48}$$

Here we see that the reversible parts of the dynamics are associated to terms that previously

made up the Alexandrov bracket in the high temperature limit (c.f. Section 5.3.5), while the irreversible part of the dynamics relates to the friction. The appearance of an anti-symmetric component of the unitary generator $G^A$ arises due the inclusion of the classical drift into the the back-reaction operators, which leads to an additional term in the unitary part of the dynamics that acts to cancel the new cross terms in the decoherence part of the dynamics.

To show that the underdamped dynamics also satisfies detailed balance, we check the dynamics against the conditions in (5.6.17) to (5.6.21). As before, the diffusion constraint is straightforward to check is satisfied, given that the only non-zero component is $D_{2,pp}$, which does not change under time-reversal. To check the reversible back-reaction constraint, we note again that the property of the $L_z$ operators (5.3.2) means that the constraint is trivially satisfied with $a(q,p) = (0,0)^T$, while the irreversible back-reaction constraint is straightforward to check is satisfied using the fact that the thermal state in this dynamics is assumed to contain a classical kinetic term $p^2/(2m)\mathbb{1}$. To check the symmetric unitary generator constraint, we first compute $O^S$, which in this case simplifies to $\beta/(16\gamma)[L_q^\dagger L_q, \pi^{1/2}]$. As in the overdamped case, comparing this to the definition of $M_{xx}$ we see that this is indeed satisfied, with $X$ identified with $H/\hbar$. Finally, we check the anti-symmetric unitary generator constraint. To do so, we first compute $O^A$. In this case, $D_2$ is not full-rank, and thus we must retain a number of terms that vanished in the overdamped case. Computing this explicitly, we find that $O^A$ takes the form $(\beta p)/(16m)[L_q^\dagger - L_q, \pi^{1/2}]$. This final constraint is therefore exactly satisfied, given the value of $G^A$, thus demonstrating that the underdamped dynamics we provide also satisfies classical-quantum detailed balance.

## 5.7 Discussion

In this chapter, we introduced classical-quantum dynamics compatible with the laws of thermodynamics. There were three main technical contributions to achieve this: (1) the proof in Section 5.2 that thermal-state preserving, completely-positive and linear dynamics necessarily obeys the second law of thermodynamics; (2) the identification in Section 5.3 of the $L_z$ and $M_{xy}$ classes of operators, given in Eqs. (5.3.1) and (5.3.3), which we showed could be used to construct such dynamics; and (3) the definition and characterisation of detailed-balance in

classical-quantum systems in Section 5.6, which we showed also applied to our $L_z$, $M_{xy}$ constructed dynamics. While we presented basic forms of such dynamics for the case of overdamped and underdamped classical systems in Eqs. (5.3.10) and (5.3.17), the $L_z$ and $M_{xy}$ operators may be used to construct dynamics to treat a wide variety of systems, with some straightforward generalisations presented in Appendix J.

One expects that these dynamics may applied in a wide range of settings. Aside from the applications to continuous measurement theory and molecular dynamics, illustrated via the analytically and numerically solved toy models in Sections 5.4 and 5.5, one could use the dynamics to study systems in quantum optics where part of the system behaves semi-classically [69], in many-body systems where local effective classical systems acting as monitoring devices, or indeed models designed to probe classical-quantum coupling [38] extended to non-perturbative regimes. The key step in any application is the identification of a fixed point of the combined system, which is then used to find the operators $L_z$ and $M_{xy}$. While the computation of these operators may in general prove challenging, the simplified forms of $L_z$ and $M_{xy}$ in the high temperature limit, given in Eqs. (5.3.9), provides a starting point for studying these dynamics that also makes connection with existing mean-field and quantum-classical Liouville approaches, as shown in Section 5.3.5. Since these models relate to both existing semi-classical methods motivated from quantum theory, and are motivated by fundamental physical principles, we expect them to be successful in describing a range of quantum systems operating in an effectively classical-quantum regime.

Aside from understanding the current thermodynamic framework as an effective theory that arises from quantum mechanics, it is interesting to consider what it may say about quantum mechanics itself. Since quantum mechanics is inherently random, at the level of the interaction between the classical measurement apparatus and the quantum system, it is reasonable to imagine that this stochastic behaviour could arise due to tracing out a number of microscopic degrees of freedom. If the underlying dynamics of these microscopic degrees of freedom is symmetric under time reversal [197], then one expects the resulting macroscopic theory of the combined classical-quantum system to satisfy detailed balance. In principle, we thus see that whether or not the detailed balance conditions (5.6.35) to (5.6.40) are satisfied in practice for classical measurement devices and quantum systems provides a test of their underlying physics.

If the dynamics satisfy detailed balance, one may be tempted to consider the possibility that quantum mechanics itself is an effective description of a microscopic T-symmetric theory, while if not, the description of quantum mechanics as the fundamental theory, in which measurement is an inherently irreversible process, becomes a more attractive option.

Finally, given that thermodynamics fundamentally is a theory that puts limitations on the allowable transformations of a system [214], it is interesting to consider what general bounds may be derivable from a consistent thermodynamic theory of classical and quantum systems. For the class of dynamics introduced in Section 5.3, it was remarked that since both the Einstein relation and the decoherence-diffusion trade-off relate back-reaction in the classical-quantum system to the diffusion, they could be used to derive bounds on decoherence rates, given in Eqs. (5.3.16) and (5.3.25) for the overdamped and underdamped cases. Beyond these basic model-dependent bounds, we expect the theory we present here to provide a number of general thermodynamic bounds on systems described by a classical-quantum framework, and thus bounds on the achievability of a number of transformations, from electronic transitions in molecules to allowable state preparation in measurement-based feedback.

# Chapter 6

# Concluding remarks

We have demonstrated in the above work that completely-positive and linear classical-quantum dynamics can appear naturally as a physically-motivated effective description of different systems. Indeed, the features in common between the dynamics we have found, despite starting each time from independent motivations, adds some support to the idea that these dynamics, rather than merely being theoretical constructs for probing our understanding of how to construct physical theories, may indeed prove useful in studying a range of physical phenomena, from gravitational systems in semi-classical regimes, to molecular dynamics and quantum measurement and control systems.

Perhaps the most remarkable aspect of our study lies in the form of operators describing back-reaction and decoherence in the effective classical-quantum dynamics we study. Writing these explicitly, the effective dynamics arising from quantum theory in Chapter 4 is determined by the operators

$$L_z^H = iE_f \frac{\partial}{\partial z}\big(e^{-\frac{i}{E_f}H}\big)e^{\frac{i}{E_f}H}, \tag{6.0.1}$$

while for the thermal state preserving dynamics of Chapter 5, the operators take the form

$$L_z = -\frac{2}{\beta}\frac{\partial}{\partial z}\big(e^{-\frac{\beta}{2}H}\big)e^{\frac{\beta}{2}H}. \tag{6.0.2}$$

It is immediate from the above definitions that these operators coincide up to the Wick rotation

$$\frac{i}{E_f} \leftrightarrow \frac{\beta}{2}. \tag{6.0.3}$$

The entirely independent appearance of the same structure of operator from both thermodynamically consistent theories and those arising from a fully quantum theory suggests some deeper relationships between the different effective theories of classical-quantum dynamics that we present here.

However, given that we did not derive the same dynamics each time, it is sensible to ask a basic question – which dynamics is relevant in different situations? As a guiding principle, one may expect that the basic dynamics of Eqs. (3.8) to (3.9) and Eq. (3.15), which provided a completely-positive and linear version of the standard mean-field and quantum-classical Liouville approaches, should provide a good description of effective classical-quantum dynamics when the noise in the classical system is large and friction is small. This is because in this case, $E_f$ is large and $\beta$ is small, and thus all three main forms of the operators determining back-reaction and decoherence become approximately equal i.e. $L_z^H \approx L_z \approx \partial_z H$. In this regime, we find that all three forms of dynamics that we introduce also take the same approximate structure i.e. that which appears in the healed semi-classical dynamics Eqs. (3.8) to (3.9) and Eq. (3.15), up to terms that do not affect the back-reaction on the classical system, nor the basis in which the quantum system decoheres.

However, outside of this regime, the three dynamics will in general differ for Hamiltonians that do not commute with themselves at different points in the classical phase space. Rather than suggesting one or the other theory is incorrect, we instead see a natural feature of effective theories arising – that the underlying theory that the effective classical-quantum description arises from has some effects on the resulting dynamics. In this case, we expect that the physically motivated dynamics of Eq. (4.4.5) coming from a full quantum theory, or the dynamics in (5.3.17) arising from a thermal environment, should provide improvements on the dynamics of Eqs. (3.8) to (3.9) and Eq. (3.15) that are not apparent at high temperatures/large noise in the classical system. Understanding which of $L_z^H$ and $L_z$ may be used in these contexts, and indeed whether linear combinations or other hybridisations of the two operators may be used, is an interesting question we leave to future work.

Of course, in practice, none of the dynamics are likely to provide an exact fit to experiment. Like for most real world models, the true dynamics will likely require a number of additional

bespoke features added, such as including additional sources of noise on the system. However, the dynamics we provide here provide a starting point for constructing such models, that are grounded in basic physical principles. Moreover, the tools we provide, such as being able to characterise purity, or move between unravelling and master equation pictures, or numerical methods for simulating the dynamics, provide basic building blocks to understand a wide range in consistent dynamics of classical and quantum systems.

Finally, we end with a somewhat philosophical remark. At the beginning of this work, it was noted that quantum theory itself suggested the correct way of coupling classical and quantum systems. While this appears in the Born rule, the sudden instantaneous nature of this collapse appeared incompatible with any standard mechanical explanation. However, after the development of continuous measurement theory, this collapse process could be effectively slowed, allowing the dynamics of the classical measuring apparatus and quantum system to be put in the setting of continuous evolution. In this work, we see that one can take this measurement process one step further into the realm of a physical theory, by treating the measuring device as a mechanical classical system that exchanges heat and information with its environment. These models of classical and quantum systems provide a version of quantum mechanics that is both mechanical at the level of unitary dynamics *and* mechanical at the level of the measurement. Whether effective classical-quantum dynamics can help render quantum theory any less strange, or suggest how it itself emerges as an effective theory remains to be seen – but they at least breathe some new life into an old theory.

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# Appendix A

# Linearity and complete-positivity

A key feature common to both classical probability theory and quantum theory is that the states in the theory, i.e. probability distributions $P(z,t)$ and density operators $\rho(t)$, are assumed to have positive and linear evolution. In this work we shall assume the same must hold for the classical-quantum state $\varrho(z,t)$, and we will take this to be required for any classical-quantum dynamics to be consistent. Since $\varrho(z,t)$ is defined as $\mathbb{E}[\delta(z-z_t)\rho_t]$, requiring the consistency of the evolution of $\varrho(z,t)$ puts constraints on the possible allowed dynamics of $\rho_t$ and $z_t$.

To see why positivity and linearity of the dynamics of $\varrho(z,t)$ are important properties for consistency, we first note that probability distributions, density operators, and classical-quantum states, all satisfy the requirements of a more general definition of *states*. Specifically, statistical mixtures of different configurations are represented by convex combinations of states, and expectation values are computed by a map that is linear on both the states and observables of the theory. This means that the classical-quantum states we present here are the same as the states discussed in a more general class of probability theories known as GPTs [215, 216, 101].

In such theories, the requirement for a consistent probabilistic interpretation of measurement outcomes leads to constraints on the evolution of states. If the evolution laws do not preserve the positivity of the state, then the theory will predict negative probabilities for some measurement outcomes. If the evolution laws of states are not linear, it leads to the non-physical result that outcomes of experiments depend on whether independent measurement records are deleted

before or after the evolution. To see this, take $\omega_1, \omega_2$ to be two states of a theory, generated with probabilities $p$ and $(1-p)$ respectively, and define the evolution map $\mathcal{E}_t$ as the map which takes every initial state to its final state at time $t$. If an observer forgets which state was prepared immediately, they predict the final state to be $\mathcal{E}_t(p\omega_1 + (1-p)\omega_2)$, which should be the same as $p\mathcal{E}_t(\omega_1)+(1-p)\mathcal{E}_t(\omega_2)$, the state they predict if they wait to delete the measurement record until after the evolution [217, 215, 218, 219].

Although we have simply stated that the dynamics of $\varrho(z,t)$ should be positive, in the context of quantum mechanics, a stronger notion of positivity is required for the dynamics to be consistent when acting on part of a larger system. This is called *complete-positivity*, and ensures that when the dynamics is applied to half of an entangled quantum state, negative probabilities do not arise [77]. We will assume the same holds in the classical-quantum case.

Taken together, we thus will state that a dynamics is *consistent with a classical-quantum description*, or simply *consistent*, whenever the dynamics of $z_t$ and $\rho_t$ lead to dynamics that is completely-positive and linear on the classical-quantum state $\varrho(z,t)$. It is worth emphasising that this is a very weak set of conditions, and indeed is a strict subset of the consistency conditions of [15]. This being said, given that it was shown in the same work that no dynamics could be constructed that satisfies the full set of these consistency conditions, we see that taking a weaker set of conditions is a necessary step to constructing examples of consistent classical-quantum dynamics.

Finally, it is important to emphasise that a consistent theory may still have primary quantities that uniquely determine the state of a system, which nevertheless do not themselves evolve linearly. For example, in the Madelung formulation of unitary quantum mechanics, an auxiliary scalar and vector field are used to describe the quantum wavefunction, and evolve according to a set of non-linear equations [220, 221]. The distinction to be drawn is that objects such as these do not define states in the sense we have so far considered, since, for example, they are not related to the expectation values of the theory via a linear map. To check the consistency of dynamics in such theories, it is necessary to directly compute the evolution of the states of the theory. In this work, this has an important consequence: the evolution equations of $z_t$ and $\rho_t$ need not necessarily be linear, provided the overall dynamics induced on $\varrho(z,t)$ is.

# Appendix B

# Conditional quantum states

When a projective measurement is made in conventional quantum mechanics, the state of the quantum system conditioned on the measurement outcome is pure. However, if the measurement outcome is not conditioned on, the act of measurement will generically cause the quantum state to lose purity i.e. decohere.

To see how this feature also arises in classical-quantum systems, we first note that when an observer has some partial information $Y$, the conditional expectation of $f(z_t, \rho_t)$, denoted $\mathbb{E}[f(z_t, \rho_t)|Y]$, defines the improved estimate based on this information. This information will typically correspond to knowing some classical quantity $y(z_t)$ for a subset of time $t \in I$, and so is formally described by the $\sigma$-algebra generated by this set of random variables, which we can denote $\sigma\{y(z_s)\}_{s\in I}$ or simply $\{y(z_s)\}_{s\in I}$ for short [222].

If an observer were to repeat an experiment many times, each time measuring the quantum system at time $t$ and recording no information about the classical system, the quantum state they would infer from their observations would be $\rho(t) = \mathbb{E}[\rho_t]$. However, if each time they performed the experiment they additionally recorded some partial information about the classical trajectory $Y = \{y(z_s)\}_{s\in I}$, the quantum state determined from their observations would be the *conditional quantum state* [223]

$$\rho(t|Y) = \mathbb{E}[\rho_t|Y]. \tag{B.1}$$

i.e. an average only over realisations of the quantum state $\rho_t$ that occur with the classical

observation $Y$. It is straightforward to prove, using the Jensen inequality [222], that the entropy $S$ of the unconditioned state will always be greater than or equal to the average entropy of the conditioned state i.e.

$$S(\rho(t)) \geq \mathbb{E}[S(\rho(t|Y))]. \tag{B.2}$$

The above inequality tells us that if there are correlations between the classical and quantum systems i.e. $\mathbb{E}[f(z_t)g(\rho_t)] \neq \mathbb{E}[f(z_t)]\mathbb{E}[g(\rho_t)]$, then conditioning on a particular outcome of the classical trajectory will generically give us an improved estimate of the state of the quantum system. This improved estimation will correspond to a state with greater purity.

An important example of a conditioned quantum state is the quantum state conditioned on the full classical trajectory up to time $t$, $\rho(t|\{z_s\}_{s\leq t}) = \mathbb{E}[\rho_t|\{z_s\}_{s\leq t}]$. The information corresponding to this state is maximal, in the sense that an observer that has access to the full classical trajectory has as much information about the combined classical-quantum system as is possible without disturbing it with a quantum measurement. Perhaps surprisingly, even in this case, there can exist classical-quantum trajectories for which $\mathbb{E}[\rho_t|\{z_s\}_{s\leq t}] \neq \rho_t$. When this is the case, the individual trajectories of $\rho_t$ are not physical. This is because in this case the entropy of the conditioned quantum state $\rho(t|Y)$ is greater than that of $\rho_t$, and thus the non-uniqueness of the decomposition of mixed quantum states means there are physically equivalent $\rho'_t$ which cannot be experimentally distinguished. This is an exact analogue of the case considered in the unravelling of quantum master equations, where individual realisations of pure states of the quantum system only take on physical meaning when they are correlated with a measurement apparatus monitoring the system [43].

