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# Adiabatic Dynamics in Closed and Open Quantum Systems

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# Abstract

This thesis is concerned with the examination of systems whose external parameters change slowly in time. The slowness assumption allows for the so called adiabatic approximation in many situations and is a useful means to study a variety of physical question. Both aspects are addressed here: On the one hand we present adiabatic theorems for linear as well as nonlinear evolution equations. On the other hand several applications are being discussed with main focus on quantum mechanical systems.

In a first – purely mathematical – part, we adopt a relatively abstract framework, namely that of time-dependent generators of contraction semigroups on a Banach space. If such generators satisfy a certain spectral gap condition there exists a perturbation expansion in the parameter measuring the slowness. The structure of the expansion has a geometric meaning entailing a distinction between terms which are local and terms which are non-local in time. If the gap condition is abandoned an adiabatic theorem can still be proved, though without information on the rate of convergence in the limit of infinite slowness. We will see that the appreciation of the geometric structure allows for fairly simple proofs in both cases.

Our theorems are likewise applicable to closed and open quantum systems described by a family of Hamiltonians or Lindbladians, respectively. A short introduction to the latter is the subject of the second part of this thesis. In view of our physical examples a particular emphasis is placed on the special class of dephasing Lindbladians. They model decoherence without dissipation: for them, a structural theorem is presented.

A third part then treats the combination of adiabatic and quantum theory resulting in a considerable range of applications: The coefficients in the above mentioned perturbation expansion have a different physical interpretation in closed as opposed to open quantum systems. After highlighting this fact in some generality we turn to more specific settings: An analogue of the Landau-Zener formula for transitions near an avoided crossings of eigenvalues is derived in the dephasing case. Furthermore, an optimization problem in adiabatic quantum computing is investigated in absence and in presence of dephasing. As a result, constraints on the physically allowed dephasing parameters are revealed in the case of Grover's search algorithm. Subsequently, we turn to slowly driven stochastic systems in order to illustrate the applicability of adiabatic perturbation expansions outside of quantum mechanics. The chapter is rounded off by a discussion of the adiabatic theorem in closed and open quantum systems without the condition of a spectral gap.

All these results are finally complemented in a forth part by an example of a nonlinear adiabatic theorem. More precisely, we study the time-dependent Gross-Pitaevskii equation which describes the dynamics of a weakly interacting Bose-Einstein condensate which is trapped by a slowly in time varying potential with exactly one eigenstate. The fact that the propagator of the linearized equation is not a contraction complicates the control of error terms considerably and asks for additional techniques in comparison to the linear case. That said however, the more concrete setting – that of a partial differential equation and a function space – allows for further structure and in particular we have dispersive estimates for the linear Schrödinger equation at hand. In connection with a bootstrap argument they enable us to prove the desired result.

# Zusammenfassung


Diese Doktorarbeit beschäftigt sich mit der Untersuchung von Systemen, deren externe Parameter sich langsam mit der Zeit ändern. Die Annahme von Langsamkeit erlaubt die sogenannte adiabatische Approximationen in zahlreichen Situationen und ist ein nützliches Mittel für das Studium einer Vielfalt physikalischer Fragen. Beide Aspekte werden hier behandelt: Einerseits präsentieren wir adiabatische Theoreme sowohl für lineare als auch für nichtlineare Evolutionsgleichungen. Andererseits werden mehrere Anwendungen diskutiert, wobei ein besonderes Augenmerk auf quantenmechanischen Systemen liegt.

In einem ersten – rein mathematischen – Teil führen wir einen relativ abstrakten Rahmen ein, nämlich denjenigen zeitabhängiger Generatoren von Kontraktionshalbgruppen auf Banachräumen. Falls solche Generatoren eine gewisse Spektrallückenbedingung erfüllen, dann existiert eine Störungsentwicklung im Parameter, welcher die Langsamkeit misst. Die Struktur der Entwicklung hat eine geometrische Bedeutung und bedingt eine Unterscheidung in Terme, welche lokal respektive nicht-lokal in der Zeit sind. Wird die Spektrallückenbedingung fallen gelassen, kann ein adiabatisches Theorem immer noch bewiesen werden; allerdings ohne Information über die Konvergenzrate im Grenzfall unendlicher Langsamkeit. Wir werden sehen, dass die Beachtung der geometrischen Struktur ziemlich einfache Beweise in beiden Fällen ermöglicht.

Unsere Theoreme sind gleichermassen anwendbar auf abgeschlossene wie auf offene Quantensysteme, welche durch eine Familie von Hamilton- respektive Lindblad-Operatoren beschrieben werden. Eine kurze Einführung in die letzteren ist Thema eines zweiten Teils dieser Doktorarbeit. Angesichts unserer physikalischen Beispiele wird eine besondere Beachtung der Klasse der phasenauslöschenden (engl. *dephasing*) Lindblad-Operatoren geschenkt. Diese modellieren Dekohärenz ohne Dissipation: für sie wird ein Strukturtheorem bewiesen.

Ein dritter Teil behandelt dann die Kombination von Adiabaten- und Quantentheorie, woraus ein beachtlicher Umfang an Anwendungen resultiert: Die Koeffizienten der oben erwähnten Störungsentwicklung haben eine unterschiedliche physikalische Interpretation für abgeschlossene im Gegensatz zu offenen Quantensystemen. Nach dem Beleuchten dieser Tatsache in einiger Allgemeinheit, wenden wir uns spezifischeren Situationen zu: Ein Analogon der Landau-Zener Formel für Übergänge nahe einem gemiedenen Kreuzen (engl. *avoided crossing*) von Eigenwerten wird hergeleitet für phasenauslöschenden Fall. Ferner wird ein Optimierungsproblem des adiabatischen Quantenrechnens (engl. *adiabatic quantum computing*) in An- und Abwesenheit von Phasenauslöschung untersucht. Als Konsequenz werden Einschränkungen für die physikalisch zulässigen Parameter, welche die Phasenauslöschung beschreiben, zutage gefördert. In der Folge wenden wir uns langsam angetriebenen stochastischen Systemen (engl. *slowly driven stochastic systems*) zu, um die Anwendbarkeit adiabatischer Störungsentwicklungen ausserhalb der Quantenmechanik zu illustrieren. Das Kapitel wird abgerundet durch eine Diskussion des adiabatischen Theorems für abgeschlossene und offene Quantensysteme ohne die Voraussetzung einer Spektrallücke.

All diese Resultate werden schlussendlich in einem vierten Teil ergänzt durch ein Beispiel eines nichtlinearen adiabatischen Theorems. Genauer gesagt studieren wir die zeitabhängige Gross-Piteavksii-Gleichung, welche die Dynamik eines schwach wechselwirkenden Bose-Einstein-Kondensats beschreibt, das gefangen ist in einem langsam zeitlich veränderlichen Potential, welches genau einen Eigenzustand zulässt. Die Tatsache, dass der Propagator der linearisierten Gleichung keine Kontraktion ist, erschwert die Kontrolle von Fehlertermen erheblich und verlangt nach zusätzlichen Techniken im Vergleich zum linearen Fall. Nichtsdestotrotz lässt der konkretere Rahmen – derjenige einer partiellen Differentialgleichung und eines Funktionen-

raums – zusätzliche Struktur zu und so haben wir insbesondere dispersive Abschätzungen für die lineare Schrödingergleichung zur Verfügung. In Verbindung mit einem Stetigkeitsargument (engl. *bootstrap argument*) ermöglichen es uns diese, das angekündigte Resultat zu beweisen.

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# Contents

# Chapter 1

# Introduction

## 1.1. Aspects of adiabatic approximation

A slow dependence on external parameters of a physical systems is conveniently formalized by introducing an adiabatic parameter $\varepsilon$, the "adiabaticity", which quantifies the slowness in an evolution equation

$$\dot{y}(t) = F(\varepsilon t, y(t)) \,. \tag{1.1.1}$$

If $\varepsilon = 0$ and $y(0) = y_0$ with $F(0, y_0) = 0$ then clearly $y(t) \equiv y_0$ is a solution of Equation (1.1.1). This leads immediately to the simple idea of adiabatic approximation in the case of finite $\varepsilon$: If the function $F$ admits a family $y_0(t)$ of instantaneous stationary states, that is, $F(\varepsilon t, y_0(t)) \equiv 0$ and if $y(0) = y_0(0)$ then it may be expected that under certain conditions $y(t)$ remains close to $y_0(t)$ for all $t$ in the limit $\varepsilon \to 0$. To give a more precise statement we note that as $\varepsilon$ gets smaller it is necessary to allow for increasingly large observation times in order to notice a nontrivial effect and it is therefore customary to go over to a macroscopic time $s := \varepsilon t \in [0, 1]$ transforming Equation (1.1.1) to

$$\varepsilon \dot{x}(s) = F(s, x(s)) \tag{1.1.2}$$

with $x(s) := y(s/\varepsilon)$. The adiabatic approximation – if it holds – then states that

$$\lim_{\varepsilon \to 0} x(s) = x_0(s) := y_0\left(\frac{s}{\varepsilon}\right)$$

for any fixed $s$. An obvious ambiguity in this discussion is the fact that the zero set of $F(\cdot, \cdot)$ need not define a unique curve $x_0(s)$ and therefore necessitates further conditions. This will incidentally almost always be the case throughout this thesis: Either $F(s, \cdot)$ is linear and has at least a one dimensional kernel, or it is part of a nonlinear partial differential equation which admits a whole manifold of instantaneous stationary states. In some cases simple arguments (e.g. unitarity in the linear, conservation laws in the nonlinear case) can almost single out the relevant curve immediately. In greater generality the situation is however less clear and we shall see that a certain notion of parallel transport will be a fruitful means to address this problem. The generally quite geometric character of the adiabatic approximation was supposedly appreciated for the first time with the discovery of Berry's phase [Ber84, Sim83] which measures the holonomy along a closed path in a space of Hamiltonians as it arises in the adiabatic limit.

Equation (1.1.2) has many faces: It may describe a classical dynamical system[1], a driven stochastic process, or a quantum evolution. Our main focus lies on the latter, where $F(s, x(s))$

[1] Finite dimensional adiabatic dynamical systems are treated in [Ber98].

is for instance replaced by $-\mathrm{i}[H(s), \rho(s)]$ or $-\mathrm{i}(H(s) - E(s))\psi(s)$ with $E(s)$ being an eigenvalue of the Hamiltonian $H(s)$. The first quantum adiabatic[2] theorem was proved by Born and Fock [BF28] in 1928 in a setting of simple eigenvalues and yielded a cornerstone of the famous Born-Oppenheimer approximation in the description of molecules. Since then, many further developments have taken place. Some of them [Kat95, ASY87, ASY93] generalized the theorem to degenerate eigenvalues or even continuous energy bands. Some of them, e.g. [Nen93, JP91], were concerned with expansions of solutions in the adiabaticity showing that error terms are exponentially small under certain conditions; just like it is the case for the Landau-Zener formula. Others [AE99, Bor98] showed that the putatively unavoidable spectral gap assumption which is usually made for the Hamiltonian $H(s)$ is unnecessary in a certain sense. In the gapped case on the other hand many of these theorems have been generalized to contracting evolutions on arbitrary Banach spaces, [Joy07, NR92, Sal07]. Such theorems are relevant if one takes into account the interaction of a quantum system with its environment. The system is then referred to as *open* quantum system and has the striking feature that pure states are transformed into mixed states during its evolution. This phenomenon is referred to as *decoherence*[3] and is of great importance both theoretically and experimentally. The dynamics of such an open quantum system can often efficiently be described by a semigroup law given by a Lindblad master equation [Lin76]; a big field of research on it own as we shall see in due course. For the time being we content ourselves with the remark that the setting is then indeed that of a contracting evolution on a Banach space and hence the above mentioned theorems apply.

As we will demonstrate the quantum adiabatic theorem can also be generalized in absence of a gap so as to be applicable to open quantum systems; a spin-off being that the proof will give a simple and new derivation even in the Hamiltonian case. At first sight the existence of such a theorem may appear a bit puzzling or even – in the words of [AE99] – "morally wrong": If a system is said to vary slowly in time any physicist will ask the just question: "slow compared to what?". Without spectral gap there is however no obvious notion of a comparison time scale. It turns out that the gap assumption is only needed to yield information on the *rate* of convergence if the adiabaticity $\varepsilon$ tends to zero. In fact, explicit expansions in $\varepsilon$ exist in that case; an observation which allows for a large range of applications, some of which will be presented in this thesis. Our own expansion result reveals geometric conditions under which the expansion terms are local, respectively non-local in time. This dichotomy applies to closed and open quantum systems at the same time, yet has a very different physical interpretation in the two cases; a feature, which will be illustrated with examples in areas as different as molecular dynamics and adiabatic quantum computing.

Notably, as for classical systems, the dynamics (1.1.2) can be nonlinear even in the quantum case: Although the time-dependent Schrödinger equation is linear, various effective evolution equations in many-body theory are not. An example is the time-dependent Gross-Pitaevskii equation

$$\mathrm{i}\varepsilon \frac{d}{ds}\psi(s) = -\Delta\psi(s) + V(s)\psi(s) + b|\psi(s)|^2\psi(s) \tag{1.1.3}$$

on $\mathbb{R}^3$ which describes the dynamics of a Bose-Einstein condensate under the influence of a time-dependent exterior potential $V(s)$. After subtracting a dynamical phase factor it can be cast in the form of Equation (1.1.2). On physical grounds the validity of the adiabatic approximation for this equation is very plausible and for instance referred to in certain interference experiments

[2] 'Adiabatic' will always be understood with respect to time. For an exposition of *space*-adiabatic theorems we refer to the monograph [Teu03].

[3] Caveat: The literature is not totally unambiguous concerning terminology.

[AK98, OTF+01]. We are however unaware of a rigorous justification and therefore made it our goal to give one in a simple model. That way we present a result which gives a contrast to other adiabatic theorems both from a mathematical as well as from a physical perspective.

## 1.2. Synopsis

This thesis is largely based on the material presented in [AFGG11b, AFGG10, AFGG11a, GG] and proceeds as follows:

### Chapter 2

In this purely functional analytic chapter a general framework for linear contracting evolutions

$$\varepsilon\dot{x}(s) = L(s)x(s)$$

is set up. It is shown that *generically* the family $L(s)$ induces a natural notion of parallel transport – an observation which appears in the proofs of all adiabatic theorems that we shall present. We then proceed with an exposition of our main results.

In the gapped case this includes the construction of the "slow manifold" which consists of special solutions that illustrate the connection between the above mentioned locality dichotomy and parallel transport. This is complemented by a theorem which – though giving less precise information – allows for arbitrary initial data.

A simple lemma on the description of the range of $L(s)$ is the key to a proof of the adiabatic theorem without spectral gap assumption which will be given thereafter.

The chapter closes with several propositions and counterexamples which specify what is meant by the "generic" occurence of parallel transport.

### Chapter 3

The main goal of Chapter 3 is to give an introduction to the theory of open quantum systems described by a Lindbladian. After introducing the central notion of complete positivity we present the axiomatic approach as well as several constructive schemes leading to Lindbladians. To avoid losing track of the thread of this thesis we only present one of them – the weak coupling limit – in some more detail.

We then develop results on the structure and physical interpretation of so called dephasing Lindbladians which prevent energy exchange between the quantum system and its environment. They will be the "drosophila" in the examples presented in Chapter 4, for which the last preparations conclude this chapter: We show as to what extent the notion of states enriches the structure of a Banach space and how it allows for more detailed results on parallel transport.

### Chapter 4

Chapter 4 combines the preceding chapters and presents several applications. We explain the implications of the locality dichotomy on physical tunneling in the Hamiltonian and Lindbladian case. We then show that the exponentially small tunneling described by the Landau-Zener formula has to be replaced by an expression which is linear in the adiabaticity once a nonzero dephasing is added. The limit of strong dephasing is shown to be in agreement with the quantum Zeno effect. Subsequently, we turn to an optimization problem in adiabatic quantum computing and show an ill-posedness result in the Hamiltonian case while establishing the contrary conclusion for dephasing Lindbladians. An optimality bound on the search time for Grover's algorithm is shown to yield restrictions on the physically allowed dephasing parameters under the assumption that the environment has no a priori knowledge of the quantum computer. As a last application of the gapped adiabatic theorem we derive formulae for integrated probability currents as they appear in driven Markov processes.

The chapter is brought to an end with a discussion of the gapless adiabatic theorem. It turns out that the existence of parallel transport in the Lindbladian case requires some care.

### Chapter 5

From a mathematical perspective Chapter 5 is slightly detached from the others in that it largely relies on results from partial differential equations. It is concerned with the proof of one single adiabatic theorem for the time-dependent Gross-Pitaevskii equation (1.1.3). Under several conditions on the external potential $V(s)$, one being that it has just one eigenstate, we show: A nonzero nonlinearity yields a whole manifold of "ground states" for the time-independent Gross-Pitaevskii equation. If the initial data $\psi(0)$ for (1.1.3) belongs to this manifold then $\psi(1)$ essentially tends to an element in the ground state manifold of equal $L^2(\mathbb{R}^3)$-norm as $\varepsilon \to 0$.

## 1.3. Notation and conventions

We have tried to use standard notation whenever possible. Hilbert spaces $\mathcal{H}$ are always assumed to be separable (although some results extend to the nonseparable case). The most important symbols are listed below.

| | |
|---|---|
| $\overline{V}$ | strong closure of a subset $V \subset \mathcal{B}$ in a Banach space $\mathcal{B}$ |
| $\|a\|_{\mathcal{B}}$ | norm of $a \in \mathcal{B}$; we simply write $\|a\|$ if no ambiguities are possible |
| $\|a\|_{\mathcal{B}_1 \cap \mathcal{B}_2}$ | $\|a\|_{\mathcal{B}_1} + \|a\|_{\mathcal{B}_2}$ |
| $\mathcal{B}^*$ | topological dual of a Banach space $\mathcal{B}$ |
| $S^\perp \subset \mathcal{B}^*$ | annihilator of $S \subset \mathcal{B}$: space of functionals $\varphi \in \mathcal{B}^*$ with $\varphi(s) = 0$ for all $s \in S$ |
| $S_\perp \subset \mathcal{B}$ | predual annihilator of $S \subset \mathcal{B}^*$: space of vectors $\phi \in \mathcal{B}$ with $s(\phi) = 0$ for all $s \in S$ |
| $V \oplus W$ | topological direct sum of vector spaces $V$ and $W$ |
| $\mathcal{L}(\mathcal{B}, \mathcal{C})$ | space of bounded linear operators $L : \mathcal{B} \to \mathcal{C}$ |

| | |
|---|---|
| $\mathcal{L}(\mathcal{B})$ | $\mathcal{L}(\mathcal{B},\mathcal{B})$ |
| $\mathcal{J}_p(\mathcal{H})$ | set of $p$-Schatten class operators $A \in \mathcal{L}(\mathcal{H})$ with $\|A\|_p := (\mathrm{tr}\,\|A\|^p)^{1/p} < \infty$. $p=1$: trace class; $p=2$: Hilbert-Schmidt class |
| $\sigma(L)$ | spectrum of a linear operator $L$ |
| $\rho(L)$ | resolvent set of a linear operator $L$ |
| $L \restriction V$ | an operator $L$ restricted to the space $V$ |
| $\ker L$ | kernel of a linear operator $L$ |
| $\mathrm{ran}\, L$ | range of a linear operator $L$ |
| $\mathbb{1}$ | unity operator |
| $\mathbb{1}_n$ | unity operator on $n$-dimensional space |
| $M'$ | commutant of a $M$ |
| $[A,B]$ | commutator $AB-BA$ for $A,B \in \mathcal{L}(\mathcal{B})$ |
| $\mathrm{tr}\, A$ | trace of $A$ |
| $\Re a$ | real part of $a$ |
| $\Im a$ | imaginary part of $a$ |
| $M_{\mathbb{R}}$ | $\Re M$ for a space of complex valued functions $M$ |
| $a \lesssim b$ | $a \le Cb$ for $C$ independent of $b$ |
| $a \simeq b$ | $a \lesssim b$ and $b \lesssim a$; if $a$, $b$ are spaces then the symbol denotes an isomorphism |
| $a \sim b$ | $a$ and $b$ share the same asymptotic behavior |
| $a \le C_{x,y} b$ | constant in $a \lesssim b$ depends on $x$ and $y$ |
| $\langle a, b\rangle$ | scalar (inner) product or duality bracket |
| $\Delta$ | Laplacian on $\mathbb{R}^n$: $\Delta f := \sum_{i=1}^n \partial_i^2 f$ |
| $\nabla$ | gradient on $\mathbb{R}^n$: $(\nabla f)_i := \partial_i f$ |
| $\nabla^2$ | Hessian on $\mathbb{R}^n$: $(\nabla^2 f)_{ij} := \partial_i \partial_j f$ |
| $\langle x\rangle$ | $\sqrt{1+\|x\|^2}$ |
| $\hat{x}$ | unit vector in direction $x$; $\hat{x} = x/\|x\|$ |
| $L^p(\Omega)$ | space of (equivalence classes of) functions $f:\Omega\to\mathbb{C}$ with $\|f\|_p < \infty$ where $\|f\|_p := \begin{cases} \left(\int dx\, \|f(x)\|^p\right)^{1/p}, & \text{if } 1 < p < \infty \\ \text{ess sup}_{x\in\Omega}\|f(x)\|, & \text{if } p = \infty. \end{cases}$ $dx$ denotes the Lebesgue measure. $\|f\|_2$ is called 'mass of $f$'. |
| $H^2(\Omega)$ | Sobolev space of functions $f:\Omega\to\mathbb{C}$ with $\|f\|_{H^2} := \|f\|_2 + \|\Delta f\|_2 < \infty$ |
| $L^{p,l}(\Omega)$ | weighted $L^p$-space of functions $f:\Omega\to\mathbb{C}$ with $\|f\|_{L^{p,l}} := \|\langle x\rangle^l f\|_p < \infty$ |
| $H^{2,l}(\Omega)$ | Sobolev space of functions $f:\Omega\to\mathbb{C}$ with $\|f\|_{H^{2,l}} := \|\langle x\rangle^l f\|_{H^2} < \infty$ |

| | |
|---|---|
| $W^{2,1}(\Omega)$ | Sobolev space of functions $f : \Omega \to \mathbb{C}$ with $\|f\|_{W^{2,1}} := \|f\|_1 + \|\Delta f\|_1 < \infty$ |
| $C([a,b];\mathcal{B})$ | continuous $\mathcal{B}$-valued functions on $[a,b]$ |
| $C^r([a,b];\mathcal{B})$ | $r$-times continuously differentiable $\mathcal{B}$-valued functions on $[a,b]$ |

# Chapter 2

# Adiabatic Theorems for Generators of Contracting Evolutions

## 2.1. Overview

In this chapter we will present adiabatic theorems for a slowly evolving family of linear operators generating a contraction in a Banach space, a setting as it is found in [Joy07,NR92,Sal07]. More precisely, we study equations of the form

$$\varepsilon \dot{x}(s) = L(s)x(s), \tag{2.1.1}$$

where $L(s)$ is, for any fixed $s$, the generator of a contraction semigroup. The initial data is assumed to be close to the manifold of instantaneous stationary vectors, that is $\ker L(s)$.

As we shall see in Chapter 4 the so adopted abstractness has the advantage that it encompasses at the same time a large variety of applications from driven stochastic systems generated in a Markovian process, through isolated quantum systems undergoing unitary evolution generated by Hamiltonians, culminating in open quantum systems whose evolution is generated by Lindblad operators.

Adiabatic evolutions have a geometric character and are closely related to parallel transport: We will demonstrate that the manifold of instantaneous stationary vectors has a distinguished complement, with the property that a vector near the former evolves with a velocity in the latter, to leading order in $\varepsilon$. Hence, to lowest order in the adiabatic limit ($\varepsilon \to 0$), the vector is parallel transported with the manifold.

We consider both the case where $\ker L(s)$ is protected by a gap condition, i.e. 0 is an isolated eigenvalue of $L(s)$, and where it is not.

In the gapped case we give an adiabatic expansion which reveals that the dynamics has distinct characters within the evolving subspace of instantaneous stationary vectors and transversal to it. Notably, as we shall see, the motion within $\ker L(s)$ is *irreversible*, whereas the motion transversal to it is *transient* in the following sense: Consider the adiabatic evolution over a finite interval, traversed at a slow rate $\varepsilon$; assume that the generator is constant near its endpoints and smooth otherwise, and let the initial state be stationary. Then the distance of the vector at the endpoint from the manifold of stationary vectors is $O(\varepsilon^N)$ for all $N$, whereas the distance covered within the manifold is typically $O(1)$ and comprises a deviation from parallel transport still as large as $O(\varepsilon)$ (see Figure 2.1).

In the gapless case we no longer obtain an expansion, however we prove that the dynamics of the system is constrained to the manifold of instantaneous stationary vectors and is parallel transported along with the manifold as $\varepsilon \to 0$. Results for the Hamiltonian case are found in [AE99, Teu01, Bor98]: Their comparison with our theorem is presented in Chapter 4.

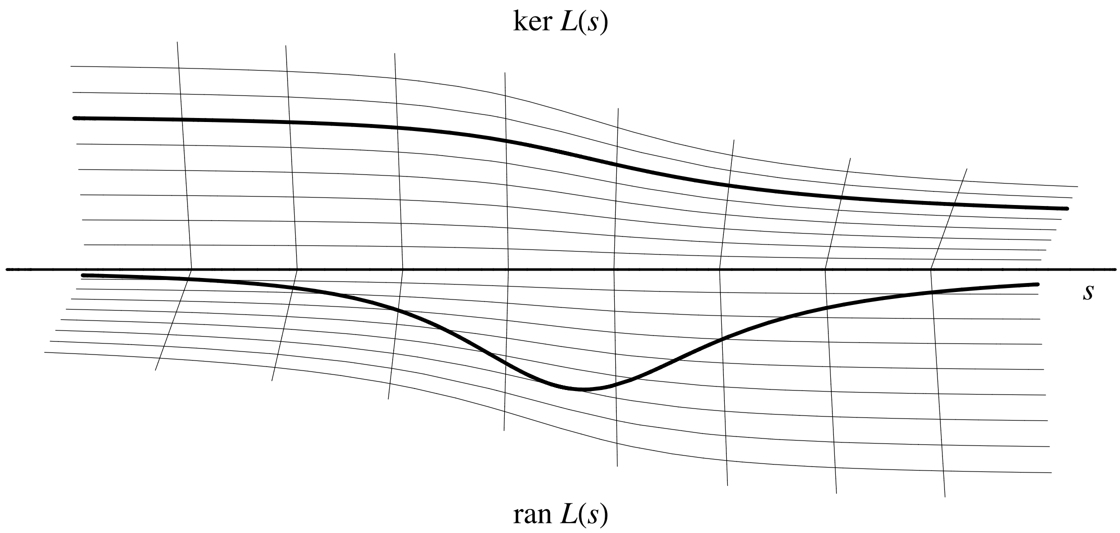


Figure 2.1: The figure illustrates the motion within the kernel and the range as described by Theorem 2.16 and Corollary 2.17 in the situation where $L(s)$ is constant near the endpoints. It shows the transient nature of the motion in the range: When $L(s)$ does not vary, the part in the range is smaller than any power.

## 2.2. Preliminaries

### 2.2.1. Existence of dynamics

We consider the evolution (2.1.1) with time-dependent generators $L(s)$ on a Banach space $\mathcal{B}$, possibly unbounded. To start it is useful to recall the following classical theorem ( [RS75], Thm. X.47a):

**Theorem 2.1** (Hille-Yosida)**.** *A closed operator $L$ on $\mathcal{B}$ generates a contraction semigroup if and only if*

$$\begin{aligned} &(a) \qquad (0,\infty) \subset \rho(L) \\ &(b) \qquad \|(L-\gamma)x\| \geq \gamma\|x\|\,, \qquad (\gamma > 0, x \in D(L))\,. \end{aligned} \tag{2.2.1}$$

**Remark 2.2.** *By definition ( [RS75], Sect. X.8), a contraction semigroup is strongly continuous. Its generator is thus closed and densely defined.*

Conditions (2.2.1) reflect the connection between the resolvent and evolution operators. For example the only if part of the Hille-Yosida theorem follows from the formula

$$-\frac{1}{L-\gamma} = \int_0^\infty \mathrm{e}^{(L-\gamma)t} dt\,, \qquad (\gamma > 0)\,. \tag{2.2.2}$$

**Definition 2.3.** *Operators $L(s)$, ($0 \leq s \leq 1$) on $\mathcal{B}$ are called a $C^k$-family or simply $C^k$ if the $L(s)$ are closed operators with a common dense domain $D$ and the function $L$, taking values in the Banach space of bounded operators $D \to \mathcal{B}$, is $k$-times differentiable in $s$ ($k$ will be specified). Here $D$ is endowed with the graph norm of $L(s)$ for any fixed $s$.*

**Lemma 2.4.** *Let $L(s)$, $(0 \le s \le 1)$ be $C^1$ and, for each $s$, the generator of a contraction semigroup on $\mathcal{B}$. Then there exist operators $U_\varepsilon(s,s') : \mathcal{B} \to \mathcal{B}$, $(0 \le s' \le s \le 1)$ with $U_\varepsilon(s,s')D \subset D$, $U_\varepsilon(s,s) = \mathbb{1}$ and*

$$\varepsilon \partial_s U_\varepsilon(s,s')x = L(s)U_\varepsilon(s,s')x\,, \qquad (x \in D)\,. \tag{2.2.3}$$

*For $x \in D$ the unique solution $x(s) \in D$ of (2.1.1) with $x(s') = x$ is $x(s) = U_\varepsilon(s,s')x$. Moreover,*

$$\|U_\varepsilon(s,s')\| \le 1 \tag{2.2.4}$$

*and*

$$\varepsilon \partial_{s'} U_\varepsilon(s,s')x = -U_\varepsilon(s,s')L(s')x\,, \qquad (x \in D)\ . \tag{2.2.5}$$

We will call $U_\varepsilon(s,s')x$ a solution of (2.1.1) even for $x \notin D$.

**Remark 2.5.** *Suppose, in alternative to the lemma, that the generator $L(s)$ is bounded and strongly continuous. Then – by an application of the uniform boundedness principle and a Dyson expansion – the propagator exists and is uniformly bounded in $0 \le s', s \le 1$, but not in $\varepsilon$ [RS75].*

Proof of Lemma 2.4. The parameter $\varepsilon$ may be absorbed in $L$ without loss of generality. The hypotheses are a convenient strenghtening of those of [RS75], Thm. X.70, including the remark thereafter. All our statements but (2.2.5) are among its claims, and that one is a consequence of its proof, as we will show. Actually, the proof in [RS75] makes the additional assumption that $0 \in \rho(L(s))$ which, as remarked there, can be arranged for by replacing $L(s)$ with $L(s) - c$, $c > 0$ (cf. Theorem 2.1). It is then shown that

$$(U(s'',s') - \mathbb{1})x = \int_{s'}^{s''} W(r,s')L(s')x\,dr\,, \qquad (x \in D)\,,$$

where $W(r,s') = L(r)U(r,s')L(s')^{-1}$ is a bounded operator on $\mathcal{B}$, jointly strongly continuous in $r$, $s'$. In particular, $W(r,r) = \mathbb{1}$. Let $0 \le s \le 1$, $x \in D$ and $\lambda > 0$ be given. For all $r, s' \in [s-\delta, s+\delta] \cap [0,1]$ we have

$$W(r,s')L(s')x - L(s)x = W(r,s')(L(s') - L(s))x + (W(r,s') - \mathbb{1})L(s)x\,,$$

which is estimated in norm as $C\|(L(s') - L(s))x\| + \|(W(r,s') - \mathbb{1})L(s)x\| \le \lambda$ for a $C \ge 0$, provided $\delta > 0$ is small enough. Hence, for $s'' \ge s \ge s'$,

$$(U(s'',s') - \mathbb{1})x = (s'' - s')L(s)x + o(s'' - s')\,, \qquad (s'' - s' \to 0)\,.$$

Equation (2.2.5) then follows by the group property of $U$. □

### 2.2.2. Parallel transport

Suppose $P(s) : \mathcal{B} \to \mathcal{B}$, $(0 \le s \le 1)$ defines a $C^1$-family of projections in norm sense. With $\dot P(s) = dP(s)/ds$ we compute the derivative of $P(s)^2 = P(s)$ and obtain

$$\dot P(s)P(s) + P(s)\dot P(s) = \dot P(s), \tag{2.2.6}$$

which, after multiplication with $P(s)$ from the left yields the simple and useful identity

$$P(s)\dot P(s)P(s) = 0. \tag{2.2.7}$$

In the language of differential geometry $P(s)$ naturally induces a subbundle $\mathfrak{P}$ of the trivial Banach bundle $[0,1]\times\mathcal{B}$:

$$(s,x)\in\mathfrak{P}\Leftrightarrow s\in[0,1] \text{ and } x\in P(s)\mathcal{B},$$

and similarly a subbundle $\mathfrak{Q}$ with respect to $Q(s):=\mathbb{1}-P(s)$. We then define a parallel transport $T(s,s'):\mathcal{B}\to\mathcal{B}$ by

$$\begin{aligned}\partial_s T(s,s') &= [\dot P(s),P(s)]T(s,s')\,,\\ T(s',s') &= \mathbb{1}\,.\end{aligned}\tag{2.2.8}$$

$T(s,s')$ respects the range of $P(s)$ and therefore induces also a parallel transport on $\mathfrak{P}$ and likewise on $\mathfrak{Q}$.