For this reason, we make a specific requirement on the representation of the classical-quantum dynamics we will study. Specifically, we will always choose to represent dynamics such that

$$\rho_t = \mathbb{E}[\rho_t|\{z_s\}_{s\leq t}], \tag{B.3}$$

where this equality is taken to hold except on a set of measure zero i.e. almost surely. In more technical language, this means restricting to stochastic processes of the quantum state $\rho_t$ such that the they are adapted to the $\sigma$-algebra $\sigma\{z_s\}_{s\leq t}$ [222]. To achieve this, it is necessary to allow the quantum system to be decomposed in terms of mixed states, $\rho_t$, rather than pure

states $|\psi\rangle_t$. In particular, if one was restricted to decompose the quantum system in terms of $|\psi\rangle_t$, one would find that in any setting where the quantum system undergoes decoherence from the perspective of an observer with maximum information, one would be forced to decompose the dynamics into a particular non-unique choice of pure quantum states. By contrast, since classical probability distributions can always be uniquely decomposed in terms of delta functions $\delta(z-z_t)$ in phase space, we suffer no loss of generality by assuming an unravelling of the classical system in terms of pure states i.e. in terms of $z_t$.

# Appendix C

# Toy models of healthier semi-classical dynamics

In this section we discuss a few simple toy models of the general dynamics illustrated above, specifically those generated by a Hamiltonian that saturate the decoherence-diffusion trade-off. Example trajectories for each of the models are simulated using basic numerical methods and the code can be found in [224]. The simulations include toy models of a Stern-Gerlach experiment, a spin confined in a potential, a mass in a superposition of two locations generating a gravitational potential, and vacuum fluctuations as a source for the expansion rate of the universe.

The forms of the dynamics that we numerically study here are closely related to those used to study unravellings of quantum dynamics (c.f. Section 2.7), which have a long history of simulation [212, 80, 160]. While it would be interesting to study further the convergence of the numerical methods used here by using these earlier models as benchmarks, and to find ways of improving upon them, here we will be content with simply extracting the qualitative behaviour of the toy models along single realisations of the dynamics. Comparing the number of timesteps that we use (around $N = 10^5$) to those in earlier work ($N = 5000$ in [212]), we see that these individual trajectories are likely to be accurate, and indeed demonstrate a number of features in common with earlier work [212, 80], such as rotation around the Bloch sphere and collapse to the $z$-axis.

## Vectorised notation

First, we restate the healed semi-classical equations (3.8) and (3.9), this time in the vectorised notation previously used for Equations (2.30) and (2.31) that is convenient for computing the dynamics in models such as these:

$$dz_t = \langle\{z, H\}\rangle dt + \sigma dW_t \tag{C.1}$$

$$\begin{aligned} d|\psi\rangle_t = -iH|\psi\rangle_t dt + \frac{1}{2} dW_t^T \sigma^{-1}\big[\{z, H\} - \langle\{z, H\}\rangle\big]|\psi\rangle_t \\ - \frac{1}{8}\big[\{z, H\} - \langle\{z, H\}\rangle\big]^T (\sigma\sigma^T)^{-1}\big[\{z, H\} - \langle\{z, H\}\rangle\big]|\psi\rangle_t dt \end{aligned} \tag{C.2}$$

where the sufficient and necessary condition for complete positivity is that $(\mathbb{I} - \sigma\sigma^{-1})\{z, H\} = a(z)\mathbb{1}$ for some $a(z) \in \mathbb{R}^n$.

## Linear Diosi model

In this section we turn our attention to a simple case of the Hamiltonian dynamics of Equations (C.1) and (C.2). In particular, we will consider a qubit coupled to a classical particle moving in one dimension. As a consequence, for any dynamics and at all times, we can characterise the classical-quantum system by a point $(q, p)$ in phase space and a point in the Bloch sphere.

We will consider dynamics generated by the Hamiltonian

$$H(q, p) = \frac{p^2}{2m}\mathbb{1} - 2\lambda q Z + \phi Z, \tag{C.3}$$

corresponding to a Stern-Gerlach type interaction. The interaction couples the classical particle by a linear potential to the Pauli $Z$ operator of the qubit, with the coupling strength determined by the parameter $\lambda \in \mathbb{R}$. Since the Hamiltonian is linear in phase-space coordinate $q$ and we use a single Lindblad operator, such CQ models which are continuous in phase space corresponds to the constant force models discussed in [25, 225, 226]. Jumping models were previously simulated in [75]. This same Hamiltonian constrains the qubit dynamics, which evolves according to both the interaction with the classical system, and a purely quantum Hamiltonian $\phi Z$, for $\phi \in \mathbb{R}$.

In this case, since backreaction is only in $p$, we see that picking noise in momentum only

i.e.

$$\sigma = \begin{pmatrix} 0 & 0 \\ 0 & \sigma_{pp} \end{pmatrix}, \tag{C.4}$$

gives

$$(\mathbb{I} - \sigma\sigma^{-1})\{z, H\} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} (p/m)\mathbb{1} \\ 2\lambda Z \end{pmatrix} = \begin{pmatrix} p/m \\ 0 \end{pmatrix} \mathbb{1}, \tag{C.5}$$

as required for complete positivity, where from now on we drop the subscript from $\sigma_{pp} \in \mathbb{R}$ for convenience. Having idenitified $H$ and a valid $\sigma$ given this, we can substitute these into Equations (C.1) and (C.2) to find the following dynamics:

$$dq_t = \frac{p_t}{m} dt \tag{C.6}$$

$$dp_t = 2\lambda \langle Z \rangle_t dt + \sigma dW_t, \tag{C.7}$$

and

$$d|\psi\rangle_t = -i(-2\lambda q_t + \phi)Z|\psi\rangle dt + \frac{\lambda}{\sigma}(Z - \langle Z \rangle)|\psi\rangle dW - \frac{\lambda^2}{2\sigma^2}(Z - \langle Z \rangle)^2|\psi\rangle dt. \tag{C.8}$$

These equations form a coupled set of stochastic differential equations, and may be easily simulated using stochastic finite difference methods such as the Euler-Maruyama or Milstein methods. An example of a classical-quantum trajectory generated by the Euler-Maruyama method for this classical-quantum dynamics is shown in Figure 3.1 for a classical particle initially at the origin in phase space and a quantum system initially in the state $|+\rangle$ for $m = \lambda = \sigma = 1$ and $\phi = 2$ between $t = 0$ and $t = 1$ for stepsize $\Delta t = 10^{-5}$. This model is also simulated in Figure C.1 for $m = \lambda = 1$, $\phi = 2$, $\sigma = 0.8$ and step size $\Delta t = 10^{-5}$ between $t = 0$ and $t = 0.45$, where dynamics given by the standard semi-classical approach, i.e. via Equations (3.4) and (3.5), is also simulated to allow a clear comparison of the two theories.

Since the current goal of simulation is only to illustrate the generic features of typical trajectories of these models, a reasonable check of the accuracy of these simulations may be made by measuring the distance of the quantum state from the surface of the Bloch sphere, which in this case has a reasonably small maximum violation of the order of $10^{-3}$. For numerical simulations leading to quantitative results, such as those requiring comparison to experiment, one would need to check the convergence in probability of the chosen numerical scheme to the random processes described by the stochastic differential equations [227].

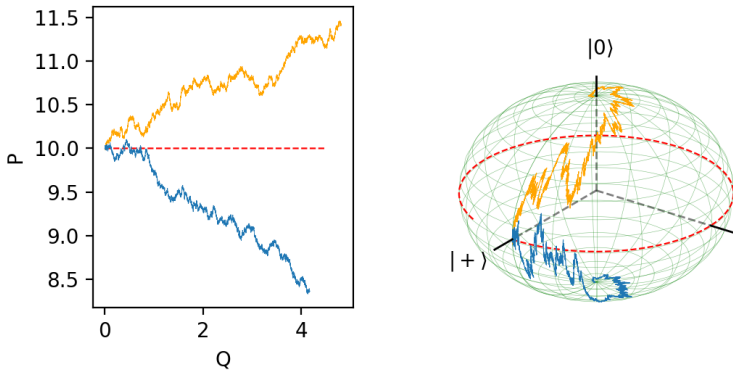


Figure C.1: Classical-quantum trajectories, represented by a classical trajectory in phase space (left) and a quantum trajectory on the Bloch sphere (right), for both the standard semi-classical equations (red, dashed lines) and two distinct realisations of their healed versions (orange upper-half lines/blue lower-half lines). Here we can clearly see that in the classical and quantum trajectories are correlated, as random variables – this should be compared to the the standard semi-classical result, for which the correlations are lost. The above figure also makes it clear that if one were to average over many quantum trajectories, the fact that half move upwards and half move downwards means that there would be a loss of purity of the quantum state, with the quantum state decohering to the centre of the Bloch sphere.

## A well and a barrier in superposition

We now come to an example that requires the general form of classical-quantum dynamics as presented in the main section, specifically by including an interaction Hamiltonian that is non-linear in $q$, and choosing a phase space-dependent diffusion process. Considering the qubit-particle set-up of the previous section, we now choose the Hamiltonian

$$H(q,p) = \frac{p^2}{2m}\mathbb{1} + \lambda\sqrt{q}Z. \tag{C.9}$$

The model describes a $\pm\lambda\sqrt{q}$ potential centred at $q = 0$, i.e. either a potential well $+\lambda\sqrt{q}$ corresponding to the state $|0\rangle$ or a potential barrier $-\lambda\sqrt{q}$ for the quantum state $|1\rangle$. Although we could consider $\sqrt{|q|}$, for simplicity we will just consider the dynamics while $q > 0$. To ensure the decoherence-diffusion trade-off is saturated, we will consider the form of Equations (C.1)/(3.8) and (C.2)/(3.9). The remaining degree of freedom is in choosing the size of the diffusion in momentum, which by the argument from the previous section is the minimal noise required, and we choose it such that $\sigma(q) = \gamma(\sqrt{q})^{-1}$ for some coupling constant $\gamma \geq 0$. This gives the following dynamics

$$dq_t = \frac{p_t}{m}dt \tag{C.10}$$

$$dp_t = -\frac{\lambda}{2\sqrt{q_t}}\langle Z\rangle dt + \frac{\gamma}{\sqrt{q_t}}dW, \tag{C.11}$$

and

$$d|\psi\rangle_t = -i\lambda\sqrt{q_t}Z|\psi\rangle dt - \frac{\lambda}{4\gamma}(Z - \langle Z\rangle)|\psi\rangle dW - \frac{\lambda^2}{32\gamma^2}(Z - \langle Z\rangle)^2|\psi\rangle dt. \tag{C.12}$$

Since the strength of the noise process also increases with proximity to the centre of the potential $q = 0$ by a factor of $\sqrt{q}$, the average rate of change of the quantum state is constant in time. In other words, even very close to a potential barrier, a strong repulsive force could equally be due to a large random kick in momentum by the diffusion process. As before, we simulate this model using the Euler-Maruyama method, and display the results in Figure C.2.

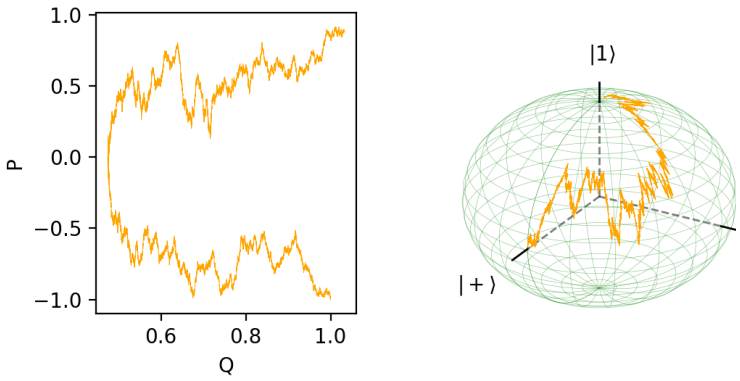


Figure C.2: A classical-quantum trajectory for the $\pm\sqrt{q}$ coupling for a step size $\Delta t = 10^{-5}$ between times $t = 0$ and $t = 2$, and parameters $m = \lambda = 1$ and $\gamma = 0.5$. Initially starting at the $q = 1$ and with momentum $p = -1$, the particle appears to rebound from a potential barrier $+\sqrt{q}$, agreeing with the evolution of the superpostion state $|+\rangle$ to a state close to $|1\rangle$ corresponding to a potential barrier, not a potential well. With probability $1/2$, the particle will instead encounter the potential well. At early times its evolution does not allow one to determine which of the two situations it is encountering.

## A toy model of a mass in superposition

We now come to a slightly more complex example, using the same philosophy as before that the quantum state of a qubit can be used to control a potential. Here we will consider the qubit to encode the position of a mass as either on the left or the right, and consider the motion of a second test mass in the Newtonian potential generated by the heavier mass. For ease of discussion one can refer to the heavier mass as the *planet*, although of course the motivation comes from interest in the gravitational field of particles which can be put in superposition [228]. The dynamics considered here can be contrasted with that of the standard semi-classical prediction where the test mass falls towards the centre of the two possible positions. Although this is a completely consistent classical-quantum theory, it is distinct from the models considered in which the gravitational field itself diffuses [125, 124, 123].

We will consider the Hamiltonian

$$H(\mathbf{r},\mathbf{p}) = \frac{\mathbf{p}\cdot\mathbf{p}}{2m}\mathbb{1} - \frac{GMm}{|\mathbf{r}-Z\mathbf{d}|} + \phi Z, \qquad Z = |L\rangle\langle L| - |R\rangle\langle R|, \tag{C.13}$$

where $\mathbf{r}$ and $\mathbf{p}$ are the position and momentum of the test mass, and $\pm\mathbf{d}$ is the position of the planet from the mean position. Choosing there to be only diffusion in momentum of the test particle that is given by a constant $\sigma$ for each direction, we find the dynamics for the components $i = x, y, z$

$$dq_t^i = \frac{p^i}{m}dt \tag{C.14}$$

$$dp_t^i = \langle \partial_i \frac{GMm}{|\mathbf{r} - Z\mathbf{d}|} \rangle + \sigma dW_i \tag{C.15}$$

and

$$d|\psi\rangle_t = -iH(z)|\psi\rangle dt + \sum_{j=x,y,z} \frac{1}{2\sigma}(\partial_j H - \langle \partial_j H \rangle)|\psi\rangle dW_j \tag{C.16}$$

$$- \sum_{j=x,y,z} \frac{1}{8\sigma^2}(\partial_j H - \langle \partial_j H \rangle)^2 |\psi\rangle dt \tag{C.17}$$

where the usual $t$ subscripts have been dropped for notational convenience, and $H(z_t)$ and $\partial_i H$ refer to the Hamiltonian and partial spatial derivatives of the Hamiltonian.

Considering first the case where $\phi = 0$, an example classical-quantum trajectory is shown for this dynamics in Figure C.3, which clearly shows the test mass approaching one planet or the other. As we can see, this model gives negligible rotation around the pole of the Bloch sphere; we may arrive at a dynamics that has a clearer representation of trajectories (and equivalent physics to an observer solely monitoring the classical test particle) by letting $\phi$ be non-zero. Such a dynamics is simulated and plotted in Figure 3.2 for $\phi = 5$, for otherwise the same choices of parameters and initial conditions as for Figure C.3.