**LEMMA 2.6** (Intertwining property)**.**

$$P(s)T(s,s')=T(s,s')P(s')\tag{2.2.9}$$

PROOF. Clearly the identity holds for $s=s'$. Using Equations (2.2.6,2.2.7) it is easy to see that the left as well as the right hand side of (2.2.9) satisfy the same differential equation. □

If $P(s)$ is a projection on the kernel of $L(s)$, as it will be, we may say that the parallel transport $T(s,s')$ is a perfect adiabatic evolution: no transitions from the bundle of projections $P(s)$ to that of the complementary projections $Q(s)=\mathbb{1}-P(s)$, nor viceversa.

In view of the proofs of our adiabatic theorems the following characterization of $T(s,s')$ restricted to $\mathfrak{P}$ turns out to be very convenient: A section $x$ on $\mathfrak{P}$ is parallel if and only if the projected velocity vanishes,

$$x(s)=T(s,0)x(0)\ \Leftrightarrow\ P(s)\dot x(s)=0\,,\tag{2.2.10}$$

and likewise for $Q$ in place of $P$. Indeed, for such sections $\dot x=\dot Px+P\dot x$ and Equation (2.2.8) reduces to

$$\partial_s T(s,s')x(s')=\dot P(s)T(s,s')x(s')\tag{2.2.11}$$

by the identity 2.2.7; hence the equivalence (2.2.10).

Yet another way to describe $T(s,s')$ is the following: As the name suggests, parallel transport is obtained by projecting vectors from either subspace at $s'$ to the corresponding one at $s$ or, more precisely, by repeating the procedure on the intervals of an ever finer partition of $[s',s]$. In fact,

$$P(s)P(s')+Q(s)Q(s')=\mathbb{1}+[\dot P(s'),P(s')](s-s')+o(|s-s'|)\,,\qquad(s\to 0)\,,\tag{2.2.12}$$

which implies

**LEMMA 2.7.**

$$\begin{aligned}T(s,s') &= \lim_{N\to\infty}\prod_{i=0}^{N-1}\left(P(s_{i+1})P(s_i)+Q(s_{i+1})Q(s_i)\right)\\ &= \lim_{N\to\infty}\Big(\prod_{i=0}^{N}P(s_i)+\prod_{i=0}^{N}Q(s_i)\Big)\,,\end{aligned}\tag{2.2.13}$$

*where $s'=s_0\le s_1\le\ldots\le s_N=s$ is a partition of $[s',s]$ into intervals of length $|s_{i+1}-s_i|=N^{-1}|s-s'|$ and $\prod_{i=0}^{N}A_i:=A_N\cdots A_0$.*

PROOF. The second equality follows immediately from the first, whose validity we now show. Define remainders $r_i, \tilde{r}_i$ so that the following equations hold for each single factor:

$$\begin{aligned} T(s,s') &= \prod_{i=0}^{N-1} T(s_{i+1}, s_i) \\ &= \prod_{i=0}^{N-1} \left(\mathbb{1} + [\dot{P}(s_i), P(s_i)](s_{i+1}-s_i) + r_i\right) \\ &= \prod_{i=0}^{N-1} \left(P(s_{i+1})P(s_i) + Q(s_{i+1})Q(s_i) + \tilde{r}_i\right) \end{aligned}$$

for arbitrary $N$. Since $P(s)$ and $T(s,s')$ both have uniformly continuous derivatives with respect to $s$ on $[0,1]$ it follows from Taylor's theorem that

$$\|r_i\|, \|\tilde{r}_i\| \leq o\left(\frac{1}{N}\right),$$

the right hand side being independent of $i$. For the same reasons also

$$\|P(s_{i+1})P(s_i) + Q(s_{i+1})Q(s_i)\|, \|P(s_{i+1})P(s_i) + Q(s_{i+1})Q(s_i) + \tilde{r}_i\| \leq 1 + C/N$$

with an $i$-independent $C$. Using the telescopic sum formula

$$\prod_{i=0}^{N-1} A_i - \prod_{i=0}^{N-1} B_i = \sum_{i=0}^{N-1} B_{N-1} \cdots B_{i+1} \left(A_i - B_i\right) A_{i-1} \cdots A_0$$

we obtain

$$\begin{aligned} &\left\| \prod_{i=0}^{N-1} \left(P(s_{i+1})P(s_i) + Q(s_{i+1})Q(s_i)\right) - \prod_{i=0}^{N-1} \left(P(s_{i+1})P(s_i) + Q(s_{i+1})Q(s_i) + \tilde{r}_i\right) \right\| \\ &\qquad \leq (N-1)\left(1 + \frac{C}{N}\right)^{N-1} o(1/N) \end{aligned}$$

which vanishes for $N \to \infty$. □

The parallel transport determined by the dual projections $P(s)^* : \mathcal{B}^* \to \mathcal{B}^*$ is

$$T^*(s,s') = T(s',s)^*, \tag{2.2.14}$$

as can be seen from Equation (2.2.8) and $\partial_s T(s',s) = -T(s',s)[\dot{P}(s), P(s)]$. The same equations show that parallel transport is unitary if $P(s)$ is an orthogonal projection on a Hilbert space. More generally, one has at least

$$\sup_{0 \leq s', s \leq 1} \|T(s,s')\| < \infty \tag{2.2.15}$$

by the remark after Lemma 2.4.

In applications we will often encounter the situation where $P(s)$ is a rank 1 projection, e.g. if a physical system admits a unique stationary state. This motivates the following lemma:

**Lemma 2.8.** *Let $P(s)$ be a $C^1$-family of rank 1 projections. If $\ker P(s)$ is independent of $s$, then $\dot{P}(s)$ vanishes on $\ker P(s)$ and $P(s) = T(s,s')P(s')$.*

Proof. Rank 1 projections $P$ are of the form $Py = \alpha(y)x$ where $x \in \mathcal{B}$ and $\alpha \in \mathcal{B}^*$ are determined up to reciprocal factors. Any $\alpha$ with $\ker \alpha = \ker P$ may thus be picked, and then $x$ normalized by $\alpha(x) = 1$. Since $\ker P(s)$ is independent of $s$, so is our choice of $\alpha$ in $P(s)y = \alpha(y)x(s)$, while $x(s)$ is $C^1$. Thus $\dot{P}(s)y = \alpha(y)\dot{x}(s)$, which vanishes for $y \in \ker P(s)$. The claim just proved states $\dot{P} = \dot{P}P$; together with (2.2.11) both sides of $P(s) = T(s,s')P(s')$ are seen to satisfy the same differential equation in $s$. □

## 2.3. Adiabatic theorem in presence of a gap

We assume that 0 is an isolated point of the spectrum of $L$, which is what we mean by a gap. Then, for small $\varepsilon$, the differential equation (2.1.1) forces a fast time scale of order $O(\varepsilon^{-1})$ on vectors transverse to the null space $\ker L(s)$. That scale reflects itself in a fast motion consisting of oscillations and decay. By contrast on vectors in the null space the dynamics is slow, for $\dot{x} = 0$. Nevertheless these vectors leak out of that subspace, because it is itself changing with $s$. The leakage however remains of order $O(\varepsilon)$, as shown by Theorem 2.19 below. We will start our discussion with a complementary result, Theorem 2.16, which constructs a "slow manifold", where solutions $x(s)$ remain suitably close to $\ker L(s)$ and the time scale is $O(1)$. Before presenting the two results, which are illustrated in Figure 4.5, we need to specify the transversal subspace complementing $\ker L(s)$.

### 2.3.1. Setup

The general assumptions on $L = L(s)$, $(0 \le s \le 1)$ are

(H1) $L$ is the generator of a contraction semigroup on a Banach space $\mathcal{B}$.

(H2) The range of $L$ is closed and complementary to the (closed) null space of $L$:

$$\mathcal{B} = \ker L \oplus \operatorname{ran} L\,, \tag{2.3.1}$$

and the corresponding projections are $P$ and $Q$.

(H3) $L(s)$ is a $C^k$-family for which 0 remains a uniformly isolated eigenvalue.

**Remark 2.9.** *We will give sufficient conditions for (H2) in Section 2.5. For short, (H2) is the regular case, given (H1) and (H3).*

Before presenting the main results of this section we formulate several direct consequences of assumptions (H1-H3) in the following sequence of Lemmata.

To start we remark that the direct sum in (2.3.1) is topological.

**Lemma 2.10.** *Let $V$ and $W$ be subspaces of $\mathcal{B}$ with $V \cap W = \{0\}$. Any two among the following statements imply the third:*

*(i)* $V$, $W$ *are closed,*

*(ii)* $V+W$ *is closed,*

*(iii) Let* $v \in V$ *and* $w \in W$*. Then* $P_V : v+w \mapsto v$ *and* $P_W : v+w \mapsto w$ *are bounded operators on* $V+W$*.*

Proof. (i) and (ii) imply (iii) by the closed graph theorem.

To see (ii) let $v_n + w_n \to x \in \overline{V+W}$ $(n \to \infty)$ with $v_n \in V$, $w_n \in W$. Then $(P_V(v_n + w_n))_{n\in\mathbb{N}} = (v_n)_{n\in\mathbb{N}}$ is a Cauchy sequence and so by (i) $v_n \to v \in V$ and similarly $w_n \to w \in W$ $(n \to \infty)$. Hence $x = v + w \in V + W$.

Finally, to prove (i) let $v_n \to v \in \overline{V}$ $(n \to \infty)$. By (ii) $v \in V+W$ and so $P_V v \in V$. Since for all $n$ we have $P_W v_n = 0$ it follows that $P_W v = 0$ and hence $P_V v = v \in V$. A similar reasoning shows that $W$ is closed. □

Conditions (H1-H3) are not independent, as the following two lemmata show.

**Lemma 2.11.** *(H1) implies*

$$\ker L \cap \operatorname{ran} L = \{0\}.$$

Proof. $La = 0$ and $a = Lb$ imply $(L-\gamma)(a+\gamma b) = -\gamma^2 b$ and by (b) in Theorem 2.1 (Hille-Yosida) $\gamma\|a+\gamma b\| \le \gamma^2\|b\|$ for $\gamma > 0$. After dividing by $\gamma$ we obtain $a = 0$ in the limit $\gamma \to 0$. □

**Lemma 2.12.** *(H1) and (H2) alone imply that* $0$ *is an isolated point of the spectrum* $\sigma(L)$*, if at all.*

Proof. By assumption (b) $\operatorname{ran} L$ reduces $L$. The restriction $L \restriction \operatorname{ran} L$ is closed and has range $\operatorname{ran}(L \restriction \operatorname{ran} L) = \operatorname{ran} L$; by Lemma 2.11 it is one-to-one. Thus $0 \notin \sigma(L \restriction \operatorname{ran} L)$. Together with $\sigma(L \restriction \ker L) \subset \{0\}$ we conclude that the resolvent set contains a punctured neighborhood of 0, which proves the presence of a gap. □

We also note that the presence of a gap has the useful consequence to be able to work with the Riesz projection.

**Lemma 2.13.** *(H1) and (H2) imply that the projection* $P$ *is given by the Riesz projection,*

$$\tilde{P} := -\frac{1}{2\pi\mathrm{i}} \oint_\Gamma (L-z)^{-1} dz; \tag{2.3.2}$$

*here* $\Gamma$ *lies in the resolvent set* $\rho(L)$ *and encircles* $0$ *in counterclockwise direction.*

Proof. We claim $\tilde{P}a = a$ for $a \in \ker L$ and $\tilde{P}b = 0$ for $b \in \operatorname{ran} L$. The first statement is evident from (2.3.2); for the second it suffices, by $\tilde{P}L \subset L\tilde{P}$, to show that $\operatorname{ran}\tilde{P} \cap \operatorname{ran} L = \{0\}$. This in turn follows because $L \restriction (\operatorname{ran}\tilde{P} \cap \operatorname{ran} L)$ is a bounded operator with empty spectrum; in fact it is contained in $\sigma(L \restriction \operatorname{ran}\tilde{P}) \cap \sigma(L \restriction \operatorname{ran} L) = \varnothing$ since the first spectrum is contained in $\{0\}$, while the second is disjoint from it. □

By the closed graph theorem $L \restriction \operatorname{ran} L$ has a bounded inverse, denoted by $L^{-1}$. In conjunction with Lemma 2.13 the uniformity of the gap, Hypothesis (H3), yields regularity in $s$.

**Lemma 2.14.** $s \mapsto P(s)$ *and* $s \mapsto L(s)^{-1}$ *are* $C^k$ *in norm.*

PROOF. We recall the formula for the inverse of $L \restriction \operatorname{ran}(1-P)$ ( [Kat95], Equation (III.6.23)):

$$L^{-1} = -\frac{1}{2\pi \mathrm{i}} \oint_\Gamma (L-z)^{-1} \frac{dz}{z} \,. \tag{2.3.3}$$

Uniformity of the gap allows us to choose $\Gamma$ independent of $s$. It is easy to see that in the norm of $\mathcal{L}(\mathcal{B}, D)$

$$\begin{aligned} \frac{1}{h}\left((L(s+h)-z)^{-1} - (L(s)-z)^{-1}\right) &= -(L(s+h)-z)^{-1}\left(\frac{L(s+h)-L(s)}{h}\right)(L(s)-z)^{-1} \\ &\to -(L(s)-z)^{-1}\dot{L}(s)(L(s)-z)^{-1} \qquad (h \to 0)\,, \end{aligned} \tag{2.3.4}$$

by assumption (H3). In fact the convergence is uniform in $z \in \Gamma$. Thus by (2.3.2) and (2.3.3) the assertion of the lemma follows: first for $k=1$ but from the explicit form of (2.3.4) also for higher derivatives. □

Finally, we give a lemma on the situation in the dual space. We denote by $L^*$ the maximal adjoint of $L$ (cf. p. 167, [Kat95]). It need not be densely defined if $\mathcal{B}$ fails to be reflexive.[1]

**LEMMA 2.15** (Dual decomposition).

$$\mathcal{B}^* = \ker L^* \oplus \operatorname{ran} L^* \tag{2.3.5}$$

*and* $\ker L^* = \operatorname{ran} P^*$, $\operatorname{ran} L^* = \operatorname{ran} Q^*$.

PROOF. By a standard duality identity (e.g. [Kat95], Problem 5.27),

$$\mathcal{B}^* = (\operatorname{ran} L)^\perp \oplus (\ker L)^\perp = \ker L^* \oplus (\ker L)^\perp \,.$$

Clearly $\operatorname{ran} L^* \subset (\ker L)^\perp$ and conversely for $x^* \in (\ker L)^\perp$ and $y \in \mathcal{B}$ we have by [Kat95], Theorem III.5.30,

$$x^*(y) = x^*(Py + Qy) = x^*(L^{-1}LQy) = L^* L^{*-1} x^*(y)$$

which proves Equation (2.3.5). Next from Lemma 2.13 it follows that $P^*x^* = 0$ for $x^* \in \ker L^*$ and similar as in the proof there it remains to show that $\operatorname{ran} P^* \cap \operatorname{ran} L^* = \{0\}$. This follows along the same lines. □

### 2.3.2. CONSTRUCTION OF THE SLOW MANIFOLD

For $\varepsilon = 0$, Equation (2.1.1) requires $x(s) \in \ker L(s)$. For small $\varepsilon$ the differential equation admits solutions which remain close to $\ker L(s)$. The construction of the "slow manifold" reduces to a differential equation for the slow variables only, with the fast ones providing the inhomogeneity. The latter, rather than being governed by a further, coupled differential equation, are enslaved to the solution at lower orders. More precisely, the solutions are described as follows.

[1] As a consequence of the fact that $L$ is closed it is however possible to show that the domain of $L^*$ is dense with respect to the ultraweak topology, [Phi55].

**THEOREM 2.16** (Slow manifold expansion)**.** *Let $L(s)$ be a $C^{N+2}$-family of operators satisfying hypotheses (H1-H3). Then*

*(i) The differential equation $\varepsilon\dot{x} = L(s)x$ admits solutions of the form*

$$x(s) = \sum_{n=0}^{N} \varepsilon^n (a_n(s) + b_n(s)) + \varepsilon^{N+1} r_N(\varepsilon, s) \tag{2.3.6}$$

*with*

- $a_n(s) \in \ker L(s),\ b_n(s) \in \operatorname{ran} L(s)$.
- *initial data $x(0)$ specified by arbitrary $a_n(0) \in \ker L(0),\ r_N(\varepsilon, 0) \in \mathcal{B}$; however, the $b_n(0)$ are determined below by the $a_n(0)$ and so together define the "slow manifold".*

*(ii) The coefficients are determined recursively through $(n = 0, \dots, N)$*

$$\begin{aligned} b_0(s) &= 0\,, \\ a_n(s) &= T(s,0)a_n(0) + \int_0^s T(s,s')\dot{P}(s')b_n(s')ds'\,, \end{aligned} \tag{2.3.7}$$

$$\begin{aligned} b_{n+1}(s) &= L(s)^{-1}Q(s)\big(\dot{P}(s)P(s)a_n(s) + \dot{b}_n(s)\big) \\ &= L(s)^{-1}\dot{P}(s)a_n(s) + L(s)^{-1}Q(s)\dot{b}_n(s)\,. \end{aligned} \tag{2.3.8}$$

*(iii) The remainder is*

$$r_N(\varepsilon, s) = U_\varepsilon(s,0)r_N(\varepsilon,0) + b_{N+1}(s) - U_\varepsilon(s,0)b_{N+1}(0) - \int_0^s U_\varepsilon(s,s')\dot{b}_{N+1}(s')ds'\,, \tag{2.3.9}$$

*where $U_\varepsilon(s,s')$ is the propagator in Lemma 2.4. It is uniformly bounded in $\varepsilon$, if $r_N(\varepsilon,0)$ is:*

$$\sup_s \|r_N(\varepsilon,s)\| \le C_N \sum_{n=0}^{N} \|a_n(0)\| + \|r_N(\varepsilon,0)\|\,,$$

*where $C_N$ depends on the family.*

Explicitly: for $a_1(0) = 0$ we have

$$a_0(s) = T(s,0)a_0(0)\,, \tag{2.3.10}$$

$$b_1(s) = L(s)^{-1}\dot{P}(s)a_0(s)\,, \tag{2.3.11}$$

$$a_1(s) = \int_0^s T(s,s')\dot{P}(s')L(s')^{-1}\dot{P}(s')a_0(s')ds'\,. \tag{2.3.12}$$

Before giving a proof of Theorem 2.16 we present two immediate corollaries.

**COROLLARY 2.17.** *If $L(s)$ is constant on an interval $I \subset [0,1]$, then*

$$b_n(s) = 0\,, \qquad (s \in I).$$

PROOF. This follows recursively from (2.3.8) by $\dot{P}(s) = 0$. □

**Corollary 2.18.** *If $P(s)$ are rank 1 projections and* $\ker P(s)$ *is independent of $s$, then* $a_n(s) = T(s,0)a_n(0)$.

Proof. In Equation (2.3.7) we have $\dot{P}(s')b_n(s') = 0$ in view of Lemma 2.8 and of $b_n(s') \in \operatorname{ran} L = \ker P$. □

Proof of Theorem 2.16. We insert the right hand side of (2.3.6) as an ansatz into (2.1.1) and equate orders $\varepsilon^n$, $(n = 0, \dots, N)$, resp. $O(\varepsilon^{N+1})$. We find

$$Lb_0 = 0,$$
$$\dot{a}_n + \dot{b}_n = Lb_{n+1}\,, \qquad (n = 0, \dots, N-1) \tag{2.3.13}$$
$$\varepsilon\dot{r}_N + \dot{a}_N + \dot{b}_N = Lr_N\,. \tag{2.3.14}$$

In particular, $b_0 = 0$. Note that $Qa = 0$ implies $\dot{Q}a + Q\dot{a} = 0$, or $Q\dot{a} = -\dot{Q}a = \dot{P}a$. Similarly, $P\dot{b} = -\dot{P}b$. Applying $Q$ and $P$ to (2.3.13) yields

$$\dot{P}a_n + Q\dot{b}_n = Lb_{n+1}\,, \tag{2.3.15}$$
$$P\dot{a}_n - \dot{P}b_n = 0. \tag{2.3.16}$$

If $b_n$ is known, (2.3.16) implies

$$\dot{a}_n = Q\dot{a}_n + P\dot{a}_n = \dot{P}a_n + \dot{P}b_n\,,$$

the solution of which is (2.3.7) by Equation (2.2.11) and the Duhamel formula. If $a_n$ and $b_n$ are known, $b_{n+1}$ follows from (2.3.15), provided $b_n$ is differentiable (see below). All this determines $b_0, a_0, b_1, \dots, a_{N-1}, b_N$. We then *define* $a_N, b_{N+1}$ by the same Equation (2.3.7, 2.3.8), which ensures $\dot{a}_N + \dot{b}_N = Lb_{N+1}$. Then (2.3.14) reads

$$\varepsilon\dot{r}_N = Lr_N - Lb_{N+1}$$

with solution

$$\begin{aligned} r_N(\varepsilon, s) &= U_\varepsilon(s,0)r_N(\varepsilon,0) - \varepsilon^{-1}\int_0^s U_\varepsilon(s,s')L(s')b_{N+1}(s')ds' \\ &= U_\varepsilon(s,0)r_N(\varepsilon,0) + \int_0^s (\frac{\partial}{\partial s'}U_\varepsilon(s,s'))b_{N+1}(s')ds'\,. \end{aligned}$$

An integration by parts yields (2.3.9) and the bound on the remainder follows by Assumption (H1) in Subsection 2.3.1 and Lemma 2.4. Inspection of the recursion relations shows $a_n, b_n \in C^{N+2-n}$, which provides the required differentiability. □

### 2.3.3. The case of general initial data: decoupling

In Theorem 2.16 the initial data $x(0) = P(0)x(0) + Q(0)x(0)$ is such that the first (slow) part is arbitrary, and it prescribes the second (fast) part, up to a remainder. The general case that both parts of the initial condition are arbitrary is addressed by a result on the decoupling of the slow variables from the fast variables:

**THEOREM 2.19** (Decoupling)**.** *Let $L(s)$ be a $C^2$-family satisfying the assumptions of Theorem 2.16. Then*

$$\|P(s)x(s) - T(s,0)P(0)x(0)\| \leq C\varepsilon\|x(0)\|\,, \qquad (0 \leq s \leq 1)\,,$$

*where $C$ depends on the family.*

**REMARK 2.20.** *Note that no statement about the fast part, $Q(s)x(s)$, is made. The proposition may in particular be applied to the difference $\tilde{x}(0) = Q(0)\tilde{x}(0)$ of initial conditions sharing the same slow part; in this case, $\|P(s)\tilde{x}(s)\| \leq C\varepsilon\|\tilde{x}(0)\|$.*

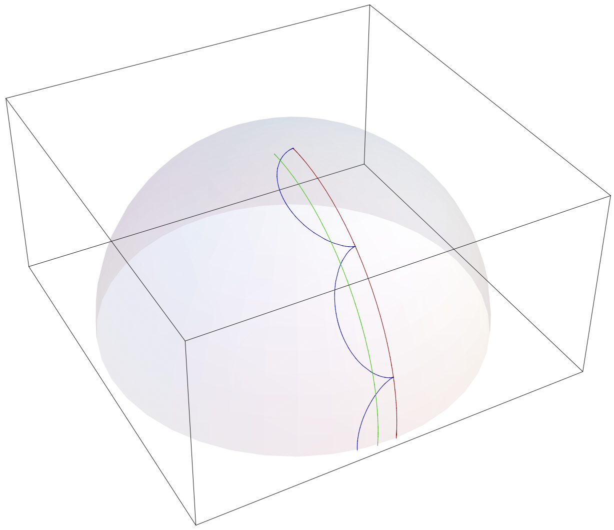

Figure 2.2: The figure shows the result of a computation of the unitary adiabatic evolution of a qubit, see Subsection 4.3.2 for details. The state is represented as a point on the Bloch sphere. The (red) meridian shows the manifold of instantaneous stationary states, i.e. $\ker L$. The parametrization corresponds to uniform speed along this path. The “slow manifold" is represented by the (green) curve essentially parallel to the (red) meridian. An orbit is shown by the (blue) cycloid. Note that the initial conditions do not lie on the slow manifold ($b_1(0) \neq 0$ when $\dot{P}(0) \neq 0$). This is the reason for the large oscillations.

The proof of Theorem 2.19 will depend on the following result. We consider linear forms $\varphi \in \mathcal{B}^*$. The duality bracket is $\langle \varphi, x\rangle$.

**PROPOSITION 2.21** (Adiabatic invariants)**.** *Let $L(s)$ be a $C^2$-family. Suppose that $\varphi(\cdot) \in C^2([0,1];\mathcal{B}^*)$ satisfies*

$$\varphi(s) \in \ker L^*(s)\,, \qquad \dot{\varphi}(s) \in \operatorname{ran} L^*(s)\,. \tag{2.3.17}$$

*Then $\varphi$ is an approximate adiabatic invariant in the sense that for any solution $x(t) \in D$ of Equation (2.1.1)*

$$\langle \varphi, x\rangle|_0^s = \varepsilon \int_0^s \langle {L^*}^{-1}\dot{\varphi}, \dot{x}\rangle ds' \tag{2.3.18}$$

*with bound*

$$|\langle \varphi, x\rangle|_0^s| \leq C\varepsilon\|\varphi(s)\|\|x(0)\|\,, \tag{2.3.19}$$

*where $C$ depends on the family $L(s)$.*

Before giving proofs we note that assumption (2.3.17) of Proposition 2.21 may be phrased differently. The projections $P^*$ and $Q^*$ are associated to $\ker L^* \oplus \operatorname{ran} L^*$, see Lemma 2.15. Thus $Q^*\varphi = 0$, $P^*\dot{\varphi} = 0$ just means that $\varphi(s) \in \operatorname{ran} P^*(s)$ is parallel transported: $\varphi(s) = T^*(s,s')\varphi(s')$.

PROOF OF PROPOSITION 2.21. Equation (2.3.18) follows from

$$\begin{aligned}\frac{d}{ds}\langle\varphi, x\rangle &= \langle\dot{\varphi}, x\rangle + \langle\varphi, \dot{x}\rangle = \langle L^* L^{*-1}\dot{\varphi}, x\rangle + \varepsilon^{-1}\langle\varphi, Lx\rangle \\ &= \langle L^{*-1}\dot{\varphi}, Lx\rangle + \varepsilon^{-1}\langle L^*\varphi, x\rangle = \varepsilon\langle L^{*-1}\dot{\varphi}, \dot{x}\rangle + 0\,.\end{aligned}$$

Integration by parts in (2.3.18) gives

$$\langle\varphi, x\rangle|_0^s = \varepsilon\left(\langle\phi, x\rangle|_0^s - \int_0^s \langle\dot{\phi}(s'), x(s')\rangle ds'\right), \tag{2.3.20}$$

where $\phi(s') = L^*(s')^{-1}\dot{\varphi}(s')$. We observe that $\|x(s')\| \leq \|x(0)\|$ by Lemma 2.4, and $\dot{\varphi}(s) = \dot{P}^*(s)\varphi(s)$ by (2.2.11). By (2.2.15) we see that $\|\varphi(s')\|, \|\phi(s')\|$ and $\|\dot{\phi}(s')\|$ are bounded by a constant times $\|\varphi(s)\|$, proving (2.3.19). □

PROOF OF THEOREM 2.19. Bound (2.3.19), together with $\langle\varphi(0), x(0)\rangle = \langle\varphi(s), T(s,0)x(0)\rangle$ yields

$$|\langle\varphi(s), x(s) - T(s,0)x(0)\rangle| \leq C\varepsilon\|\varphi(s)\|\|x(0)\|\,.$$

The claim follows from $\|P(s)x\| = \sup\{|\langle\varphi, x\rangle| \mid \varphi \in \ker L^*(s), \|\varphi\| = 1\}$. □

## 2.4. Adiabatic theorem in absence of a gap

In this section we no longer assume that $\operatorname{ran} L$ is closed. By Lemma 2.12 and Assumptions (H1) and (H2') below this intimately connected with the absence of a spectral gap. Remarkably, an adiabatic theorem can still be proved in this setting as has been discovered independently by Avron and Elgart [AE99] as well as Bornemann [Bor98] in the Hamiltonian case. A characteristic feature of such theorems is the fact that no information on the rate of convergence as $\varepsilon \to 0$ is obtained unless further assumption on $L$ are made.

In what follows we provide a shorter proof which in addition does not require anti-self-adjointness of $L$ and therefore allows for a wider range of applications, such as open quantum systems described by a Lindbladian, see Chapter 4.

Assumptions (H1-H3) of Subsection 2.3.1 are relaxed in a natural way:

(H1) $L$ is the generator of a contraction semigroup on a Banach space $\mathcal{B}$.

(H2')

$$\mathcal{B} = \ker L \oplus \overline{\operatorname{ran} L}. \tag{2.4.1}$$

(H3') $L(s)$ is a $C^1$-family.

**REMARK 2.22.** *Sufficient conditions for (H2') are given in Section 2.5.*

The proof of our adiabatic theorem without gap condition depends on the 'if'-part of the following key observation.

**LEMMA 2.23.** *(H1) implies*

$$b \in \overline{\operatorname{ran} L} \Leftrightarrow \lim_{\gamma \searrow 0} \frac{\gamma}{L-\gamma} b = 0, \qquad (b \in \mathcal{B}).$$

PROOF. By Theorem 2.1 (Hille-Yosida) $\gamma(L-\gamma)^{-1}$ is uniformly bounded in $\gamma > 0$. By density it suffices to prove the direct implication for $b = Lx$, for which it follows from $\gamma(L-\gamma)^{-1}Lx = \gamma(x + \gamma(L-\gamma)^{-1}x)$. Conversely, set $x_\gamma := (L-\gamma)^{-1}b$; then $Lx_\gamma = b + \gamma(L-\gamma)^{-1}b \to b$. □

Lemma 2.23 allows for the following strengthening of Lemma 2.11.