## A toy model of vacuum fluctuations sourcing expansion

In this toy model, we consider $n$ qubits, each coupled to a local classical degree of freedom. This provides a discretized toy model of a quantum field interacting with a classical field. We will consider the quantum system to initially be in an entangled Greenberger–Horne–Zeilinger (GHZ) or *cat* state [229], and dynamics such that each subsystem back-reacts locally on a classical degree of freedom. Since the vacuum is a highly entangled state, this simulation serves as a very crude toy model for vacuum fluctuations which source the expansion of the universe

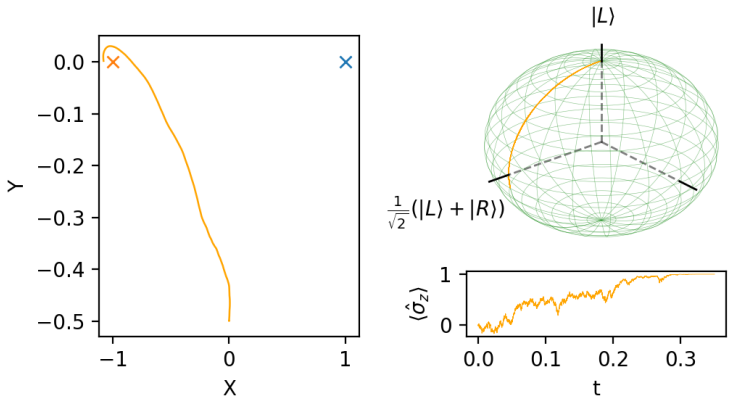


Figure C.3: A classical-quantum trajectory for a test mass and a planet in superposition, for a step size $\Delta t = 10^{-5}$ between times $t = 0$ and $t = 0.35$, and parameters $G = 1$, $M = 10$, $m = 0.01$, $\sigma = 2m$, $\phi = 0$ and $d = 1$, with the momentum dimensions of phase space suppressed. Initially starting at rest at $X = 0$ and $Y = -0.5$, the initial motion of the test mass towards the centre of the two masses (as predicted by the standard semi-classical theory) is due to a large random kick in momentum in the simulated realisation of the noise process. Due to negligible rotation around the z axis, the z component on the Bloch sphere is inset.

during inflation. Here, we find that the initially entangled quantum state back-reacts locally on a classical degree of freedom, so that the configurations of the classical degrees of freedom become correlated and the quantum state becomes unentangled. In the same way, we expect local expansion factors during inflation to be imprinted with correlations of the vacuum.

Let the local classical degrees of freedom be denoted $(\phi_i, \pi_i)$ for $i = 1, \ldots, n$, and the local Pauli operator be $Z^i$. We will then take the system to evolve under the Hamiltonian

$$H(\phi_1, \ldots, \phi_n, \pi_1, \ldots, \pi_n) = \lambda \sum_{i=1}^{n} \phi_i Z^i + \frac{\pi^2}{2m} \mathbb{1}. \tag{C.18}$$

Here $\lambda \in \mathbb{R}$ controls the strength of the coupling between the classical and quantum fields. As before, we will use the purity preserving Hamiltonian theory of equations (C.1)/(3.8) and (C.2)/(3.9), and so the only remaining freedom is in choosing the $\sigma_{ij}$. The situation here is more interesting than in the previous models, since the noise process on different lattice sites can be chosen to be correlated. Here however we will take the simplest case and assume that the noise in momentum is uncorrelated between lattice points with $\sigma_{p_i,p_j} = \delta_{ij}\sigma$, and that there

is no diffusion in $\phi$, arriving at the dynamics

$$d\phi_t^i = \frac{\pi_t^i}{m} dt \tag{C.19}$$

$$d\pi_t^i = -\lambda \langle Z^i \rangle dt + \sigma dW_t^i, \tag{C.20}$$

and

$$d|\psi\rangle_t = -i\lambda \sum_{i=1}^{n} \phi_t^i Z^i |\psi\rangle_t dt - \frac{\lambda}{2\sigma} \sum_{i=1}^{n} (Z^i - \langle Z^i \rangle)|\psi\rangle dW_i - \frac{\lambda^2}{8\sigma^2} \sum_{i=1}^{n} (Z^i - \langle Z^i \rangle)^2 |\psi\rangle_t dt, \tag{C.21}$$

where the usual $t$ subscripts have been dropped for notational convenience. While the classical degrees of freedom evolve based on the local noise and reduced quantum state, the evolution of the total n-partite quantum state is highly non-local and preserves the initial purity of the quantum state for all times.

An example classical-quantum trajectory, where a highly entangled GHZ or *cat* state evolves to a local state with no entanglement, and the local classical degrees of freedom exhibit fluctuations about a mean value, is shown in Figure 3.3. The simulation used a step size $\Delta t = 5 \times 10^{-6}$, and parameters $m = \sigma = \lambda = 1$. Note that each local degree of freedom $\phi_i$ is correlated. Here the evolution of the quantum trajectory is represented by the vector $(\langle \hat{\sigma}_x^{\otimes n} \rangle, \langle \hat{\sigma}_y^{\otimes n} \rangle, \langle Z^{\otimes n} \rangle)$, which captures the non-local dynamics that take an initial cat state $\frac{1}{\sqrt{2}}(|0\rangle^{\otimes n} + |1\rangle^{\otimes n})$ to the $|0\rangle^{\otimes n}$ state – this follows a path on the surface of the Bloch sphere for odd $n$. Had the cat state collapsed to the $|1\rangle^{\otimes 5}$ state instead, the particle positions would be driven on average in the opposite direction.

It is important to note that the fluctuations here are entirely due to the noise process, rather than the initial state, which here provides the same force at each site. These models thus, when the low noise, $\sigma \to 0$, limit is not taken, provide additional fluctuations on top of the purely "quantum" fluctutations due to the inital quantum state alone.

# Appendix D

# Pawula and CQ Pawula theorems

For convenience, we reproduce the two theorems relevant for characterising positivity of dynamics, namely the Pawula theorem [47] and the CQ Pawula theorem [45]. We then explain how the Liouville equation (4.2.4), quantum-classical Liouville equation (4.2.9), and the classical-quantum generator (4.4.5) satisfy (or not) the various required forms for positivity.

**Pawula (1957)** The general form of Markovian, linear, trace-preserving and positive dynamics of a real-valued function of phase space $P$ is either of Fokker-Planck form

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial z_i}(D_{1,i}P) + \frac{1}{2}\frac{\partial^2}{\partial z_i \partial z_j}(D_{2,ij}P) \tag{D.1}$$

or it contains an infinite number of higher order derivative terms in phase space. The $i, j, \ldots$ indices run from 1 to $n$, the number of phase space degrees of freedom $z_i$, and there is summation of repeated indices. Here, $D_{1,i}$ are the elements of a real vector of length $n$, $D_1$, and $D_{2,ij}$ are the elements of a real positive semi-definite $n \times n$ matrix $D_2$. All of the $D$ coefficients are allowed to have dependence on phase space.

**CQ Pawula (2022)** The general form of Markovian, linear, trace-preserving and completely-positive dynamics of an operator-valued function of phase space $\varrho$ is either of the form

$$\begin{aligned}\frac{\partial \varrho}{\partial t} =& -\frac{\partial}{\partial z_i}(D^C_{1,i}\varrho) + \frac{1}{2}\frac{\partial^2}{\partial z_i \partial z_j}(D_{2,ij}\varrho) \\ & - i[\bar{H}, \varrho] + D_0^{\alpha\beta}\big(L_\alpha \varrho L_\beta^\dagger - \frac{1}{2}\{L_\beta^\dagger L_\alpha, \varrho\}_+\big) \\ & - \frac{\partial}{\partial z_i}\left(D_{1,i}^{\alpha}{}^* L_\alpha \varrho + \varrho D_{1,i}^\alpha L_\alpha^\dagger\right),\end{aligned} \tag{D.2}$$

where

$$D_0 \succeq D_1^\dagger D_2^{-1} D_1, \quad (\mathbb{I} - D_2 D_2^{-1}) D_1 = 0, \tag{D.3}$$

or it contains an infinite number of higher order derivative terms in phase space. Here, the $i, j, \ldots$ indices run from 1 to $n$, the number of phase space degrees of freedom $z_i$, while the $\alpha, \beta, \ldots$ indices run from 1 to $p$, the number of traceless and orthogonal Lindblad operators $L_\alpha$ in Hilbert space. We assume summation over repeated indices of either kind. The various $D$ coefficients are organised as follows: $D_0^{\alpha\beta}$ are the elements of an $p \times p$ complex positive semi-definite matrix $D_0$, $D_{1,i}^\alpha$ are the elements of a complex $n \times p$ matrix $D_1$, which has conjugate transpose $D_1^\dagger$, while ${D_{1,i}^\alpha}^*$ denotes the complex conjugate of $D_{1,i}^\alpha$. Additionally, $D_{1,i}^C$ are the elements of a real vector of length $n$, $D_1^C$, and $D_{2,ij}$ are the elements of a real positive semi-definite $n \times n$ matrix $D_2$, which has the generalised inverse $D_2^{-1}$. Finally, $\bar{H}$ is Hermitian operator. All the $D$ coefficients and $\bar{H}$ may have arbitrary dependence on $z$.

When the Lindblad operators are not chosen traceless and orthogonal, the above conditions on the dynamics can be shown to still be sufficient for complete-positivity, even when dependent on phase space. In this case, the role of classical drift vector $D_1^C$ is essentially played by the component of the $L_\alpha$ proportional to the identity.

### Liouville equation

The Liouville equation (4.2.4) satisfies the Fokker-Planck form given by (D.1) for

$$\begin{gathered} D_{1,q} = \frac{\partial H}{\partial p} \qquad D_{1,p} = -\frac{\partial H}{\partial q} \\ D_2 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \end{gathered} \tag{D.4}$$

where here $H$ is the classical Hamiltonian.

### Quantum-classical Liouville equation

The quantum-classical Liouville equation, when written in the form of (D.2) with phase space dependent Lindblad operators, has

$$\begin{gathered} L_q = \frac{\partial H}{\partial p}, \quad L_p = -\frac{\partial H}{\partial q}, \quad \bar{H} = \frac{H}{\hbar}, \quad D_1^C = (0,0)^T \\ D_0 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \quad D_1 = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \quad D_2 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}. \end{gathered} \tag{D.5}$$

where $H$ is the classical-quantum Hamiltonian. Since $D_2$ and $D_0$ are zero everywhere, but $D_1$ is not, the positivity conditions (D.3) are not satisfied, and thus the dynamics is not completely-positive.

### Classical-quantum dynamics of $\mathcal{L}$

By the same reasoning as above, one may read from (4.4.5) the three matrices $D_0$, $D_1$ and $D_2$ given in (4.4.10),(4.4.11),(4.4.12) by taking the Lindblad operators to be $L_q^H$ and $L_p^H$. The remaining degrees of freedom are $\bar{H} = (H + H_{eff})/\hbar$ and $D_1^C = (0,0)^T$. Since $\bar{H}$ is Hermitian and the $D$ coefficients satisfy the requirements of (D.3), the dynamics is completely-positive.

# Appendix E

# Derivation of the classical-quantum limit generator $\mathcal{L}$

In this appendix, we provide the technical details needed to go from the dynamical map of equation (4.4.1) to the form of generator given in equation (4.4.3) and equation (4.4.5).

To compute $\mathcal{L}$ given by equations (4.4.3) and (4.4.5) we first write out the evolution map $\mathcal{E}_\tau = \mathcal{E}_\tau^{E_f \tau}$ explicitly as

$$\mathcal{E}_\tau = e^{\frac{1}{2}(\frac{E_f s^2}{2}\frac{\partial^2}{\partial q^2}+\frac{E_f}{2s^2}\frac{\partial^2}{\partial p^2})\tau} e^{-\frac{i}{E_f}[H,\,\cdot\,]+\frac{1}{2}(\{H,\,\cdot\,\}-\{\,\cdot\,,H\})\tau+O(\tau^2)} e^{\frac{1}{2}(\frac{E_f s^2}{2}\frac{\partial^2}{\partial q^2}+\frac{E_f}{2s^2}\frac{\partial^2}{\partial p^2})\tau}. \tag{E.1}$$

The most important part of this expression to notice immediately is that the first term in the middle exponential has no $\tau$ dependence – this term is ultimately responsible for most of the subsequent structure of the generator $\mathcal{L}$.

To go from this dynamical map to a generator, we will use equation (4.4.2). This expression generalises the standard method for constructing generators to the case where the dynamical maps which do not reduce to the identity map at $\tau = 0$. This arises by identifying two separate contributions to the short-time dynamics, $\mathcal{L}_1$ and $\mathcal{L}_2$, corresponding to the first and second terms of (4.4.2). The first part $\mathcal{L}_1$ can be understood as the standard one, defined as $\mathcal{L}_1 = \lim_{\tau\to 0} \mathcal{L}_{1,\tau}$, where $\mathcal{L}_{1,\tau}\varrho(\tau) = \partial_\tau \varrho(\tau)$. This describes how the state of the system changes

from $t = 0$ to a short time $t = \tau$ later as $\tau \to 0$. This may be computed from the dynamical map by noting that $\varrho(\tau) = \mathcal{E}_\tau \varrho(0)$ and $\varrho(0) = \mathcal{E}_\tau^{-1}\varrho(\tau)$, which may be substituted into the definition of $\mathcal{L}_{1,\tau}$ to arrive at the first term of (4.4.2). The second part of the generator $\mathcal{L}_2$ can be understood as arising from the part of the dynamical map at $\tau = 0$, which in contrast to standard treatments, is not proportional to the identity. That the map is not proportional to the identity here occurs as a result of inadvertently taking $\hbar \to 0$ even for purely quantum degrees of freedom, and so should be corrected for by restoring $E_f = \hbar/\tau$.

We first turn to explicitly finding an expression for the second term of equation (4.4.2), and providing further justification for its appearance, using equation (E.1). As described above, this term arises from the part of the dynamical map at $\tau = 0$, which is given

$$\mathcal{E}_0 = e^{-\frac{i}{E_f}[H,\ \cdot\ ]}. \tag{E.2}$$

After $N = t/\tau$ evolution steps, the total contribution of this part of the dynamics is

$$\mathcal{E}_0^N = \mathcal{E}_0^{t/\tau} = e^{-\frac{i}{E_f \tau}[H,\ \cdot\ ]t} \tag{E.3}$$

and thus is generated by the unitary term $-\frac{i}{\hbar}[H,\ \cdot\ ]$ if we restore $\hbar = E_f\tau$. This agrees with the expression given by the second term of equation (4.4.2). Although in principle the unitary steps occur in between steps generated by the $\tau$-dependent part of the generator, any changes to the generator from the non-commutativity of these terms are of $O(\tau)$, and thus vanish in the $\tau \to 0$ limit, meaning that the resulting dynamics is captured by the generator $\mathcal{L}_2 = -\frac{i}{\hbar}[H,\ \cdot\ ]$.

To compute the first part of the generator $\mathcal{L}$, denoted above as $\mathcal{L}_1$, we take the derivative of $\mathcal{E}_\tau$ to give

$$\begin{aligned}\frac{\partial}{\partial\tau}\mathcal{E}_\tau =& \frac{1}{2}\Big(\frac{E_f s^2}{2}\frac{\partial^2}{\partial q^2} + \frac{E_f}{2s^2}\frac{\partial^2}{\partial p^2}\Big)\mathcal{E}_\tau \\ &+ e^{\frac{E_f}{2}D\tau}\frac{e^{\mathrm{ad}_{\frac{-i}{E_f}[H,\cdot]+O(\tau)}}-1}{\mathrm{ad}_{\frac{-i}{E_f}[H,\cdot]+O(\tau)}}\left(\frac{1}{2}\{H,\cdot\} - \frac{1}{2}\{\cdot,H\} + O(\tau)\right)e^{-\frac{E_f}{2}D\tau}\mathcal{E}_\tau \\ &+ \frac{1}{2}\mathcal{E}_\tau\Big(\frac{E_f s^2}{2}\frac{\partial^2}{\partial q^2} + \frac{E_f}{2s^2}\frac{\partial^2}{\partial p^2}\Big),\end{aligned} \tag{E.4}$$

where here $D = \frac{E_f s^2}{2}\frac{\partial^2}{\partial q^2} + \frac{E_f}{2s^2}\frac{\partial^2}{\partial p^2}$. This gives the first component of the generator $\mathcal{L}$ as

$$\begin{aligned}\lim_{\tau\to 0}\left(\frac{\partial}{\partial\tau}\mathcal{E}_\tau\right)\mathcal{E}_\tau^{-1} =& \frac{1}{2}\left(\frac{E_f s^2}{2}\frac{\partial^2}{\partial q^2} + \frac{E_f}{2s^2}\frac{\partial^2}{\partial p^2}\right) \\ &+ \frac{e^{\mathrm{ad}_{\frac{-i}{E_f}[H,\cdot]}} - 1}{\mathrm{ad}_{\frac{-i}{E_f}[H,\cdot]}}\left(\frac{1}{2}\{H,\cdot\} - \frac{1}{2}\{\cdot, H\}\right) \\ &+ \frac{1}{2}e^{-\frac{i}{E_f}[H,\ \cdot\ ]}\left(\frac{E_f s^2}{2}\frac{\partial^2}{\partial q^2} + \frac{E_f}{2s^2}\frac{\partial^2}{\partial p^2}\right)e^{\frac{i}{E_f}[H,\ \cdot\ ]}\end{aligned} \tag{E.5}$$

where the $O(\tau)$ terms disappear in the $\tau \to 0$ limit and we have used the fact that $\lim_{\tau\to 0} e^{\pm\frac{E_f}{2}D\tau}$ is the identity operator. Noting that we may use the following equality between the exponential of the adjoint and the adjoint of the exponential

$$e^{\mathrm{ad}_{\mathcal{B}}}\mathcal{A} = e^{\mathcal{B}}\mathcal{A}e^{-\mathcal{B}} \tag{E.6}$$

we find the quoted form of the generator in equation (4.4.3).

To compute the form of the generator given in (4.4.5) is a little more work. Denoting the following term $\mathcal{T}_1$

$$\mathcal{T}_1\varrho = \frac{1}{2}e^{\mathrm{ad}_{\frac{-i}{E_f}[H,\cdot]}}\left(\frac{E_f s^2}{2}\frac{\partial^2}{\partial q^2} + \frac{E_f}{2s^2}\frac{\partial^2}{\partial p^2}\right)\varrho \tag{E.7}$$

where we introduce an aribtrary CQ state $\varrho$ to make the action of this generator explicit, one may use the equality between the exponential of the adjoint and the adjoint of the exponential as in equation (E.6) to rewrite this as

$$\frac{1}{2}e^{-\frac{i}{E_f}[H,\ \cdot\ ]}\left(\frac{E_f s^2}{2}\frac{\partial^2}{\partial q^2} + \frac{E_f}{2s^2}\frac{\partial^2}{\partial p^2}\right)e^{+\frac{i}{E_f}[H,\ \cdot\ ]}\varrho \tag{E.8}$$

and then use it *again*, noting that $\pm\frac{i}{E_f}[H,\ \cdot\ ] = \mathrm{ad}_{\frac{\pm i}{E_f}H}$, to give

$$\frac{1}{2}e^{\frac{-i}{E_f}H}\left(\frac{E_f s^2}{2}\frac{\partial^2}{\partial q^2} + \frac{E_f}{2s^2}\frac{\partial^2}{\partial p^2}\right)\left(e^{\frac{i}{E_f}H}\varrho e^{\frac{-i}{E_f}H}\right)e^{\frac{i}{E_f}H}. \tag{E.9}$$

One may then compute this expression explicitly, taking care to note that whenever a derivative is made of the exponential of a $z = q, p$ dependent operator, that

$$\begin{aligned}\frac{\partial}{\partial z}e^{-\frac{i}{E_f}H} &= -\frac{i}{E_f}\frac{e^{\mathrm{ad}_{\frac{-i}{E_f}H}} - 1}{\mathrm{ad}_{\frac{-i}{E_f}H}}\left(\frac{\partial H}{\partial z}\right)e^{-\frac{i}{E_f}H} \\ &= -\frac{i}{E_f}L_z^H e^{-\frac{i}{E_f}H},\end{aligned} \tag{E.10}$$

and

$$\begin{aligned}\frac{\partial}{\partial z}e^{\frac{i}{E_f}H} &= \frac{i}{E_f}e^{\frac{i}{E_f}H}\ \frac{e^{\mathrm{ad}_{\frac{-i}{E_f}H}}-1}{\mathrm{ad}_{\frac{-i}{E_f}H}}\left(\frac{\partial H}{\partial z}\right)\\ &= \frac{i}{E_f}e^{\frac{i}{E_f}H}L_z^H.\end{aligned} \tag{E.11}$$

Using these formulae, one may show that

$$\begin{aligned}\frac{1}{2}e^{-\frac{i}{E_f}H}\frac{\partial^2}{\partial z^2}(e^{\frac{i}{E_f}H}\varrho e^{-\frac{i}{E_f}H})e^{\frac{i}{E_f}H} =& -\frac{i}{2E_f}[\frac{\partial L_z^H}{\partial z},\varrho]+\frac{i}{E_f}\frac{\partial}{\partial z}[L_z^H,\varrho]\\ &+\frac{1}{E_f^2}\big(L_z^H\varrho L_z^H-\frac{1}{2}\{L_z^{H^2},\varrho\}_+\big)+\frac{1}{2}\frac{\partial^2\varrho}{\partial z^2},\end{aligned} \tag{E.12}$$

which gives the overall generator $\mathcal{T}_1$ as

$$\begin{aligned}\mathcal{T}_1\varrho =& -i[\frac{s^2}{4}\frac{\partial L_q^H}{\partial q}+\frac{1}{4s^2}\frac{\partial L_p^H}{\partial p},\varrho]+\frac{is^2}{2}\frac{\partial}{\partial q}[L_q^H,\varrho]+\frac{i}{2s^2}\frac{\partial}{\partial p}[L_p^H,\varrho]\\ &+\frac{s^2}{2E_f}(L_q^H\varrho L_q^H-\frac{1}{2}\{L_q^{H^2},\varrho\}_+)+\frac{1}{2E_fs^2}(L_p^H\varrho L_p^H-\frac{1}{2}\{L_p^{H^2},\varrho\}_+)\\ &+\frac{1}{2}\big(\frac{E_fs^2}{2}\frac{\partial^2\varrho}{\partial q^2}+\frac{E_f}{2s^2}\frac{\partial^2\varrho}{\partial p^2}\big).\end{aligned} \tag{E.13}$$

The other component of $\mathcal{L}$ that remains to be computed we will denote $\mathcal{T}_2$ and is given

$$\mathcal{T}_2\varrho = \frac{e^{\mathrm{ad}_{\frac{-i}{E_f}[H,\cdot]}}-1}{\mathrm{ad}_{\frac{-i}{E_f}[H,\cdot]}}\left(\frac{1}{2}\{H,\ \cdot\ \}-\frac{1}{2}\{\ \cdot\ ,H\}\right)\varrho. \tag{E.14}$$

Since the fraction $\frac{e^{\mathrm{ad}}-1}{\mathrm{ad}}$ is to be interpreted as describing a power series, and using the symmetry of second derivatives of $H$ to rewrite the Alexandrov-bracket as the derivatives of anticommutators, we may rewrite this generator more explicitly as

$$\mathcal{T}_2\varrho = \sum_{n=0}^{\infty}\frac{1}{(n+1)!}\mathrm{ad}^n_{\frac{-i}{E_f}[H,\cdot]}\left(-\frac{1}{2}\frac{\partial}{\partial q}\{\frac{\partial H}{\partial p},\ \cdot\ \}_+ +\frac{1}{2}\frac{\partial}{\partial p}\{\frac{\partial H}{\partial q},\ \cdot\ \}_+\right)\varrho. \tag{E.15}$$

To compute this infinite series, we will first need to find the commutation relations of the algebra generated by $-\frac{i}{E_f}[H,\cdot]$, as one would do for the case for a Lie algebra of a Lie group – for some related work in the purely quantum case, see [230]. To simplify this subsequent analysis, we will use a shorthand $\mathbb{L}(A,\ \cdot\ ,B)$ to denote a generic component of a Lindblad decoherence generator i.e.

$$\mathbb{L}(A,\varrho,B) = A\varrho B-\frac{1}{2}BA\varrho-\frac{1}{2}\varrho BA. \tag{E.16}$$

One may then compute the commutation relations between $-\frac{i}{E_f}[H,\cdot]$ and the various terms that appear: (a) with the derivative of an anticommuator

$$\mathrm{ad}_{\frac{-i}{E_f}[H,\,\cdot\,]}\frac{\partial}{\partial z}\{A,\,\cdot\,\}_+ = \frac{\partial}{\partial z}\{\mathrm{ad}_{\frac{-i}{E_f}H}A,\,\cdot\,\}_+ + \frac{i}{E_f}\mathbb{L}(\frac{\partial H}{\partial z},\,\cdot\,,A) - \frac{i}{E_f}\mathbb{L}(A,\,\cdot\,,\frac{\partial H}{\partial z}) + \frac{i}{E_f}[\frac{1}{2}\{A,\frac{\partial H}{\partial z}\}_+,\,\cdot\,], \tag{E.17}$$

(b) with the component of the Lindblad decoherence generator

$$\mathrm{ad}_{\frac{-i}{E_f}[H,\,\cdot\,]}\mathbb{L}(A,\,\cdot\,,B) = \mathbb{L}(\mathrm{ad}_{\frac{-i}{E_f}H}A,\,\cdot\,,B) + \mathbb{L}(A,\,\cdot\,,\mathrm{ad}_{\frac{-i}{E_f}H}B), \tag{E.18}$$

and (c) with a unitary generator

$$\mathrm{ad}_{\frac{-i}{E_f}[H,\,\cdot\,]} - i[A,\,\cdot\,] = -i[\mathrm{ad}_{\frac{-i}{E_f}H}A,\,\cdot\,]. \tag{E.19}$$

Since the above generators are closed under the repeated action of $\mathrm{ad}_{\frac{-i}{E_f}[H,\,\cdot\,]}$, these relations are sufficient to compute the above series.

To actually compute the series, we will consider each kind of generator (a)-(c) separately. Starting with (a), the derivative of an anticommutator, we note that the adjoint action of the commutator with $H$ is equivalent to the adjoint action with $H$ on the operator in question. This gives the first part of $\mathcal{T}_2$ as

$$\begin{aligned}\mathcal{T}_2^{(a)} &= \sum_{n=0}^{\infty}\frac{1}{(n+1)!}\Big(-\frac{1}{2}\frac{\partial}{\partial q}\{\mathrm{ad}^n_{\frac{-i}{E_f}H}\frac{\partial H}{\partial p},\,\cdot\,\}_+ + \frac{1}{2}\frac{\partial}{\partial p}\{\mathrm{ad}^n_{\frac{-i}{E_f}H}\frac{\partial H}{\partial q},\,\cdot\,\}_+\Big)\\ &= -\frac{1}{2}\frac{\partial}{\partial q}\{L_p^H,\,\cdot\,\}_+ + \frac{1}{2}\frac{\partial}{\partial p}\{L_q^H,\,\cdot\,\}_+,\end{aligned} \tag{E.20}$$

where we have again used the series expansion of $\frac{e^{\mathrm{ad}}-1}{\mathrm{ad}}$.

To compute $\mathcal{T}_2^{(b)}$, the part corresponding to the Lindblad terms, we first write down the form of the $O(E_f^{-n})$ order term, which is given

$$\begin{aligned}\frac{i}{2E_f}\sum_{k=0}^{n-1}\Big\{&\mathbb{L}(\frac{1}{(k+1)!}\mathrm{ad}^k_{\frac{-i}{E_f}H}\frac{\partial H}{\partial p},\,\cdot\,,\frac{1}{(n-k)!}\mathrm{ad}^{n-1-k}_{\frac{-i}{E_f}H}\frac{\partial H}{\partial q})\\ &-\mathbb{L}(\frac{1}{(k+1)!}\mathrm{ad}^k_{\frac{-i}{E_f}H}\frac{\partial H}{\partial q},\,\cdot\,,\frac{1}{(n-k)!}\mathrm{ad}^{n-1-k}_{\frac{-i}{E_f}H}\frac{\partial H}{\partial p})\Big\}\end{aligned} \tag{E.21}$$

We will now show by induction that this is true for all $n \geq 1$. When $n = 1$, all the Lindblad terms come from the application of (E.17) on the Alexandrov-bracket, which one can check

agrees with the above expression (being careful to include the factor of $1/(1+1)!$ coming from (E.15)). For an arbitrary term of order $n+1$, it follows from (E.17)-(E.19) that all terms must come from the application of $\frac{1}{n+2}\mathrm{ad}_{\frac{-i}{E_f}[H,\,\cdot\,]}$ to either the previous $n$th order term in (E.21) or to the $n$th order term of (E.20). This gives the $(n+1)$th order term in total as

$$\begin{aligned}
\frac{i}{2E_f}\frac{1}{n+2}\sum_{k=0}^{n-1}\Big\{&\mathbb{L}(\frac{1}{(k+1)!}\mathrm{ad}^{k+1}_{\frac{-i}{E_f}H}\frac{\partial H}{\partial p},\ \cdot\ ,\frac{1}{(n-k)!}\mathrm{ad}^{n-1-k}_{\frac{-i}{E_f}H}\frac{\partial H}{\partial q})\\
&+\mathbb{L}(\frac{1}{(k+1)!}\mathrm{ad}^{k}_{\frac{-i}{E_f}H}\frac{\partial H}{\partial p},\ \cdot\ ,\frac{1}{(n-k)!}\mathrm{ad}^{n-k}_{\frac{-i}{E_f}H}\frac{\partial H}{\partial q})\\
&-\mathbb{L}(\frac{1}{(k+1)!}\mathrm{ad}^{k+1}_{\frac{-i}{E_f}H}\frac{\partial H}{\partial q},\ \cdot\ ,\frac{1}{(n-k)!}\mathrm{ad}^{n-1-k}_{\frac{-i}{E_f}H}\frac{\partial H}{\partial p})\\
&-\mathbb{L}(\frac{1}{(k+1)!}\mathrm{ad}^{k}_{\frac{-i}{E_f}H}\frac{\partial H}{\partial q},\ \cdot\ ,\frac{1}{(n-k)!}\mathrm{ad}^{n-k}_{\frac{-i}{E_f}H}\frac{\partial H}{\partial p})\Big\}\\
+\frac{i}{2E_f}\frac{1}{(n+2)!}\Big\{&\mathbb{L}(\frac{\partial H}{\partial p},\ \cdot\ ,\mathrm{ad}^{n}_{\frac{-i}{E_f}H}\frac{\partial H}{\partial q})+\mathbb{L}(\mathrm{ad}^{n}_{\frac{-i}{E_f}H}\frac{\partial H}{\partial p},\ \cdot\ ,\frac{\partial H}{\partial q})\\
&-\mathbb{L}(\frac{\partial H}{\partial q},\ \cdot\ ,\mathrm{ad}^{n}_{\frac{-i}{E_f}H}\frac{\partial H}{\partial p})-\mathbb{L}(\mathrm{ad}^{n}_{\frac{-i}{E_f}H}\frac{\partial H}{\partial q},\ \cdot\ ,\frac{\partial H}{\partial p})\Big\}.
\end{aligned}\tag{E.22}$$

Considering first the Lindblad terms with one entry $\mathrm{ad}^n$ and the other $\mathrm{ad}^0$, we see that the numerical prefactors of these terms are given

$$\frac{1}{n+2}\frac{1}{n!}+\frac{1}{(n+2)!}=\frac{1}{(n+1)!},\tag{E.23}$$

with the term on the left hand side coming from $k=n-1$ or 0 terms, and the right hand side coming from the bottom two lines. Analogously, for a generic Lindblad term with one entry $\mathrm{ad}^m$ and the other $\mathrm{ad}^{n-m}$ for $0<m<n$ we have two terms coming from the sum over $k$, given

$$\frac{1}{n+2}\left(\frac{1}{m!}\frac{1}{(n-m+1)!}+\frac{1}{(m+1)!}\frac{1}{(n-m)!}\right)=\frac{1}{(m+1)!(n+1-m)!},\tag{E.24}$$

which implies that the $(n+1)$th order terms may be written as

$$\begin{aligned}
\frac{i}{2E_f}\sum_{k=0}^{n}\Big\{&\mathbb{L}(\frac{1}{(k+1)!}\mathrm{ad}^{k}_{\frac{-i}{E_f}H}\frac{\partial H}{\partial p},\ \cdot\ ,\frac{1}{(n+1-k)!}\mathrm{ad}^{n-k}_{\frac{-i}{E_f}H}\frac{\partial H}{\partial q})\\
&-\mathbb{L}(\frac{1}{(k+1)!}\mathrm{ad}^{k}_{\frac{-i}{E_f}H}\frac{\partial H}{\partial q},\ \cdot\ ,\frac{1}{(n+1-k)!}\mathrm{ad}^{n-k}_{\frac{-i}{E_f}H}\frac{\partial H}{\partial p})\Big\}
\end{aligned}\tag{E.25}$$

which indeed is the expression (E.21) with $n\to n+1$. Since this expression is only the $n$th

order term, we may write $\mathcal{T}_2^{(b)}$ as the sum over all these terms

$$\frac{i}{2E_f}\sum_{n=1}^{\infty}\sum_{k=0}^{n-1}\Big\{\mathbb{L}(\frac{1}{(k+1)!}\mathrm{ad}^k_{\frac{-i}{E_f}H}\frac{\partial H}{\partial p},\ \cdot\ ,\frac{1}{(n-k)!}\mathrm{ad}^{n-1-k}_{\frac{-i}{E_f}H}\frac{\partial H}{\partial q}) \\ -\mathbb{L}(\frac{1}{(k+1)!}\mathrm{ad}^k_{\frac{-i}{E_f}H}\frac{\partial H}{\partial q},\ \cdot\ ,\frac{1}{(n-k)!}\mathrm{ad}^{n-1-k}_{\frac{-i}{E_f}H}\frac{\partial H}{\partial p})\Big\} \tag{E.26}$$

which noting that $\mathbb{L}$ is linear each of its arguments can be simplified to

$$\mathcal{T}_2^{(b)} = \frac{i}{2E_f}\mathbb{L}(L_p^H,\ \cdot\ ,L_q^H) - \frac{i}{2E_f}\mathbb{L}(L_q^H,\ \cdot\ ,L_p^H) \tag{E.27}$$

i.e.