**LEMMA 2.24.** *(H1) implies*

$$\ker L \cap \overline{\operatorname{ran} L} = \{0\}. \tag{2.4.2}$$

PROOF. Let $b$ be in the intersection (2.4.2): we holds that $(L-\gamma)b = -\gamma b$, and therefore $b = -\gamma(L-\gamma)^{-1}b$, which vanishes for $\gamma \searrow 0$. □

**THEOREM 2.25** (Gapless). *Let $L(s)$ satisfy hypotheses (H1), (H2'), (H3') and let $\mathbb{1} = P(s) + Q(s)$ be the projections associated to Equation (2.4.1) for almost all $s$; moreover let $P(s)$ be defined for all $0 \le s \le 1$ and $C^1$ as a bounded operator on $\mathcal{B}$. Then the solution of $\varepsilon\dot{x} = L(s)x$ with initial data $x(0) = P(0)x(0)$ satisfies*

$$\sup_{0 \le s \le 1} \|x(s) - T(s,0)x(0)\| \to 0\,, \qquad (\varepsilon \to 0)\,. \tag{2.4.3}$$

**REMARK 2.26.**

1) *Since we do no longer have the Riesz projection formula 2.3.2 at our disposal regularity of $P(s)$ has to be assumed.*

2) *The regularity assumption is as mild as $C^1$ thanks to a remark by Elgart, reported in [Teu01].*

PROOF. We observe that, by continuity, $L(s)P(s) = 0$ holds for all $0 \le s \le 1$. In particular, $L(s)x_0(s) = 0$ for $x_0(s) = T(s,0)x(0)$. The remainder to be estimated is $r(s) = x(s) - x_0(s)$. By Equation (2.1.1) it satisfies the differential equation $\varepsilon\dot{r}(s) = L(s)r(s) - \varepsilon\dot{x}_0(s)$ with solution

$$\begin{aligned} r(s) &= -\int_0^s U_\varepsilon(s,s')\dot{x}_0(s')ds' \\ &= -\int_0^s U_\varepsilon(s,s')L(s')(L(s')-\gamma)^{-1}\dot{x}_0(s')ds' + \int_0^s U_\varepsilon(s,s')\gamma(L(s')-\gamma)^{-1}\dot{x}_0(s')ds'\,, \end{aligned}$$

for $\gamma > 0$. By Equations (2.2.10, 2.4.1) we have $\dot{x}_0(s) \in \overline{\operatorname{ran} L(s)}$ for almost all $s$. Therefore, by an appropriate choice of $\gamma > 0$, the second integral can be made arbitrarily small by means of Lemma 2.23 and dominated convergence; in fact, uniformly in $\varepsilon$ due to $\|U_\varepsilon(s,s')\| \le 1$.

It remains to show that, for fixed $\gamma > 0$, the first integral vanishes with $\varepsilon \to 0$. To illustrate the argument, let us temporarily pretend that $z(s) := (L(s)-\gamma)^{-1}\dot{x}_0(s)$ is $C^1$. Since $\varepsilon\partial_{s'}U_\varepsilon(s,s') = -U_\varepsilon(s,s')L(s')$ an integration by parts yields for that integral

$$\varepsilon\int_0^s \partial_{s'}U_\varepsilon(s,s')z(s')ds' = \varepsilon U_\varepsilon(s,s')z(s')|_{s'=0}^{s'=s} - \varepsilon\int_0^s U_\varepsilon(s,s')\frac{d}{ds'}z(s')ds'\,,$$

and exhibits the desired property for $\varepsilon \to 0$.

Finally, we get rid of the additional assumption by amending the argument as follows. We introduce a mollifier $j$, ($j \in C_0^\infty(\mathbb{R})$, $\int j(x)dx = 1$) and set $j_\delta(x) = \delta^{-1}j(x/\delta)$, ($\delta > 0$); we extend $\dot{x}_0$ continuously outside of the interval $[0,1]$; and split

$$z = (L-\gamma)^{-1}(\dot{x}_0 - j_\delta * \dot{x}_0) + (L-\gamma)^{-1}(j_\delta * \dot{x}_0)\,.$$

Since $\dot{x}_0 - j_\delta * \dot{x}_0 \to 0$, ($\delta \to 0$) and $\|L(L-\gamma)^{-1}\|$ is bounded, both uniformly in $s$, the first term contributes arbitrary little to the integral, uniformly in $\varepsilon$, if $\delta$ is picked small enough. The preliminary argument can now be applied to the second term in place of $z$. □

In view of our applications we present the following variant of Proposition 2.21. Its assumptions allow to estimate the error to be of order $O(\varepsilon)$ even in the gapless case.

**Proposition 2.27.** *Let $L(s)$ be a $C^1$-family satisfying (H1). Suppose the family $\varphi(s) \in \mathcal{B}^*$, $(0 \le s \le 1)$ satisfies*

$$\varphi(s) \in \ker L^*(s)\,, \qquad \dot{\varphi}(s) = L^*(s)\phi(s) \tag{2.4.4}$$

*with uniformly bounded $\phi(s)$ and $\dot{\phi}(s)$. Then*

$$|\langle\varphi, x\rangle|_0^s| \le 3\varepsilon \sup_{0\le s'\le 1}\big(\|\phi(s')\| + \|\dot{\phi}(s')\|\big)\|x(0)\|\,. \tag{2.4.5}$$

Proof. Equation (2.3.20) can be obtained from the present assumptions by replacing $\phi$ for $L^{*-1}\dot{\varphi}$ in the previous derivation. □

## 2.5. Complementarity of subspaces

In this section we give sufficient conditions for the Complementarity Assumptions (H2) of Section 2.3 in relation with a spectral gap, and (H2') of Section 2.4 otherwise. Counterexamples matching the two cases are also given. Related results are found in [HP57], Section 18.8. In either case the two subspaces in Equations (2.3.1, 2.4.1) are transversal,

$$\ker L \cap \overline{\operatorname{ran} L} = \{0\}\,,$$

as a consequence of assumption (H1), cf. Lemmata 2.11 and 2.24. However they may fail to generate $\mathcal{B}$ without further hypotheses.

**Example 2.28.** *[Gan] Consider the operator $L$ defined by $(Lf)(x) = -xf(x)$ for $f \in L^\infty(0,1) = \mathcal{B}$. Obviously, $L$ has trivial kernel and $(\mathrm{e}^{Lt}f)(x) = \mathrm{e}^{-xt}f(x)$, which makes $L$ the generator of a contraction semigroup. However, for $1 \equiv g \in L^\infty(0,1)$ one has*

$$\|g - Lf\|_{L^\infty} \ge 1\,, \qquad (f \in L^\infty(0,1))\,.$$

*Thus $\overline{\operatorname{ran} L}$ is a proper subspace of $L^\infty(0,1)$.*

*Notation:* As before, a prime indicates a hypothesis tailored to the second, gapless case; a sufficient condition for an earlier hypothesis is noted by an added roman numeral.

### 2.5.1. Complementarity in presence of a gap

In this case the Riesz projection plays a crucial role.

**Proposition 2.29.** *Let $\mathcal{B}$ be a Banach space and $L$ a closed operator on $\mathcal{B}$. Assume*

*(H1)* *$L$ is the generator of a contraction semigroup;*

*(H2i)* *$0 \in \sigma(L)$ is isolated and that $\operatorname{ran} \tilde{P} = \ker L$, where $\tilde{P}$ is the Riesz projection (2.3.2).*

*Then*

$$\mathcal{B} = \ker L \oplus \operatorname{ran} L \,,$$

*and in particular $\operatorname{ran} L$ is closed.*

PROOF. Note

$$L \frac{1}{2\pi \mathrm{i}} \oint_\Gamma (L-z)^{-1} \frac{dz}{z} = \frac{1}{2\pi \mathrm{i}} \oint_\Gamma \frac{1}{z} dz + \frac{1}{2\pi \mathrm{i}} \oint_\Gamma (L-z)^{-1} dz = \mathbb{1} - \tilde{P}$$

and so $\operatorname{ran} L \supset \operatorname{ran}(\mathbb{1} - \tilde{P})$, which implies

$$\mathcal{B} = \operatorname{ran} \tilde{P} \oplus \operatorname{ran}(\mathbb{1} - \tilde{P}) = \ker L \oplus \operatorname{ran} L$$

in view of Lemma 2.11; $\operatorname{ran} L$ is closed by Lemma 2.10. □

If $\mathcal{B}$ is a Hilbert space and $L$ an anti-self-adjoint operator on $\mathcal{B}$ with 0 being an isolated eigenvalue it is always true that $\mathcal{B} = \ker L \oplus \overline{\operatorname{ran} L}$ and $\operatorname{ran} \tilde{P} = \ker L$. Lemma 2.12 and Proposition 2.29 then imply

$$\operatorname{ran} L \text{ is closed } \Leftrightarrow 0 \in \sigma(L) \text{ is isolated.}$$

In general the situation is more subtle since $\ker L$ may indeed be a proper subspace of $\operatorname{ran} \tilde{P}$ even if $L$ generates a contraction semigroup as the following example from [LP61], Theorem 2.2, shows.

**EXAMPLE 2.30.** *There exists a non-trivial generator $L$ of a contraction semigroup with trivial null space, yet with $\sigma(L) = \{0\}$.*

However, if $\tilde{P}$ is finite-dimensional (i.e. if $0 \in \sigma(L)$ then 0 is a discrete eigenvalue[2]) such a thing cannot happen:

**LEMMA 2.31.** *Suppose $L$ is the generator of a contraction semigroup on a Banach space $\mathcal{B}$ and*

*(H2ii)* *If $0 \in \sigma(L)$, then 0 is a discrete eigenvalue.*

*Then*

$$\operatorname{ran} \tilde{P} = \ker L \,.$$

PROOF. Clearly $\operatorname{ran} \tilde{P} \supset \ker L$ and $\sigma(L \restriction \operatorname{ran} \tilde{P}) \subset \{0\}$, in particular $L \restriction \operatorname{ran} \tilde{P}$ is finite-dimensional and nilpotent. Assuming that there is $b \in \operatorname{ran} \tilde{P} \setminus \ker L$ it follows that $0 \neq Lb \in \operatorname{ran} L$ and in fact, by Lemma 2.11, $0 \neq L^n b \; \forall n \in \mathbb{N}$: a contradiction.

Alternatively, the claim follows from the observation that $\mathrm{e}^{Lt}$ exhibits polynomial growth on $\operatorname{ran} \tilde{P}$ if $L$ is a nontrivial nilpotent which is again a contradiction. □

[2]Note that for non-self-adjoint operators the discrete spectrum need not be the complement of the essential spectrum. In fact, several, inequivalent, definitions of the essential spectrum (=complement of the discrete spectrum) exist in this case, cf. [EE87].

A combination of Proposition 2.29 and Lemma 2.31 can also be derived by means of stability theorems in Fredholm theory which is shown in the remainder of this subsection. We recall that $L$ is semi-Fredholm if and only if $\operatorname{ran} L$ is closed and $\ker L$ or $\mathcal{B}/\operatorname{ran} L$ are finite-dimensional. If both are, $L$ is called Fredholm.

**Proposition 2.32.** *Let $\mathcal{B}$ be a Banach space and $L$ a closed operator on $\mathcal{B}$. Assume*

*(H1)* *$L$ is the generator of a contraction semigroup;*

*(H2ii)* *If $0 \in \sigma(L)$, then $0$ is a discrete eigenvalue.*

*Then $\mathcal{B} = \ker L \oplus \operatorname{ran} L$, cf. Equation (2.3.1).*

*Property (H2ii) implies that $L$ is Fredholm, and hence*

*(H2iii)* *$L$ is semi-Fredholm.*

*In conjunction with (H1), properties (H2ii) and (H2iii) are equivalent.*

Proof. Suppose a closed operator $L$ has 0 as an isolated point in its spectrum with associated Riesz projection $\tilde{P}$. Then $\tilde{P}$ decomposes $L$ with $\sigma(L \restriction \operatorname{ran} \tilde{P}) = \{0\}$ and $\sigma(L \restriction \operatorname{ran}(1 - \tilde{P})) = \sigma(L) \setminus \{0\}$ ( [Kat95], Theorem III.6.17). Furthermore $\operatorname{ran} L$ is closed being the direct sum of a closed and a finite dimensional vector space. As a result, (H2ii) implies that $L$ is Fredholm as it is the direct sum of two Fredholm operators. In particular (H2iii) holds, regardless of (H1).

From now on we assume (H1), which implies Equation (2.4.2), and (H2iii). By the stability theorem ( [Kat95], Theorem IV.5.31) $L - z$ remains semi-Fredholm for $z$ in a complex neighborhood of 0 and the index $\dim\ker(L - z) - \dim(\mathcal{B}/\operatorname{ran}(L - z))$ is constant; moreover the two dimensions are separately constant in a punctured neighborhood $U$. By (2.2.1) in Theorem 2.1 (Hille-Yosida), they both vanish there, and so does the index at $z = 0$. This has the following implications: First, if $0 \in \sigma(L)$, then it is isolated. Second, the map $\ker L \to \mathcal{B}/\operatorname{ran} L$, $a \mapsto a + \operatorname{ran} L$ is one-to-one by (2.4.2) and thus onto by the vanishing index. This proves $\ker L + \operatorname{ran} L = \mathcal{B}$, completing the proof of Equation (2.3.1).

Finally in order to prove (H2ii), we observe that the Riesz projection is given by $P$, as established in Lemma 2.13. Thus it is finite-dimensional because $\ker L$ is. □

**Example 2.30 (revisited).** For the mentioned operator the Riesz projection cannot be finite-dimensional. Hence (H2ii) fails there. By the equivalence with (H2iii), $\operatorname{ran} L$ is not closed, spoiling (2.3.1).

### 2.5.2. Complementarity in absence of a gap

In absence of a gap the Riesz projection is no longer available as a tool and a different approach is needed. It turns out that reflexivity of the Banach space $\mathcal{B}$ is a key property.

**Proposition 2.33.** *If $\mathcal{B}$ is a reflexive Banach space and $L$ the generator of a contraction semigroup on $\mathcal{B}$, then $\ker L + \overline{\operatorname{ran} L} \subset \mathcal{B}$ is dense. Thus, in particular, if $\ker L + \overline{\operatorname{ran} L}$ is closed, then*

$$\mathcal{B} = \ker L \oplus \overline{\operatorname{ran} L}.$$

**REMARK 2.34.**

1) *Recall that P(s) in Theorem 2.25 was required to be $C^1$ in norm sense. Under this hypothesis* $\ker L + \overline{\operatorname{ran} L}$ *is closed as a consequence of Lemma 2.10.*

2) $L^\infty(0,1)$ *in Example 2.28 is not reflexive.*

PROOF. By the Hahn-Banach theorem it suffices to show that $x^* \in (\ker L)^\perp \cap (\operatorname{ran} L)^\perp$ implies $x^* = 0$. Here $S^\perp \subset \mathcal{B}^*$ is the annihilator of a subspace $S \subset \mathcal{B}$. We have $(\operatorname{ran} L)^\perp = \ker L^*$ and, in the reflexive case, $(\ker L)^\perp = \overline{\operatorname{ran} L^*}$. The last equality is due to $(S^\perp)_\perp = \overline{S}$ ( [Kat95], Equation III.1.24), where $S_\perp \subset \mathcal{B}$ denotes the predual annihilator in $\mathcal{B}$ for $S \subset \mathcal{B}^*$. The properties (2.2.1) are inherited by $L^*$, and hence so is (2.4.2). We conclude that $x^* = 0$. (As a matter of fact, $L^*$ is also densely defined ( [Kat95], Theorem III.5.29) by reflexivity, and hence is the generator of a contraction semigroup). □

### 2.5.3. SUMMARY

For convenience we collect here the most important results on the Decomposition (H2) resp. (H2'). Let $L$ be the generator of a contraction semigroup on a Banach space $\mathcal{B}$. Then it holds that

(i) $\ker L \cap \overline{\operatorname{ran} L} = \{0\}$.

(ii) $\mathcal{B} = \ker L \oplus \overline{\operatorname{ran} L}$ if in addition one of the following conditions is satisfied:

- $0 \in \sigma(L)$ is isolated and $\operatorname{ran} \tilde{P} = \ker L$, which holds in particular if $0 \in \sigma(L)$ is discrete or, equivalently, if $L$ is semi-Fredholm. As a consequence, $\operatorname{ran} L$ is closed.
- $\mathcal{B}$ is reflexive and $\ker L + \overline{\operatorname{ran} L}$ is closed.

Now *assume* also $\mathcal{B} = \ker L \oplus \overline{\operatorname{ran} L}$ and let $P$ be the associated projection onto $\ker L$. Then it holds that:

| | | |
|---|---|---|
| $\operatorname{ran} L$ is closed | $\Rightarrow$ | $0 \in \sigma(L)$ is isolated. |
| $0 \in \sigma(L)$ is isolated and $P = \tilde{P}$ | $\Rightarrow$ | $\operatorname{ran} L$ is closed. |

Specifically, if $0 \in \sigma(L)$ and $L$ is semi-Fredholm or anti-self-adjoint (in which case $\mathcal{B}$ is a Hilbert space):

| | | |
|---|---|---|
| $\operatorname{ran} L$ is closed | $\Leftrightarrow$ | $0 \in \sigma(L)$ is isolated. |

# Chapter 3

# Quantum Dynamical Semigroups

## 3.1. Interaction of a physical system with its environment

In most textbooks on quantum mechanics the usual setting is given by some physical system $\Sigma$ described by a Hamiltonian $H_\Sigma$ which acts on an appropriate Hilbert space $\mathcal{H}_\Sigma$. Recall that Hilbert spaces are always assumed to be separable without further notice. A common assumption is that the interaction of $\Sigma$ with its environment[1] $\mathcal{E}$ (described by a Hilbert space $\mathcal{H}_\mathcal{E}$ and a Hamiltonian $H_\mathcal{E}$) can be neglected.

In principle however the full Hamiltonian

$$H_{\Sigma\vee\mathcal{E}} = H_\Sigma \otimes \mathbb{1} + H_I + \mathbb{1} \otimes H_\mathcal{E} \qquad \text{on } \mathcal{H}_\Sigma \otimes \mathcal{H}_\mathcal{E}\,, \tag{3.1.1}$$

with $H_I$ describing the interaction, has to be taken into account. It is of course still the dynamics of the system $\Sigma$ itself in which we are interested: If $\Sigma \vee \mathcal{E}$ is prepared in an initial state described by a density matrix $\rho \otimes \rho_\mathcal{E} \in \mathcal{J}_1(\mathcal{H}_\Sigma \otimes \mathcal{H}_\mathcal{E})$ then the dynamics on $\Sigma$ is described by tracing out the degrees of freedom of the environment,

$$\Phi_t(\rho) = \mathrm{tr}_\mathcal{E}\left(\mathrm{e}^{-\mathrm{i}H_{\Sigma\vee\mathcal{E}}t} \rho \otimes \rho_\mathcal{E} \mathrm{e}^{\mathrm{i}H_{\Sigma\vee\mathcal{E}}t}\right)\,. \tag{3.1.2}$$

If $H_I = 0$ then $\Phi_t(\rho) = \mathrm{e}^{-\mathrm{i}H_\Sigma t}\rho \mathrm{e}^{\mathrm{i}H_\Sigma t}$ and in particular $\Phi_t(\rho)$ is a pure state if $\rho$ is. In general though, correlations between $\Sigma$ and $\mathcal{E}$ will build up such that a pure state on $\Sigma$ is transformed into a mixed state under the evolution $\Phi_t$; a phenomenon referred to as *decoherence* and not always negligible. Its inclusion may rather change the physical picture. This is corroborated in Chapter 4 by several examples.

Tracing out the degrees of freedom of the environment yields a complicated integro-differential equation for $\Phi_t$. Its complexity is due to the fact that the interaction between $\Sigma$ and $\mathcal{E}$ causes memory effects and destroys the Markovian structure of the Heisenberg equation $\mathrm{i}\frac{d}{dt}\rho(t) = [H_{\Sigma\vee\mathcal{E}}, \rho(t)]$ once the dynamics is reduced to the system $\Sigma$.

For those reasons approximations for (3.1.2) which still account for the effect of decoherence are necessary. This is most commonly achieved by the *assumption* of a semigroup law

$$\Phi_t(\rho) = \mathrm{e}^{t\mathcal{L}}\rho$$

in place of (3.1.2) and applies to many physical systems. It can be be justified in certain limiting regimes as we shall see in Section 3.4.

Before asking about the structure of the generator $\mathcal{L}$ it pays to examine the properties of $\Phi_t$ more closely. The key notion turns out to be that of complete positivity.

[1] E.g. a heat bath or measurement apparatus.

## 3.2. Completely positive maps

### 3.2.1. Motivation

To have better accordance with the existing literature we find it convenient to go over to the Heisenberg picture. Let $\mathcal{L}(\mathcal{H}_\Sigma)$ be the $C^*$-algebra of bounded operators whose self-adjoint elements are the observables of $\Sigma$. Equation (3.1.2) induces a dynamical map

$$\Phi_t^* : \mathcal{L}(\mathcal{H}_\Sigma) \to \mathcal{L}(\mathcal{H}_\Sigma)$$

which is the Banach space dual of $\Phi_t$ and is defined by

$$\mathrm{tr}(\Phi_t(\rho)A) = \mathrm{tr}\left(\rho\Phi_t^*(A)\right), \qquad \rho \in \mathcal{J}_1(\mathcal{H}_\Sigma)\,,\ A \in \mathcal{L}(\mathcal{H}_\Sigma)\,.$$

It follows immediately that $\Phi_t^*$ preserves positivity since $\Phi_t$ does and this is certainly a necessary requirement for any reasonable approximative scheme for (3.1.2). Interestingly the following argument suggests a stronger notion of positivity (see [Lin76]). Imagine a second system $\Sigma_n$ with $n$-dimensional Hilbert space $\mathcal{H}_{\Sigma_n}$ which is governed by the trivial Hamiltonian $H_{\Sigma_n} = 0$ and assume that it does neither interact with the system $\Sigma$ nor with the environment $\mathcal{E}$. For $A \in \mathcal{L}(\mathcal{H}_\Sigma)$, $B \in \mathcal{L}(\mathcal{H}_{\Sigma_n})$ the dynamics on $\Sigma \vee \Sigma_n$ is then given by

$$\Phi^*_{\Sigma\vee\Sigma_n,t}(A \otimes B) := (\Phi_t^* \otimes \mathbb{1}_n)(A \otimes B) = (\Phi_t^* A) \otimes B\,.$$

By construction $\Phi^*_{\Sigma\vee\Sigma_n,t}$ is positivity preserving (short: positive). Remarkably the mere fact that $\Phi_t^*$ is positive is not sufficient to draw this conclusion as is seen in the following standard example.

**Example 3.1.** *Consider the transpose map $T$ on the space of complex $n \times n$-matrices $M_n(\mathbb{C}) \simeq \mathcal{L}(\mathcal{H}_n)$: For $n = 2$*

$$T : \begin{pmatrix} a & b \\ c & d \end{pmatrix} \mapsto \begin{pmatrix} a & c \\ b & d \end{pmatrix}.$$

*Clearly $T$ is positive, however*

$$(T \otimes \mathbb{1}_2) \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

*shows that $T \otimes \mathbb{1}_2$ is not positive.*

### 3.2.2. Definition and Kraus maps

**Definition 3.2** (Complete positivity)**.** *For a map $\Psi : \mathcal{A} \to \mathcal{B}$ between two $C^*$-algebras $\mathcal{A}$, $\mathcal{B}$ we define*

$$\Psi_n := \Psi \otimes \mathbb{1}_n : \mathcal{A} \otimes M_n(\mathbb{C}) \to \mathcal{B} \otimes M_n(\mathbb{C}).$$

*$\Psi$ is called completely positive if and only if $\Psi_n$ is positive for all $n \in \mathbb{N}$ and in that case we write $\Psi \in CP(\mathcal{A}, \mathcal{B})$;*

- *if $\mathcal{A} = \mathcal{B} = \mathcal{L}(\mathcal{H})$ where $\mathcal{H}$ is a Hilbert space we simply write $\Psi \in CP(\mathcal{H})$.*
- *if $\mathcal{A}$ and $\mathcal{B}$ are $W^*$-algebras then $CP(\mathcal{A},\mathcal{B})_\sigma$ denotes the set of ultraweakly continuous elements in $CP(\mathcal{A},\mathcal{B})$.*

To understand the significance of the ultraweak topology think of a norm convergent net $A_i \to A \in \mathcal{L}(\mathcal{H})$. Physically, we require convergence of expectation values: $\mathrm{tr}(\rho\Psi A_i) \to \mathrm{tr}(\rho\Psi A)$ for every $\rho \in \mathcal{J}_1(\mathcal{H})$. However, this is precisely ultraweak continuity by the duality relation $\mathcal{J}_1(\mathcal{H})^* \simeq \mathcal{L}(\mathcal{H})$.

As an important structure theorem we present the following useful characterization of completely positive maps due to Kraus [Kra71].

**Theorem 3.3** (Kraus maps). *$\Psi \in CP(\mathcal{H})_\sigma$ if and only if*

$$\Psi(A) = \sum_{i\in I} V_i^* A V_i$$

*where $V_i, \sum_{i\in I} V_i^* V_i \in \mathcal{L}(\mathcal{H})$. $I$ is finite or countably infinite and in the latter case convergence of the sum is to be understood with respect to the ultraweak topology.*

## 3.3. Lindblad-GKS generators

As announced we now replace the dynamics in Equation (3.1.2) on $\Sigma$ by the semigroup law

$$\Phi_t(\rho) = \mathrm{e}^{t\mathcal{L}}\rho \tag{3.3.1}$$

on the $W^*$-algebra of bounded operators $\mathcal{L}(\mathcal{H})$.[2] Under natural assumptions on $\Phi_t$, such as the aforementioned complete positivity, Lindblad [Lin76] described the general form of all possible generators $L$. In fact some of his results even apply at the level of abstract $C^*/W^*$-algebras. Independently, and by a different method, the same structural result was obtained in the case $\dim \mathcal{H} < \infty$ by Gorini, Kossakowski and Sudarshan [GKS76].

To state their theorem recall that we adopted the Heisenberg picture. By the previous section the natural postulates for $\Phi_t^*$ are

(i) $\Phi_t^* \in CP_\sigma(\mathcal{H})$ ,

(ii) $\Phi_t^*(\mathbb{1}) = \mathbb{1}$ (trace conservation) ,

(iii) $\Phi_s^*\Phi_t^* = \Phi_{s+t}^*$ ,

(iv) $\lim_{t\searrow 0} \|\Phi_t^* - \mathbb{1}\| = 0$ .

If (i-iv) are satisfied we call $\Phi_t^*$ a *quantum dynamical semigroup*. By (i) $\Phi_t^*$ is in particular positive and in conjunction with (ii) it follows that $\|\Phi_t^*\| = 1$ ( [BR79], Corollary 3.2.6). Hence $\Phi_t^*$ is a norm continuous contraction semigroup and therefore possesses a bounded generator $\mathcal{L}$.

**Theorem 3.4** (Lindblad [Lin76]). *If $\Phi_t^*$ satisfies (i-iv) then its generator $\mathcal{L}^*$ is of the form*

$$\mathcal{L}^*(A) = \mathrm{i}[H,A] + \sum_{i\in I}(V_i^* A V_i - \frac{1}{2}\{V_i^* V_i, A\}) \tag{3.3.2}$$

*where $H = H^* \in \mathcal{L}(\mathcal{H})$ and $V_i$, $I$ as in Theorem 3.3. Conversely, if $\mathcal{L}^*$ satisfies (3.3.2) then $\Phi_t^*$ is a quantum dynamical semigroup.*

[2] The subscript $\Sigma$ is from now on omitted.

**Remark 3.5.** *In the Schrödinger picture the corresponding formula reads*

$$\mathcal{L}(\rho) = -\mathrm{i}[H,\rho] + \frac{1}{2}\sum_{i\in I}\left([V_i\rho, V_i^*] + [V_i, \rho V_i^*]\right) \tag{3.3.3}$$

*and is an operator on* $\mathcal{J}_1(\mathcal{H})$*. We call* $\mathcal{L}$ *a Lindbladian.*

**Remark 3.6.** *Note that* $\mathcal{L}$ *does not determine the* $V_i$ *and* $H$ *uniquely: the transformation*

$$\begin{aligned} V_i &\mapsto V_i + \beta_i \mathbb{1} \\ H &\mapsto H + \frac{\mathrm{i}}{2}\sum_{i\in I}\left(\beta_i V_i^* - \overline{\beta}_i V_i\right) \end{aligned}$$

*leaves* $\mathcal{L}$ *invariant. Another example for an invariance transformation is*

$$V_i \mapsto \sum_{j\in I} U_{ij} V_j$$

*for* $I$ *finite and* $(U_{ij})$ *unitary.*

In the case of unbounded generators a classification of the kind of Theorem 3.4 is unknown. However there exist concrete physical models where a generator of the form (3.3.2, 3.3.3), yet unbounded, arises [Dav77].

## 3.4. Quantum dynamical semigroups as a limiting regime

Lindblad's result leaves the question unanswered as to what extent the evolution law (3.3.1) really captures the physical situation or, to be more precise, how it relates to the "true" dynamics described by Equation (3.1.2). It turns out that the reduced dynamics (3.1.2) can be shown to become Markovian in certain limiting regimes such as the weak coupling limit [Dav74, Dav76, Dav75], the singular coupling limit [HL73, GK76, Pal77], or the low density limit [Düm85]. Exemplarily we will discuss this matter in the first scheme in what follows.

To prevent this digression to distract too much from the main goals of this thesis we stress that for our applications we take up on the position that we are simply given a quantum dynamical semigroup without further asking about its origin.

### 3.4.1. Weak coupling limit

Following the pioneering work of Davies [Dav74, Dav76, Dav75] we first adopt a rather abstract framework. In a second step we shall translate the results to the context of composite quantum systems.

Let $P_0$ be a projection on a Banach space $\mathcal{B}$ and $P_1 := \mathbb{1} - P_0$. On $\mathcal{B}$ there exists a free evolution given by a strongly continuous one-parameter semigroup $U_t$ which leaves $P_0\mathcal{B}$ as well as $P_1\mathcal{B}$ invariant; its closed and densely defined generator is denoted by $Z$. Under the assumption that $P_0$ respects the domain of $Z$ we may put $Z_i = P_i Z P_i = Z P_i$. Furthermore let $A$ be a bounded perturbation of $Z$ and put $A_{ij} = P_i A P_j$. Finally let $V_t^\lambda$ describe the full evolution generated by $Z + \lambda A$, $U_t^\lambda$ the diagonal evolution generated by $(Z + \lambda A_{00} + \lambda A_{11})$, and $W_t^\lambda$ the full dynamics restricted to $P_0\mathcal{B}$, that is $W_t^\lambda = P_0 V_t^\lambda P_0$. By Duhamel's principle

$$V_t^\lambda = U_t^\lambda + \lambda \int_0^t ds\ U_{t-s}^\lambda (A_{01} + A_{10}) V_s^\lambda$$

which yields the restricted evolutions

$$\begin{aligned} P_0 V_t^\lambda P_0 &= P_0 U_t^\lambda P_0 + \lambda \int_0^t ds\ U_{t-s}^\lambda A_{01} P_1 V_s^\lambda P_0\,, \\ P_1 V_t^\lambda P_0 &= \lambda \int_0^t ds\ U_{t-s}^\lambda A_{10} W_s^\lambda\,. \end{aligned}$$

Therefore, with $X_t^\lambda = P_0 U_t^\lambda = P_0 \mathrm{e}^{(Z_0 + \lambda A_{00})t}$,

$$\begin{aligned} W_t^\lambda &= X_t^\lambda + \lambda^2 \int_0^t ds \int_0^s du\ X_{t-s}^\lambda A_{01} U_{s-u}^\lambda A_{10} W_u^\lambda && (3.4.1) \\ &= X_t^\lambda + \lambda^2 \int_0^t ds \int_s^t du\ X_{t-u}^\lambda A_{01} U_{u-s}^\lambda A_{10} W_s^\lambda && (3.4.2) \\ &= X_t^\lambda + \lambda^2 \int_0^t ds\ X_{t-s}^\lambda K^\lambda (t-s) W_s^\lambda, && (3.4.3) \end{aligned}$$

where

$$K^\lambda(t) = \int_0^t ds\ X_{-s}^\lambda A_{01} U_s^\lambda A_{10}\,.$$

With $\varphi$ in the domain of $Z_0$ and $\varphi_t = W_t^\lambda \varphi$ we arrive by differentiation of Equation (3.4.1) at an abstract formulation of the so called Nakajima-Zwanzig equation

$$\frac{d}{dt}\varphi_t = (Z_0 + A_{00})\varphi_t + \lambda^2 \int_0^t du\ A_{01} U_{t-u}^\lambda A_{10} \varphi_u \qquad (3.4.4)$$

which is manifestly non-Markovian since it contains a memory term in form of an integral. We now turn to the regime of weak coupling. In order to see an effect of the perturbation $A$ it is necessary that we look at very large times. In fact from Equation (3.4.1) we deduce that the right scaling is $\tau = \lambda^2 t$ for fixed $\tau$ and $\lambda \to 0$. This is known as the *van Hove limit.* A change of variables transforms Equation (3.4.3) into

$$W_{\lambda^{-2}\tau}^\lambda = X_{\lambda^{-2}\tau}^\lambda + \int_0^{\lambda^{-2}\tau} d\sigma\ X_{\lambda^{-2}(\tau-\sigma)}^\lambda K^\lambda \left(\lambda^{-2}(\tau-\sigma)\right) W_{\lambda^{-2}\sigma}^\lambda\,. \qquad (3.4.5)$$

In the regime $\lambda \to 0$ Davies showed the following theorem.

**Theorem 3.7** (Davies, [Dav76]). *Suppose that $X_t^\lambda$ is a one-parameter group of isometries on $P_0\mathcal{B}$ for all real $\lambda$. Suppose that for all $\tau_1 > 0$ the norm of $K^\lambda(\lambda^{-2}\tau)$ is uniformly bounded in $\lambda$ and $\tau$ for $|\lambda| \leq 1$ and $0 \leq \tau \leq \tau_1$. Furthermore suppose that there is a bounded operator $K$ on $P_0\mathcal{B}$ such that if $0 < \tau_0 < \tau_1 < \infty$ then*

$$\lim_{\lambda \to 0} \sup_{\tau_0 \leq \tau \leq \tau_1} \|K^\lambda(\lambda^{-2}\tau) - K\| = 0.$$

*Then*

$$\lim_{\lambda\to 0}\sup_{0\le t\le \lambda^{-2}\tau_1}\|W_t^\lambda-\tilde W_t^\lambda\|=0$$

*where*

$$\tilde W_t^\lambda=\mathrm{e}^{(Z_0+\lambda A_{00}+\lambda^2K)t}\,.$$

Now suppose that $P_0\mathcal{B}$ is finite dimensional and $A_{00}=0$. Then there is a simpler generator than $K$ which still approximates the full dynamics. It is convenient to change to the interaction picture. Note that now $X_t=X_t^\lambda$ does no longer depend on $\lambda$ and with $Y_t^\lambda=X_{-t}W_t^\lambda$ it follows from (3.4.5) that

$$Y^\lambda_{\lambda^{-2}\tau}=\mathbb{1}+\int_0^{\lambda^{-2}\tau}d\sigma\;X_{-\lambda^{-2}\sigma}K^\lambda\left(\lambda^{-2}(\tau-\sigma)\right)X_{\lambda^{-2}\sigma}Y^\lambda_{\lambda^{-2}\sigma}\,.$$

Since $K^\lambda$ is intertwined by $X$ we expect that oscillations will make off-diagonal terms of $K^\lambda$ negligible (in the literature this is sometimes referred to as coarse-graining or rotating wave approximation): Denote the spectral projections of $Z_0$ on $P_0\mathcal{B}$ by $Q_\alpha$ and introduce

$$B^\natural=\sum_\alpha Q_\alpha BQ_\alpha$$

or, equivalently,

$$B^\natural=\lim_{t\to\infty}\frac{1}{2t}\int_{-t}^{t}dx\;X_xBX_{-x}\,.$$

**THEOREM 3.8** (Davies, [Dav74]). *Let $A_{00}=0$ and $P_0\mathcal{B}$ be finite dimensional. Furthermore let the same assumptions as in Theorem 3.7 be valid. Then*

$$\lim_{\lambda\to 0}\sup_{0\le t\le \lambda^{-2}\tau_1}\|Y_t^\lambda-\tilde Y_t^\lambda\|=0$$

*where*

$$\tilde Y_t^\lambda=\mathrm{e}^{\lambda^2K^\natural t}\,. \tag{3.4.6}$$

Note that $K^\natural$ is simpler than $K$ and that it commutes with the free evolution. To appreciate the significance of these theorems we first have to translate the abstract theory to the more concrete framework of Section 3.1.

*Dictionary:* $\mathcal{B}$ is identified with $\mathcal{J}_1(\mathcal{H}_\Sigma\otimes\mathcal{H}_\mathcal{E})$ and we have $Z=-\mathrm{i}[H_\Sigma\otimes\mathbb{1}+\mathbb{1}\otimes H_\mathcal{E},\cdot]$, at least formally in the case of unbounded Hamiltonians. Furthermore, $A=-\mathrm{i}[H_I,\cdot]$ with $H_I=Q\otimes\phi$, where $Q$, $\phi$ are bounded symmetric operators on $\mathcal{H}_\Sigma$ and $\mathcal{H}_\mathcal{E}$ respectively. The state of the system $\Sigma$ is given by $\rho$ and that of the environment by $\rho_\mathcal{E}$ for which we assume

$$[\rho_\mathcal{E},\mathrm{e}^{\mathrm{i}t\mathcal{H}_\mathcal{E}}]=0\,, \tag{3.4.7}$$

$$\mathrm{tr}(\phi\rho_\mathcal{E})=0\,. \tag{3.4.8}$$

The projection $P_0:\mathcal{B}\to\mathcal{B}$ is essentially the partial trace, $P_0a:=\mathrm{tr}_\mathcal{E}(a)\otimes\rho_\mathcal{E}$, and by (3.4.7) it commutes with the free evolution generated by $Z$. This is for instance the case if $\mathcal{E}$ is a certain thermal heat bath and $\rho_{\mathcal{E}}$ one of its thermal equilibrium states [Dav74]. In addition (3.4.8) implies $A_{00} = 0$.

Davies noted that the existence of a limit operator $K$ in Theorems 3.7, 3.8 depends on the decay of the environment correlation function

$$\mathrm{tr}(\rho_{\mathcal{E}} \mathrm{e}^{itH_{\mathcal{E}}} \phi \mathrm{e}^{-itH_{\mathcal{E}}} \phi) = \mathrm{tr}\left(\rho_{\mathcal{E}} \phi(t) \phi\right) . \tag{3.4.9}$$

This however is not granted if the environment is finite due to Poincaré recurrences [AL07]: Note that Davies chose a Fermion gas described by a quasi-free representation of the canonical anticommutation relations with an *infinite* number of degrees of freedom [Dav74].

Comparing Theorem 3.7 with Theorem 3.8 it is interesting to note, as shown by Dümcke and Spohn [DS79], that $K$ generically does not give rise to a positivity preserving semi-group. On the other hand $\mathrm{e}^{K^\natural \tau}$ arises as the limit of completely positive maps by Equation (3.4.6) and is therefore itself completely positive: we remark that $K^\natural$ is the natural generator in the van Hove limit.

### 3.4.2. Other limiting regimes

Apart from the weak coupling limit there exist other regimes in which quantum dynamical semigroups arise. Physically speaking, the Markovian approximation is expected to be valid if the typical time $\tau_\Sigma$ of variation of quantities of the physical system $\Sigma$ (relaxation time of $\Sigma$) is much larger than the decay time $\tau_{\mathcal{E}}$ of the environment correlation functions: Under such conditions we may expect to get rid of memory terms. The van Hove limit corresponds to the situation where $\tau_{\mathcal{E}}$ is finite and fixed while $\tau_\Sigma$ tends to infinity.

The *singular coupling limit* corresponds to the situation where $\tau_\Sigma$ fixed and $\tau_{\mathcal{E}} \to 0$. It appears in the study of strongly driven systems such as lasers [HL73] and yields quantum dynamical semigroups under suitable conditions, see also [GFV⁺78, GK76]. The Hamiltonian is rescaled to

$$H = H_\Sigma \otimes \mathbb{1} + \lambda^{-1} Q \otimes \phi + \lambda^{-2} \mathbb{1} \otimes H_{\mathcal{E}}$$

with the effect that the decay time $\tau_{\mathcal{E}}$ of the correlation function (3.4.9) acquires a factor of $\lambda^2$. The rescaling of the interaction term produces a finite Fourier transform of the correlation function which is needed to see a nonzero effect. A rigorous mathematical treatment can be inferred from Davies' theory for the weak coupling limit as has been pointed out by Palmer [Pal77].

We refer to [AL07, BP02] and references therein for more details on various procedures (e.g. *low density limit* or *dilation techniques*[3]) which deduce a quantum dynamical semigroup from an underlying Hamiltonian dynamics.

## 3.5. Dephasing Lindbladians

### 3.5.1. General structure

In our applications we will particularly focus on the special class of *dephasing* Lindbladians. Their defining property is the assumption that all observables which are conserved by the

[3] This is not a limiting procedure, to be precise.

Hamiltonian $H$ are so by the Lindbladian $\mathcal{L}^*$. In particular $H$ itself is conserved; if one interprets the energy of the system in terms of $H$ and $V_i$ (caveat: cf. Remark 3.6) then one learns that, although the system $\Sigma$ is open, it does not exchange energy with its environment $\mathcal{E}$. Formally, this amounts to the following

**Definition 3.9.** *A Lindbladian $\mathcal{L}$ is called dephasing if*

$$\ker \mathcal{L}^* \supset \ker[H, \cdot]\,. \tag{3.5.1}$$

Despite the lack of dissipation dephasing Lindbladians induce decoherence. A (non-rigorous) scenario where they may arise is discussed in [PZ99]. The following lemma shows how the manifolds of stationary states of the two evolutions, generated by $H$ and $\mathcal{L}$ respectively, relate.

**Proposition 3.10.** *In connection with Equations (3.3.2, 3.3.3) we have:*

*(i)* $\ker \mathcal{L}^* \supset \ker([H,\cdot])$ *is equivalent to* $V_i = f_i(H)$ *for some bounded Borel functions* $f_i$.

*(ii)* $V_i = f_i(H)$ *implies* $\ker \mathcal{L} = \ker([H,\cdot])$.

*(iii) If the spectrum of $H$ is pure point, then the last implication is an equivalence. This applies in particular to the finite-dimensional case.*

Proof. To begin we write Equations (3.3.2, 3.3.3) as

$$\mathcal{L}\rho = -\mathrm{i}[H,\rho] + \frac{1}{2}\sum_{i\in I}\big(2V_i\rho V_i^* - \{\rho, V_i^*V_i\}\big)\,,$$

and hence

$$\mathcal{L}^*A = \mathrm{i}[H,A] + \frac{1}{2}\sum_{i\in I}\big(2V_i^*AV_i - \{A, V_i^*V_i\}\big)\,.$$

It is evident that $V_i = f_i(H)$ implies $\ker \mathcal{L}^* \supset \ker([H,\cdot])$ and, through $[V_i^*, V_i] = 0$, also $\ker \mathcal{L} \supset \ker([H,\cdot])$. By an elaborate version of the spectral theorem and von Neumann's bicommutant theorem it holds that $\{f(H) \in \mathcal{L}(\mathcal{H}) | f \text{ a bounded Borel function}\} =: \{f(H)\} = \{f(H)\}''$ (cf. [Con90], Chapter IX, Theorems 6.4 and 8.10). Here a prime denotes the commutant.

The three claims then reduce to the following ones:

(i) $\ker \mathcal{L}^* \supset \ker([H,\cdot])$ implies $V_i \in \{f(H)\}''$.

(ii) $V_i = f_i(H)$ implies $\ker \mathcal{L} \subset \ker([H,\cdot])$.

(iii) If the spectrum of $H$ is pure point and if $\ker \mathcal{L} \supset \ker([H,\cdot])$, then $V_i \in \{f(H)\}''$.

The implications (i-iii) are based on the readily verified identity [Lin76]

$$\mathcal{L}^*(A^*A) - A^*\mathcal{L}^*(A) - \mathcal{L}^*(A^*)A = \sum_{i\in I}[A, V_i]^*[A, V_i]\,. \tag{3.5.2}$$

(i): Let $A \in \ker([H,\cdot]) = \{f(H)\}'$. Since that subspace of $\mathcal{L}(\mathcal{H})$ is closed under taking adjoints and products, the left hand side of Equation (3.5.2) vanishes by assumption, implying $V_i \in \{f(H)\}''$.

(ii): Under the assumption, $\mathcal{L}$ acts as $\mathcal{L}^*$ under the replacement $H \to -H$, $V_i \to V_i^*$. Since $\operatorname{tr}\mathcal{L}(\rho) = 0$ for $\rho \in \mathcal{J}_1(\mathcal{H})$, Equation (3.5.2) implies

$$-\operatorname{tr}\rho^*\mathcal{L}(\rho) - \operatorname{tr}\rho\mathcal{L}(\rho^*) = \sum_{i\in I}\operatorname{tr}[\rho, V_i^*]^*[\rho, V_i^*]\,.$$

Thus $\rho \in \ker \mathcal{L}$ implies $[\rho, V_i^*] = 0$ and, by $\mathcal{L}(\rho^*) = \mathcal{L}(\rho)^*$, also $[\rho, V_i] = 0$. We conclude $[H, \rho] = 0$.

(iii): By the first assumption we can pick a sequence of finite-dimensional projections $(P_n)_{n\in\mathbb{N}}$, which are sums of eigenprojections of $H$ or of subprojections thereof, such that $P_n \to \mathbb{1}$ strongly as $n \to \infty$. In particular $[H, P_n] = 0$.

If $A \in \mathcal{J}_1(\mathcal{H})$ then $\mathcal{L}^*(A) \in \mathcal{J}_1(\mathcal{H})$ and, we claim, $\operatorname{tr} \mathcal{L}^*(A) = 0$ by our second assumption. Indeed, it implies $\mathcal{L}(P_n) = 0$ and hence

$$\operatorname{tr} \mathcal{L}^*(A) = \lim_{n\to\infty} \operatorname{tr}(\mathcal{L}^*(A)P_n) = \lim_{n\to\infty} \operatorname{tr}(A\mathcal{L}(P_n)) = 0\,.$$

Let now $A \in \mathcal{J}_1(\mathcal{H}) \cap \{f(H)\}'$. Then $\mathcal{L}(A) = 0$ and $\operatorname{tr}(\mathcal{L}^*(A^*)A) = \operatorname{tr}(A^*\mathcal{L}(A)) = 0$. By taking the trace of Equation (3.5.2) we conclude $[A, V_i] = 0$. The conclusion extends to $A \in \{f(H)\}'$ since $P_nA \to A$ strongly as $n \to \infty$. This proves the claim. □

### 3.5.2. An example

Our main applications will concern the simplest (nontrivial) of all dephasing Lindbladians, namely those which describe 2-level systems (qubits). They can be viewed as a 4-parameter family: The Hamiltonian is determined by the 3-vector $b$

$$2H = b \cdot \sigma \qquad (b \in \mathbb{R}^3,\ \sigma = (\sigma_1, \sigma_2,\ \sigma_3)^\mathsf{T})\,,$$

where the $\sigma_i$ are the Pauli matrices. With the dephasing parameter $\gamma \geq 0$

$$\mathcal{L}\rho = -\mathrm{i}[H, \rho] + \frac{\gamma}{|b|^2}\big[[H, \rho], H\big]\,. \tag{3.5.3}$$

Recall that by $4H^2 = (b \cdot b)\mathbb{1}$ any function of $H$ is of the form $f(H) = \alpha H + \beta\mathbb{1}$. If $P_+$, $P_-$ denote the eigenprojections of $H = \frac{|b|}{2}(P_+ - P_-)$, (3.5.3) takes the form

$$\mathcal{L}\rho = -\mathrm{i}[H, \rho] - \gamma\,(P_-\rho P_+ + P_+\rho P_-)\,. \tag{3.5.4}$$

The canonical map from the set of normalized states to the Bloch ball,

$$\rho \mapsto n \in \mathbb{R}^3,\ |n| \leq 1 : \quad \rho = \frac{\mathbb{1} + n \cdot \sigma}{2}\,,$$

maps the evolution equation $\dot\rho = \mathcal{L}\rho$ to the Bloch equation [GKS76]

$$\begin{aligned}\dot n &= b \times n + \frac{\gamma}{|b|^2} b \times (b \times n)\\ &= b \times n - \gamma\left(n - (n \cdot \hat b)\hat b\right)\,,\end{aligned} \tag{3.5.5}$$

where $\hat b = b/|b|$ is the unit vector of $b$.

By Equation (3.5.4) dephasing Lindbladians can be interpreted as a model for a continuous energy measurement in the following sense: Imagine that the energy $H$ is measured with probability $\gamma\delta t$ after a short waiting time $\delta t$. In the process the state is changed from $\rho$ first to $\tilde\rho = e^{-iH\delta t}\rho e^{iH\delta t}$. If a measurement takes place, its outcome shall not be recorded which means that a state $\tilde\rho$ is replaced by the incoherent superposition $\sum_{i=\pm} P_i\tilde\rho P_i$. This explains the word *dephasing*.

The full measurement prescription then amounts to

$$\rho \mapsto (1-\gamma\delta t)\tilde{\rho} + \gamma\delta t \sum_{i=\pm} P_i\tilde{\rho}P_i = \rho - \mathrm{i}[H,\rho]\delta t + \gamma\Big(\sum_{i=\pm} P_i\rho P_i - \rho\Big)\delta t + O((\delta t)^2)\,. \tag{3.5.6}$$

In the limit $\delta t \to 0$ the resulting dynamics is generated by Equation (3.5.4). Hence the dephasing term in the Lindblad generator can be viewed as a continuous monitoring of the state of the system at rate $\gamma$.

A different interpretation of Equation (3.5.4) applies to nuclear magnetic resonance (NMR) where it models *transversal relaxation processes*; a terminology which is natural in view of Equation (3.5.5). The corresponding relaxation time $\gamma^{-1}$ is commonly denoted by $T_2$ and is usually smaller than the longitudinal relaxation time $T_1$. The latter arises if dissipative effects are taken into account as well [Lev08].

## 3.6. States, duality, and parallel transport

We conclude this chapter with a brief discussion of the concept of states in a physical system and we shall first adopt the fairly general setting of abstract $C^*$-algebras. We will then compare this with the more concrete algebras already encountered, such as $\mathcal{L}(\mathcal{H})$ and $\mathcal{J}_1(\mathcal{H})$. With this at hand we finally revisit the concept of parallel transport from Chapter 2 in order to prepare the ground for the applications in the next chapter.

### 3.6.1. States on $C^*$-algebras

Let $\mathcal{A}$, $\tilde{\mathcal{A}}$ be two unital $C^*$-algebras and consider linear maps $\Phi : \mathcal{A} \to \widetilde{\mathcal{A}}$ enjoying

(i) $\Phi$ is positive ($\Phi \geq 0$): $a \geq 0 \Rightarrow \Phi a \geq 0$ ;

(ii) $\Phi(\mathbb{1}) = \mathbb{1}$ (normalization).

The maps are automatically bounded and in fact satisfy $\|\Phi\| = 1$ ( [BR79], Corollary 3.2.6). For $\widetilde{\mathcal{A}} = \mathbb{C}$ one is considering linear functionals, denoted $\rho \in \mathcal{A}^*$, and (i, ii) define *states*, $\rho \in \mathcal{A}^*_{+,1}$ (The subscripts indicate that the functionals are positive and normalized). For $\widetilde{\mathcal{A}} = \mathcal{A}$, the dual maps $\Phi^* : \mathcal{A}^* \to \mathcal{A}^*$ satisfy the corresponding properties

(i) $\rho \geq 0 \Rightarrow \Phi^*\rho \geq 0$ ,

(ii) $(\Phi^*\rho)(\mathbb{1}) = \rho(\mathbb{1})$ .

We call them *state preserving* maps. By an application of the Hahn-Banach theorem,

$$\|\Phi^*\| = 1\,. \tag{3.6.1}$$

The maps $\Phi$ and $\Phi^*$ then refer to the Heisenberg and the Schrödinger picture (in the sense that $\Phi$ acts on observables and $\Phi^*$ acts on states).

In case $\mathcal{A}$ is not unital, we obtain $\hat{\mathcal{A}}$ by adjoining a unity ( [BR79], Definition 2.1.6). We consider maps defined on $\hat{\mathcal{A}}$ satisfying (i, ii), provided they are compatible with the adjunction.

More precisely, we consider linear functionals $\rho \in \hat{\mathcal{A}}^*$ (and in particular, *states*), provided they arise by canonical extension from $\rho \in \mathcal{A}$ ( [BR79], p. 52). Of a *state preserving* map it is then required to be so with respect to the amended sense of states.

Of particular interest in connection with parallel transport are those state preserving maps which are projections $\mathcal{P} : \mathcal{A}^* \to \mathcal{A}^*$ (for economy of notation we omit the star and write $\mathcal{P}_*$ for the predual, if need arises). Associated to them is the norm closed[4] convex set of states in their ranges,

$$\mathcal{S} := \mathcal{A}^*_{+,1} \cap \operatorname{ran} \mathcal{P} . \tag{3.6.2}$$

Such projections naturally arise through the mean ergodic theorem [HP57] as projections on stationary states of state preserving semigroups $\Phi^*_t$,

$$\mathcal{P} = \lim_{\gamma \searrow 0} \gamma \int_0^\infty dt \ \mathrm{e}^{-\gamma t} \Phi^*_t , \tag{3.6.3}$$

provided the limit exists in a certain sense. Exemplarily we demonstrate how this relates to Hypotheses (H1) and (H2') on p. 18. If $\Phi^*_t$ is strongly continuous with generator $\mathcal{L}$ then the following formula is a standard fact, cf. (2.2.2)

$$\int_0^\infty dt \ \mathrm{e}^{-\gamma t} \Phi^*_t(\rho) = -(\mathcal{L} - \gamma)^{-1} \rho \qquad \forall \rho \in \mathcal{A}^* .$$

For $\rho \in \ker \mathcal{L}$ we obtain

$$-\gamma(\mathcal{L} - \gamma)^{-1}\rho = \rho - (\mathcal{L} - \gamma)^{-1} \mathcal{L} \rho = \rho$$

whereas for $\rho \in \overline{\operatorname{ran} \mathcal{L}}$ it holds that

$$-\gamma(\mathcal{L} - \gamma)^{-1}\rho \to 0 \qquad (\gamma \searrow 0)$$

by Lemma 2.23. Together with (H2') we conclude that (3.6.3) converges strongly to the projection onto $\ker \mathcal{L}$ associated to the decomposition $\mathcal{A}^* = \ker \mathcal{L} \oplus \overline{\operatorname{ran} \mathcal{L}}$.

**Example 3.11.** *Let $\rho \in \mathcal{J}_1(\mathcal{H})$ satisfy $\rho \geq 0$ and $\operatorname{tr} \rho = 1$. Then $\operatorname{tr}(\rho \ \cdot)$ is a state[5] on $\mathcal{L}(\mathcal{H})$. An example of a state preserving projection $\mathcal{P}$ is given by its action on density matrices $\rho$,*

$$\mathcal{P}\rho = \sum_{i \in K} P_i \rho P_i , \tag{3.6.4}$$

*where $K = \{1, \dots, M\}$ resp. $K = \mathbb{N}$ is a countable index set and the $P_i$ are mutually orthogonal projections on $\mathcal{H}$ with $\sum_{i \in K} P_i = \mathbb{1}$ in strong sense. For finite $I$ the projection $\mathcal{P}$ is well-defined and so it is if $K = \mathbb{N}$: the infinite sum converges strongly for every $\rho$. Indeed, for arbitrary $y \in \mathcal{H}$ and $N \in \mathbb{N}$ we obtain by Pythagoras*

$$\left\| \sum_{i=1}^N P_i \rho P_i y \right\|^2 = \sum_{i=1}^N \| P_i \rho P_i y \|^2 \leq \|\rho\|^2 \cdot \left\| \sum_{i=1}^N P_i y \right\|^2 \leq \|\rho\|^2 \|y\|^2$$

*which implies that $\sum_{i=1}^N P_i \rho P_i y$ is a Cauchy sequence and hence convergent.*

[4] Since $\mathcal{P}$ is bounded.

[5] Of course the state is usually simply identified with $\rho$ itself.

*As required by the definition of state preserving maps, $\mathcal{P}$ arises from the dual of a positive normalized map on $\mathcal{L}(\mathcal{H})$; explicitly*

$$\mathcal{P}_* A = \sum_{i \in K} P_i A P_i$$

*which is well-defined for the same reasons as $\mathcal{P}$ is.*

For clarity we recall that $\mathcal{L}(\mathcal{H})^* \supsetneq \mathcal{J}_1(\mathcal{H})$ and hence $\mathcal{P}$ defined on density matrices in Example 3.11 does strictly speaking not yield the whole dual. This issue is discussed in the next subsection. Note that density matrices naturally induce linear functionals on $\mathcal{L}(\mathcal{H})$ in the sense that

$$\|\rho\|_{\mathcal{J}_1(\mathcal{H})} = \| \operatorname{tr}(\rho\ \cdot)\|_{\mathcal{L}(\mathcal{L}(\mathcal{H});\mathbb{C})} =: \| \operatorname{tr}(\rho\ \cdot)\| \,. \tag{3.6.5}$$

This follows form

$$\sup_{\|A\|_{\mathcal{L}(\mathcal{H})}=1} |\operatorname{tr}(\rho A)| \leq \|\rho\|_{\mathcal{J}_1(\mathcal{H})}$$

which can be improved to an equality by choosing $A = \mathbb{1}$.

### 3.6.2. Normal states and the operator algebras $\mathcal{L}(\mathcal{H})$, $\mathcal{J}_1(\mathcal{H})$, $\mathcal{K}(\mathcal{H})$

As we have seen a Lindbladian $\mathcal{L}$ acts on density matrices $\rho \in \mathcal{J}_1(\mathcal{H})$ if regarded in the Schrödinger picture while its dual $\mathcal{L}^*$ acts on $\mathcal{L}(\mathcal{H})$ which corresponds to the Heisenberg picture. In that sense the duality $\mathcal{J}_1(\mathcal{H})^* = \mathcal{L}(\mathcal{H})$ is seemingly converse to the general notion of states on a $C^*$-algebra.

One possible reconciliation is to restrict the algebra of observables to the compact operators $\mathcal{K}(\mathcal{H})$ for it holds that

$$\mathcal{K}(\mathcal{H})^* = \mathcal{J}_1(\mathcal{H})\,.$$

Since $\mathbb{1} \notin \mathcal{K}(\mathcal{H})$ if $\dim \mathcal{H} = \infty$, a unity has to be adjoined in that case in order to embed $\mathcal{K}(\mathcal{H})$ in a unital $C^*$-algebra.

Another option is to note that $\mathcal{L}(\mathcal{H})$ is in fact a $W^*$-algebra (von Neumann algebra) and hence carries the following refined notion of a state [BR79].

**Definition 3.12.** *A state $\rho$ on the $W^*$-algebra $\mathcal{L}(\mathcal{H})$ is called normal if and only if it is ultraweakly continuous.*

Thus normal states are induced by elements in the predual and therefore by $\mathcal{J}_1(\mathcal{H})^* = \mathcal{L}(\mathcal{H})$ they are precisely those which can be identified with density matrices. Note that the normal states are ultraweakly dense in the set of all states [Thi02].

### 3.6.3. Parallel transport on states

The fact that states enjoy more properties than mere vectors in a Banach space can be used to investigate the parallel transport as defined in Subsection 2.2.2 in more detail. The family of projections $P(s)$ is now in addition assumed to be state preserving and therefore denoted by $\mathcal{P}(s)$. The associated parallel transport and states are denoted by $\mathcal{T}(s,s')$ and $\mathcal{S}(s)$ (cf. Equations (2.2.8, 3.6.2)).

The following proposition shows that the action of $\mathcal{T}(s,s')$ on $\mathcal{S}(s)$ is that of a rigid motion. In the context of Example 3.11 this is illustrated in Figure 3.1.

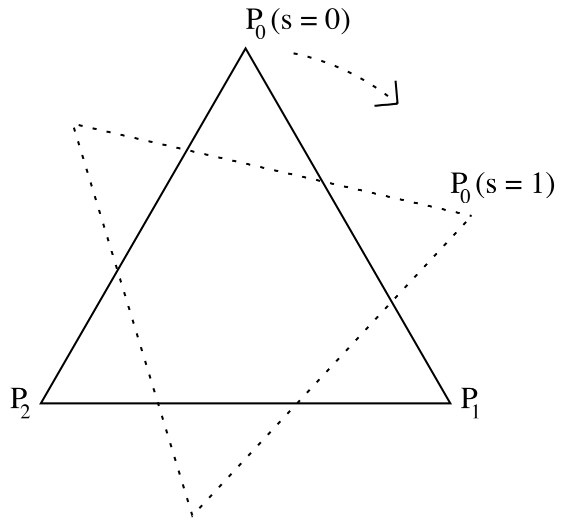


Figure 3.1: An example where the set of instantaneous stationary states, given by $\mathcal{P}\rho = \rho$, form a simplex, here a triangle. The extreme points are the simple spectral projections $P_i(s)$, $i = 1,2,3$. Parallel transport rotates the triangle at time $s = 0$ (triangle whose boundary is the full line) to the triangle at time $s = 1$ (triangle whose boundary is the dashed line) as a rigid body.

**Proposition 3.13.** *Let the $C^1$-family of projections $\mathcal{P}(s) : \mathcal{A}^* \to \mathcal{A}^*$, $(0 \le s \le 1)$ be state preserving. Then so is $\mathcal{T}(s,s')$. In particular, $\mathcal{T}(s,s')$ maps*

*(i) $\mathcal{S}(s')$ to $\mathcal{S}(s)$ isometrically;*

*(ii) (isolated) extreme points of $\mathcal{S}(s')$ to corresponding ones of $\mathcal{S}(s)$.*

*Moreover, if $\rho(s) \in \operatorname{ran}\mathcal{P}(s)$, depending continuously on $s$, is an isolated extreme point of $\mathcal{S}(s)$, then $\rho(s) = \mathcal{T}(s,s')\rho(s')$.*

Proof. The first claim follows from Equation (2.2.13). As a result $\mathcal{T}(s,s')\mathcal{P}(s')$ maps $\mathcal{S}(s') \to \mathcal{S}(s)$, with inverse $\mathcal{T}(s',s)\mathcal{P}(s)$. Next, (i) follows from Equation (3.6.1) for the two maps since for arbitrary $\rho \in \mathcal{S}(s')$

$$\|\mathcal{T}(s,s')\rho\| \le \|\rho\| = \|\mathcal{T}(s',s)\mathcal{T}(s,s')\rho\| \le \|\mathcal{T}(s,s')\rho\|.$$

Any convex decomposition of $\mathcal{T}(s,s')\rho(s')$, $(\rho(s') \in \mathcal{S}(s'))$ entails one of $\rho(s')$, which yields (ii) in the variant where the bracketed word is omitted. Since $\mathcal{T}(s,s')$ is a homeomorphism the other variant is also proved.