$$\mathcal{T}_2^{(b)}\varrho = -\frac{i}{2E_f}(L_q^H\varrho L_p^H - \frac{1}{2}\{L_p^H L_q^H,\varrho\}_+) + \frac{i}{2E_f}(L_p^H\varrho L_q^H - \frac{1}{2}\{L_q^H L_p^H,\varrho\}_+). \tag{E.28}$$

The final component of $\mathcal{T}_2$ to compute is the unitary part, which we will keep track of by defining an associated Hamiltonian $H_{qp+pq}$ via $\mathcal{T}_2^{(c)} = -i[H_{qp+pq},\ \cdot\ ]$. From (E.17)-(E.19) it is apparent that any contributions to $H_{qp+pq}$ are generated by the action of $\mathrm{ad}_{\frac{-i}{E_f}[H,\ \cdot\ ]}$ on derivatives of anticommutator terms, given by (E.20), and then the subsequent action of $\mathrm{ad}_{\frac{-i}{E_f}[H,\ \cdot\ ]}$ on the unitary terms generated by these. The numerical factor coming from the repeated action in (E.15) may be kept track of by simply noting that the $O(E_f^{-n})$ terms have a factor $1/(n+1)!$. This lets us write down the Hamiltonian $H_{qp+pq}$ as

$$H_{qp+pq} = \frac{1}{4E_f}\sum_{n,m=0}^{\infty}\frac{1}{(n+m+2)!}\mathrm{ad}^n_{\frac{-i}{E_f}H}\Big[\{\mathrm{ad}^m_{\frac{-i}{E_f}H}\frac{\partial H}{\partial p},\frac{\partial H}{\partial q}\}_+ - \{\mathrm{ad}^m_{\frac{-i}{E_f}H}\frac{\partial H}{\partial q},\frac{\partial H}{\partial p}\}_+\Big], \tag{E.29}$$

with the sum over $m$ indicating the initial creation of a unitary term via (E.17), and the sum over $n$ giving the subsequent action via (E.19). Using the fact that

$$\mathrm{ad}^n_{\frac{-i}{E_f}H}\{A,B\}_+ = \sum_{k=0}^{n}\binom{n}{k}\{\mathrm{ad}^{n-k}_{\frac{-i}{E_f}H}A,\mathrm{ad}^k_{\frac{-i}{E_f}H}B\}_+ \tag{E.30}$$

where $\binom{n}{k}$ is the binomial coefficient, and collecting terms, we finally arrive at the form

$$H_{qp+pq} = \frac{1}{4E_f}\sum_{n,m=0}^{\infty}\frac{C_{nm}}{(n+m+2)!}\{\mathrm{ad}^n_{\frac{-i}{E_f}H}\frac{\partial H}{\partial q},\mathrm{ad}^m_{\frac{-i}{E_f}H}\frac{\partial H}{\partial p}\}_+. \tag{E.31}$$

Here the coefficients $C_{nm}$, explicitly given by

$$C_{nm} = \sum_{r=0}^{m}\frac{(r+n)!}{r!n!} - \sum_{r=0}^{n}\frac{(r+m)!}{r!m!}, \tag{E.32}$$

may be written out pictorially to show that they are generated by a version of the Pascal triangle, here with the same addition rules but with the boundary elements given by the integers $\mathbb{Z}$ i.e.

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | 0 | | | | | | | |
| | | | | -1 | | 1 | | | | | | |
| | | | -2 | | 0 | | 2 | | | | | |
| | | -3 | | -2 | | 2 | | 3 | | | | |
| | -4 | | -5 | | 0 | | 5 | | 4 | | | |
| -5 | | -9 | | -5 | | 5 | | 9 | | 5 | | |
| -6 | -14 | | -14 | | 0 | | 14 | | 14 | | 6 | |

Finally, combining the components $-\frac{i}{\hbar}[H,\ \cdot\ ]$, $\mathcal{T}_1$ and $\mathcal{T}_2$, using the definition

$$H_{\text{eff}} = \frac{\hbar s^2}{4}\frac{\partial L_q^H}{\partial q} + \frac{\hbar}{4s^2}\frac{\partial L_p^H}{\partial p} + \hbar H_{qp+pq} \tag{E.33}$$

gives the form quoted in (4.4.5).

# Appendix F

# Including $O(\hbar)$ contributions in the classical-quantum Hamiltonian

If instead of assuming $H^W = H + O(\hbar^2)$ we had assumed $H^W = H + \hbar H^1 + O(\hbar^2)$, we would find that the equations of motion for the Liouville equation are unchanged, but that there is a change in the quantum-classical Liouville equation. Specifically, the $O(\hbar^0)$ part of the partial Wigner generator now takes the form

$$\mathcal{L}^W = -\frac{i}{\hbar}[H,\ \cdot\ ] - i[H^1,\ \cdot\ ] + \frac{1}{2}(\{H,\ \cdot\ \} - \{\ \cdot\ , H\}) + O(\hbar). \tag{F.1}$$

Following the same steps as before in computing the generator, the only change is found at the level of the $\mathcal{T}_2$ component given in (E.14), which now has the additional term $\mathcal{T}_2^1$

$$\mathcal{T}_2^1 = \frac{e^{\mathrm{ad}_{\frac{-i}{E_f}[H,\cdot]}} - 1}{\mathrm{ad}_{\frac{-i}{E_f}[H,\cdot]}}\Big(-i[H^1,\ \cdot\ ]\Big). \tag{F.2}$$

To put this in canonical form, we note that $\mathrm{ad}_{[A,\ \cdot\ ]}[B,\ \cdot\ ] = [\mathrm{ad}_A B,\ \cdot\ ]$, which follows from the Jacobi identity, and thus using the series expansion of $\frac{e^x-1}{x}$ and resumming we find

$$\mathcal{T}_2^1 = -i[\frac{e^{-\frac{i}{E_f}H} - 1}{\mathrm{ad}_{\frac{-i}{E_f}H}}H^1,\ \cdot\ ]. \tag{F.3}$$

Considering an $H^W$ with $O(\hbar)$ terms thus simply leads to an additional unitary term, and does not affect the resulting complete-positivity of the dynamics.

# Appendix G

# Double scaling limit of a continuous Lindbladian evolution

In this appendix we consider a double scaling limit of a continuous time Lindbladian dynamics, and illustrate the difference with the classical-quantum limit we present. In particular, we show that while this set-up can reproduce the stochastic classical dynamics of (4.8.1), it does not coincide with (4.4.5) and in fact does not describe completely-positive dynamics. This example illustrates that one must be careful in constructing classical-quantum limits simply by identifying scaling limits that leave diffusion in the classical degrees of freedom.

To start with, consider the following model of bipartite dynamics on the $C$ and $Q$ subsystems

$$\frac{\partial\hat{\rho}}{\partial t} = -\frac{i}{\hbar}[\hat{H},\hat{\rho}] + \frac{\gamma}{s^2}(\hat{q}\hat{\rho}\hat{q} - \frac{1}{2}\{\hat{q}^2,\hat{\rho}\}_+) + \gamma s^2(\hat{p}\hat{\rho}\hat{p} - \frac{1}{2}\{\hat{p}^2,\hat{\rho}\}_+). \tag{G.1}$$

where $\gamma$ is positive parameter controlling the overall rate of decoherence, while $s$ is a positive parameter controlling the relative strength of decoherence between position and momentum. This model is of the GKSL form [231, 232], and is thus completely-positive at the level of the quantum dynamics. To consider how this dynamics appears in the partial Wigner representation, we first rewrite each Lindblad term as a double commutator with $-i/\hbar$ prefactors i.e.

$$\hat{z}\hat{\rho}\hat{z} - \frac{1}{2}\{\hat{z}^2,\hat{\rho}\}_+ = \frac{\hbar^2}{2}\big(-\frac{i}{\hbar}[\hat{z},\ -\frac{i}{\hbar}[\hat{z},\hat{\rho}]\ ]\big), \tag{G.2}$$

for $\hat{z} = \hat{q},\hat{p}$. Using the mapping of operators to the partial Wigner representation $\hat{f}\hat{g} \mapsto f \star g$,

which here amounts to identifying the commutators with $-i/\hbar$ prefactors with Poisson brackets, one arrives at the partial Wigner representation of this dynamics

$$\begin{aligned}\frac{\partial \varrho^W}{\partial t} =& -\frac{i}{\hbar}[H, \varrho^W] + \frac{1}{2}(\{H, \varrho^W\} - \{\varrho^W, H\}) \\ &+ \frac{\gamma\hbar^2}{2s^2}\{q, \{q, \varrho^W\} + \frac{\gamma\hbar^2 s^2}{2}\{p, \{p, \varrho^W\} \\ &+ O(\hbar),\end{aligned} \tag{G.3}$$

where the $O(\hbar)$ terms are those truncated in (4.2.7) to arrive at (4.2.9).

In this case, the natural limit to take if one wishes to remove the $O(\hbar)$ terms and additionally preserve the terms containing $\gamma$ is the double scaling limit

$$\hbar \to 0,\ \gamma \to \infty \quad s.t. \quad \gamma\hbar^2 = E_f. \tag{G.4}$$

Doing so with the above dynamics whilst naively ignoring $O(\hbar^{-1})$ terms gives the final form of master equation as

$$\begin{aligned}\frac{\partial \varrho^W}{\partial t} =& -\frac{i}{\hbar}[H, \varrho^W] + \frac{1}{2}(\{H, \varrho^W\} - \{\varrho^W, H\}) \\ &+ \frac{E_f}{2s^2}\frac{\partial^2 \varrho^W}{\partial p^2} + \frac{E_f s^2}{2}\frac{\partial^2 \varrho^W}{\partial q^2}.\end{aligned} \tag{G.5}$$

At first glance, this appears to be a valid classical-quantum limit incorporating the affects of decoherence. Indeed, substituting in a trivial Hamiltonian $H = H(q,p)\mathbb{1}$ as in 4.8, one finds that this dynamics reduces exactly to the stochastic Liouville dynamics given in (4.8.1). However, comparing the form of this dynamics to the general form of completely-positive Markovian classical-quantum dynamics given in Appendix D, one sees that the dynamics is in fact not a valid dynamics; it has non-zero back-reaction and diffusion, but without any decoherence on the quantum degrees of freedom. Moreover, repeating the above steps in either the partial Husimi $\varrho^Q$ or the partial Glauber-Sudarshan $\varrho^P$ representations using (4.6.1) and (4.6.2), one can see that the resulting form of dynamics is dependent on the choice of phase space representation used, even in the $\hbar \to 0$ limit. This example suggests some importance of the specific model of decoherence that is used to construct the classical-quantum limit we propose.

# Appendix H

# Effective classicality via representations of states and measurements

In this subsection, we show how the framework of characterising the non-classicality of a quantum system in terms of its states and measurements [59, 61] can be used to motivate the definition of effective classicality of a subsystem as the positivity of the partial Glauber-Sudarshan representation $\varrho^P$. In particular, we see that our definition coincides with an operational definition of classicality: that regardless of the measurements performed on a bipartite quantum system, the statistics are indistinguishable from that of an underlying classical-quantum probability distribution.

### Quasi-probability representations of states and measurements

We consider first a single quantum system denoted $C$ as in section 4.2. First, note that the general framework for discussing measurements is that of POVMs $\{\hat{E}_i\}$, where $\hat{E}_i$ denote the POVM elements [77]. A quasiprobability representation $R$ is the assignment to every state $\hat{\rho}$ and every set of POVM elements $\hat{E}_i$ the real-valued functions of phase space $R(z)$ and $E_i^R(z)$

respectively, such that

$$\mathrm{tr}[\hat{\rho}\hat{E}_i] = \int dz\ R(z)E_i^R(z). \tag{H.1}$$

This allows for the statistics of every measurement performed on the quantum system to be represented in terms of functions in phase space, with the Wigner representation introduced in section 4.2 providing one such example. As in the case of the Wigner representation, the functions $R(z)$ and $E_i^R(z)$ will not be positive for all states and measurements, and thus cannot always be interpreted as a classical probability distribution with an associated distribution over classical measurement outcomes. However, when a restricted set of states $\{\hat{\rho}_\lambda\}$ and measurements $\{\{\hat{E}_i\}, \{\hat{F}_i\}, \ldots\}$ are considered, it turns out it is possible to find subtheories for which both states and measurements are represented positively. In particular, we will say that *a set of states and POVMs admit a classical description* when there exists a representation $R$ such that $R_\lambda(z)$ and $E_i^R(z), F_i^R(z), \ldots$ are non-negative for all $z$. Important examples of subtheories that admit classical descriptions are the measurements and states associated with Gaussian quantum optics [61, 172] and stabilizer circuits in quantum computing [233, 234].

The above framework allows one to distinguish when a set of states and measurements in a quantum theory can be explained by a classical one. However, since a non-contextual theory of classical physics does not need to make reference to measurements, it is reasonable to expect that for taking a classical limit, one should use a definition of classicality that is independent of any choice of measurements performed on the system. In order to do so, we note that a special case of a quasiprobability representation is one for which every set of POVM elements $\{\hat{E}_i\}$ is specified by a set of non-negative real-valued functions $E_i^R(z)$ i.e. every measurement has a classical representation. In such a representation, any states for which $R(z) \geq 0$ for all $z$ necessarily permit a classical explanation, and we will refer to quantum states which satisfy this property as *effectively classical states*. Providing a measurement-independent notion of classicality, the advantage of this approach is that one may guarantee the effective classicality of dynamics without needing to additionally study the choice of measurements being performed.

To study the representation of measurements, and in particular POVMs, one may ask what form $E_i^Q(q,p)$ and $E_i^P(q,p)$ must take, given the definitions of $Q(q,p)$ and $P(q,p)$ above, in order for equation (H.1) to hold. By substitution and using the linearity of the trace, it is

straightforward to check that the form of POVMs is reversed compared to the states between the two representations: namely that $E_i^P(q,p)$ is obtained by using $\hat{E}_i$ in place of $\hat{\rho}$ in equation (4.5.1), while $E_i^Q(q,p)$ is defined implicitly by equation (4.5.2) but with $\hat{E}_i$ in place of $\hat{\rho}$. Just as the $Q$ distribution is positive for all quantum states, this means that the $P$ representations of measurements, $E_i^P(q,p)$, are always positive functions of phase space. Given the definition of effective classicality given above, this means that states which have positive $P$ distributions should be considered to be effectively classical according to this definition.

### Partial quasi-probability representations of states and measurements

We will now generalise the above discussion to study the effective classicality of subsystems. To make this concrete, we begin by defining in general terms the notion of a *partial quasiprobability representation*. Recall that a more general treatment of measurements is that of POVMs $\{\hat{E}_i\}$, where $\hat{E}_i$ denote the POVM elements. A partial quasiprobability representation $R$ is the assignment to every state $\hat{\rho}$ and every set of POVM elements $\hat{E}_i$ the operator-valued functions of phase space $\varrho^R$ and $E_i^R$ acting on $\mathcal{H}^Q$, in such a way that

$$\mathrm{tr}[\hat{\rho}\hat{E}_i] = \int dz \ \mathrm{tr}[\varrho^R(z)E_i^R(z)]. \tag{H.2}$$

Here the trace on the left-hand side is over the $C$ and $Q$ subsystem Hilbert spaces, while the trace on the right-hand side is just over $\mathcal{H}^Q$. By definition, every measurement may be represented in this way, and thus the partial quasiprobability representation provides an entirely equivalent description of bipartite quantum mechanics. The partial Wigner representation described in Section 4.2 provides an example of this. Note that in this example the same map is applied to both states $\hat{\rho}$ and POVM elements $\hat{E}_i$ to generate the representation, but in general the states and observables are treated differently.

To identify when a given set of bipartite quantum states $\{\hat{\rho}_\lambda\}$ and measurements $\{\{\hat{E}_i\},\{\hat{F}_i\}$ $,\ldots\}$ may be described using an effectively classical subsystem, it is necessary to study the positivity of their representations. This was first demonstrated in [59], where the criterion for whether a given set of quantum states and measurements could be modelled classically was identified as when the representations of both the states and POVM elements were non-negative real-valued functions of phase space. To generalise to the case of an effectively classical

subsystem, we will say that *a set of states and POVMs admit an effective classical-quantum description* whenever there exists a representation $R$ in which $\varrho^R$ and $E_i^R$ are positive semi-definite for all $z$ in phase space, by direct analogue with the purely classical case. As in the case of defining an effective classical description of a quantum system [59, 61], only a restricted set of all measurements and states in quantum theory permit an effective classical-quantum description.