To obtain the last statement we note that $\mathcal{T}(s,s')\rho(s')$ is, for fixed $s$ and all $s'$, an isolated extreme point in $\mathcal{S}(s)$, just like $\rho(s)$. They agree, since they do for $s' = s$. □

**Example 3.14** (continuing Example 3.11). *With respect to the Hilbert-Schmidt inner product induced by the inclusion $\mathcal{J}_1(\mathcal{H}) \subset \mathcal{J}_2(\mathcal{H})$, the projection $\mathcal{P}$ is orthogonal and the transport $\mathcal{T}$ unitary: Indeed, its generator $[\dot{\mathcal{P}}(s), \mathcal{P}(s)]$ is anti-self-adjoint. In particular, the motion seen in Figure 3.1 is rigid with respect to the norms of both $\mathcal{J}_1(\mathcal{H})$, see Equation (3.6.5), and $\mathcal{J}_2(\mathcal{H})$. Explicitly, if $\rho(s) = \sum_{i\in K} \lambda_i P_i(s)$ then $\rho(s') = \sum_{i\in K} \lambda_i P_i(s')$ for the same $\lambda_i$, while the projections retain their distances in both norms.*

We conclude with a consideration about rank 1 projections, which is linked to Lemma 2.8. In the present setting its hypothesis is satisfied:

**Lemma 3.15.** *Consider state preserving projections $\mathcal{P}$ of rank 1. Then* $\operatorname{ran}\mathcal{P}_* = \operatorname{span}\{\mathbb{1}\}$ *and* $\ker\mathcal{P}$ *is independent of $\mathcal{P}$. In particular, if $\mathcal{P}(s)$ is a $C^1$-family of such projections, then $\mathcal{P}(s) = \mathcal{T}(s,s')\mathcal{P}(s')$ and $\rho(s) = \mathcal{T}(s,s')\rho(s')$, where $\rho(s)$ is the unique state in* $\operatorname{ran}\mathcal{P}(s)$.

Proof. $\mathcal{P}$ has a predual $\mathcal{P}_*$, which is also of rank 1: Since $\mathcal{P}_*(\mathbb{1}) = \mathbb{1}$ by the normalization condition its rank is at least one. If it were larger then $(\ker\mathcal{P}_*)^\perp$ would contain at least two linearly independent vectors as is seen from the decomposition $\mathcal{B} = \ker\mathcal{P}_* \oplus \operatorname{ran}\mathcal{P}_*$. This contradicts $(\ker\mathcal{P}_*)^\perp = (\operatorname{ran}(\mathbb{1} - \mathcal{P}_*))^\perp = \ker(\mathbb{1} - \mathcal{P}) = \operatorname{ran}\mathcal{P}$ and hence we have $\operatorname{ran}\mathcal{P}_* = \operatorname{span}\{\mathbb{1}\}$. Therefore $\ker\mathcal{P} = (\operatorname{ran}\mathcal{P}_*)^\perp$ is independent of $\mathcal{P}$. The remaining claims follow from Lemma 2.8 and Proposition 3.13. □

**Example 3.16.** *Let $\mathcal{A} = \mathcal{L}(\mathcal{H})$ and let $\rho_0 \in \mathcal{J}_1(\mathcal{H})$ be a normal state*[6]*. Consider the positive and normalized projection*

$$\begin{aligned} \mathcal{P}_* : \mathcal{A} &\to \mathcal{A} \\ A &\mapsto \operatorname{tr}(A\rho_0)\mathbb{1}. \end{aligned}$$

*Its state preserving dual acts on normal states by $\mathcal{P} : \rho \mapsto (\operatorname{tr}\rho)\rho_0$ with $\ker\mathcal{P} = \{\rho \mid \operatorname{tr}\rho = 0\}$. If $\rho_0 = \rho_0(s)$ is a $C^1$-family, then $\dot{\mathcal{P}}(s)\rho = (\operatorname{tr}\rho)\dot{\rho}_0(s)$ and the statements of the lemma are evident. Note however that, in contrast to the Projection (3.6.4), the actions of $\mathcal{P}$ and of $\mathcal{P}_*$ are different if considered on $\mathcal{J}_2(\mathcal{H})$. Hence $\mathcal{P}$ is not orthogonal there.*

[6]Alternatively, let $\mathcal{A} = \mathcal{K}(\mathcal{H})$ with adjoined unity and let $\rho_0$ be a state which is a canonical extension.

# Chapter 4

# Applications of Linear Adiabatic Theorems

## 4.1. Overview

With the background on quantum dynamical semigroups developed in the previous chapter we can now appreciate the significance of the adiabatic theorems of Chapter 2 when applied to closed and open quantum systems.

In the gapped case Theorems 2.16, 2.19 can be applied to time-dependent Hamiltonians $H(s)$ as well as Lindbladians $\mathcal{L}(s)$. We will explain that although both setups can be formulated as an equation of the form (2.1.1),

$$\varepsilon\dot{x}(s) = L(s)x(s)\,,$$

the physical interpretation is different. For short, the key to this difference is that when both systems are phrased in terms of Equation (2.1.1) the manifolds of instantaneous stationary states are not matching and this has interesting consequences for the magnitude of physical tunneling. We shall explain this feature in the Hamiltonian case and illustrate it also for general dephasing Lindbladians in some detail before specializing to two concrete applications.

The first is concerned with the Landau-Zener formula for the tunneling in a unitary adiabatic evolution in a generic situation of nearly crossing eigenvalues. It was found in 1932 by Landau [Lan32] and independently by Zener [Zen32], Majorana [Maj32], and Stückelberg [Stü32]. We shall describe the corresponding result for the non-unitary case associated with a dephasing Lindbladian.

The second application is concerned with adiabatic quantum computing. There one is given a Hamiltonian $H_1$ whose ground state is interpreted to be the solution of a computational problem. This ground state is aimed at by an adiabatic interpolation of $H_1$ with another Hamiltonian $H_0$ whose ground state is easy to prepare. This procedure naturally implies optimization problems: On the one hand one is interested in short computation times while on the other hand one needs to control the tunneling out of the ground state in order to make the computation reliable. The *time-scheduling problem* is concerned with the determination of optimal time parametrization of a given interpolating path between $H_0$ and $H_1$. We will address this question both in absence and in presence of dephasing and discuss some of its consequences.

We finally point out that the applications of Theorems 2.16, 2.19 are not restricted to quantum mechanics; this will be illustrated at the example of a driven stochastic system.

As for the adiabatic theorem without gap condition, Theorem 2.25, examples will be different in nature due to the absence of knowledge on the rate of convergence: in particular there is no formula for a next to leading order correction. However, as in the gapped case, Theorem 2.25 applies to closed *and* open quantum systems. We discuss this in sufficient detail in order to explain the appropriate notions of convergence.

## 4.2. Time-dependent Hamiltonians I

Let $H(s)$ be a $C^{N+2}$-family[1] of self-adjoint operators on a Hilbert space $\mathcal{H}$ and let $E_*(s)$ be an eigenvalue with degeneracy $n$ which is uniformly separated from the rest of the spectrum of $H(s)$. Technically,

$$\operatorname{dist}(\{E_*(s)\}, \sigma(H(s))\backslash\{E_*(s)\}) \geq g_0 > 0. \tag{4.2.1}$$

By Lemma 2.14 uniformity of the gap implies that the associated eigenprojection $P_*(s)$ is $C^{N+2}$ (in norm sense) and hence so is $E_*(s)$ by $nE_*(s) = \operatorname{tr}(P_*(s)H(s))$. It follows that the operator

$$L_0(s) := -\mathrm{i}\,(H(s) - E_*(s)) \tag{4.2.2}$$

satisfies the conditions of Theorem 2.16. Starting the evolution at $s = 0$ the solutions of $\varepsilon\dot{x}(s) = L_0(s)x(s)$ differ from those of the Schrödinger equation,

$$\mathrm{i}\varepsilon\dot{\psi}(s) = H(s)\psi(s)\,, \tag{4.2.3}$$

only by a dynamical phase factor $\psi(s) = \mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon}\int_0^s E_*(s')ds'}x(s)$.

### 4.2.1. Reversible tunneling

If $E_*(s)$ is simple then any associated normalized eigenfunction $\psi_*(s)$ spans the manifold of instantaneous stationary states, i.e. the kernel of $L_0(s)$. The tunneling $T(s)$ is defined as the leaking out from this manifold,

$$T(s) := 1 - |(\psi(s), \psi_*(s))|^2\,. \tag{4.2.4}$$

There is extensive literature ( [Nen93, HJ06], and references therein) which is concerned with estimates of the tunneling amplitude at all orders in $\varepsilon$, or beyond. A simple, yet still remarkable, version of these results can be seen to be an immediate consequence of Corollary 2.17.

**Theorem 4.1.** *Suppose that $H(s)$ is $C^\infty$ and constant near the endpoints $s = 0$ and $s = 1$. Suppose further that $E_*(s)$ is simple. Then $T(1) = O(\varepsilon^k)$, for any $k$, see Figure 2.1.*

We refer to this subpertubatively small tunneling as *reversible*. Interestingly, when Theorem 2.16 is applied to open quantum systems, described by a dephasing Lindbladian one reaches the opposite conclusion! Before coming to this point in Section 4.3 we comment on some caveats when going over to a formulation which uses density matrices and the von Neumann equation.

[1] Recall Definition 2.3.

### 4.2.2. Hilbert-Schmidt formulation

To avoid domain questions we assume $H$ to be bounded for the sake of the argument. An equivalent description of the above can be given on the level of density matrices $\rho \in \mathcal{J}_1(\mathcal{H})$ with $L_1(s)\rho := -\mathrm{i}[H(s), \rho]$ or, more elegantly, on Hilbert-Schmidt operators $k \in \mathcal{J}_2(\mathcal{H})$ with $L_2(s)k := L_1(s)k$, $k^*k = \rho$ and scalar product $\langle k_1, k_2 \rangle := \mathrm{tr}\, k_1^* k_2$. The dynamics is governed by

$$\varepsilon \dot{k}(s) = -\mathrm{i}[H(s), k(s)].$$

Clearly, $P_*(s) \in \ker L_3(s)$ but even more we have:

**Lemma 4.2.** *The section $s \mapsto P_*(s)$ is parallel with respect to the transport induced by the orthogonal decomposition $\mathcal{J}_2(\mathcal{H}) = \ker L_2(s) \oplus \overline{\mathrm{ran}\, L_2(s)}$.*

Proof. Omitting the time-dependence it suffices by (2.2.10) to show that

$$\dot{P}_* \perp \ker L_2.$$

For $k \in \ker L_2(s)$ and $Q_* := \mathbb{1} - P_*$ it holds that $HP_*kQ_* = P_*kQ_*H$ and hence

$$P_*kQ_*(H - E_*) = 0$$

which in turn implies $P_*kQ_* = Q_*kP_* = 0$. Finally, by $\dot{P}_* = P_*\dot{P}_*Q_* + Q_*\dot{P}_*P_*$,

$$\mathrm{tr}(k\dot{P}_*) = \mathrm{tr}\left((P_*kP_* + Q_*kQ_*)(P_*\dot{P}_*Q_* + Q_*\dot{P}_*P_*)\right) = 0$$

where we applied the cyclicity of the trace. □

**Remark 4.3.** *We stress that the gap assumption (4.2.1) was irrelevant in the proof. Only the fact that $P_*(s)$ is an eigenprojection was needed.*

With the Hilbert-Schmidt formulation one might suspect to get to following well known improvement of Theorem 4.1 ( [ASY87, ASY93, Nen93]) as an easy application of Theorem 2.16.

**Theorem 4.4.** *Suppose $H(s)$ is $C^\infty$ and constant near the endpoints $s = 0$ and $s = 1$. Suppose further that $P_{\Delta_s}(s)$ is the spectral projection for a uniformly isolated energy band $\Delta_s \subset \sigma(H(s))$; i.e. there exist continuous real valued functions $g_+(s) > g_-(s)$ such that $\Delta_s \subset [g_-(s), g_+(s)]$ and*

$$\mathrm{dist}([g_-(s), g_+(s)], \sigma(H(s)) \backslash \Delta_s) \geq g_0 > 0.$$

*Then for $\rho(0) = P_{\Delta_0}(0)$ it holds in norm sense that*

$$\rho(1) = P_{\Delta_1}(1) + O(\varepsilon^k), \qquad \textit{for any } k.$$

However in contrast to Theorem 4.1 it turns out that Theorem 2.16 is not an efficient means to tackle this problem.

*Reason 1.* If $\Delta_s$ is a proper energy band in the sense that it contains continuous spectrum then $P_{\Delta_s}(s) \notin \mathcal{J}_2(\mathcal{H})$. Moreover 0 cannot be an isolated eigenvalue of $L_2(s)$ due to

$$\sigma(L_2) = \{-\mathrm{i}(E - E') : E, E' \in \sigma(H)\}.$$

Thus by reformulating the problem in a Hilbert-Schmidt setting the gap condition is 'lost'; in the gapless case however, the approach is still feasible, cf. Section 4.7.

*Reason 2.* Even if $\Delta_s$ consist only of a finite number of discrete eigenvalues it not obvious that the second term in the formula for the $a_n$,

$$a_n(s) = \mathcal{T}(s,0)a_n(0) + \int_0^s \mathcal{T}(s,s')\dot{\mathcal{P}}(s')b_n(s')ds',$$

will vanish at the endpoints (in order to avoid confusion we use script characters). The kernel of $L_2$ is far from being one dimensional and in general $\dot{\mathcal{P}}b_n$ need not be 0, though $\dot{\mathcal{P}}b_1$ is. More importantly, $\mathcal{P}(s)$ is not even continuous if $\Delta_s$ contains crossing eigenvalues.

It turns out that if one is only interested in the Hamiltonian case a different iterative procedure [Nen93] is more efficient: Under the assumption that $k(0) = P_*(0)$ it then holds that $k(s)^2 = k(s)$ which implies the additional relation

$$a_n + b_n = \sum_{i=0}^{n} (a_i a_{n-i} + a_i b_{n-i} + b_i a_{n-i} + b_i b_{n-i}) \qquad (n \leq N) \tag{4.2.5}$$

for the ansatz (2.3.6). It is then possible to solve for the $a_n$ without appealing to Duhamel's formula and so expressions which are local in time are obtained. For details and estimates on the remainder we refer to [Nen93]. We stress however that Equation (4.2.5) is a special feature of the Hamiltonian structure of the problem.

## 4.3. Time-dependent Lindbladians I

We now consider

$$\varepsilon\dot{\rho}(s) = \mathcal{L}(s)\rho(s)\,, \tag{4.3.1}$$

where $\mathcal{L}(s)$ is a family of Lindbladians depending smoothly on $s$. Davies and Spohn [DS78] derived similar models from Hamiltonian dynamics by considering a joint limit of adiabatic driving and weak coupling of a system interacting with its environment. However we will simply take Equation (4.3.1) as the definition of our model.[2] In addition we will consider only finite dimensional Hilbert spaces $\mathcal{H}$ unless otherwise stated; in particular $\mathcal{J}_1(\mathcal{H}) \cong \mathcal{K}(\mathcal{H}) \cong \mathcal{L}(\mathcal{H})$.

### 4.3.1. Tunneling in the generic case

Generically $\ker \mathcal{L}(s)$ is one-dimensional and hence so is $\ker \mathcal{L}^*(s) = \mathrm{span}\{\mathbb{1}\}$. The state in $\ker \mathcal{L}(s)$ is denoted by $\rho_*(s)$. The tunneling in Equation (4.2.4) is generalized to $T = 1 - F^2$, where the fidelity is

$$F(s) := \mathrm{tr}\left((\rho_*(s)^{1/2}\rho(s)\rho_*(s)^{1/2})^{1/2}\right) = \|\rho_*(s)^{1/2}\rho(s)^{1/2}\|_{J_1(\mathcal{H})}\,. \tag{4.3.2}$$

As an immediate consequence of Corollaries 2.17, 2.18 and Lemma 3.15 we obtain

**Theorem 4.5.** *Let $\mathcal{L}(s)$ be as above and assume in addition that it is constant near the endpoints $s = 0$ and $s = 1$. Then*

$$\rho(1) = \rho_*(1) + O(\varepsilon^k) \qquad \textit{(for any } k\textit{)}$$

*and in particular, $T(1) = O(\varepsilon^k)$ for any $k$.*

[2] This is not an unusual procedure in mathematical physics. As a prominent example we mention that the validity of the Boltzmann equation is only established rigorously for very small times [Lan75,Lan76] even though it is successfully applied to describe also large time-behavior in many situations.

### 4.3.2. Adiabatic expansion for dephasing Lindbladians

The situation changes drastically if dephasing Lindbladians are considered. For simplicity we consider a smooth family of Hamiltonians $H = H(s)$ with simple eigenvalues $E_0, \dots, E_{d-1}$ and corresponding normalized eigenvectors $\psi_i$:

$$H = \sum_i E_i P_i \,, \qquad P_i = |\psi_i\rangle\langle\psi_i| \,,$$

$\dim \mathcal{H} = d$. The operators $E_{ij} := |\psi_i\rangle\langle\psi_j|$ form a basis of $\mathcal{L}(\mathcal{H})$ which is orthonormal once that space is endowed with the Hilbert-Schmidt inner product. A straightforward computation using Proposition 3.10 shows that the $E_{ij}$ are eigenvectors of $\mathcal{L}$ and the eigenvalues in $\mathcal{L}E_{ij} = \lambda_{ij} E_{ij}$ satisfy

(i) $\lambda_{ij} = \overline{\lambda}_{ji}$ since $\mathcal{L}$ is a $*$-map,

(ii) $\Re\lambda_{ij} \le 0$ since $\mathcal{L}$ generates a contraction,

(iii) $\lambda_{ij} = 0$ if and only if $i = j$ since the eigenvalues are simple.

It follows that $\ker \mathcal{L}$ is spanned by $E_{ii} = P_i$ and $\operatorname{ran} \mathcal{L}$ by $E_{ij}$ $(i \neq j)$ with the corresponding projections (cf. (3.6.4))

$$\mathcal{P}\rho = \sum_i P_i \rho P_i \,, \qquad \mathcal{Q}\rho = \sum_{i \neq j} P_i \rho P_j \,.$$

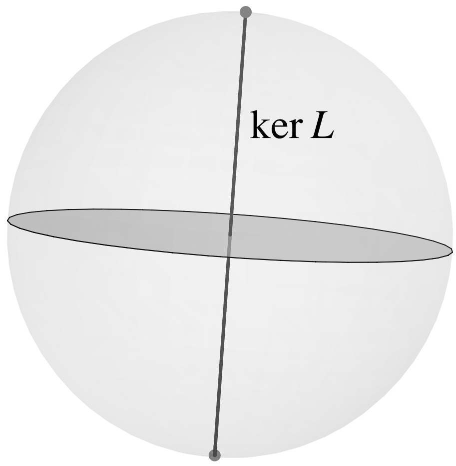


Figure 4.1: The states of a qubit (2-level system) can be represented as the three dimensional ball, the convex hull of the Bloch sphere. For a dephasing Lindbladian, the set of stationary states is the indicated axis whose extreme points (dots) are spectral projections for the Hamiltonian $H$.

**Theorem 4.6.** *The equation*

$$\varepsilon \dot\rho(s) = \mathcal{L}(s)\rho(s)$$

*admits solutions of the form*

$$\rho(s) = P_0(s) + \varepsilon \sum_{j\neq 0} \left( \frac{P_j \dot{P}_0}{\lambda_{j0}} + \frac{\dot{P}_0 P_j}{\lambda_{0j}} \right) - \varepsilon \sum_{j\neq 0} (P_0(s) - P_j(s)) \int_0^s \alpha_j(s')ds' + O(\varepsilon^2) \qquad (4.3.3)$$

*with*

$$\alpha_j(s) = \mathrm{tr}(P_0(s)\dot{P}_j(s)^2 P_0(s)) \cdot \frac{(-2\Re\lambda_{0j}(s))}{|\lambda_{0j}(s)|^2} \geq 0 \,.$$

*More generally, the expansion applies to any solution for which it does at $s = 0$, e.g. for the one with initial condition $\rho(0) = P_0(0)$, if $\dot{P}_0(0) = 0$.*

The expansion (4.3.3) is just $\rho(s) = a_0(s) + \varepsilon(b_1(s) + a_1(s)) + O(\varepsilon^2)$, in this order, with coefficients given in (2.3.10-2.3.12). Like in the Hamiltonian case, $b_1(s) \in \mathrm{ran}\, \mathcal{Q}(s)$ describes the shift of the slow manifold relative to the manifold of instantaneous stationary states which is *reversible* in the sense of Corollary 2.17. Unlike there, $a_1(s) \in \mathrm{ran}\, \mathcal{P}(s)$ now describes *irreversible* tunneling by means of a loss and a gain term involving $P_0(s)$ and $P_j(s)$, $(j \neq 0)$ respectively. Note also that $\alpha_j(s)$ vanishes in the Hamiltonian case in agreement with Theorem 4.4.

Proof. Clearly,

$$\begin{aligned} \dot{\mathcal{P}}\rho &= \sum_i (\dot{P}_i \rho P_i + P_i \rho \dot{P}_i) \,, \\ \mathcal{L}^{-1} E_{ij} &= \lambda_{ij}^{-1} E_{ij} \,, \qquad (i \neq j) \,. \end{aligned} \qquad (4.3.4)$$

We note that

$$\mathcal{T}(s, s')P_k(s') = P_k(s) \,,$$

which follows directly from Lemma 4.2 since the projection $\mathcal{P}$ here is a simple example for the one considered there.

Alternatively, we can argue that the left hand side satisfies the differential equation (2.2.8), viz.

$$\begin{aligned} \frac{d}{ds}\rho(s) &= \dot{\mathcal{P}}(s)\rho(s) \,, \\ \rho(s') &= P_k(s') \,, \end{aligned}$$

and so does the right hand side, since

$$\dot{\mathcal{P}} P_k = \sum_i \dot{P}_i P_k P_i + P_i P_k \dot{P}_i = \dot{P}_k P_k + P_k \dot{P}_k = \dot{P}_k \,.$$

The claim now follows from (2.3.10-2.3.12) with $a_0(0) = P_0(0)$. Indeed, the middle term of (4.3.3) follows from (2.3.11) and (4.3.4):

$$\begin{aligned} \mathcal{L}^{-1}\dot{\mathcal{P}} P_0 = \mathcal{L}^{-1}\dot{P}_0 &= \mathcal{L}^{-1} \sum_{j\neq 0} P_j \dot{P}_0 P_0 + P_0 \dot{P}_0 P_j \\ &= \sum_{j\neq 0} \lambda_{j0}^{-1} P_j \dot{P}_0 P_0 + \lambda_{0j}^{-1} P_0 \dot{P}_0 P_j = \sum_{j\neq 0} \lambda_{j0}^{-1} P_j \dot{P}_0 + \lambda_{0j}^{-1} \dot{P}_0 P_j \,. \end{aligned} \qquad (4.3.5)$$

For the last term of (4.3.3) we compute with (4.3.5)

$$\begin{aligned}\dot{\mathcal{P}}\mathcal{L}^{-1}\dot{\mathcal{P}}P_0 &= \sum_{j\neq 0}\dot{\mathcal{P}}(\lambda_{j0}^{-1}P_j\dot{P}_0P_0 + \lambda_{0j}^{-1}P_0\dot{P}_0P_j)\\ &= \sum_{j\neq 0}(\lambda_{j0}^{-1}+\lambda_{0j}^{-1})(P_0\dot{P}_j^2P_0 - P_j\dot{P}_0^2P_j)\\ &= \sum_{j\neq 0}\alpha_j(P_j - P_0)\,,\end{aligned}$$

(with termwise equality) where we have used $\dot{P}_iP_k = -P_i\dot{P}_k$ and $\mathrm{tr}(P_j\dot{P}_0^2P_j) = \mathrm{tr}(P_0\dot{P}_j^2P_0)$. Together with (2.3.12) the expansion follows. The generalization follows because of the contraction property of the propagator, Equation (2.2.4). □

If $\dot{P}_0(0)$ is arbitrary we have the following result about tunneling (cf. Equation (4.3.2)):

**Corollary 4.7.** *The solution of $\varepsilon\dot{\rho}(s) = \mathcal{L}(s)\rho(s)$ with the initial condition $\rho(0) = P_0(0)$ has, to leading order in the adiabaticity, a non-negative tunneling*

$$T(s) = \varepsilon\sum_{j\neq 0}\int_0^s ds'\ \alpha_j(s') + O(\varepsilon^2)\,, \qquad \alpha_j(s') \geq 0\ :$$

*Tunneling is irreversible and $O(\varepsilon)$.*

This result should be contrasted with the subperturbatively small tunneling in the unitary case, Theorem 4.1.

Proof. For the given initial data we denote the corresponding trajectory in the slow manifold, Equation 4.3.3, by $\rho_M(s)$. It holds that

$$\mathcal{P}(0)\left(\rho_M(0) - \rho(0)\right) = \varepsilon\mathcal{P}(0)\sum_{j\neq 0}(\lambda_{j0}^{-1}P_j\dot{P}_0 + \lambda_{0j}^{-1}\dot{P}_0P_j) + O(\varepsilon^2) = O(\varepsilon^2)$$

and by Theorem 2.19 for small $\varepsilon$

$$\begin{aligned}\|\mathcal{P}(s)(\rho_M(s)-\rho(s))\| \leq &\|\mathcal{P}(s)(\rho_M(s)-\rho(s)) - \mathcal{T}(s,0)\mathcal{P}(0)(\rho_M(0)-\rho(0))\|\\ &+ \|\mathcal{T}(s,0)\mathcal{P}(0)(\rho_M(0)-\rho(0))\| \leq C\varepsilon^2\,,\end{aligned}$$

hence

$$F(s)^2 = \mathrm{tr}(P_0\rho(s)P_0) = 1 - \sum_{j\neq 0}\int_0^s ds'\alpha_j(s') + O(\varepsilon^2)\,.$$

□

**Example 4.8** (Continuing the example in Subsection 3.5.2 in a time-dependent setting). *The adiabatic expansion, Equation (4.3.3), takes a rather simple form for the Bloch equations (3.5.5). With $\dot{n}$ replaced by $\varepsilon\dot{n}$ in (3.5.5), the assumption $\dot{b}(0) = 0$ and initial condition $n(0) = -\hat{b}(0)$ ($\hat{b} = b/|b|$) one finds*

$$n(s) = -\hat{b}(s) + \varepsilon\left(\frac{\gamma(s)\dot{\hat{b}}(s) + b(s)\times\dot{\hat{b}}(s)}{|b(s)|^2+\gamma^2(s)} + \hat{b}(s)\int_0^s\alpha(t)dt\right) + O(\varepsilon^2)\,. \tag{4.3.6}$$

*where*

$$\alpha(t) = \frac{\gamma(t)|\dot{\hat{b}}(t)|^2}{|b(t)|^2 + \gamma^2(t)} \, .$$

*The terms in brackets, in the order as they appear, have the following interpretation: The first term, being proportional to $\gamma\dot{\hat{b}}(s)$, describes friction that causes lagging behind the driver $\hat{b}$. The second term describes "geometric magnetism", a term introduced in [BR93]. The third term is tunneling and describes a motion along the axis towards the center, see Figure 4.1. While the first two terms describe an instantaneous response in the plane perpendicular to the stationary axis $\hat{b}(s)$, the last term describes irreversible motion inside the Bloch sphere along the axis, Figure 4.1.*

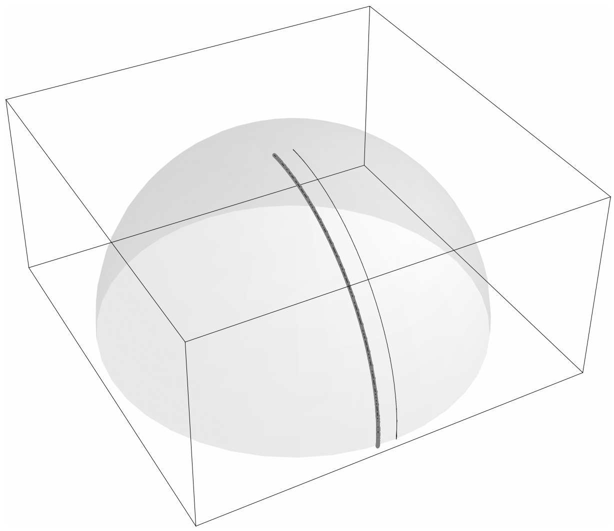

Figure 4.2: The figure illustrates the adiabatic expansion in Example 4.8 in the case of no dephasing $\gamma = 0$. It shows the northern hemisphere of the Bloch sphere. The orbit of $H(s)$ is represented by the (thin) meridian starting at the north pole. The parallel (thick) curve shows the shift due to the term describing "geometric magnetism".

Proof. Write (4.3.3) in the form

$$\rho(s) = P_-(s) + \frac{\varepsilon}{|\lambda|^2}\big(\Re\lambda\{P_+, \dot{P}_-\} + \mathrm{i}\,\Im\lambda[P_+, \dot{P}_-]\big) - \varepsilon(P_-(s) - P_+(s)) \int_0^s \alpha(s')ds' + O(\varepsilon^2)$$

and use $\lambda = \mathrm{i}|b| - \gamma$ as well as the (anti-)commutation relations

$$\{P_+, \dot{P}_-\} = -\frac{1}{2}\dot{\hat{b}} \cdot \sigma \, , \qquad [P_+, \dot{P}_-] = -\frac{\mathrm{i}}{2}(\hat{b} \times \dot{\hat{b}}) \cdot \sigma \, , \qquad (\dot{P}_+)^2 = \frac{|\dot{\hat{b}}|^2}{4}$$

to get the first order correction terms exactly in the same order as they appear in (4.3.6). □

Solutions of the Bloch equations are illustrated in Figure 4.5.