For a restricted set of measurements, many quantum states may admit an effective classical-quantum description of the combined set of measurements and states. However, a special class of states are those which may be modelled using a classical-quantum description for all possible bipartite measurements on the system. Translated to the technical language above, we will call a bipartite density operator $\hat{\rho}$ an *effective classical-quantum state* whenever there exists a representation where the corresponding partial quasiprobability distribution is positive semi-definite $\varrho^R \succeq 0$ and the representation of all POVMs are positive semi-definite. This provides an operationally relevant definition of states with an effective classical subsystem, since it means that regardless of the form of measurement performed on the joint bipartite quantum system, the statistics are reproducible via an underlying classical-quantum (or partially non-contextual) model [59].

Using this definition, it is straightforward to see that the positivity of $\varrho^P$ gives sufficient and necessary conditions for the effective classicality of the $C$ subsystem. To see this, we may substitute the definition of $\varrho^P$ given in equation (4.5.4) into equation (H.2) to see that the representation of POVM elements in the partial $P$ representation are in fact given by the partial $Q$ representation, and thus are always positive semi-definite. By the definition given above, if the partial Glauber-Sudarshan representation $\varrho^P$ for a bipartite state $\hat{\rho}$ is positive, this state must therefore be an effective classical-quantum state.

# Appendix I

# Relating states and dynamics in partial quasiprobability representations

A well known property of the three common quasiprobability distributions is that they may be related via convolution with a Gaussian (also known as a Weierstrass transform). Specifically, the Wigner distribution $W$ may be obtained from the Glauber-Sudarshan $P$ distribution by a convolution with a Gaussian with variance $\frac{1}{2}\hbar s^2$ in $q$ and $\frac{1}{2}\hbar s^{-2}$ in $p$, and in turn the Husimi $Q$ representation may be obtained from the Wigner representation by the same convolution [152, 43, 151]. These relations are unchanged by when one considers instead the partial quasiprobability representations $\varrho^W, \varrho^P, \varrho^Q$, and so using the differential operator representation [153] of the convolution

$$\mathcal{D}^{\frac{1}{2}} = e^{\frac{1}{2}(\frac{\hbar s^2}{2}\frac{\partial^2}{\partial q^2}+\frac{\hbar}{2s^2}\frac{\partial^2}{\partial p^2})}, \tag{I.1}$$

we may write them as

$$\begin{aligned} \varrho^W(q,p) &= \mathcal{D}^{\frac{1}{2}}\varrho^P(q,p) \\ \varrho^Q(q,p) &= \mathcal{D}^{\frac{1}{2}}\varrho^W(q,p). \end{aligned} \tag{I.2}$$

For the different representations to be all equivalent, the mapping between the quasiprobability distributions must be bijective, and thus the convolutions must be invertible. While this is not

possible for general functions on phase space [153], in this case it is possible on the restricted domain formed by the sets of all possible partial Husimi and Wigner distributions [171]. In terms of the differential operator $\mathcal{D}$, these inverse maps may be written in terms of the differential operator

$$\mathcal{D}^{-\frac{1}{2}} = e^{-\frac{1}{2}(\frac{\hbar s^2}{2}\frac{\partial^2}{\partial q^2}+\frac{\hbar}{2s^2}\frac{\partial^2}{\partial p^2})} \tag{I.3}$$

which gives

$$\begin{aligned} \varrho^P(q,p) &= \mathcal{D}^{-\frac{1}{2}}\varrho^W(q,p) \\ \varrho^W(q,p) &= \mathcal{D}^{-\frac{1}{2}}\varrho^Q(q,p). \end{aligned} \tag{I.4}$$

Having specified the maps between states in the three representations, one may construct the dynamics in any representation from another by mapping the state, evolving in that representation, and then mapping back to the original representation. In particular, using the form of the generator in the partial Wigner representation $\mathcal{L}^W$, given in (4.2.8), one may construct generators for $\mathcal{L}^Q$ and $\mathcal{L}^P$, which take the form

$$\mathcal{L}^Q = \mathcal{D}^{\frac{1}{2}}\mathcal{L}^W\mathcal{D}^{-\frac{1}{2}} = e^{\mathrm{ad}_{\frac{\hbar s^2}{4}\frac{\partial^2}{\partial q^2}+\frac{\hbar}{4s^2}\frac{\partial^2}{\partial p^2}}}\mathcal{L}^W \tag{I.5}$$

$$\mathcal{L}^P = \mathcal{D}^{-\frac{1}{2}}\mathcal{L}^W\mathcal{D}^{\frac{1}{2}} = e^{-\mathrm{ad}_{\frac{\hbar s^2}{4}\frac{\partial^2}{\partial q^2}+\frac{\hbar}{4s^2}\frac{\partial^2}{\partial p^2}}}\mathcal{L}^W, \tag{I.6}$$

where we have used the relation $e^{\mathrm{ad}_{\mathcal{B}}}\mathcal{A} = e^{\mathcal{B}}\mathcal{A}e^{-\mathcal{B}}$. To compute the generators to $O(1)$ in $\hbar$, one can use the definition of the exponential of the adjoint, and the generator of $\mathcal{L}^W$, and expand in orders of $\hbar$. Taking first the generator of partial Husimi dynamics, we find

$$\begin{aligned} \mathcal{L}^Q &= \left[1 + \mathrm{ad}_{\frac{\hbar s^2}{4}\frac{\partial^2}{\partial q^2}+\frac{\hbar}{4s^2}\frac{\partial^2}{\partial p^2}} + \frac{1}{2}\mathrm{ad}^2_{\frac{\hbar s^2}{4}\frac{\partial^2}{\partial q^2}+\frac{\hbar}{4s^2}\frac{\partial^2}{\partial p^2}} + \dots\right]\left(-\frac{i}{\hbar}[H,\,\cdot\,] + \frac{1}{2}(\{H,\,\cdot\,\} - \{\,\cdot\,,H\}) + \dots\right) \\ &= -\frac{i}{\hbar}[H,\,\cdot\,] + \frac{1}{2}(\{H,\,\cdot\,\} - \{\,\cdot\,,H\}) + \mathrm{ad}_{\frac{\hbar s^2}{4}\frac{\partial^2}{\partial q^2}+\frac{\hbar}{4s^2}\frac{\partial^2}{\partial p^2}}\left(-\frac{i}{\hbar}[H,\,\cdot\,]\right) + O(\hbar). \end{aligned} \tag{I.7}$$

Computing the adjoint action explicitly gives

$$\begin{aligned} \mathcal{L}^Q\big|_{O(\hbar^0)} = &-\frac{i}{\hbar}[H,\,\cdot\,] + \frac{1}{2}(\{H,\,\cdot\,\} - \{\,\cdot\,,H\}) \\ &- \frac{is^2}{2}[\frac{\partial H}{\partial q},\frac{\partial\,\cdot}{\partial q}] - \frac{i}{2s^2}[\frac{\partial H}{\partial p},\frac{\partial\,\cdot}{\partial p}] - \frac{is^2}{4}[\frac{\partial^2 H}{\partial q^2},\,\cdot\,] - \frac{i}{4s^2}[\frac{\partial^2 H}{\partial p^2},\,\cdot\,], \end{aligned} \tag{I.8}$$

as given in (4.6.1). Similarly, one may compute the same for the partial Glauber-Sudarshan dynamics, which differs only by a minus sign, giving

$$\begin{aligned}\mathcal{L}^P\big|_{O(\hbar^0)} = &-\frac{i}{\hbar}[H,\ \cdot\ ] + \frac{1}{2}(\{H,\ \cdot\ \} - \{\ \cdot\ , H\}) \\ &+ \frac{is^2}{2}[\frac{\partial H}{\partial q}, \frac{\partial\ \cdot}{\partial q}] + \frac{i}{2s^2}[\frac{\partial H}{\partial p}, \frac{\partial\ \cdot}{\partial p}] + \frac{is^2}{4}[\frac{\partial^2 H}{\partial q^2},\ \cdot\ ] + \frac{i}{4s^2}[\frac{\partial^2 H}{\partial p^2},\ \cdot\ ],\end{aligned} \tag{I.9}$$

as in (4.6.2).

# Appendix J

# A broader class of thermal state preserving dynamics

In this appendix we provide a explicit forms of dynamics satisfying both $\mathcal{L}(\pi) = 0$ and detailed balance that generalise the models provided in Section 5.3.

## Overdamped dynamics with correlated noise

Consider a thermal fixed point $\pi = e^{-\beta H(z)}/\mathcal{Z}$ and consider a general classical-quantum dynamics that both saturates the trade-off and satisfies detailed balance i.e. takes the form (2.20) and satisfies the equations (5.6.17) to (5.6.21). If we additionally assume that $D_2$ is full rank, $K^{rev} = 0$ and $K_i^{irr}\pi^{1/2} = \pi^{1/2}K_i^{irr\dagger}$, then the dynamics significantly simplifies, and may be written in a closed form.

To begin with, one may use $K^{rev} = 0$ and $K_i^{irr}\pi^{1/2} = \pi^{1/2}K_i^{irr\dagger}$ to show that the Lindblad operators $K_i$ take the form

$$K_i = \frac{1}{4}\frac{\partial D_{2,ij}}{\partial z_j} + \frac{1}{2}D_{2,ij}\frac{\partial \pi^{\frac{1}{2}}}{\partial z_j}\pi^{-1/2} = \frac{1}{4}\frac{\partial D_{2,ij}}{\partial z_j} - \frac{\beta}{4}D_{2,ij}L_j, \tag{J.1}$$

where here we use $L_j$ to denote the $L_z$ operator for $z = z_j$. On the other hand, since $D_2$ is full rank, $\mathbb{I} - D_2 D_2^{-1} = 0$, which along with $K^{rev} = 0$ and $K_i^{irr}\pi^{1/2} = \pi^{1/2}K_i^{irr\dagger}$ implies that $O^A = 0$. This means that there are no additional constraints on $K_i$ in terms of $D_{2,ij}$, and

additionally that $G^A$ is 0 up to an arbitrary component that we set equal to zero. This means that the unitary part of the dynamics is described by a unitary generator $G$ that is purely symmetric under time-reversal, which takes the form

$$G = H - \frac{i\hbar\beta}{32} D_{2,ij} \frac{\partial D_{2,il}}{\partial z_l} D_{2,jk} (L_k^\dagger - L_k) + \frac{\beta^2}{16} D_{2,ij} M_{ij}, \tag{J.2}$$

where $M_{ij}$ is $M_{xy}$ for $x = z_i$ and $y = z_j$. When we take the case of uncorrelated noise that satisfies the Einstein relation $D_{2,ij} = \frac{2\mu}{\beta}\delta_{ij}$, and take the number of degrees of freedom $n = 1$, we recover the model given in (5.3.10).

## Underdamped dynamics for arbitrary $H(q, p)$

Consider a thermal fixed point $\pi = e^{-\beta H(q,p)}/\mathcal{Z}$, where $H(q, p)$ may have any functional dependence on $q$ and $p$ provided it is invariant under time-reversal. In this case, there may be backreaction on both the classical momentum $p$ and classical position $q$, and thus for positivity of the dynamics, there must be corresponding diffusion in both momentum and position. Although phase-dependent and correlated noise may be studied using the methods discussed in the previous section, a simple choice is

$$D_2 = \frac{2}{\beta} \begin{pmatrix} \gamma_q & 0 \\ 0 & \gamma_p \end{pmatrix}, \tag{J.3}$$

where $\gamma_q$ and $\gamma_p$ are constants. Taking the following choices for $K = K^{rev} + K^{irr}$ and $S$

$$K^{rev} = \frac{1}{2} \begin{pmatrix} L_p \\ -L_q \end{pmatrix} \qquad K^{irr} = \frac{1}{2} \begin{pmatrix} -\gamma_q L_q \\ -\gamma_p L_p \end{pmatrix} \qquad S = \frac{\beta}{8}(\gamma_q + \gamma_p^{-1}) M_{pp} + \frac{\beta}{8}(\gamma_p + \gamma_q^{-1}) M_{qq} + H, \tag{J.4}$$

it is straightforward to check that these satisfy the detailed balance constraints, and thus that the dynamics satisfies detailed balance, and hence $\mathcal{L}(\pi) = 0$.

# Appendix K

# Invariance of interaction under changes to the classical Hamiltonian

For the interaction between the classical and quantum subsystems to be meaningfully defined, it is reasonable to expect that it is independent of the particular choice of classical Hamiltonian. In other words, changing the classical potential should only affect the drift of the classical system, and not affect the structure of the dynamics related to the quantum system.

To see that this is indeed the case, consider the affect of modifying the classical-quantum Hamiltonian by

$$H \mapsto H + V(z)\mathbb{I}. \tag{K.1}$$

The corresponding change to $L_z$ is easily computed to be

$$L_z \mapsto L_z + \frac{\partial V}{\partial z}\mathbb{1}, \tag{K.2}$$

and the change in $M_{zz}$ may also be solved, using (5.3.4) and (5.3.2), to give

$$M_{zz} \mapsto M_{zz} - \frac{i\hbar}{2}\frac{\partial V}{\partial z}(L_z - L_z^\dagger). \tag{K.3}$$

As expected, the change to $L_z$ leads to an additional drift term in the classical part of the dynamics. However, at first glance the change in $M_{zz}$ makes it appear that the unitary part of the quantum dynamics is affected by the choice of classical potential $V$. However, the change in $L_z$ also affects the decoherence part of the dynamics, and it turns out that the additional

term that arises exactly cancels the change in $M_{zz}$ described above. The overall effect of the transformation (K.1) is thus simply captured by

$$\mathcal{L}(\varrho) \mapsto \mathcal{L}(\varrho) + \mu\partial_x((\partial_x V)) \tag{K.4}$$

or

$$\mathcal{L}(\varrho) \mapsto \mathcal{L}(\varrho) + \{V, \varrho\}. \tag{K.5}$$

Aside from being physically reasonable, this property means that purely classical parts of the dynamics may be included by including additional classical drift terms, independent of $L_z$ and $M_{zz}$, rather than needing to include such effects directly via these operators.

# Appendix L

# Thermalisation additional material

In this appendix, we include additional material showing evidence that the coherences in the adiabatic basis, correlations between position and momentum, and the correlations between the classical and quantum systems, all vanish over time in the relative position representation. Along with the thermalisation properties shown in Section 5.5.6, this provides evidence that the classical-quantum state for this model does indeed thermalise for typical initial conditions and model parameters.

We first turn to look at the coherences in the adiabatic basis in the relative position representation i.e. the coherences in the number state basis when expressed in terms of $|\psi^{\mathfrak{r}}\rangle$. To study this, we consider a pure state whose probabilities of occupying the adiabatic basis states is given by the thermal state, namely that $|\psi^{\mathfrak{r}}\rangle = \sum_n \sqrt{p_n}|n\rangle$ where $p_n \propto \exp(-\beta\epsilon_n)$. Plotting the coherences between the first 5 adiabatic energy levels in Fig. L.1 we see that their each of their values appear to tend to zero. The same behaviour may be found for other initial conditions with coherence in this basis.

We must also check that the classical variables $q_t$ and $p_t$ are indeed uncorrelated at long times. To check this, we plot the covariance function between the two variables in Figure L.2 for an initial condition in which the system either starts at $q_0 = p_0 = 1$ with $|\psi^{\mathfrak{r}}\rangle = |1\rangle$ or $q_0 = p_0 = -1$ with $|\psi^{\mathfrak{r}}\rangle = |0\rangle$ with equal probability i.e. with the initial condition

$$\hat{\varrho}^{\mathfrak{r}}(q,p) = \frac{1}{2}\delta(q-1)\delta(p-1)|1\rangle\langle 1| + \frac{1}{2}\delta(q+1)\delta(p+1)|0\rangle\langle 0|. \tag{L.1}$$

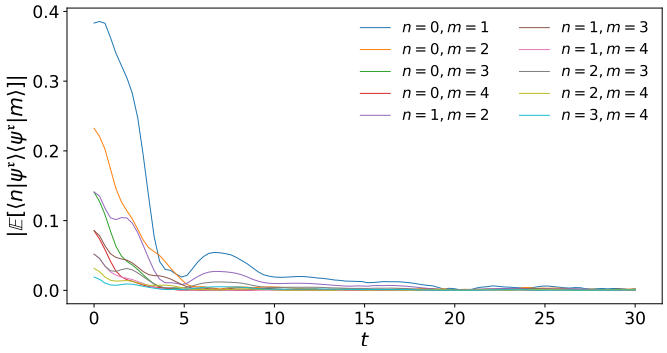


Figure L.1: Absolute value of the coherences between the first five energy levels plotted from $t = 0$ to $t = 30$. Here we take parameters $\omega = m_C = m_Q = \hbar = \beta = \gamma = \Omega = 1$, while $N_{max} = 20$ and $N_{steps} = 10^4$, and compute the average over $10^4$ trajectories.