## 4.4. An analogue of the Landau-Zener formula

Zener and independently Landau [Lan32, Zen32] modeled a generic situation of an avoided crossing of eigenvalues as it appears in the transition of a polar and homopolar state of a molecule treated in the time-dependent Born-Oppenheimer approximation. The transition region is so small that the Hamiltonian may be assumed to be linear in time. More precisely, by an appropriate choice of basis and of the zero of energy the relevant dynamics is governed by the Landau-Zener Hamiltonian

$$H_{LZ}(s, g_0) = \frac{1}{2}\begin{pmatrix} s & g_0 \\ g_0 & -s \end{pmatrix} = \frac{1}{2}\begin{pmatrix} g_0 \\ 0 \\ s \end{pmatrix} \cdot \sigma\,, \qquad (s = \varepsilon t)$$

where $g_0$ is the minimal gap and $\sigma = (\sigma_1, \sigma_2, \sigma_3)^\intercal$, where the $\sigma_i$ denote the Pauli matrices. The tunneling probability $T$ is the probability of a state, which originates asymptotically on

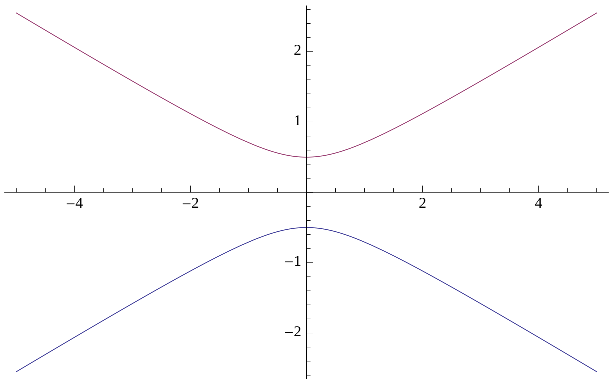


Figure 4.3: The avoided crossing of the two eigenvalue branches $E_\pm(s)$ for $g_0 = 1$.

one eigenvalue branch, to end up in the other at late times: Let $P_\pm(s)$ be the eigenprojections corresponding to the eigenvalues $E_\pm(s) = \pm\frac{1}{2}\sqrt{g_0^2 + s^2}$ and $\rho(s)$ the solution of

$$\varepsilon\dot{\rho} = -\mathrm{i}[H_{LZ}, \rho] \tag{4.4.1}$$

with

$$\lim_{s\to-\infty} \rho(s) = \lim_{s\to-\infty} P_-(s)\,.$$

Then

$$T := \lim_{s\to\infty} \mathrm{tr}(\rho(s)P_+(s))\,,$$

cf. Equation (4.2.4). Landau and Zener found the following formula:

$$T = e^{-\pi g_0^2/2\varepsilon}\,. \tag{4.4.2}$$

**Remark 4.9.** *Landau, who used semiclassical methods did not actually attempt to calculate the multiplicative overall factor in front of the exponential in Equation (4.4.2). Fortunately, this factor happens to be unity. Zener solved the differential equation in terms of Weber functions and derived Equation (4.4.2) exactly. He was aware of Landau's solution but for some reason, incorrectly, believed that Landau missed a factor of $2\pi$ in the exponent.*

### 4.4.1. The Landau-Zener formula with dephasing

Formula (4.4.2) holds for arbitrary $\varepsilon$ and shows that for fast driving a transition takes place with high probability. However we are particularly interested in the regime of small $\varepsilon$ in order to compare it with the tunneling results obtained for dephasing Lindbladians. The situation then changes radically: The exponentially small tunneling in Equation (4.4.2) is exchanged for an irreversible one. More precisely, we have

**Theorem 4.10.** *Suppose $T$ is defined as above with the single exception that Equation (4.4.1) is exchanged for a dephasing Lindblad evolution,*

$$\varepsilon\dot{\rho} = -\mathrm{i}[H_{LZ}, \rho] - \gamma\,(P_-\rho P_+ + P_+\rho P_-) = \mathcal{L}\rho\,,$$

*with time-independent $\gamma$. Then for $\varepsilon \to 0$*

$$T = \frac{\varepsilon}{2g_0^2} Q\left(\frac{\gamma}{g_0}\right) + O(\varepsilon^2)\,, \tag{4.4.3}$$

*where $Q$ is the function (shown in Figure 4.4.1):*

$$Q(x) = \frac{\pi}{2}\frac{x(2+\sqrt{1+x^2})}{\sqrt{1+x^2}(\sqrt{1+x^2}+1)^2}. \tag{4.4.4}$$

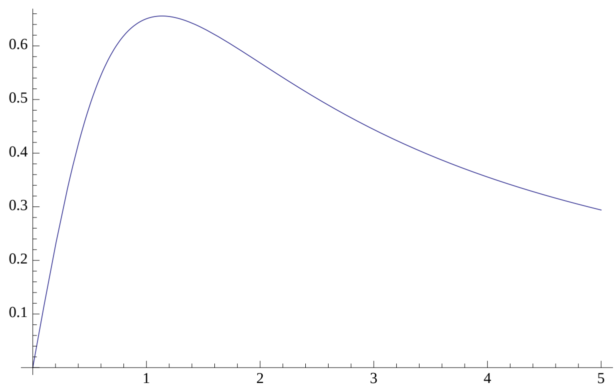


Figure 4.4: The function $Q(x)$. The argument is the ratio of dephasing rate to the minimal gap. The function has a maximum at $x = 1.14$.

Proof. Letting $s_0$ and $s_1$ be the initial and end times instead of $s = 0, 1$ the theorem is formally a direct application of Corollary 4.7 and Example 4.8 with

$$b = \begin{pmatrix} g_0 \\ 0 \\ s \end{pmatrix} \qquad \text{and} \qquad \rho(s_0) = P_-(0).$$

Indeed, if we define $g := E_+ - E_-$ and $x := \frac{\gamma}{g_0}$ we obtain $|\dot{\hat{b}}|^2 = \frac{g_0^2}{g^4}$ and

$$\begin{aligned} T_{[s_0,s_1]} &:= \operatorname{tr}(\rho(s_1), P_+(s_1)) = \operatorname{tr}\left(\frac{\mathbb{1} + n(s_1)\cdot\sigma}{2} P_+(s_1)\right) + O(\varepsilon^2) \\ &= \frac{1}{2}(1 + n(s_1)\cdot \hat{b}(s_1)) + O(\varepsilon^2) \\ &= \frac{\varepsilon}{2}\int_{s_0}^{s_1} \frac{\gamma|\dot{\hat{b}}(s)|^2}{|b(s)|^2+\gamma^2} + O(\varepsilon^2) \\ &= \frac{\varepsilon}{2}\int_{s_0}^{s_1} \frac{\gamma g_0^2}{g(s)^6 + \gamma^2 g(s)^4} ds + O(\varepsilon^2) \\ &= \frac{\varepsilon}{2g_0^2} x \int_{s_0/g_0}^{s_1/g_0} (1+u^2)^{-2}(1+x^2+u^2)^{-1} du + O(\varepsilon^2)\,. \end{aligned} \tag{4.4.5}$$

The last integral can be calculated explicitly if its boundaries extend to $\pm\infty$ and this will explain expression (4.4.4).

However it remains to justify that the error of order $\varepsilon^2$ is uniform in $s_0$, $s_1$ and this can be seen as follows: Clearly $P_+(s)$ is an approximate adiabatic invariant in the sense of Proposition 2.21 and it is readily checked that the adjoint acts like $\mathcal{L}^* A = \mathrm{i}[H, A] - \gamma(P_- A P_+ + P_+ A P_-)$ and so

$$X = \mathcal{L}^{*-1}\dot{P}_+ = -\mathrm{i}\sum_{k\neq j} \frac{P_k \dot{P}_+ P_j}{E_k - E_j + \mathrm{i}\gamma}. \tag{4.4.6}$$

Integrating Equation (2.3.18) by parts yields

$$\operatorname{tr}(\rho P_+)|_{s_0}^{s_1} = \varepsilon \operatorname{tr}(\rho X)|_{s_0}^{s_1} - \varepsilon \int_{s_0}^{s_1} \operatorname{tr} \rho \dot{X} ds.$$

Note that $X(s) = O(s^{-3})$, $\dot{X}(s) = O(s^{-4})$ as $s \to \pm\infty$ (this follows for instance by looking at the Riesz formulae for $P_\pm$). Theorem 4.10 is then an immediate consequence of the claim

$$\rho(s) - P_-(s) = O(\varepsilon) \qquad \text{uniformly in } s_0,\ s,$$

for which we argue as follows: Note that

$$\hat{X} = \mathcal{L}^{-1}\dot{P}_- = \mathrm{i}\sum_{k\neq j} \frac{P_k \dot{P}_- P_j}{E_k - E_j - \mathrm{i}\gamma}$$

yields by Equation (2.3.9) in Theorem (2.16) for $N = 1$

$$\rho(s) - P_-(s) = \varepsilon \mathcal{U}_\varepsilon(s,s')\hat{X}(s')|_{s'=s_0}^{s'=s} - \varepsilon \int_{s_0}^{s} \mathcal{U}_\varepsilon(s,s')\dot{\hat{X}}(s') ds'.$$

Since $\mathcal{U}_\varepsilon(s,s')$ is a contraction the uniformity follows from the decay of $\hat{X}$, $\dot{\hat{X}}$. □

### 4.4.2. Discussion

*Units.* We chose units where $\hbar = 1$ and $s$ has the dimension of an energy: $[s] = [g_0] = [\gamma]$. Hence $[\varepsilon] = [st^{-1}] = [g_0^2]$. This yields two independent dimensionless parameters and it is therefore not obvious what the correct dimensionless expression corresponding to $O(\varepsilon^2)$ is. We read off from Equations (4.4.3, 4.4.4) that by $Q(x) \sim \frac{x}{1+x^2}$ for small and large $x$ we can interpret $O(\varepsilon)$ as $O(\frac{\varepsilon}{\gamma^2+g_0^2}\frac{\gamma}{g_0})$. In general, the adiabatic limit means that $\sqrt{\varepsilon}$ is the smallest energy scale in the problem: $\varepsilon \ll \gamma^2$, $\varepsilon \ll g_0^2$.

*Weak dephasing.* If dephasing is weak, $\gamma \ll g_0$, Equation (4.4.3) reduces to

$$T = \frac{3\pi}{16} \cdot \frac{\varepsilon\gamma}{g_0^3} + O\left(\frac{\gamma^3}{g_0^3}\right)\frac{\varepsilon}{g_0^2} + O(\varepsilon^2).$$

The leading order has the same form as one of the tunneling terms found by Shimshoni and Stern [SS93] in a (different) model where a two-level system is dephased by noise. The method they use cannot give the overall constant $3\pi/16$ [Ber90], nor does it allow investigating the full range of $\gamma/g_0$.

*Strong dephasing.* When $\gamma \gg g_0$, Equation (4.4.3) reduces to

$$T = \frac{\pi\varepsilon}{4g_0\gamma} + O\left(\frac{g_0^3}{\gamma^3}\right)\frac{\varepsilon}{g_0^2} + O(\varepsilon^2). \tag{4.4.7}$$

This may be understood as a manifestation of the quantum Zeno effect [MS77] by the following interpretation: In Subsection 3.5.2 we argued how a dephasing Lindbladian can be interpreted to model a continuous energy measurement of a 2-level system: coherent superpositions $\rho$ of $P_\pm$, which are reflected in $P_\pm\rho P_\mp$, get destroyed in the sense that the evolution drives them towards incoherent superpositions at a rate $\gamma$. Transitions between the states $P_\pm$, which the changing Hamiltonian term potentially induces, are suppressed at high measurement rates as stated in Equation (4.4.7) and in line with the Zeno effect.

## 4.5. Optimal schedule in presence of dephasing

Quantum computation holds a promise to solve some of the most challenging problems in computational science: e.g. integer factorization [NC00]. The adiabatic model of quantum computation introduced by Farhi et al. [FGGS02] is equivalent [AvDK+07, MLM07] to the standard circuit model of a quantum computer [NC00] while having a built in protection from decoherence associated with the exchange of energy with the environment. The simplicity and physical character of the model led to a resurgence of interest in adiabatic control of both isolated [JRS07, AR06] and open quantum systems [SL05] and gave rise to new and interesting optimization problems in the context of adiabatic evolutions [RKH+09]: One is interested in minimizing the requisite time to reach a target state with given fidelity and given cap on the available energy. Equivalently, one is interested in minimizing the tunneling out of the ground state given a cap on the energy and the time duration $\tau$. For unitary evolution path optimization problems have been studied by several authors analyzing various *upper bounds* on the tunneling, see [JRS07] and references therein. A variational ansatz for the optimal path has been proposed by Rezakhani et al. [RKH+09].

As indicated in the overview to this chapter the *time-scheduling problem* is to determine the optimal time-parameterization of a *given* path of Hamiltonians. Theorem 4.11 below states that in absence of dephasing, there is no unique optimizer – there are plenty of them. On the other hand we will demonstrate that under reasonable conditions the presence of dephasing singles out a unique optimizer. This optimizer turns out to have a "local" characterization: It has *fixed tunneling rate* along the path. This means that monitoring the tunneling rate (or, equivalently, the purity of the state) allows one to adhere to an optimal time-schedule. In particular no a-priori knowledge about the governing dynamics is required.

As an application we derive relations between dephasing rates of Lindblad evolutions and Grover's bound [Gro97] on the time for searching an unstructured data base. We show that Markovian environments which are universal, i.e. environments which do not anticipate any properties of the system, must have dephasing rates that are bounded by the spectral gaps in the Hamiltonian for consistency with Grover's bound.

### 4.5.1. Rules of the game

Let $H_q$, $q \in [0,1]$ be a smooth path in the space of bounded Hamiltonians, e.g. a linear interpolation

$$H_q = (1-q)H_0 + qH_1\,, \quad (0 \le q \le 1)\,. \tag{4.5.1}$$

For the sake of simplicity we assume that the associated Hilbert space has a dimension $d < \infty$ and that $H_q$ is a smooth self-adjoint matrix-valued function of $q$ with ordered simple eigenvalues $E_{i,q}$, $0 \le i \le d-1$, so that

$$H_q = \sum_i E_{i,q} P_{i,q}\,,$$

where the $P_{i,q}$ are the corresponding spectral projections. Furthermore let $q = q(s)$ be a timetable ($q(0) = 0$, $q(1) = 1$), parametrized by the slow time $s = \varepsilon t = t/\tau$. The cost function is the tunneling, $T_q(1)$, at the end point defined by

$$T_q(s) = 1 - \mathrm{tr}\big(P_{0,q(s)}\rho_q(s)\big)\,,$$

cf. Equation (4.2.4). Here $\rho_q(s)$ is the state at time $s$ which has evolved from the initial condition $\rho_q(0) = P_{0,0}$ either under Hamiltonian evolution,

$$\varepsilon\dot\rho_q(s) = -\mathrm{i}[H_{q(s)}, \rho_q(s)]\,, \tag{4.5.2}$$

or under a dephasing Lindblad evolution with a single smooth dephasing rate $\gamma_q > 0$,

$$\varepsilon\dot\rho_q(s) = -\mathrm{i}[H_{q(s)}, \rho_q(s)] - \gamma_{q(s)} \sum_{i \ne j} P_{i,q(s)}\rho_q(s)P_{j,q(s)}\,. \tag{4.5.3}$$

The time-scheduling problem in both cases amounts to the following question:

*Which timetable $q = q(s)$ minimizes the tunneling $T_q(1)$?*

### 4.5.2. Time-scheduling problem in Hamiltonian dynamics

We show ill-posedness of the time-scheduling problem in the Hamiltonian case by demonstrating that paths with zero tunneling are ubiquitous for $\varepsilon \to 0$.

**Theorem 4.11.** *Let $q(s)$ be a $C^1$ timetable and let the dynamics be Hamiltonian, i.e. given by Equation (4.5.2), with*

$$2H_{q(s)} = g(q(s)) \cdot \sigma \,,$$

*where $g \in C^1([0,1];\mathbb{R}^3)$ satisfies the gap condition $|g(q)| \geq g_0 > 0$. Then for $\varepsilon \leq g_0/(2\pi)$ there is a timetable $q_\varepsilon(s)$ such that*

*(i)* $T_{q_\varepsilon}(1) = 0$,

*(ii)* $\|q - q_\varepsilon\|_\infty \leq \|\dot{q}\|_\infty \frac{2\pi\varepsilon}{g_0}$.

**Remark 4.12.** *The function $q_\varepsilon$ is not smooth. Convolution with a mollifier yields smooth timetables with arbitrarily small tunneling. They are however no longer close to $q$ with respect to $\|\cdot\|_\infty$.*

Proof. Since our argument will be geometric it is convenient to translate Equation (4.5.2) to the Bloch sphere with $\rho_q = \frac{1}{2}(\mathbb{1} + n \cdot \sigma)$, cf. Equation (3.5.5):

$$\varepsilon \dot{n}(s) = g(q(s)) \times n(s)\,. \tag{4.5.4}$$

To avoid unnecessary signs we may assume $n(0) = \hat{g}(0)$ even though this corresponds to the excited state. For $\varepsilon$ as in the hypothesis choose $1 \leq C_\varepsilon \leq 2$ such that the slow time interval $[0,1]$ can be partitioned into intervals of length $C_\varepsilon \frac{\pi\varepsilon}{g_0}$ and let $[s_-, s_+]$ be an arbitrary exemplar of those intervals.

Applying the intermediate value theorem to $s \mapsto \hat{g}(q(s)) \cdot (\hat{g}(q(s_+)) - \hat{g}(q(s_-)))$ yields the existence of a time $s_* \in [s_-, s_+]$ such that $g(q(s_*))$ is a point of intersection of the path $g(q(s))$ with the equatorial plane orthogonal to $\hat{g}(q(s_+)) - \hat{g}(q(s_-))$, see Figure 4.1. As a consequence of Equation (4.5.4) the time-independent Hamiltonian $H_{q(s_*)}$ rotates the vector $\hat{g}(q(s_-))$ to $\hat{g}(q(s_+))$ after a time duration $\delta s = \frac{\varepsilon\pi}{|g(s_*)|} \leq \frac{\varepsilon\pi}{g_0}$.

Since $s_- + \delta s \in [s_-, s_+]$ we may define on that interval

$$q_\varepsilon(s) := \begin{cases} q(s_*) & \text{if } s \in [s_-, s_- + \delta s] \\ q(s_+) & \text{if } s \in [s_- + \delta s, s_+] \end{cases}$$

from which it is obvious that the so constructed $H_{q_\varepsilon(s)}$ yields (i). The second point follows from the mean value theorem and $C_\varepsilon \leq 2$. □

### 4.5.3. Time-scheduling problem with dephasing

The dynamics shall now be given by Equation (4.5.3). Corollary 4.7 then takes the following form.

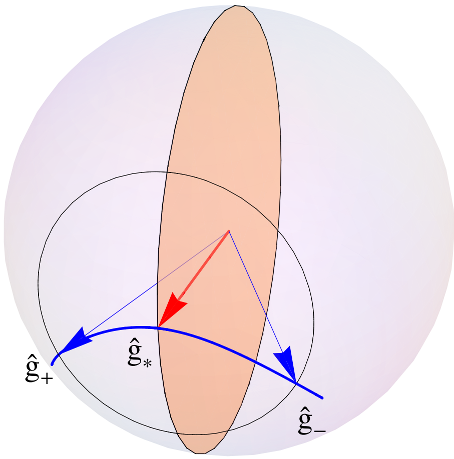


Figure 4.5: $\hat{g}_\pm := \hat{g}(q(s_\pm))$ are the images on the Bloch sphere of the end points of an interval of size $C_\varepsilon \frac{\pi\varepsilon}{g_0}$ of a given parameterization (blue). The intersection of the associated interpolating path with the equatorial plane (shaded) determines the time $s_*$ and thereby the axis of precession $\hat{g}_* := \hat{g}(q(s_*))$ (red) that maps the instantaneous state at the initial end point to the corresponding state at the final end point.

**Corollary 4.13.**

$$T_q(1) = 2\varepsilon \int_0^1 M(q)\dot{q}^2 ds + O(\varepsilon^2)\,,$$

*with the $q$-dependent* mass *term*

$$M(q) = \sum_{i\neq 0} \frac{\gamma_q \operatorname{tr}(P_{i,q} {P'_{0,q}}^2)}{(E_{0,q} - E_{i,q})^2 + \gamma_q^2} \geq 0\,.$$

$P'_{0,q}$ *denotes a derivative with respect to $q$. For a 2-level system, by Equation (4.4.5),*

$$M(q) = \frac{\gamma_q}{4} \frac{|\hat{g}'(q)|^2}{|g(q)|^2 + \gamma_q^2}\,.$$

The leading order functional

$$T_q^{(1)} := \lim_{\varepsilon\to 0} \frac{T_q(1)}{\varepsilon} = 2\int_0^1 M(q)\dot{q}^2 ds$$

has the standard form of variational Euler-Lagrange problems with fixed boundaries and therefore generically possesses a unique minimizer (in contrast to Theorem 4.11). More precisely, considering $T_q^{(1)}$ on the set of $C^1$-timetables, the following holds.

**Theorem 4.14.** *Suppose $M(q) > 0$ for all $0 \leq q \leq 1$. Then $T_q^{(1)}$ has a unique minimizing timetable $q_0$; in fact $q_0$ is smooth and the optimal tunneling to leading order is*

$$\varepsilon T_{q_0}^{(1)} = 2\varepsilon A \qquad \text{where } \sqrt{A} = \int_0^1 \sqrt{M(q)}dq\,. \tag{4.5.5}$$

**Remark 4.15.**

1) *We refer to the positivity assumption in Theorem 4.14 as generic since it corresponds to the fact that the path $\frac{1}{2}g(q)\cdot\sigma$ is nowhere tangent to a simple rescaling of the Hamiltonian (characterized by $\hat{g}'(q)=0$). For a 2-level system this amounts to the statement that the projection of the path on the Bloch sphere is a regular curve.*

2) *The constancy of the tunneling rate is due to the fact that the Lagrangian is s-independent and hence its "energy" $2M(q_0)\dot{q}_0^2$ is conserved. This gives a local algorithm for optimizing the parametrization: Adjust the speed $\dot{q}$ to keep the tunneling rate constant.*

Proof. For an arbitrary $C^1$-timetable $q$ Hölder's inequality yields

$$\int_0^1 \sqrt{2M(q)}dq = \int_0^1 \sqrt{2M(q)}\dot{q}ds \le \left(2\int_0^1 M(q)\dot{q}^2 ds\right)^{\frac{1}{2}} = (T_q^{(1)})^{\frac{1}{2}} \tag{4.5.6}$$

and equality holds if and only if $\sqrt{M(q)}\dot{q}$ is constant. Together with the boundary conditions $q(0)=0$, $q(1)=1$ the only candidate for a minimizer is the inverse of

$$s(q) = \frac{\int_0^q \sqrt{M(q')}dq'}{\int_0^1 \sqrt{M(q')}dq'} \tag{4.5.7}$$

which apparently exists and is $C^\infty$ by the inverse function theorem. □

### 4.5.4. Apparent speedup of Grover's algorithm and dephasing rates

From now on we assume that the dephasing rate $\gamma=\gamma_q$ is constant. Note that it is in principle arbitrary and not subject to any restrictions. However we shall show that if one makes some natural assumptions about the environment, it is constrained by the minimal gap of $H(s)$.

To see this we turn to quantum search with dephasing [ÅKS05, BKS09, CDF+02]. Grover has shown [Gro97] that $O(\sqrt{N})$ queries of an oracle suffice to search an unstructured data base of size $N \gg 1$. In the adiabatic formulation [JRS07, VDM01, RC02] of the problem one considers the $N=2^n$ dimensional Hilbert space $\mathcal{H}=(\mathbb{C}^2)^{\otimes n}$ of $n$ qubits. Let $|0\rangle$, $|1\rangle$ be an orthonormal basis on $\mathbb{C}^2$ and for $w\in\{0,1\}^n$ define $|w\rangle := |w_1\rangle\otimes\cdots\otimes|w_n\rangle$. Then initial and final Hamiltonian are given by

$$H_0 := \mathbb{1} - |\hat{0}\rangle\langle\hat{0}|, \qquad H_1 := \mathbb{1} - |u\rangle\langle u|,$$

where $|\hat{0}\rangle = 2^{-n/2}\sum_{w\in\{0,1\}^n}|w\rangle$ and $u\in\{0,1\}^n$ encodes the object in the data base we are searching for. The family of Hamiltonians is then given by linear interpolation as in Equation (4.5.1),

$$H_q = \mathbb{1} + (q-1)|\hat{0}\rangle\langle\hat{0}| - q|u\rangle\langle u|.$$

Clearly $\operatorname{span}\{|\hat{0}\rangle, |u\rangle\}$ and its orthogonal complement reduce $H_q$ for all $q$ and hence 1 is an $(N-2)$-fold degenerate eigenvalue. We replace $|u\rangle$, $|\hat{0}\rangle$ by the orthonormal basis

$$|\pm\rangle := \frac{1}{\sqrt{2\pm 2N^{-1/2}}}\left(|\hat{0}\rangle \pm |u\rangle\right)$$

with inverse relations

$$|\hat{0}\rangle = \frac{1}{\sqrt{2}}\left(\sqrt{1+N^{-1/2}}\,|+\rangle + \sqrt{1-N^{-1/2}}\,|-\rangle\right),$$
$$|u\rangle = \frac{1}{\sqrt{2}}\left(\sqrt{1+N^{-1/2}}\,|+\rangle - \sqrt{1-N^{-1/2}}\,|-\rangle\right).$$

Therefore

$$\begin{aligned} H_q = \mathbb{1} - &\frac{1+N^{-1/2}}{2}\,|+\rangle\langle+| - \frac{1-N^{-1/2}}{2}\,|-\rangle\langle-| \\ &+(q-\frac{1}{2})\sqrt{1-N^{-1}}\,(|-\rangle\langle+| + |+\rangle\langle-|)\,. \end{aligned}$$

It follows that on $\mathrm{span}\{|\hat{0}\rangle, |u\rangle\}$

$$2H_q = 2\cdot\mathbb{1} + \begin{pmatrix} (2q-1)\sqrt{1-N^{-1}} \\ 0 \\ -N^{-1/2} \end{pmatrix}\cdot\sigma \equiv 2\cdot\mathbb{1} + g(q)\cdot\sigma$$

which yields the gap function

$$|g(q)|^2 = 4\frac{(1-q)q}{N} + (1-2q)^2 \tag{4.5.8}$$

as well as the velocity on the Bloch sphere

$$|\hat{g}'(q)| = \sqrt{\frac{1}{N} - \frac{1}{N^2}}\,\frac{2}{|g(q)|^2}\,. \tag{4.5.9}$$

The constant $A$ which determines the optimal tunneling is given by

$$\begin{aligned} \sqrt{A} &= \sqrt{\frac{\gamma}{N}}\sqrt{1-\frac{1}{N}}\int_0^1 \frac{dq}{4\frac{(1-q)q}{N} + (1-2q)^2\sqrt{4\frac{(1-q)q}{N} + (1-2q)^2 + \gamma^2}} \\ &= \sqrt{\frac{\gamma}{4}}\sqrt{1-\frac{1}{N}}\int_{-\sqrt{N}}^{\sqrt{N}} \frac{dx}{(x^2+1-\frac{x^2}{N})\sqrt{\frac{1}{N}(1-\frac{x^2}{N}+x^2)+\gamma^2}} \\ &\to \frac{1}{2\sqrt{\gamma}}\int_{-\infty}^{\infty}\frac{1}{x^2+1}dx \qquad (N\to\infty) \\ &= \frac{\pi}{2\sqrt{\gamma}} \end{aligned} \tag{4.5.10}$$

where we applied the change of variables $x = \sqrt{N}(2q-1)$ and used dominated convergence. More precisely, we read of from (4.5.10) that $A$ can be estimated by evaluating the integrand in Equation (4.5.5) at its maximum, $q = 1/2$, and taking the width to be $1/\sqrt{N}$. This gives

$$A = O\left(\frac{M(1/2)}{N}\right). \tag{4.5.11}$$

The exact result is

$$A = \gamma^{-1}\arctan^2\left(\gamma\sqrt{\frac{N-1}{1+\gamma^2}}\right).$$

The adiabatic formulation of Grover's search [FGGS02] fixes the scaling of the minimal gap $g_0 = \frac{1}{\sqrt{N}}$ but does not fix the scaling of the dephasing rate $\gamma$ with $N$. We shall now address the issue of what physical principles determine the scaling of the dephasing with $N$. To this end we consider various cases.

The regime $\gamma \ll \varepsilon$ is a priori outside the framework of the adiabatic theory described here: Note that for $\varepsilon T_q^{(1)}$ to be a good approximation for $T_q(1)$, $\varepsilon$ should be the smallest energy scale in the problem. Even Lemma 4.16 below, which holds for arbitrary $\varepsilon$, yields no information in this regime. However, $\gamma \ll \varepsilon$ is essentially the unitary scenario [FGGS02, JRS07].

The regime $\varepsilon \ll \gamma \ll g_0$ is trivially consistent with Grover's bound since $\tau \gg \gamma^{-1} \gg O(\sqrt{N})$.

Optimal scheduling recovers Grover's bound when dephasing is comparable to the gap, $\gamma \sim g_0$, at least within the framework of a first order approximation by means of $T_q^{(1)}$. One finds $M(1/2) \sim 1/g_0^3$ and from Equations (4.5.8, 4.5.11) the search time

$$\tau = O\left(\frac{1}{g_0^3 N}\right) = O(\sqrt{N}) . \tag{4.5.12}$$

The most interesting regime is the dominant dephasing case: $\gamma \gg g_0$. Here $M(1/2) \sim \gamma^{-1}/g_0^2$ and from Equations (4.5.8, 4.5.11) one finds

$$\tau = O\left(\gamma^{-1}\right) . \tag{4.5.13}$$

If $\gamma$ is scaled like $\gamma \sim N^{-\alpha/2}$ then $\tau = O\left(N^{\alpha/2}\right)$ which seems to beat Grover's time whenever $\alpha < 1$ .

The accelerated search enabled by strong dephasing is in apparent conflict with the optimality of Grover's bound [FG98, BBBV97]: Consider the joint Hamiltonian dynamics of the system (computer) and its environment, which underlies the Lindblad evolution. By an argument of [RC02] for a universal environment, the Grover search time is optimal. How can one reconcile Equation (4.5.13) with this result? Before giving an answer, however, we want to point out that Equation (4.5.13) is essentially not an artefact of perturbation theory. This follows from Lemma 4.16 below. In particular, while $T_{q_0}(1) = 2\varepsilon A$ is valid to first order in $\varepsilon$, an estimate $T_{q_0}(1) \lesssim N^{\alpha/2}\varepsilon$ remains true up to a logarithmic correction for all $\varepsilon$ provided $\gamma \sim N^{-\alpha/2}$ for $\alpha < 1$.

The resolution is that a Markovian environment with $\gamma \gg g_0$ cannot be universal and must be system specific: The bath has a premonition of what the solution to the problem is. (Formally, this "knowledge" is reflected in the dephasing in the instantaneous eigenstates of $H_q$.) Lindbladians with dephasing rates that dominate the gaps mask resources hidden in the bath. This can also be seen by the following argument: As we have seen dephasing can be interpreted as the monitoring of the observable $H_q$. The *time-energy* uncertainty principle [AMP02] says that if $H_q$ is unknown, then the rate of monitoring is bounded by the gap. The accelerated search occurs when the monitoring rate exceeds this bound, which is only possible if the bath already "knows" what $H_q$ is. If $H_q$ is known, the bath can freeze the system in the instantaneous ground state arbitrarily fast. Consequently, the Zeno effect [MS77] then allows for the speedup of the evolution without paying a large price in tunneling.

It remains to prove the following

**Lemma 4.16.** *If $g_0 \le \gamma$ then $T_{q_0}(1) \le C(\gamma)\varepsilon$ where $C(\gamma)$ has the following behavior:*

$C(\gamma) \sim 1/\gamma \log(1/\gamma)$ *if $\gamma = \gamma(N) \to 0$ as $N \to \infty$,*

$C(\gamma) \sim 1/\gamma$ *if $\gamma = \gamma(N) \ge c > 0$ where $c$ does not depend on $N$.*

**Remark 4.17.** *In the critical scaling $\gamma \sim g_0 = 1/\sqrt{N}$ we obtain a logarithmic correction with respect to (4.5.13). It is conceivable that this would vanish with sharper estimates at our disposal. Note however that the Grover bound still gets apparently beaten as soon as $N\gamma^2 \to \infty$.*

Proof. By definition of $T_q(1)$ and Theorem 2.16, using the setting of Example 4.8, it suffices to estimate the right hand side of

$$|n(1) - (-\hat{g}(q_0(1))| \le \varepsilon \left|\frac{\gamma\hat{g}'(1) + g(1)\times\hat{g}'(1)}{|g(1)|^2+\gamma^2}\right| |\dot{q}_0(1)| + \varepsilon \left|\frac{\gamma\hat{g}'(0) + g(0)\times\hat{g}'(0)}{|g(0)|^2+\gamma^2}\right| |\dot{q}_0(0)|$$
$$+ \varepsilon \int_0^1 ds \left|\frac{d}{ds}\frac{\{\gamma\hat{g}'(q_0(s)) + g(q_0(s))\times\hat{g}'(q_0(s))\}\dot{q}_0(s)}{|g(q_0(s))|^2+\gamma^2}\right| . \tag{4.5.14}$$

Henceforth we omit the $s$-dependence, introduce $f := |g(q_0)|^2$, and recall

$$f(q) = 4\frac{(1-q)q}{N} + (1-2q)^2 ,$$
$$|\hat{g}'(q_0)| = \sqrt{\frac{1}{N} - \frac{1}{N^2}\frac{2}{f}} \sim \frac{1}{\sqrt{Nf}} ,$$
$$g(q_0) = \begin{pmatrix} (2q_0-1)\sqrt{1-N^{-1}} \\ 0 \\ -N^{-1/2} \end{pmatrix} ,$$

as well as

$$A \sim \gamma^{-1} ,$$
$$M(q_0) = \frac{\gamma}{4}\frac{|\hat{g}'(q_0)|^2}{f+\gamma^2} .$$

Therefore

$$\dot{q}_0(s(q_0)) = \sqrt{\frac{A}{M(q_0)}} \sim \frac{1}{|\hat{g}'(q_0)|} \sim \sqrt{N}f .$$

The first line in (4.5.14) is then estimated by the bounds in the assertion. For the second we note

$$\int_0^1 ds \left|\frac{d}{ds}\frac{\{\gamma\hat{g}'(q_0(s)) + g(q_0(s))\times\hat{g}'(q_0(s))\}\dot{q}_0(s)}{f(q_0(s))+\gamma^2}\right| = \int_0^1 dq \left|\left(\frac{\gamma\hat{g}'(q) + g(q)\times\hat{g}'(q)}{f(q)+\gamma^2}\sqrt{\frac{A}{M(q)}}\right)'\right|$$
$$= 2\sqrt{\frac{A}{\gamma}}\int_0^1 dq \left|\left(\frac{\gamma\frac{\hat{g}'(q)}{|\hat{g}'(q)|} + g(q)\times\frac{\hat{g}'(q)}{|\hat{g}'(q)|}}{\sqrt{f(q)+\gamma^2}}\right)'\right| . \tag{4.5.15}$$

We need

$$\left|\left(\frac{\hat{g}'}{|\hat{g}'|}\right)'\right|^2 = \left|\frac{\hat{g}''}{|\hat{g}'|} - \frac{\hat{g}'(\hat{g}'\cdot\hat{g}'')}{|\hat{g}'|^3}\right|^2 = \frac{|\hat{g}''|^2|\hat{g}'|^2 - (\hat{g}''\cdot\hat{g}')^2}{|\hat{g}'|^4} = \frac{|\hat{g}'\times\hat{g}''|^2}{|\hat{g}'|^4} ,$$

where

$$\begin{aligned}\hat{g}'' &= \left(\frac{g'}{|g|} - \frac{g}{|g|^3}(g\cdot g')\right)' \\ &= \frac{g''}{|g|} - \frac{2g'(g\cdot g') + g|g'|^2 + g(g\cdot g'')}{|g|^3} + 3\frac{g(g\cdot g')^2}{|g|^5} \\ &= 3\frac{g(g\cdot g')^2}{|g|^5} - \frac{2g'(g\cdot g') + g|g'|^2}{|g|^3}\,,\end{aligned}$$

and so

$$\begin{aligned}|\hat{g}' \times \hat{g}''|^2 &= \left|\left(\frac{g'}{|g|} - \frac{g(g\cdot g')}{|g|^3}\right) \times \left(3\frac{g(g\cdot g')^2}{|g|^5} - \frac{2g'(g\cdot g') + g|g'|^2}{|g|^3}\right)\right|^2 \\ &= \left|3\frac{g'\times g(g\cdot g')^2}{|g|^6} - \frac{g'\times g|g'|^2}{|g|^4} - 2\frac{g'\times g(g\cdot g')}{|g|^6}\right|^2 \\ &= \frac{|g'\times g|^6}{|g|^{12}}\,.\end{aligned}$$

With

$$|g'\times g| = 2\sqrt{N^{-1} - N^{-2}} \sim 1/\sqrt{N}$$

we obtain

$$\left|\left(\frac{\hat{g}'}{|\hat{g}'|}\right)'\right| = \frac{|g'\times g|^3}{|g|^6|\hat{g}'|^2} \lesssim \frac{1}{\sqrt{N}f}\,.$$

Ultimately,

$$g \wedge \frac{\hat{g}'}{|\hat{g}'|} = g \wedge \left(\frac{g'}{|\hat{g}'||g|}\right) \sim \sqrt{N f} g \wedge g'$$

which implies

$$|\left(g \wedge \frac{\hat{g}'}{|\hat{g}'|}\right)'| \lesssim \sqrt{N}\frac{f'}{\sqrt{f}}\frac{1}{\sqrt{N}} + \sqrt{N f}\left(g'\wedge g' + g\wedge g''\right) = \frac{f'}{\sqrt{f}} + 0$$

We can now estimate Expression (4.5.15):

$$\begin{aligned}2\sqrt{\frac{A}{\gamma}}\int_0^1 dq\,\left|\left(\frac{\gamma\frac{\hat{g}'(q)}{|\hat{g}'(q)|} + g(q)\times\frac{\hat{g}'(q)}{|\hat{g}'(q)|}}{\sqrt{f(q)+\gamma^2}}\right)'\right| &\lesssim \int_0^1 dq\,\Big(\frac{1/(\sqrt{N}f(q))}{\sqrt{f(q)+\gamma^2}} + \frac{f'}{\gamma\sqrt{f}\sqrt{f(q)+\gamma^2}} \\ &\qquad + \left|\frac{f'(q)}{\sqrt{f(q)+\gamma^2}^3}\right|\Big) \\ &= (\mathrm{I}) + (\mathrm{II}) + (\mathrm{III})\,.\end{aligned}$$

We estimate the three integrals separately:

$$\begin{aligned}
|(\mathrm{I})| &\lesssim \frac{1}{\gamma\sqrt{N}} \int_0^1 \frac{1}{f} dq \\
&\lesssim \frac{1}{\gamma\sqrt{N}} \int_0^1 dq \, \frac{1}{4\frac{(1-q)q}{N} + (1-2q)^2} \\
&= \frac{1}{\gamma\sqrt{N}} \int_0^1 dq \, \frac{1}{(1-\frac{1}{N})(2q-1)^2 + \frac{1}{N}} \\
&= \frac{1}{\gamma} \int_{-\sqrt{N}}^{\sqrt{N}} dx \, \frac{1}{(1-\frac{1}{N})x^2 + 1} \\
&\sim \frac{\pi}{\gamma} \qquad (N \to \infty)\,.
\end{aligned}$$

$$|(\mathrm{II})| \lesssim \frac{1}{\gamma} \int_{1/N}^1 \frac{dx}{\sqrt{x(x+\gamma^2)}} = \frac{2}{\gamma} \log\left(\frac{\sqrt{N} + \sqrt{N + N\gamma^2}}{1 + \sqrt{1 + N\gamma^2}}\right)$$

By inspection we see that this expression can be estimated by the bounds in the assertion of the lemma. Finally,

$$|(\mathrm{III})| \lesssim \int_{1/N}^1 \frac{dx}{\sqrt{x+\gamma^2}^3} = \frac{2}{\sqrt{\gamma^2 + \frac{1}{N}}} - \frac{2}{\sqrt{\gamma^2+1}}\,,$$

which again has the asserted asymptotics. □

## 4.6. Driven Markov processes

Theorem 2.16 may be applied to an evolution of the probability distribution of a continuous-time Markov process. In particular, we shall describe below an application to (stochastic) molecular pumps [RHJ08].

Let $X$ be a random variable on a finite state space $S = (1, 2, \ldots, d)$ and denote

$$p_i = \mathrm{Prob}(X = i)\,.$$

The evolution of $X$ is governed by

$$\dot{p}_i = \sum_{j=1}^{d} L_{ij} p_j\,, \tag{4.6.1}$$

where the transition rate $j \to i$, $L_{ij}\,(i \neq j)$, is non-negative and $L_{jj} := -\sum_{i\neq j} L_{ij}$. For convenience we collect some standard facts in the following lemma.

**Lemma 4.18.** *The transition matrix $\phi(t) := \exp(Lt)$ is*

*(i) a left-stochastic matrix ($0 \leq \phi_{ij} \leq 1$, $\sum_{i=1}^d \phi_{ij} = 1$),*

*(ii) a contraction with respect to the norm $\|x\|_1 = \sum_{j=1}^d |x_j|$,*

*(iii) and converges to a projection, $\phi(t) \to P^+$, $(t \to \infty)$. The range of $P^+$ is spanned by stationary probability distributions, meaning $\sum_{j=1}^d L_{ij}\pi_j = 0$.*

PROOF. Note that whenever $p_i = 0$ for a probability distribution $p$ then $\dot{p}_i = \sum_{j\neq i} L_{ij}p_j \geq 0$ and hence $p_i(t) \geq 0$ for all $t$ which implies that the entries of $\phi$ are non-negative. By $\sum_{i,j} L_{ij}p_j = 0$ it follows that $\phi$ is trace preserving, which implies (i); (ii) is seen by $\sum_{i=1}^d |\sum_{j=1}^d \phi_{ij}x_j| \leq \sum_{i,j}\phi_{ij}|x_j| = \|x\|_1$ which yields also $\mathbb{R}^d = \ker L \oplus \operatorname{ran} L$ by Proposition 2.29 and Lemma 2.31. Hence for (iii) it suffices to show that $L$ cannot have purely imaginary eigenvalues. If it did then $\phi(t)$ would possess an eigenvalue $e_{*,t}$ on the unit circle different from 1 for arbitrarily small nonzero $t$. However since the diagonal elements of $\phi(t)$ are nonzero for small $t$ the Gershgorin discs for $\phi(t)$ cannot cover $e_{*,t}$ by (i). □

We assume that the state space $S$ is indecomposable and denote by $\pi$ the unique stationary distribution of $L$, whence $\ker L = \operatorname{span}\{\pi\}$ and $\operatorname{ran} L = \{p \mid \sum p_i = 0\}$. In line with Equation (2.3.1), let $P$ be the rank 1 projection associated to that pair of subspaces, which are left invariant by $L$. We identify $L^{-1}$ with the map $(1-P)L^{-1}(1-P)$ defined on all of $\mathbb{C}^d$, and denote its matrix elements by $L^{-1}_{ij}$.

Now we consider a smooth family of generators $L(s)$ with corresponding stationary states $\pi(s)$. The following result generalizes one by [RHJ08] (see also [Par98, HJ09]).

**THEOREM 4.19.** *Assume that $S$ is irreducible for $L(s)$ and that $\dot{\pi}_i(0) = 0$. The solution of*

$$\varepsilon\dot{p}_i(s) = \sum_{j=1}^d L_{ij}(s)p_j(s) \tag{4.6.2}$$

*with initial condition $p_i(0) = \pi_i(0)$ is*

$$p_i(s) = \pi_i(s) + \varepsilon\sum_{j=1}^d L^{-1}_{ij}(s)\dot{\pi}_j(s) + O(\varepsilon^2)\,. \tag{4.6.3}$$

PROOF. The expansion (4.6.3) is just that of Theorem 2.16. Note that by $\ker P(s) = \operatorname{ran} L(s)$ (or, more abstractly, by Lemma 3.15 for $\mathcal{A} = \ell^\infty(S)$) the hypothesis of Corollary 2.18 is satisfied. Thus $T(s, s')\pi(s') = \pi(s)$ and $a_1(s) = 0$. □

We say that $L$ satisfies a *detailed balance* if

$$M_{ij} := L_{ij}\pi_j\,. \tag{4.6.4}$$

is a symmetric matrix for some $\pi$, in which case that is the stationary distribution. This can be interpreted as the statement that the current through any link $j \to i$

$$J_{ij}(p) = L_{ij}p_j - L_{ji}p_i \tag{4.6.5}$$

vanishes at equilibrium, $J_{ij}(\pi) = 0$.

We now strengthen the assumption on $S$ from indecomposable to irreducible, meaning that $\pi_j > 0$ for all $j$. Then $\ker M = \operatorname{span}\{(1, 1, \dots 1)\}$, $\operatorname{ran} M = \operatorname{ran} L$, and the two subspaces decompose $M$ as a linear map. At first $M^{-1}$ is defined on $\operatorname{ran} M$, and it may be extended afterwards, arbitrarily but linearly, to all of $\mathbb{C}^d$, e.g. by having it vanish on $\ker M$.

In applications to (stochastic) molecular pumps (see [RHJ08] and references therein) one is interested in systems that carry no current in their equilibrium states, but can be induced to yield net particle transport in an adiabatic pump cycle. Note that $M$ and $\pi$ provide natural coordinates for those irreducible processes $L$ which satisfy a detailed balance condition. We set the pump period (in scaled time) to be unity.

The net transport across the link $j \to i$ is expressed in terms of the integrated probability current

$$T_{ij} := \frac{1}{\varepsilon}\int_0^1 J_{ij}\big(p(s)\big)\, ds\,.$$

The following result is due to [RHJ08].

**Corollary 4.20.** *Let $s \mapsto (M(s), \pi(s))$ be a pump cycle with $\pi(s)$ the unique equilibrium state for every $s$. Assume that $\dot\pi_j(0) = 0$. Then the transport is geometric to leading order, given by*

$$T_{ij} = \int_0^1 \sum_{k=1}^{d} \Big(M_{ij}(s)M^{-1}_{jk}(s) - M_{ji}(s)M^{-1}_{ik}(s)\Big)\, d\pi_k(s) \;+ O(\varepsilon)\,. \tag{4.6.6}$$

*In particular, $T_{ij} = O(\varepsilon)$ if $\pi$ is constant or, in the periodic case $L(0) = L(1)$, if $M$ is.*

**Remark 4.21.**

1) *Here, geometric means that the transport is independent of the parametrization of the pumping cycle. This is evident in Equation (4.6.6).*
2) *Corollary 4.20 says that* effective pump cycles *require the variation of both $\pi$ and $M$.*

Proof. The contribution to $T_{ij}$ of order $\varepsilon^{-1}$ vanishes due to the detailed balance condition. To next order Equations (4.6.5, 4.6.3) yield

$$T_{ij} = \int_0^1 \sum_{k=1}^{d} \big(L_{ij}(s)L^{-1}_{jk}(s) - L_{ji}(s)L^{-1}_{ik}(s)\big)\dot\pi_k(s)\, ds + O(\varepsilon)\,.$$

Equation (4.6.4) may be written as $M = (1-P)L(1-P)\Pi$, where $\Pi_{ij} = \pi_i\delta_{ij}$, implying $L^{-1} = (1-P)\Pi M^{-1}(1-P)$. Thus, with $P_{jl} = \pi_j$, we have

$$L_{ij}L^{-1}_{jk}\dot\pi_k = L_{ij}\sum_{l=1}^{d}(1-P)_{jl}\pi_l M^{-1}_{lk}\dot\pi_k = M_{ij}M^{-1}_{jk}\dot\pi_k - \sum_{l=1}^{d} M_{ij}\pi_l M^{-1}_{lk}\dot\pi_k\,.$$

After interchanging $i, j$ and taking the difference, the second term cancels and we are left with (4.6.6). The additional claim in the periodic case follows by the fundamental theorem of calculus. □

## 4.7. Time-dependent Hamiltonians II

Theorem 2.25 can be applied to evolutions generated by either a Hamiltonian or a Lindbladian, just like Theorem 2.16 was in Sections 4.2 and 4.3, respectively. The Hilbert space $\mathcal{H}$ is, again, infinite dimensional.

In this section we discuss the first case where the result provides a simple proof of the adiabatic theorem for the Schrödinger equation

$$\mathrm{i}\varepsilon\dot{\psi}(s) = H(s)\psi(s) \tag{4.7.1}$$

or, in density matrix language, the von Neumann equation

$$\mathrm{i}\varepsilon\dot{\rho}(s) = [H(s), \rho(s)]\,. \tag{4.7.2}$$

Without the gap assumption for the family of Hamiltonian $H(s)$ we have, as in [AE99, Teu01] (with slightly weakened assumptions):

**Theorem 4.22.** *Let $H(s)$ be a $C^1$-family of Hamiltonians with eigenvalue $E_*(s)$ and let $P(s)$ be a $C^1$-family of finite rank projections such that $H(s)P(s) = E_*(s)P(s)$ for all $s \in [0,1]$ and $P(s)$ is the spectral projection of $H(s)$ associated to $E_*(s)$ for almost all $s \in [0,1]$. Then if $P(0)\psi(0) = \psi(0)$ the solution of Equation (4.7.1) satisfies*

$$\sup_{0\le s\le 1} \|\mathrm{e}^{\frac{\mathrm{i}}{\varepsilon}\int_0^s E_*(s')ds'}\psi(s) - T(s,0)\psi(0)\| \to 0\,, \qquad (\varepsilon \to 0)\,. \tag{4.7.3}$$

*$T(s,s')$ is the parallel transport on pure states given by $\partial_s T(s,s') = \dot{P}(s)T(s,s')$. In terms of density matrices it holds that for $\rho(0) = P(0)$ in Equation (4.7.2)*

$$\sup_{0\le s\le 1} \|\rho(s) - P(s)\|_{\mathcal{J}_1(\mathcal{H})} \to 0\,, \qquad (\varepsilon \to 0)\,. \tag{4.7.4}$$

Proof. The eigenvalue $E_*(s)$ is differentiable by $E_*(s) = \mathrm{tr}(H(s)P(s))/\mathrm{tr}\,(P(s))$ and therefore Theorem (2.25) implies (4.7.3) immediately by considering $L(s) := -\mathrm{i}(H(s) - E_*(s))$. From this, (4.7.4) follows by decomposing $\rho(s)$ into a finite convex combination of pure states. □

**Remark 4.23.**

1) *The "almost all" formulation [Bor98, Teu01] allows for eigenvalue crossings.*

2) *(4.7.3) also holds for projections of infinite rank if $E_*(s)$ is* assumed *to be continuously differentiable.*

3) *It is instructive to note that (4.7.4) can be also be proved directly by considering*

$$\mathrm{i}\varepsilon\dot{k}(s) = [H(s), k(s)]$$

*with $k(s) = \sqrt{\rho(s)} \in \mathcal{J}_2(\mathcal{H})$: With respect to the projection onto the kernel of this generator the projection $P(s)$ is automatically parallel transported, cf. Lemma 4.2*[3].

## 4.8. Time-dependent Lindbladians II

We now turn to a discussion of gapless adiabatic theorems for open quantum systems. One can adopt the point of view that they are more generic than their Hamiltonian counterpart for the following reason: Consider a closed quantum system described by a family of Hamiltonians

[3] to be fair: that $H(s)$ was bounded there.

$H(s)$ with nonempty continuous spectrum and an isolated eigenvalue $E(s)$. Then 0 is a *non-isolated* eigenvalue for the corresponding Liouvillian[4] $\mathcal{L}(s) = -\mathrm{i}[H(s), \cdot]$ which acts on $\mathcal{J}_1(\mathcal{H})$[5]. In that sense the transition to a picture of density matrices may cloud the existence of a spectral gap in the Hamiltonian case, cf. page 41. If in addition the interaction of the system with its environment is taken into account (that is the Liouvillian becomes a "genuine" Lindbladian) then – generically – 0 will still be a non-isolated point of the spectrum. However, the alternative of working at the level of pure states is no longer available and hence the nonexistence of a gap cannot be circumvented by the above "algebraic" measure.

As a first theorem we present the following somewhat generic case:

**THEOREM 4.24.** *Let $\mathcal{L}(s)$, $0 \le s \le 1$, be a $C^1$-family of Lindbladians with* $\dim\ker\mathcal{L}^*(s) = 1$ *for almost all $s$. Furthermore assume the existence of a $C^1$-section of instantaneous stationary states $\rho_*(s)$. Then the solution of $\varepsilon\dot\rho(s) = \mathcal{L}(s)\rho(s)$ with initial data $\rho(0) = \rho_*(0)$ satisfies*

$$\sup_{0\le s\le 1} \|\rho(s) - \rho_*(s)\|_{\mathcal{J}_1(\mathcal{H})} \to 0\,, \qquad (\varepsilon \to 0)\,.$$

PROOF. Inspection of the proof of Theorem 2.25 shows that we only need to show that $\dot\rho_*(s) \in \overline{\operatorname{ran}\mathcal{L}(s)} = (\ker\mathcal{L}^*(s))_\perp = (\operatorname{span}\{\mathbb{1}\})_\perp$ (the last equality is due to $\dim\ker\mathcal{L}^*(s) = 1$). This however is nothing but the normalization condition for states: $\operatorname{tr}(\mathbb{1}\dot\rho_*(s)) = \frac{d}{dt}\operatorname{tr}(\rho_*(s)) = 0$. □

More generally some care is required: Since $\mathcal{J}_1(\mathcal{H})$ is not reflexive the decomposition condition

$$\mathcal{J}_1(\mathcal{H}) = \ker\mathcal{L} \oplus \overline{\operatorname{ran}\mathcal{L}} \tag{4.8.1}$$

is not ensured by Proposition 2.33 and therefore needs to be implemented by assumption. In that case the formulation of Theorem 2.25 translates directly to Lindbladians if $L = \mathcal{L}$, $P = \mathcal{P}$, $Q = \mathcal{Q}$ and $\mathcal{B} = \mathcal{J}_1(\mathcal{H})$. Unfortunately, Decomposition (4.8.1) will generically be false (!) as follows from the subsequent example, cf. also Example 2.28.

**EXAMPLE 4.25.** *Consider the Liouvillian $\mathcal{L} : \rho \mapsto -\mathrm{i}[H, \rho]$ defined for $\rho \in \mathcal{J}_1(\mathcal{H})$ with a bounded Hamiltonian $H$. Let $H$ have nonempty continuous spectrum with associated projection $P_c$ and possibly also eigenvalues with associated eigenprojections $\{P_i\}_{i\in I}$, $I$ a countable index set. Note that on* $\operatorname{ran}\mathcal{L}$ *we have* $\operatorname{tr} P_c\mathcal{L}\rho = 0$ *because* $\operatorname{tr} P_c H\rho = \operatorname{tr} P_c\rho H$ *( [Sim05], Corollary 3.8). Then* $\operatorname{tr} P_c\chi = 0$ *extends to* $\chi \in \overline{\operatorname{ran}\mathcal{L}}$. *In addition,* $\operatorname{tr} P_c\rho = 0$ *for* $\rho \in \ker\mathcal{L} = \operatorname{span}\{P_i\}_{i\in I}$. *By considering any finite subprojection of $P_c$ it follows that* $\mathcal{J}_1(\mathcal{H}) = \ker\mathcal{L} \oplus \overline{\operatorname{ran}\mathcal{L}}$ *is impossible.*

**REMARK 4.26.** *The example has also a noteworthy consequence in relation with Theorem 4.24: There one might be tempted to translate the dimensionality assumption to the Schrödinger picture: "*$\dim\ker\mathcal{L} = \dim\ker\mathcal{L}^* = 1$*" . However, the first equality can be violated for the following reason: Since* $\overline{\operatorname{ran}\mathcal{L}}$ *is a proper subspace of $\mathcal{J}_1(\mathcal{H})$ it follows from the Hahn-Banach theorem that there exists* $0 \neq y^* \in \mathcal{J}_1(\mathcal{H})^* = \mathcal{L}(H)$ *such that* $0 = y^*(\mathcal{L}f) = \mathcal{L}^*y^*(f)$ *for all* $f \in \mathcal{J}_1(\mathcal{H})$. *But then* $y^* \in \ker\mathcal{L}^*$ *and hence* $\dim\ker\mathcal{L} < \dim\ker\mathcal{L}^*$.

[4]Recall that $H$ is – as always when we refer to Lindbladians in this thesis – bounded and hence the expression for the Liouvillian is well-defined.

[5]In fact the spectrum of $\mathcal{L}$ consists precisely of i times the differences of elements in $\sigma(H)$. This follows from the spectral theorem if $\mathcal{L}$ is considered on $\mathcal{J}_2(\mathcal{H})$, see [Spo76, Spo77]. If we restrict to $\mathcal{J}_1(\mathcal{H})$ the same can be seen to hold: $\sigma(\mathcal{L} \upharpoonright \mathcal{J}_1(\mathcal{H})) \subset \sigma(\mathcal{L} \upharpoonright \mathcal{J}_2(\mathcal{H}))$ is obvious. Conversely, the fact that $\mathrm{i}\sigma(\mathcal{L} \upharpoonright \mathcal{J}_1(\mathcal{H}))$ contains all energy differences is seen by considering Weyl sequences (which is admissible even though $\mathcal{J}_1(\mathcal{H})$ is not a Hilbert space).

In the absence of (4.8.1) an alternative approach can be a remedy: Consider the Lindblad evolution

$$\varepsilon\dot{\rho}(s) = \mathcal{L}(s)\rho(s) = -\mathrm{i}[H(s),\rho(s)] + \frac{1}{2}\sum_{i\in I}\left([V_i(s)\rho(s),V_i^*(s)] + [V_i(s),\rho(s)V_i^*(s)]\right) \qquad (4.8.2)$$

on any $p$-Schatten class $\mathcal{J}_p(\mathcal{H})$, $1 < p \leq \infty$[6], with $\mathcal{L}(s)$ being a $C^1$-family. Recall that $H$, $V_i \in \mathcal{L}(\mathcal{H})$. To avoid topological complications we assume that the index set $I$ is finite. In fact, this will be a standing hypothesis for the remainder of this section. Equation (4.8.2) is well-defined since all $p$-Schatten classes are two-sided ideals in $\mathcal{L}(\mathcal{H})$. To apply Theorem 2.25 on $\mathcal{J}_p(\mathcal{H})$, $1 < p < \infty$, we use the following result.

**Lemma 4.27.** *The propagator to Equation (4.8.2) is contracting on $\mathcal{J}_p(\mathcal{H})$ for any $1 \leq p \leq \infty$ if*

$$\sum_{i\in I}[V_i(s),V_i^*(s)] = 0 \qquad (4.8.3)$$

*for all $s \in [0,1]$.*

**Remark 4.28.** *Note that Condition (4.8.3) is satisfied for normal $V_i$ and in particular for dephasing Lindbladians, cf. Proposition 3.10.*

Proof. We first consider the case $p = \infty$. We need to check that for fixed $s$ the Lindbladian generates a contraction. Equation (4.8.3) allows to write for $A \in \mathcal{L}(\mathcal{H})$

$$\begin{aligned}\mathcal{L}(A) &= -\mathrm{i}[H,A] + \frac{1}{2}\sum_{i\in I}\left(2V_iAV_i^* - V_i^*V_iA - AV_i^*V_i\right)\\ &= -\mathrm{i}[H,A] + \sum_{i\in I}\left(V_iAV_i^* - \frac{1}{2}\{V_iV_i^*,A\}\right)\end{aligned}$$

which is of the standard form in the Heisenberg picture, cf. Equation (3.3.2), for $H \to -H$ and $V_i \to V_i^*$. By Theorem 3.4 this generates a quantum dynamical semigroup and therefore proves the contraction property on $\mathcal{L}(\mathcal{H})$. The assertion of the Lemma follows by the $p$-Schatten class analogue of the Riesz-Thorin interpolation theorem ( [Zhu90], Theorem 2.2.7). □

We mention that on $\mathcal{J}_2(\mathcal{H})$ a more direct proof can be given:

Alternative proof for the case $p = 2$. We verify the conditions for the Lumer-Phillips Theorem [LP61]. Clearly $\mathcal{L} - \lambda$ is surjective for $\lambda$ large enough and it suffices to show that $\mathcal{L}$

[6] $\mathcal{J}_\infty(\mathcal{H}) := \mathcal{L}(\mathcal{H})$.

is dissipative. For any $A \in \mathcal{J}_2(\mathcal{H})$,

$$
\begin{aligned}
\Re \operatorname{tr}(A^*\mathcal{L}(A)) &= \Re \frac{1}{2} \sum_{i\in I} \left(\operatorname{tr}(A^*[V_iA, V_i^*]) + \operatorname{tr}(A^*[V_i, AV_i^*])\right) \\
&= \Re \frac{1}{2} \sum_{i\in I} \left(2 \operatorname{tr}(A^* V_i A V_i^*) - \|V_iA\|^2_{\mathcal{J}_2(\mathcal{H})} - \|V_iA^*\|^2_{\mathcal{J}_2(\mathcal{H})}\right) \\
&\leq \frac{1}{2} \sum_{i\in I} \left(\|V_i^*A\|^2_{\mathcal{J}_2(\mathcal{H})} + \|AV_i^*\|^2_{\mathcal{J}_2(\mathcal{H})} - \|V_iA\|^2_{\mathcal{J}_2(\mathcal{H})} - \|V_iA^*\|^2_{\mathcal{J}_2(\mathcal{H})}\right) \\
&= \frac{1}{2} \sum_{i\in I} \left(\|V_i^*A\|^2_{\mathcal{J}_2(\mathcal{H})} - \|V_iA\|^2_{\mathcal{J}_2(\mathcal{H})}\right) \\
&= \frac{1}{2} \operatorname{tr}\left(AA^* \sum_{i\in I} (V_iV_i^* - V_i^*V_i)\right) = 0\,.
\end{aligned}
$$

In the third line we used Hölder's and Young's inequality; the fourth line follows by duality. □

Lemma 2.10, Proposition 2.33 and Theorem 2.25 imply:

**Theorem 4.29.** *Assume the conditions of Lemma 4.27 for a $C^1$-family of Lindbladians $\mathcal{L}(s)$, $0 \leq s \leq 1$, considered on the reflexive Banach space $\mathcal{B} = \mathcal{J}_p(\mathcal{H})$, $1 < p < \infty$. Let $\mathcal{L}(s)$ be $C^1$ and let $\mathbb{1} = \mathcal{P}(s) + \mathcal{Q}(s)$ for almost all $s$ be the projections associated to the Decomposition (2.4.1); moreover let $\mathcal{P}(s)$ be defined for all $0 \leq s \leq 1$ and $C^1$ as a bounded operator on $\mathcal{J}_p(\mathcal{H})$. Then the solution of $\varepsilon\dot{\rho}(s) = \mathcal{L}(s)\rho(s)$ with initial data $\rho(0) = \mathcal{P}(0)\rho(0) \in \mathcal{J}_p(\mathcal{H})$ satisfies*

$$
\sup_{0\leq s\leq 1} \|\rho(s) - \mathcal{T}(s,0)\rho(0)\|_{\mathcal{J}_p(\mathcal{H})} \to 0\,, \qquad (\varepsilon \to 0)\,. \tag{4.8.4}
$$

*$\mathcal{T}(s,s')$ is the parallel transport on density matrices given by $\partial_s\mathcal{T}(s,s') = \dot{\mathcal{P}}(s)\mathcal{T}(s,s')$.*

This theorem can be interpreted to imply convergence of the evolved state towards the instantaneous stationary state in "almost" the physically natural topology.

A different point of view applies in the case of dephasing Lindbladians where many *pure* instantaneous stationary states are present. Satisfactorily, this case is covered due to Remark 4.28. In what follows we shall explain how the case $p = 2$ in Theorem 4.29 can be naturally applied to tunneling, cf. Equation (4.3.2). As a preparation we state the following observation:

**Lemma 4.30.** *Let $\mathcal{L}$ be a dephasing Lindbladian considered on $\mathcal{J}_2(\mathcal{H})$. Associated to it is a Hamiltonian $H$ with eigenprojections $\{P_i\}_{i\in K}$, where $K = \{1,\dots,M\}$ resp. $K = \mathbb{N}$ is a countable index set. Then*

*(i) $\mathcal{J}_2(\mathcal{H}) = \ker\mathcal{L} \oplus \overline{\operatorname{ran}\mathcal{L}}$ is an orthogonal direct sum and*

*(ii) the projection onto the first component has the explicit form $\mathcal{P}\rho = \sum_{i\in K} P_i\rho P_i$ where $\rho \in \mathcal{J}_2(\mathcal{H})$.*

*(iii) Time-dependence: If $H(s)$ is $C^1$ then so is $\mathcal{L}(s)$. If the $P_i(s)$ are $C^1$, uniformly in $i$, then so is $\mathcal{P}(s)$.*

Proof. By Proposition 2.33 and Lemma 4.27, $\mathcal{J}_2(\mathcal{H}) = \overline{\ker\mathcal{L} \oplus \overline{\operatorname{ran}\mathcal{L}}}$ and hence (i) follows by showing that $\ker\mathcal{L} \perp \operatorname{ran}\mathcal{L}$ and application of Lemma 2.10: In fact, for a dephasing Lindbladian the statement $\ker\mathcal{L} = \ker([H,\cdot])$ from Proposition 3.10 also holds true as subspaces of $\mathcal{J}_2(\mathcal{H})$, as inspection of the proof shows. Thus $\ker\mathcal{L}\subset\ker\mathcal{L}^*$ by Inclusion (3.5.1). Then $\mathcal{L}a=0$ and $b=\mathcal{L}\tilde{b}$ imply $\langle a,b\rangle_{\mathcal{J}_2(\mathcal{H})}=\langle\mathcal{L}^*a,\tilde{b}\rangle_{\mathcal{J}_2(\mathcal{H})}=0$.