We see here that the initially non-zero covariance between the two classical variables vanishes at long times, up to remaining fluctuations limited by the achievable number of trajectories in the simulation.

Finally, we study the correlations between the classical and quantum degrees of freedom in the relative position representation, using the same correlated distribution as described by Eq. (L.1). As before, we may compute the covariance, here between the random variable $q_t$ or $p_t$ and the density matrix $\hat{\rho}^{\mathfrak{r}}_t = |\psi^{\mathfrak{r}}\rangle_t\langle\psi^{\mathfrak{r}}|_t$. Since this gives in both cases a Hermitian matrix, plotting the eigenvalues of this matrix provides a measure of the covariance between the classical and quantum degrees of freedom – if all of the eigenvalues tend to zero then this is sufficient to conclude that the covariance between the classical and quantum degrees vanishes. Plotting the first five eigenvalues of these matrices in Figure L.3 we see that the initial correlations due to the initial conditions rapidly die off, again up to fluctuations due to limitations in the number of trajectories that are averaged over.

Strictly speaking, the vanishing of the covariance function in the above two cases does not guarantee that the two variables in each case are not correlated, since we have not also demonstrated that they also are not jointly Gaussian distributed. While this appears likely, given that the drift and back-reaction operators are linear in both $q, p$ and in $\hat{q}, \hat{p}$, we leave this, and a more rigorous theoretical characterisation of thermalisation, to future work.

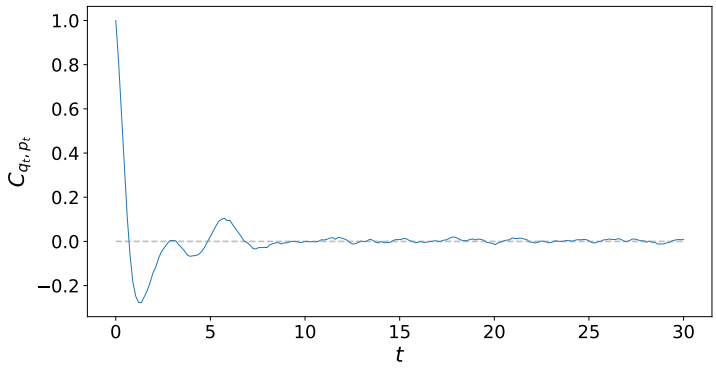


Figure L.2: The covariance between $q_t$ and $p_t$ from $t = 0$ to $t = 30$ for an initial state given in Eq. (L.1) with $\omega = m_C = m_Q = \hbar = \beta = \gamma = \Omega = 1$, while $N_{max} = 10$ and $N_{steps} = 5000$, and computed over $2 \times 10^4$ trajectories.

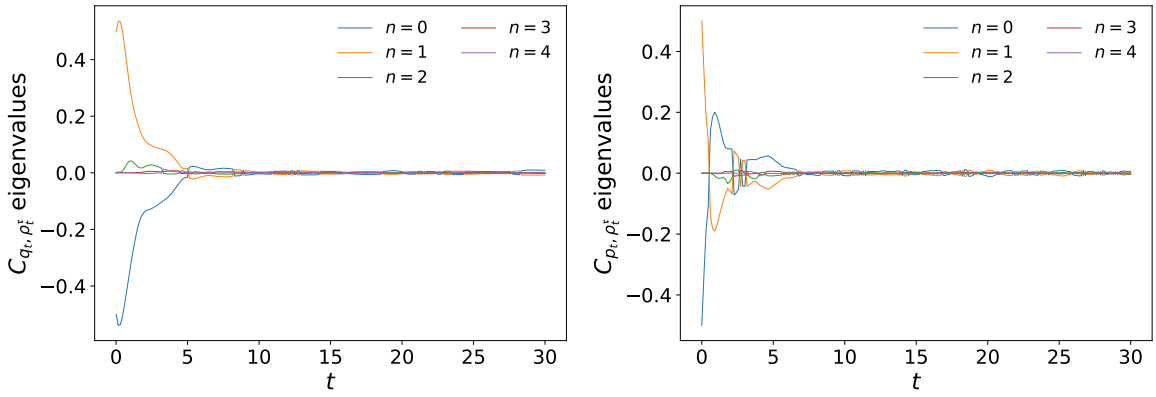


Figure L.3: Eigenvalues of the covariance between $q_t$ (left) and $q_t$ (right) with the quantum state in the relative position basis $\rho_t^{\mathfrak{r}}$, with the same initial conditions and parameters as in Figure L.2.

# Appendix M

# Derivation of the detailed balance conditions

In this section we demonstrate how the detailed balance conditions (5.6.17) to (5.6.21) may be derived from the definition of detailed balance (5.6.5), using the positivity conditions of (2.21) and (2.22). Note that here we assume the trade-off is saturated i.e. $\tilde{L}_\alpha = 0$.

We start by explicitly writing out the forms of both the generator $\pi^{-\frac{1}{2}}\mathcal{L}(\pi^{\frac{1}{2}}A\pi^{\frac{1}{2}})\pi^{-\frac{1}{2}}$ and the adjoint generator under time-reversal $\mathcal{L}_\epsilon^\dagger(A)$, in terms of the operators $K_i^{rev}$, $K_i^{irr}$, $G^S$, and $G^A$. It is straightforward to check that these take the form

$$\begin{aligned}
&\pi^{-\frac{1}{2}}\mathcal{L}(\pi^{\frac{1}{2}}A\pi^{\frac{1}{2}})\pi^{-\frac{1}{2}} = \\
&-\frac{i}{\hbar}\pi^{-\frac{1}{2}}[G^S+G^A,\pi^{\frac{1}{2}}A\pi^{\frac{1}{2}}]\pi^{-\frac{1}{2}} - \pi^{-\frac{1}{2}}\frac{\partial}{\partial z_i}\left(K_i^{rev}\pi^{\frac{1}{2}}A\pi^{\frac{1}{2}} + \pi^{\frac{1}{2}}A\pi^{\frac{1}{2}}K_i^{rev\dagger}\right)\pi^{-\frac{1}{2}} \\
&-\pi^{-\frac{1}{2}}\frac{\partial}{\partial z_i}\left(K_i^{irr}\pi^{\frac{1}{2}}A\pi^{\frac{1}{2}} + \pi^{\frac{1}{2}}A\pi^{\frac{1}{2}}K_i^{irr\dagger}\right)\pi^{-\frac{1}{2}} + \frac{1}{2}\pi^{-\frac{1}{2}}\frac{\partial^2}{\partial z_i\partial z_j}(D_{2,ij}\pi^{\frac{1}{2}}A\pi^{\frac{1}{2}})\pi^{-\frac{1}{2}} \\
&+D_{2,ij}^{-1}\pi^{-\frac{1}{2}}\big[(K_i^{rev}+K_i^{irr})\pi^{\frac{1}{2}}A\pi^{\frac{1}{2}}(K_j^{rev}+K_j^{irr})^\dagger - \frac{1}{2}\{(K_j^{rev}+K_j^{irr})^\dagger(K_i^{rev}+K_i^{irr}),\pi^{\frac{1}{2}}A\pi^{\frac{1}{2}}\}_+\big]\pi^{-\frac{1}{2}}
\end{aligned} \tag{M.1}$$

$$\mathcal{L}_\epsilon^\dagger(A) - 2i[X,A] =$$
$$-2i[X,A] + \frac{i}{\hbar}[G^S - G^A, A] + (K_i^{irr} - K_i^{rev})^\dagger \frac{\partial A}{\partial z_i} + \frac{\partial A}{\partial z_i}(K_i^{irr} - K_i^{rev}) + \frac{1}{2}\epsilon_i\epsilon_j D_{2,ij}(\epsilon z)\frac{\partial^2 A}{\partial z_i \partial z_j}$$
$$+ \epsilon_i\epsilon_j D_{2,ij}^{-1}(\epsilon z)\big[(K_i^{irr} - K_i^{rev})^\dagger A (K_j^{irr} - K_j^{rev}) - \frac{1}{2}\{(K_j^{irr} - K_j^{rev})^\dagger (K_i^{irr} - K_i^{rev}), A\}_+\big], \tag{M.2}$$

where here all quantities are dependent on $z$ rather than $\epsilon z$ unless indicated otherwise.

Since the detailed balance condition (5.6.5) must hold for all $A$, the terms containing each order of derivative of $A$ must cancel separately. Starting with the second order derivative terms, we see that all the dependence on $\pi$ cancels to give

$$\frac{1}{2}D_{2,ij}\frac{\partial^2 A}{\partial z_i \partial z_j} = \frac{1}{2}\epsilon_i\epsilon_j D_{2,ij}(\epsilon z)\frac{\partial^2 A}{\partial z_i \partial z_j}. \tag{M.3}$$

This holds for all $A$ if and only if

$$D_{2,ij}(z) = \epsilon_i\epsilon_j D_{2,ij}(\epsilon z) \tag{M.4}$$

which is exactly equivalent to the diffusion constraint of (5.6.17).

Turning now to the first derivatives of $A$, collecting terms and defining the operators $B_i$ as

$$B_i = -\pi^{-\frac{1}{2}} K_i^{rev} \pi^{\frac{1}{2}} - \pi^{-\frac{1}{2}} K_i^{irr} \pi^{\frac{1}{2}} + \frac{1}{2}\frac{\partial D_{2,ij}}{\partial z_j} + D_{2,ij}\pi^{-\frac{1}{2}}\frac{\partial \pi^{\frac{1}{2}}}{\partial z_j} - K_i^{irr\dagger} + K_i^{rev\dagger}, \tag{M.5}$$

we see that

$$B_i \frac{\partial A}{\partial z_i} + \frac{\partial A}{\partial z_i} B_i^\dagger = 0 \tag{M.6}$$

must hold for every choice of operator $A$, which is true if and only if $B_i C + C B_i^\dagger = 0$ holds for every choice of operator $C$. Taking the trace with $C = \mathbb{1}$, we see that each $B_i$ must be anti-Hermitian. Decomposing this as $B = iJ$ where $J = J^\dagger$, we see that the above relation implies that $J$ commutes with every operator i.e. is proportional to the identity operator. We thus see that we can write this condition in the form

$$-\pi^{-\frac{1}{2}}(K_i^{rev} + K_i^{irr})\pi^{\frac{1}{2}} + \frac{1}{2}\frac{\partial D_{2,ij}}{\partial z_j} + D_{2,ij}\pi^{-\frac{1}{2}}\frac{\partial \pi^{\frac{1}{2}}}{\partial z_j} - (K_i^{irr} - K_i^{rev})^\dagger = -ia_i\mathbb{1}, \tag{M.7}$$

where here $a_i$ is some real number that may depend on phase space. Acting on the left with the operator $\pi^{\frac{1}{2}}$ and setting the Hermitian and anti-Hemtitian parts equal separately, we see that we recover the reversible and irreversible backreaction constraints given in (5.6.18) and

(5.6.19). For these constraints to be self-consistent, we see that $a_i$ must transform as the reversible back-reaction operators do i.e. $a_i(\epsilon z) = -\epsilon_i a_i(z)$.

The final conditions that follow from the terms proportional to $A$ are a little more complex to compute. To start with, we consider the expression $\mathcal{E}_1$, made up of moving all the terms which have operators acting on both sides of $A$ to the left hand side of the equation, which takes the form

$$\begin{aligned}\mathcal{E}_1 = \\ &- \pi^{-\frac{1}{2}}(K_i^{rev} + K_i^{irr})\pi^{\frac{1}{2}} A \frac{\partial \pi^{\frac{1}{2}}}{\partial z_i}\pi^{-\frac{1}{2}} - \pi^{-\frac{1}{2}}\frac{\partial \pi^{\frac{1}{2}}}{\partial z_i} A \pi^{\frac{1}{2}}(K_i^{rev} + K_i^{irr})^\dagger \pi^{-\frac{1}{2}} + D_{2,ij}\pi^{-\frac{1}{2}}\frac{\partial \pi^{\frac{1}{2}}}{\partial z_i} A \frac{\partial \pi^{\frac{1}{2}}}{\partial z_i}\pi^{-\frac{1}{2}} \\ &+ D_{2,ij}^{-1}\big[\pi^{-\frac{1}{2}}(K_i^{rev} + K_i^{irr})\pi^{\frac{1}{2}}\big] A \big[\pi^{\frac{1}{2}}(K_i^{rev} + K_i^{irr})^\dagger \pi^{-\frac{1}{2}}\big] - D_{2,ij}^{-1}(K_i^{irr} - K_i^{rev})^\dagger A (K_i^{irr} - K_i^{rev}).\end{aligned} \tag{M.8}$$

Here we have here used the diffusion constraint (M.4) to rewrite $\epsilon_i\epsilon_j D_{2,ij}^{-1}(\epsilon z)$ as simply $D_{2,ij}^{-1}$. From the above expression, it is apparent that some of the terms will cancel upon replacing appearances of $\pi^{-\frac{1}{2}}(K_i^{rev} + K_i^{irr})\pi^{\frac{1}{2}}$ and its conjugate with $(K_i^{irr} - K_i^{rev})^\dagger$ and its conjugate using Eq. (M.7). Substituting these in, and using the properties of $D_2$ and its pseudoinverse that follow from the positivity condition $D_2 \succeq 0$, such as $D_2 D_2^{-1} = D_2^{-1} D_2$ and $D_2 D_2 D_2^{-1} = D_2$, we find that this expression takes the form

$$\begin{aligned}\mathcal{E}_1 = &- (\mathbb{I} - D_2 D_2^{-1})_{ij}\big[(K_i^{rev} - K_i^{irr})^\dagger + \frac{1}{2}\frac{\partial D_{2,ik}}{\partial z_k} + i a_i\big] A \frac{\partial \pi^{\frac{1}{2}}}{\partial z_j}\pi^{-\frac{1}{2}} + h.c. \\ &+ D_{2,ij}^{-1}(K_i^{rev} - K_i^{irr})^\dagger(\frac{1}{2}\frac{\partial D_{2,jk}}{\partial z_k} - i a_j) A + \frac{1}{8} D_{2,ij}^{-1}\frac{\partial D_{2,ik}}{\partial z_k}\frac{\partial D_{2,jl}}{\partial z_l} A + \frac{1}{2} D_{2,ij}^{-1} a_i a_j A + h.c.\end{aligned} \tag{M.9}$$

where here $h.c.$ denotes the Hermitian conjugate (treating $A$ as Hermitian) of all of the terms explicitly written on a given line. We see from this expression that the only terms that are not of the form of only a single operator to the left or right of $A$ are on the top line. However, let us recall that in addition to the positivity condition $D_2 \succeq 0$, we also have the condition of (2.22). Writing this out explicitly, we see that this implies the existence of a phase space dependent vector $v$ such that

$$(\mathbb{I} - D_2 D_2^{-1})(K^{rev} + K^{irr}) = v\mathbb{1}. \tag{M.10}$$

Acting on the left with $\pi^{-\frac{1}{2}}$ and the right with $\pi^{\frac{1}{2}}$, we may use the expression in (M.7) to

rewrite this as

$$(\mathbb{I} - D_2 D_2^{-1})\big[(K^{rev} - K^{irr})^\dagger + \frac{1}{2}\frac{\partial D_2}{\partial z} + ia\big] = v\mathbb{1}, \tag{M.11}$$

where here we have dropped a term using $D_2 D_2^{-1} D_2 = D_2$. We thus see that the main expression of the top line of (M.9) is proportional to the identity, and thus may be commuted with $A$ to give an expression of $\mathcal{E}_1$ entirely in the form of operators on the left or right hand side of $A$. Returning now to include the terms already of this form, we see that the constraint setting the entirety of the terms proportional to $A$ to zero takes the form

$$FA + AF^\dagger = 0 \tag{M.12}$$

for all operators $A$, where $F$ is defined as the operator

$$\begin{aligned}
F =& -\frac{i}{\hbar}(\pi^{-\frac{1}{2}} G^S \pi^{\frac{1}{2}} + G^S) - \frac{i}{\hbar}(\pi^{-\frac{1}{2}} G^A \pi^{\frac{1}{2}} - G^A) + 2iX \\
&- \pi^{-\frac{1}{2}} \frac{\partial}{\partial z_i}\left((K_i^{rev} + K_i^{irr})\pi^{\frac{1}{2}}\right) + \frac{1}{4}\frac{\partial^2 D_{2,ij}}{\partial z_i \partial z_j} + \pi^{-\frac{1}{2}}\frac{\partial D_{2,ij}}{\partial z_i}\frac{\partial \pi^{\frac{1}{2}}}{\partial z_j} + \frac{1}{2}\pi^{-\frac{1}{2}} D_{2,ij}\frac{\partial^2 \pi^{\frac{1}{2}}}{\partial z_i \partial z_j} \\
&- \frac{1}{2} D_{2,ij}^{-1}\left[\pi^{-\frac{1}{2}}(K_i^{rev} + K_i^{irr})^\dagger (K_j^{rev} + K_j^{irr})\pi^{\frac{1}{2}} + (K_i^{irr} - K_i^{rev})^\dagger (K_j^{irr} - K_j^{rev})\right] \\
&- (\mathbb{I} - D_2 D_2^{-1})_{ij}\big[(K_i^{rev} - K_i^{irr}) + \frac{1}{2}\frac{\partial D_{2,ik}}{\partial z_k} - ia_i\big]\pi^{-\frac{1}{2}}\frac{\partial \pi^{\frac{1}{2}}}{\partial z_j} \\
&+ D_{2,ij}^{-1}(K_i^{rev} - K_i^{irr})^\dagger(\frac{1}{2}\frac{\partial D_{2,jk}}{\partial z_k} - ia_j) + \frac{1}{8} D_{2,ij}^{-1}\frac{\partial D_{2,ik}}{\partial z_k}\frac{\partial D_{2,jl}}{\partial z_l} + \frac{1}{2} D_{2,ij}^{-1} a_i a_j.
\end{aligned} \tag{M.13}$$

Noting as before that this implies that $F = ib\mathbb{1}$, where $b$ is a real number dependent on phase-space, we may act with $\pi^{\frac{1}{2}}$ on the left to find the analogue of (M.7) for the zeroth order derivative terms

$$\begin{aligned}
&- \frac{i}{\hbar}(G^S \pi^{\frac{1}{2}} + \pi^{\frac{1}{2}} G^S) - \frac{i}{\hbar}(G^A \pi^{\frac{1}{2}} - \pi^{\frac{1}{2}} G^A) + i(X\pi^{\frac{1}{2}} + \pi^{\frac{1}{2}} X) \\
&- \frac{\partial}{\partial z_i}\left((K_i^{rev} + K_i^{irr})\pi^{\frac{1}{2}}\right) + \frac{1}{4}\pi^{\frac{1}{2}}\frac{\partial^2 D_{2,ij}}{\partial z_i \partial z_j} + \frac{\partial D_{2,ij}}{\partial z_i}\frac{\partial \pi^{\frac{1}{2}}}{\partial z_j} + \frac{1}{2} D_{2,ij}\frac{\partial^2 \pi^{\frac{1}{2}}}{\partial z_i \partial z_j} \\
&- \frac{1}{2} D_{2,ij}^{-1}[K_i^{rev\dagger} K_j^{rev} + K_i^{irr\dagger} K_j^{irr}, \pi^{\frac{1}{2}}] - \frac{1}{2} D_{2,ij}^{-1}\{K_i^{rev\dagger} K_j^{irr} + K_i^{irr\dagger} K_j^{rev}, \pi^{\frac{1}{2}}\}_+ \\
&- (\mathbb{I} - D_2 D_2^{-1})_{ij}\big[(K_i^{rev} - K_i^{irr}) + \frac{1}{2}\frac{\partial D_{2,ik}}{\partial z_k} - ia_i\big]\frac{\partial \pi^{\frac{1}{2}}}{\partial z_j} \\
&+ D_{2,ij}^{-1}(\frac{1}{2}\frac{\partial D_{2,ik}}{\partial z_k} - ia_i)\pi^{\frac{1}{2}}(K_j^{rev} - K_j^{irr})^\dagger + \frac{1}{8} D_{2,ij}^{-1}\frac{\partial D_{2,ik}}{\partial z_k}\frac{\partial D_{2,jl}}{\partial z_l}\pi^{\frac{1}{2}} + \frac{1}{2} D_{2,ij}^{-1} a_i a_j \pi^{\frac{1}{2}} = ib\pi^{\frac{1}{2}}.
\end{aligned} \tag{M.14}$$

In the above, we have used the property that $X$ commutes with $\pi$ to rewrite the term containing $X$ as an anti-Hermitian term, as well as rewriting the $D_{2,ij}^{-1}$ term into commutator and anti-commutator parts. To derive the symmetric and anti-symmetric unitary generator constraints from this expression, we consider the anti-Hermitian and Hermitian parts of the above expression separately. The anti-Hermitian part of this equation takes the form

$$
\begin{aligned}
&-\frac{i}{\hbar}(G^S\pi^{\frac{1}{2}}+\pi^{\frac{1}{2}}G^S)+i(X\pi^{\frac{1}{2}}+\pi^{\frac{1}{2}}X)\\
&-\frac{1}{2}\frac{\partial}{\partial z_i}(K_i^{rev}\pi^{\frac{1}{2}}-\pi^{\frac{1}{2}}K_i^{rev\dagger})-\frac{1}{2}\frac{\partial}{\partial z_i}(K_i^{irr}\pi^{\frac{1}{2}}-\pi^{\frac{1}{2}}K_i^{irr\dagger})\\
&-\frac{1}{2}D_{2,ij}^{-1}[K_i^{rev\dagger}K_j^{rev}+K_i^{irr\dagger}K_j^{irr},\pi^{\frac{1}{2}}]\\
&-\frac{1}{2}(\mathbb{I}-D_2D_2^{-1})_{ij}\big[(K_i^{rev}-K_i^{irr})\frac{\partial\pi^{\frac{1}{2}}}{\partial z_j}-\frac{\partial\pi^{\frac{1}{2}}}{\partial z_j}(K_i^{rev}-K_i^{irr})^\dagger\big]+ia_i(\mathbb{I}-D_2D_2^{-1})_{ij}\frac{\partial\pi^{\frac{1}{2}}}{\partial z_j}\\
&-\frac{i}{2}a_iD_{2,ij}^{-1}(K_j^{rev}\pi^{\frac{1}{2}}+\pi^{\frac{1}{2}}K_j^{rev\dagger})+\frac{i}{2}a_iD_{2,ij}^{-1}(K_j^{irr}\pi^{\frac{1}{2}}+\pi^{\frac{1}{2}}K_j^{irr\dagger})\\
&-\frac{1}{4}D_{2,ij}^{-1}\frac{\partial D_{2,ij}}{\partial z_k}(K_j^{rev}\pi^{\frac{1}{2}}-\pi^{\frac{1}{2}}K_j^{rev\dagger})+\frac{1}{4}D_{2,ij}^{-1}\frac{\partial D_{2,ij}}{\partial z_k}(K_j^{irr}\pi^{\frac{1}{2}}-\pi^{\frac{1}{2}}K_j^{irr\dagger})=ib\pi^{\frac{1}{2}}.
\end{aligned}
\tag{M.15}
$$

Substituting in the reversible and irreversible backreaction constraints (5.6.18) and (5.6.19) wherever $K_i^{rev}\pi^{1/2}-\pi^{1/2}K_i^{rev\dagger}$ or $K_i^{irr}\pi^{1/2}+\pi^{1/2}K_i^{irr\dagger}$ explicitly appear, one finds that the equation simplifies to

$$
\begin{aligned}
&-\frac{i}{\hbar}(G^S\pi^{\frac{1}{2}}+\pi^{\frac{1}{2}}G^S)=\\
&-i(X\pi^{\frac{1}{2}}+\pi^{\frac{1}{2}}X)+\frac{1}{2}\frac{\partial}{\partial z_i}(K_i^{irr}\pi^{1/2}-\pi^{1/2}K_i^{irr\dagger})\\
&-\frac{1}{2}(\mathbb{I}-D_2D_2^{-1})_{ij}(K_i^{irr}\frac{\partial\pi^{\frac{1}{2}}}{\partial z_j}-\frac{\partial\pi^{\frac{1}{2}}}{\partial z_j}K_i^{irr\dagger})-\frac{1}{4}D_{2,ij}^{-1}\frac{\partial D_{2,ik}}{\partial z_k}(K_j^{irr}\pi^{1/2}-\pi^{1/2}K_j^{irr\dagger})\\
&+\frac{i}{2}D_{2,ij}^{-1}a_i(K_i^{rev}\pi^{1/2}+\pi^{1/2}K_i^{rev\dagger})+\frac{1}{2}D_{2,ij}^{-1}[K_i^{rev\dagger}K_j^{rev}+K_i^{irr\dagger}K_j^{irr},\pi^{1/2}]\\
&-\frac{i}{2}a_i(\mathbb{I}-D_2D_2^{-1})_{ij}\frac{\partial\pi^{\frac{1}{2}}}{\partial z_j}+\frac{1}{2}(\mathbb{I}-D_2D_2^{-1})_{ij}(K_i^{rev}\frac{\partial\pi^{\frac{1}{2}}}{\partial z_j}-\frac{\partial\pi^{\frac{1}{2}}}{\partial z_j}K_i^{rev\dagger})+i(b+\frac{1}{2}\frac{\partial a_i}{\partial z_i})\pi^{\frac{1}{2}}
\end{aligned}
\tag{M.16}
$$

Since the left-hand side of this equation is symmetric under time-reversal, the right-hand side must also be. Performing the time-reversal transformation, noting the previously found form of time-reversal for $a_i$, we see that all of the terms are symmetric, other than the three terms on the final line. Returning to the positivity condition (M.10), we note that since this holds for

both the reversible and irreversible components separately i.e.

$$(\mathbb{I} - D_2 D_2^{-1})K^{rev} = v^{rev}\mathbb{1}, \qquad (\mathbb{I} - D_2 D_2^{-1})K^{irr} = v^{irr}\mathbb{1}, \tag{M.17}$$

one may rearrange the two terms containing $\mathbb{I} - D_2 D_2^{-1}$ on the final line into the form

$$\frac{1}{2}(\mathbb{I} - D_2 D_2^{-1})_{ij}\big[K_i^{rev}\pi^{\frac{1}{2}} - \pi^{\frac{1}{2}}K_i^{rev} - ia_i\pi^{\frac{1}{2}}\big]\pi^{-\frac{1}{2}}\frac{\partial \pi^{\frac{1}{2}}}{\partial z_j}, \tag{M.18}$$

which clearly vanishes due to the reversible back-reaction constraint. For the final term containing $b$ to vanish, we see that $b$ must have an anti-symmetric component equal to $-\frac{1}{2}\partial_i a_i$ such that this final term cancels. Since the remaining component is purely symmetric and real, this term can be absorbed into the definition of $X$ by including a term $\frac{b}{2}\mathbb{1}$; since the above condition required the existence of a real-number $b$, and detailed balance required the existence of the operator $X$, we see that we may do this without loss of generality. Doing so, and defining the operator $O^S$ as in (5.6.22), we find the form of the symmetric unitary generator constraint quoted in (5.6.20).

Finally, turning to the Hermitian part of (M.14), we find this takes the form

$$\begin{aligned}
&-\frac{i}{\hbar}(G^A\pi^{\frac{1}{2}} - \pi^{\frac{1}{2}}G^A)\\
&-\frac{1}{2}\frac{\partial}{\partial z_i}(K_i^{rev}\pi^{\frac{1}{2}} + \pi^{\frac{1}{2}}K_i^{rev\dagger}) - \frac{1}{2}\frac{\partial}{\partial z_i}(K_i^{irr}\pi^{\frac{1}{2}} + \pi^{\frac{1}{2}}K_i^{irr\dagger})\\
&+\frac{1}{4}\pi^{\frac{1}{2}}\frac{\partial^2 D_{2,ij}}{\partial z_i \partial z_j} + \frac{\partial D_{2,ij}}{\partial z_i}\frac{\partial \pi^{\frac{1}{2}}}{\partial z_j} + \frac{1}{2}D_{2,ij}\frac{\partial^2 \pi^{\frac{1}{2}}}{\partial z_i \partial z_j}\\
&-\frac{1}{2}D^{-1}_{2,ij}\{K_i^{rev\dagger}K_j^{irr} + K_i^{irr\dagger}K_j^{rev}, \pi^{\frac{1}{2}}\}_+\\
&-\frac{1}{2}(\mathbb{I} - D_2 D_2^{-1})_{ij}\big[(K_i^{rev} - K_i^{irr})\frac{\partial \pi^{\frac{1}{2}}}{\partial z_j} + \frac{\partial \pi^{\frac{1}{2}}}{\partial z_j}(K_i^{rev} - K_i^{irr})^\dagger\big] - \frac{1}{2}(\mathbb{I} - D_2 D_2^{-1})_{ij}\frac{\partial D_{2,ik}}{\partial z_k}\frac{\partial \pi^{\frac{1}{2}}}{\partial z_j}\\
&+\frac{i}{2}a_i D^{-1}_{2,ij}(K_j^{rev}\pi^{\frac{1}{2}} - \pi^{\frac{1}{2}}K_j^{rev\dagger}) - \frac{i}{2}a_i D^{-1}_{2,ij}(K_j^{irr}\pi^{\frac{1}{2}} - \pi^{\frac{1}{2}}K_j^{irr\dagger})\\
&+\frac{1}{4}D^{-1}_{2,ij}\frac{\partial D_{2,ij}}{\partial z_k}(K_j^{rev}\pi^{\frac{1}{2}} + \pi^{\frac{1}{2}}K_j^{rev\dagger}) - \frac{1}{4}D^{-1}_{2,ij}\frac{\partial D_{2,ij}}{\partial z_k}(K_j^{irr}\pi^{\frac{1}{2}} + \pi^{\frac{1}{2}}K_j^{irr\dagger})\\
&+\frac{1}{8}D^{-1}_{2,ij}\frac{\partial D_{2,ik}}{\partial z_k}\frac{\partial D_{2,jl}}{\partial z_l}\pi^{\frac{1}{2}} + \frac{1}{2}D^{-1}_{2,ij}a_i a_j \pi^{\frac{1}{2}} = 0.
\end{aligned} \tag{M.19}$$

As before, substituting in the expressions for $K_i^{rev}\pi^{1/2} - \pi^{1/2}K_i^{rev\dagger}$ or $K_i^{irr}\pi^{1/2} + \pi^{1/2}K_i^{irr\dagger}$ from

(5.6.18) and (5.6.19), we find that this equation simplifies to take the form

$$
\begin{aligned}
-\frac{i}{\hbar}(G^A\pi^{\frac{1}{2}}-\pi^{\frac{1}{2}}G^A) = &\frac{1}{2}\frac{\partial}{\partial z_i}(K_i^{rev}\pi^{1/2}+\pi^{1/2}K_i^{rev\dagger}) \\
&+\frac{1}{2}(\mathbb{I}-D_2D_2^{-1})_{ij}(K_i^{rev}\frac{\partial\pi^{\frac{1}{2}}}{\partial z_j}+\frac{\partial\pi^{\frac{1}{2}}}{\partial z_j}K_i^{rev\dagger}) \\
&-\frac{1}{4}D_{2,ij}^{-1}\frac{\partial D_{2,ik}}{\partial z_k}(K_j^{rev}\pi^{1/2}+\pi^{1/2}K_j^{rev\dagger}) \\
&+\frac{i}{2}D_{2,ij}^{-1}a_i(K_i^{irr}\pi^{1/2}-\pi^{1/2}K_i^{irr\dagger}) \\
&+\frac{1}{2}D_{2,ij}^{-1}\{K_i^{rev\dagger}K_j^{irr}+K_i^{irr\dagger}K_j^{rev},\pi^{1/2}\}_+ \\
&+\frac{1}{4}(\mathbb{I}-D_2D_2^{-1})_{ij}\frac{\partial D_{2,ik}}{\partial z_k}\frac{\partial\pi^{\frac{1}{2}}}{\partial z_j}-\frac{1}{2}(\mathbb{I}-D_2D_2^{-1})_{ij}(K_i^{irr}\frac{\partial\pi^{\frac{1}{2}}}{\partial z_j}+\frac{\partial\pi^{\frac{1}{2}}}{\partial z_j}K_i^{irr\dagger}).
\end{aligned}
\tag{M.20}
$$

As before, we perform the time-reversal operation on both sides to see that all but the final line as written are antisymmetric under time-reversal. Using now the relation for $K^{irr}$ in (M.17) we see that this final time-reversal symmetric line vanishes in an analogous way to before, this time by using the irreversible back-reaction constraint. Defining the operator $O^A$ in (5.6.23), we thus recover the antisymmetric unitary generator constraint (5.6.21).