To prove (ii) it suffices to show that

$$\rho\in\ker\mathcal{L}\qquad\text{if and only if}\qquad\rho=\sum_{i\in K}P_i\rho P_i\ : \tag{4.8.5}$$

The last expression defines an orthogonal projection on $\mathcal{J}_2(\mathcal{H})$, cf. Example 3.14, and so the claim follows from (i). The "if" part in (4.8.5) is immediate; to understand the "only if" part note that for a Hilbert-Schmidt operator $\rho\in\ker\mathcal{L}=\ker[H,\cdot]$ it holds that

$$\begin{aligned}\rho&=\lim_{T\to\infty}\frac{1}{T}\int_0^T\mathrm{e}^{\mathrm{i}Ht}\rho\mathrm{e}^{-\mathrm{i}Ht}\\&=\lim_{T\to\infty}\frac{1}{T}\int_0^T\sum_{i,j\in K}\mathrm{e}^{\mathrm{i}E_it}P_i\rho P_j\mathrm{e}^{-\mathrm{i}E_jt}\\&=\sum_{i\in K}P_i\rho P_i\,.\end{aligned}$$

The second equality is due to the RAGE theorem ( [CFKS87], Theorem 5.8 (3)).

Finally, for (iii), the statement for $\mathcal{L}(s)$ is immediate. For $\mathcal{P}(s)$ we have (for notational convenience choose without loss of generality $\rho=\rho^*\in\mathcal{J}_2(\mathcal{H})$ and $K=\mathbb{N}$)

$$\begin{aligned}\limsup_{s\to s'}&\left\|\frac{\mathcal{P}(s)\rho-\mathcal{P}(s')\rho}{s-s'}-\sum_{i\in\mathbb{N}}\Big(\dot{P}_i(s')\rho P_i(s')-P_i(s')\rho\dot{P}_i(s')\Big)\right\|^2_{\mathcal{J}_2(\mathcal{H})}\\&\le\limsup_{s\to s'}\sum_{i\in\mathbb{N}}\left(\left\|\left(\frac{P_i(s)-P_i(s')}{s-s'}-\dot{P}_i(s')\right)\rho P_i(s')\right\|^2_{\mathcal{J}_2(\mathcal{H})}+\|\text{c.c.}\|^2_{\mathcal{J}_2(\mathcal{H})}\right)\\&\le o(1)\sum_{i\in\mathbb{N}}\|\rho P_i(s')\|^2_{\mathcal{J}_2(\mathcal{H})}=o(1)\|\rho\|^2_{\mathcal{J}_2(\mathcal{H})}\qquad(s\to s')\,.\end{aligned}$$

In the first inequality we applied Pythagoras. The $o(1)$ in the third line is independent of $i$ due to the uniformity assumption. □

Now let $H(s)$ and $P_i(s)$ be $C^1$, uniformly in $i$. It follows by regularity that $\mathcal{P}(s)\rho=\sum_{i\in K}P_i(s)\rho P_i(s)$ *for all* $s\in[0,1]$. Since $\mathcal{P}(s)$ is also the projection onto the kernel of $[H(s),\cdot]$ it induces a parallel transport which preserves the purity of states.[7] Then, if $\rho(0)$ is a pure state the tunneling in Equation (4.3.2) has a very simple form and converges to zero by Theorem 4.29 and Equation (2.2.15):

$$\begin{aligned}T(1)&:=1-\mathrm{tr}(\rho(1)\mathcal{T}(1,0)\rho(0))\\&=\underbrace{1-\mathrm{tr}(\mathcal{T}(1,0)\rho(0)\mathcal{T}(1,0)\rho(0))}_{=0}+\mathrm{tr}((\rho(1)-\mathcal{T}(1,0)\rho(0))\mathcal{T}(1,0)\rho(0))\\&\le\|\rho(1)-\mathcal{T}(1,0)\rho(0)\|_{\mathcal{J}_2(\mathcal{H})}\|\mathcal{T}(1,0)\rho(0)\|_{\mathcal{J}_2(\mathcal{H})}\to0\,,\qquad(\varepsilon\to0)\,.\end{aligned}$$

Note that if in particular $\rho(0)=P_i(0)$ is one-dimensional the above formula applies with $\mathcal{T}(1,0)\rho(0)=P_i(1)$ as follows from Lemma 4.2.

[7] This can also be shown explicitly by computing $\frac{d}{dt}\operatorname{tr}\rho^2=2\operatorname{tr}\rho\dot{\rho}=2\operatorname{tr}\rho[\dot{\mathcal{P}},\mathcal{P}](\rho)=0$ using Lemma 4.30 (ii).

We conclude the discussion of gapless Lindbladians with an example which illustrates that, although the tunneling out of the initial state is of order $o(1)$, an adiabatic invariant is conserved up to order $O(\varepsilon)$.

**Example 4.31.** *Consider the Hamiltonians* $H(s) = V(s)HV^*(s)$ *arising from a* $C^2$*-family of unitaries* $V(s)$ *and from a bounded* $H$*. Let* $\rho(s)$ *solve the equation* $\varepsilon\dot{\rho} = -\mathrm{i}[H, \rho]$*. Then the energy is an adiabatic invariant in the sense that*

$$\left|\operatorname{tr}(H(1)\rho(1)) - \operatorname{tr}(H(0)\rho(0))\right| = O(\varepsilon)\,.$$

*This follows from Equation (2.4.5) in Proposition 2.27. We may in fact apply that estimate to* $x(s) = \rho(s)$*,* $\varphi(s) = H(s)$*,* $\langle\varphi,\, x\rangle = \operatorname{tr}(H\rho)$ *and* $\mathcal{L} = -\mathrm{i}[H, \cdot]$*, since the Assumptions (2.4.4) hold true by*

$$\mathcal{L}^*(s)(H(s)) = 0\,, \qquad \dot{H}(s) = -[H(s), \dot{V}(s)V^*(s)] = \mathcal{L}^*(s)(\mathrm{i}\dot{V}(s)V^*(s))\,.$$

# Chapter 5

# A nonlinear adiabatic theorem

## 5.1. Introduction

We contrast our results of the previous chapters by an adiabatic theorem for the non-autonomous Gross-Pitaevskii equation (nonlinear Schrödinger equation) with a time-dependent external potential $V_s = V_s(x)$,

$$\mathrm{i}\varepsilon\partial_s\Psi_s = -\Delta\Psi_s + V_s\Psi_s + b|\Psi_s|^2\Psi_s\,, \tag{5.1.1}$$

and initial data $\Psi_0$ which is small in $L^2(\mathbb{R}^3)$ and $b = \pm 1$ (focusing resp. defocusing nonlinearity)[1]. As before the microscopic time $s = \varepsilon t$ takes values in $[0, 1]$. The stationary equation reads

$$-\Delta\psi_{E,s} + V_s\psi_{E,s} + b|\psi_{E,s}|^2\psi_{E,s} = E\psi_{E,s} \tag{5.1.2}$$

and its solutions are referred to as *ground states* since they solve the Euler-Lagrange equation for the Gross-Pitaevskii energy functional

$$I[\psi_{E,s}] := \int_{\mathbb{R}^3} d^3x\ \left(\frac{1}{2}|\nabla\psi_{E,s}|^2 + V_s|\psi_{E,s}|^2 + \frac{b}{4}|\psi_{E,s}|^4\right), \tag{5.1.3}$$

with $\|\psi_{E,s}\|_2^2 = \eta$ fixed.

Equation (5.1.1) constitutes an effective description for the dynamics of a Bose-Einstein condensate in an external trap $V_s$ and can be rigorously derived from the many-body Schrödinger dynamics in the limit of large particle numbers $N \to \infty$ if the interaction potential among the particles is scaled suitably with $N$; see [Sch09] for a survey yet also [Pic10] for a recent theorem. Such results however are not uniform in the macroscopic time $t = s/\varepsilon$ and hence we will - in the spirit of Chapter 4 - take Equation (5.1.1) as our starting point: Issues concerning the interchangeability of adiabatic and particle number limit will not be addressed.

Physically speaking we consider a situation where the experimentalist is allowed to slowly tune the parameters which determine the shape of the trapping potential $V_s$. For our main result we shall assume that $V_s$ decays at infinity ("weak trap") and that the linear Hamiltonian $-\Delta + V_s$ admits exactly one bound state for each $s$. After adding the nonlinearity this bifurcates into a whole manifold of ground states. Under the assumption that $\Psi_0$ belongs to this manifold we will show that, up to phase, $\Psi_1$ converges to an element in the ground state manifold at $s = 1$ with equal mass as $\varepsilon \searrow 0$. In fact the error term will be $O(\varepsilon)$ and is thus reminiscent of linear adiabatic theorems in presence of a gap condition.

[1] Equivalently $\|\Psi_0\|_2 = 1$ and $|b| \ll 1$ as is seen from the replacements $\Psi_s \rightsquigarrow \Psi_s/\|\Psi_s\|_2$ and $b \rightsquigarrow b\|\Psi_s\|_2^2$ and mass conservation.

To our knowledge the non-autonomous setting considered here - contrary to the autonomous case (e.g. [SW90, SW92, YT02, FGJS04, SW04]) - has not yet been subject to intensive investigations: A *space*-adiabatic theorem is found in [Sal08], however we are not aware of nonlinear *time*-adiabatic theorems for the Gross-Pitaevskii equation.

Interestingly, the techniques we apply differ from the ones in the linear case. The main difficulty is that by linearizing the Gross-Pitaevskii equation around a ground state one obtains an operator which does no longer give rise to a unitary evolution on $L^2(\mathbb{R}^3)$ and therefore makes it more delicate to estimate the error terms. This problem however can be dealt with by a bootstrap argument where we will make use of the dispersive behavior of the *linear* Schrödinger equation (see [Sch05] for a survey and [Gol06] for a recent result).

The organization of this chapter is as follows. We start in Section 5.2 with a proposition that establishes the existence and regularity of a ground state manifold for Equation (5.1.2). This enables us to give a precise statement of the main theorem in Section 5.3. In order to be able to prove it we show $H^2(\mathbb{R}^3)$-wellposedness for Equation (5.1.1) in Section 5.4 and discuss the relevant properties of an appropriate linearization in Section 5.5. This allows us to cast the main theorem in a more convenient form which we then prove (Sections 5.6 and 5.7). To improve the readability we have placed the proofs concerning the ground state manifold and several auxiliary results in Section 5.8.

## 5.2. Ground state manifold: Existence and regularity

### 5.2.1. Hypotheses on the potential

Here we state the general assumptions for the potential $V_s$. *Unless stated otherwise they will be standing hypotheses throughout this chapter.*

We use the standard notation $H^{2,\sigma}(\mathbb{R}^3) := \{\phi : \mathbb{R}^3 \to \mathbb{C} | \|\phi\|_{H^{2,\sigma}} := \|\langle x\rangle^\sigma \phi\|_{H^2} < \infty\}$, $\langle x\rangle := \sqrt{1+|x|^2}$.

($\mathrm{H_d}$) $V_\cdot \in C([0,1]; H^{2,\sigma}(\mathbb{R}^3)) \cap C^2([0,1]; L^\infty(\mathbb{R}^3))$ *for a* $\sigma > 2$.

($\mathrm{H_e}$) *For every* $s \in [0,1]$, $-\Delta + V_s$ *admits exactly one eigenstate* $v_{*,s}$. *The associated eigenvalue* $E_{*,s}$ *is separated from the rest of the spectrum of* $-\Delta + V_s$, *uniformly in* $s$: *there is* $G_0 > 0$ *such that* $E_{*,s} \leq -G_0$ *for all* $s$.

($\mathrm{H_r}$) *For every* $s \in [0,1]$, $V_s$ *admits no zero energy resonance, that is, the equation*

$$(-\Delta + V_s)\, g = 0$$

*admits no distributional solution* $g \notin L^2(\mathbb{R}^3)$ *such that* $\langle x\rangle^{-\beta} g \in L^2(\mathbb{R}^3)$ *for every* $\beta > 1/2$.

**Remark 5.1.** *Note that* ($\mathrm{H_d}$) *implies a spatial decay of* $V_s(x) \sim \langle x\rangle^{-\sigma}$ *due to Sobolev's embedding:*

$$\sup_{x\in\mathbb{R}^3} |\langle x\rangle^\sigma V_s(x)| = \|\langle x\rangle^\sigma V_s\|_\infty \lesssim \|V_s\|_{H^{2,\sigma}} .$$

*We will prove in Subsection 5.8.1 that this implies pointwise exponential decay estimates for* $v_{*,s}$ *resp.* $\Delta v_{*,s}$.

### 5.2.2. Ground state manifold

We present the proposition which establishes in particular the existence of a curve of constant mass in the manifold of instantaneous stationary states for Equation (5.1.1). More generally, our result yields a differentiable manifold of nonlinear ground states. Before stating it we introduce some notation. By

$$P^d_{H_s} := |v_{*,s}\rangle \langle v_{*,s}| \,, \tag{5.2.1}$$

$$P^c_{H_s} := \mathbb{1} - P^d_{H_s} \tag{5.2.2}$$

we denote the spectral projections on the eigenvector space of $-\Delta + V_s$ and its orthogonal complement. Moreover, we declare that a subindex in Landau's $O$-symbol denotes the space in which the statement is to be understood.

**Proposition 5.2.** *Let $s \in [0,1]$, $\eta \ll 1$, $0 \leq (E - E_{*,s})/b \ll 1$ and $l \in \mathbb{R}$.*

*(i) The "time-independent" Gross-Pitaevskii equation (5.1.2) admits a family of nonlinear ground states $\psi_{E,s} > 0$ which bifurcate from the zero solution:*

$$\psi_{E,s} = \sqrt{\frac{E - E_{*,s}}{b}} \frac{1}{\sqrt{\langle v^2_{*,s}, v^2_{*,s}\rangle}} v_{*,s} + O_{H^{2,l}}(E - E_{*,s})\,.$$

*In fact, $\psi_{E,s}$ is analytic in $\sqrt{\frac{E-E_{*,s}}{b}}$ and $P^c_{H,s}\psi_{E,s} = O_{H^{2,l}}\left( \left(\frac{E-E_*}{b}\right)^{\frac{3}{2}}\right)$.*

*(ii) The ground states $\psi_{E,s}$ form a two-dimensional Banach manifold $\mathcal{M} \subset H^{2,l}(\mathbb{R}^3)$. For fixed $s$ the assertions in (i) hold and the map $s \mapsto \psi_{E,s} \in H^{2,l}(\mathbb{R}^3)$ is $C^2$.*

*(iii) There exists a unique positive family of ground states $s \mapsto \psi_{E_s,s} \in C^2([0,1]; H^{2,l}(\mathbb{R}^3))$ with constant mass, $\|\psi_{E_s,s}\|_2^2 \equiv \eta$.*

The proof is somewhat lengthy and therefore deferred to Subsection 5.8.1.

## 5.3. Main theorem

The notion of a family of ground states allows to formulate the following adiabatic theorem.

**Theorem 5.3.** *Let $\Psi_0 = \psi_{E_0,0}$ with $\|\psi_{E_0,0}\|_2^2 = \eta \ll 1$ as above and $\varepsilon \ll 1$. Then Equation (5.1.1) possesses a unique solution $s \mapsto \Psi_s$ in $C^1([0,1]; H^2(\mathbb{R}^3))$ with the property that*

$$\sup_{0\leq s\leq 1} \|\Psi_s - \mathrm{e}^{-\mathrm{i}\zeta_s}\psi_{E_s,s}\|_{H^2} \lesssim \varepsilon\,.$$

*Here, $\zeta_s := \xi^\varepsilon_s + \frac{1}{\varepsilon}\int_0^s E_{s'}ds'$ and $\xi^\varepsilon_s$ is a real function, uniformly bounded in $s$ and $\varepsilon$.*

The unaesthetic factor $\mathrm{e}^{\mathrm{i}\zeta_s}$ is avoided by going over to projectors. Dirac notation allows us to formulate the following immediate corollary of Theorem 5.3.

**Corollary 5.4.** *Under the assumptions in Theorem 5.3*

$$\sup_{0\leq s\leq 1} \|\, |\Psi_s\rangle \langle \Psi_s| - |\psi_{E_s,s}\rangle \langle \psi_{E_s,s}|\, \|_{L^2\to L^2} \lesssim \varepsilon\,.$$

## 5.4. Local well-posedness

The local existence of solutions for the nonlinear Schrödinger equation is well known even in the energy class $H^1(\mathbb{R}^3)$, see e.g. [GV84a, GV84b]. The case considered here is easier[2] and for convenience we present our own argument for it.

**Proposition 5.5** (Local Well-Posedness in $H^2(\mathbb{R}^3)$). *Let $\varepsilon > 0$. For $\Psi_0 \in H^2(\mathbb{R}^3)$ and $\tau = \tau(\varepsilon) \ll 1$,*

$$\mathrm{i}\varepsilon\partial_s\Psi_s = -\Delta\Psi_s + V_s\Psi_s + b|\Psi_s|^2\Psi_s.$$

*has a unique solution in $C^1([0,\tau];H^2(\mathbb{R}^3))$. Furthermore, every solution can be extended uniquely to a maximal (forward) time inverval $[0,T) \subset [0,1]$ or $[0,1]$ and in the first case*

$$\lim_{s\nearrow T} \|\Psi_s\|_{H^2} = \infty \qquad \textit{(blow-up alternative).}$$

Proof. The proof is an application of the Banach fixed point theorem. To cast the equation into a convenient form we use Duhamel's formula to obtain

$$\Psi_s = (\mathcal{T}\Psi)(s) := \mathrm{e}^{\mathrm{i}\Delta s/\varepsilon}\Psi_0 - \frac{\mathrm{i}}{\varepsilon}\int_0^s du\ \mathrm{e}^{\mathrm{i}\Delta(s-u)/\varepsilon}\left(V_u\Psi_u + b|\Psi_u|^2\Psi_u\right). \tag{5.4.1}$$

Now we study the map

$$\mathcal{T} : C([0,\tau];H^2(\mathbb{R}^3)) \to C([0,\tau];H^2(\mathbb{R}^3)).$$

To make the fixed point theorem applicable we have to verify that $\mathcal{T}$ meets two criteria:

(i) $\mathcal{T}$ maps a small ball around 0 in $C([0,\tau];H^2(\mathbb{R}^3))$ to itself,

(ii) $\mathcal{T}$ is contractive on that ball.

For the first use Lemma 5.6 below and $\|\mathrm{e}^{\frac{\mathrm{i}\Delta s}{\varepsilon}}\Psi_0\|_{H^2} = \|\Psi_0\|_{H^2}$ to obtain

$$\sup_{0\le u\le\tau} \|(\mathcal{T}\Psi)(u)\|_{H^2} \le C\left(\|\Psi_0\|_{H^2} + \frac{\tau}{\varepsilon}\left(\sup_{0\le u\le 1}\|V_u\|_{H^2}M_\tau + M_\tau^3\right)\right)$$

where $M_\tau := \sup_{0\le u\le\tau}\|\Psi_u\|_{H^2} = \|\Psi\|_{C([0,\tau];H^2(\mathbb{R}^3))}$. For

$$\tau \le \frac{\varepsilon/2}{\sup_{0\le s\le 1}\|V_s\|_{H^2} + (2C\|\Psi_0\|_{H^2})^2}$$

$\mathcal{T}$ is indeed a map from to complete metric space

$$B_{2C\|\Psi_0\|_{H^2}} := \{\Psi \in C([0,\tau];H^2(\mathbb{R}^3)) : \Psi(0) = \Psi_0 \text{ and } \|\Psi\|_{C([0,\tau];H^2(\mathbb{R}^3))} \le 2C\|\Psi_0\|_{H^2}\}$$

to itself.

Now we verify the contractiveness. For $\Psi,\ \tilde{\Psi} \in B_{2C\|\Psi_0\|_{H^2}}$

$$\|\mathcal{T}\Psi - \mathcal{T}\tilde{\Psi}\|_{C([0,\tau];H^2(\mathbb{R}^3))} \le \frac{\tau}{\varepsilon}C'\left(\sup_{0\le u\le 1}\|V_u\|_{H^2} + \|\Psi_0\|_{H^2}^2\right)\|\Psi - \tilde{\Psi}\|_{C([0,\tau];H^2(\mathbb{R}^3))}.$$

[2] A remark for the time-independent, defocusing case: Note that the *global* existence theory is harder on $H^2(\mathbb{R}^3)$ since energy conservation no longer controls the norm.

Thus by choosing $\tau$ to satisfy

$$\tau < \min\{\frac{\varepsilon}{C'\left(\sup_{0\le u\le 1}\|V_u\|_{H^2}+\|\Psi_0\|_{H^2}^2\right)}, \frac{\varepsilon/2}{\sup_{0\le u\le 1}\|V_u\|_{H^2}+(2C\|\Psi_0\|_{H^2})^2}\} \tag{5.4.2}$$

we see that $\mathcal{T}$ defines a strict contraction on $B_{2C\|\Psi_0\|_{H^2}}$ and hence has a fixed point $\Psi$. Inspection of (5.4.1) yields $\Psi \in C^1([0,\tau]; H^2(\mathbb{R}^3))$.

Next, the maximal time interval of existence is open in $[0,1]$ for if it were $[0,T]$ for a $T<1$, we could extend it at $t=T$ by the just established local existence result.

Finally, assume that the blow-up alternative is wrong, that is, there is a finite number $M$ such that $\|\Psi_s\|_{H^2} \le M$ for all $s$ in the maximal interval of existence $[0,T)$. Note that in (5.4.2) $\tau$ depends on the *norm* of the initial data only. Thus exchanging $\|\Psi_0\|_{H^2}$ for $M$ there defines a $\tau^*$ and applying local existence to $\Psi_{T-\tau^*/2}$ as initial data implies a contradiction to the maximality of $[0,T)$. □

In the proof of Proposition 5.5 we have used the following well-known results, some of which will also be important later on.

**Lemma 5.6.**

*(i)* $\|\phi\|_{H^2} \simeq \|\phi\|_2 + \|(-\Delta+V)\phi\|_2$.

*(ii) For any* $l\in\mathbb{R}$

$$\|\phi\|_{H^{2,l}} \simeq \|\langle x\rangle^l\phi\|_2 + \|\langle x\rangle^l\Delta\phi\|_2 .$$

*(iii) Product estimates (*$\|\phi\|_{W^{2,1}} := \|\phi\|_1 + \|\Delta\phi\|_1$*):*

$$\|\phi\chi\|_{W^{2,1}} \lesssim \|\phi\|_{H^2}\|\chi\|_{H^2}, \tag{5.4.3}$$

$$\|\phi\chi\|_{H^2} \lesssim \|\phi\|_{H^2}\|\chi\|_{H^2}, \tag{5.4.4}$$

$$\|\phi\chi\|_{H^{2,l}} \lesssim \|\phi\|_{H^{2,l}}\|\chi\|_{H^{2,l}}, \qquad \text{(if } l\ge 0\text{)}. \tag{5.4.5}$$

A proof is given in Subsection 5.8.2.

## 5.5. Linearization around the ground state

We start with linearizing around the ground state and make a naive[3] ansatz

$$\Psi_s = e^{-\frac{i}{\varepsilon}\int_0^s E_{s'}ds'}(\psi_{E_s,s}+\varphi_s) \tag{5.5.1}$$

in order to linearize Equation (5.1.1) around the ground state. Note that since the nonlinearity in (5.1.1) is not complex analytic in the wave function $\Psi_s$, the linearized operator will only be real linear. It is thus favorable to adopt the notation

$$\vec{\varphi}_s = \begin{pmatrix}\Re\varphi_s\\ \Im\varphi_s\end{pmatrix} = \begin{pmatrix}\varphi_{1,s}\\ \varphi_{2,s}\end{pmatrix} \tag{5.5.2}$$

[3] The ansatz is arguably very naive as it does not reflect possible geometric phase changes (geometric as in the sense of Berry's phase). This will be made good for in Lemma 5.9.

and likewise for any other complex quantity. Plugging (5.6.3) into (5.1.1) yields

$$\dot{\vec{\varphi}}_s = -\frac{1}{\varepsilon} J \begin{pmatrix} -\Delta + V_s - E_s + 3b\psi_{E_s,s}^2 & 0 \\ 0 & -\Delta + V_s - E_s + b\psi_{E_s,s}^2 \end{pmatrix} \vec{\varphi}_s \tag{5.5.3}$$

$$- \frac{d}{ds}\vec{\psi}_{E_s,s} - \frac{1}{\varepsilon} J \begin{pmatrix} b\psi_{E_s,s}|\vec{\varphi}_s|^2 + 2b\psi_{E_s,s}(\varphi_{1,s})^2 + b|\vec{\varphi}_s|^2\varphi_{1,s} \\ 2b\psi_{E_s,s}\varphi_{1,s}\varphi_{2,s} + b|\vec{\varphi}_s|^2\varphi_{2,s} \end{pmatrix} \tag{5.5.4}$$

$$=: \frac{1}{\varepsilon} L_{E_s,s}\vec{\varphi}_s - \frac{d}{ds}\vec{\psi}_{E_s,s} - \frac{1}{\varepsilon} N(\vec{\psi}_{E_s,s}, \vec{\varphi}_s)\,. \tag{5.5.5}$$

Here the linear operator $L_{E,s}$ is naturally defined by (5.5.3) and the nonlinearity $N = N(\vec{\psi}_{E_s,s}, \vec{\varphi}_s)$ by (5.5.4). We used the notation

$$J := \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},$$

and moreover $L_{E,s}$ is considered as an unbounded operator on the Hilbert space $L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$. To facilitate later discussions we define operators $L^+_{E,s}, L^-_{E,s}$ so that $L_{E,s}$ takes the form

$$L_{E,s} = \begin{pmatrix} 0 & L^-_{E,s} \\ -L^+_{E,s} & 0 \end{pmatrix}. \tag{5.5.6}$$

In the rest of this section we study various aspects of $L_{E,s}$. This will eventually yield a convenient reformulation of Theorem 5.3.

### 5.5.1. The zero eigenspace of the linearized operator $L_{E,s}$

Now we study the eigenvalues of the operator $L_{E,s}$. By a direct computation we find that

$$L^-_{E,s}\psi_{E,s} = 0\,.$$

Hence $\left(0, \psi_{E,s}\right)^\intercal$ is an eigenvector of $L_{E,s}$ with eigenvalue 0. Differentiation of the left hand side with respect to $E$ yields

$$L^+_{E,s}\partial_E\psi_{E,s} = \psi_{E,s}\,.$$

It follows that $\left(-\partial_E\psi_{E,s}, 0\right)^\intercal$ is an associated generalized eigenvector of $\left(0, \psi_{E,s}\right)^\intercal$ for $L_{E,s}$. Similarly,

$$L^*_{E,s}\begin{pmatrix} \psi_{E,s} \\ 0 \end{pmatrix} = \begin{pmatrix} 0 & -L^+_{E,s} \\ L^-_{E,s} & 0 \end{pmatrix}\begin{pmatrix} \psi_{E,s} \\ 0 \end{pmatrix} = 0$$

and

$$L^*_{E,s}\begin{pmatrix} 0 \\ \partial_E\psi_{E,s} \end{pmatrix} = -\begin{pmatrix} \psi_{E,s} \\ 0 \end{pmatrix}.$$

**LEMMA 5.7.** *0 is the only eigenvalue of $L_{E,s}$ in the ball of radius $G_0/2$ around zero (cf. ($\mathrm{H_e}$)). More precisely, if $\Gamma$ parametrizes its boundary in counterclockwise direction then*

$$P^d_{E,s} := -\frac{1}{2\pi \mathrm{i}} \oint_\Gamma (L_{E,s} - z)^{-1} dz = \frac{2}{\partial_E \|\psi_{E,s}\|_2^2} \left( \left| \begin{matrix} \partial_E \psi_{E,s} \\ 0 \end{matrix} \right\rangle \left\langle \begin{matrix} \psi_{E,s} \\ 0 \end{matrix} \right| + \left| \begin{matrix} 0 \\ \psi_{E,s} \end{matrix} \right\rangle \left\langle \begin{matrix} 0 \\ \partial_E \psi_{E,s} \end{matrix} \right| \right). \tag{5.5.7}$$

PROOF. By the above considerations

$$\mathrm{span} \left( \left| \begin{matrix} 0 \\ \psi_{E,s} \end{matrix} \right\rangle, \left| \begin{matrix} \partial_E \psi_{E,s} \\ 0 \end{matrix} \right\rangle \right) \subset \mathrm{ran}\, P^d_{E,s},$$
$$\mathrm{span} \left( \left| \begin{matrix} \psi_{E,s} \\ 0 \end{matrix} \right\rangle, \left| \begin{matrix} 0 \\ \partial_E \psi_{E,s} \end{matrix} \right\rangle \right) \subset \mathrm{ran} (P^d_{E,s})^*.$$

*Claim:* These two inclusion are equalities.

To see the claim note that

$$JL_{E,s} = \begin{pmatrix} -\Delta + V_s - E_{*,s} & 0 \\ 0 & -\Delta + V_s - E_{*,s} \end{pmatrix} + A_{E,s} = H_{E_{*,s},s} + A_{E,s},$$

where

$$A_{E,s} = \begin{pmatrix} E_{*,s} - E + 3b\psi^2_{E,s} & 0 \\ 0 & E_{*,s} - E_s + b\psi^2_{E,s} \end{pmatrix} \tag{5.5.8}$$

is a small perturbation with $\|A_{E,s}\|_{L^2 \to L^2} \sim |E_{*,s} - E| \ll 1$. For $z \in \Gamma$,

$$JL_{E,s} - z = H_{E_{*,s},s} + A_{E,s} - z = (H_{E_{*,s},s} - z)(\mathbb{1} + (H_{E_{*,s},s} - z)^{-1} A_{E,s}) \tag{5.5.9}$$

is invertible on $L^2(\mathbb{R}^3)$ by $\|(H_{E_{*,s},s} - z)^{-1}\|_{L^2 \to L^2} = 2/G_0$ and using a Neumann series, in particular

$$\|(JL_{E,s} - z)^{-1}\|_{L^2 \to L^2} \lesssim 1/G_0. \tag{5.5.10}$$

This justifies to write

$$(JL_{E,s} - z)^{-1} - (H_{E_{*,s},s} - z)^{-1} = -(JL_{E,s} - z)^{-1} A_{E,s} (H_{E_{*,s},s} - z)^{-1},$$

and so

$$\begin{aligned} &\Big\| \frac{1}{2\pi \mathrm{i}} \oint_\Gamma (JL_{E,s} - z)^{-1} dz - \frac{1}{2\pi \mathrm{i}} \oint_\Gamma (H_{E_{*,s},s} - z)^{-1} dz \Big\|_{L^2 \to L^2} \\ &\qquad \le \Big\| \frac{1}{2\pi \mathrm{i}} \oint_\Gamma (JL_{E,s} - z)^{-1} A_{E,s} (H_{E_{*,s},s} - z)^{-1} dz \Big\|_{L^2 \to L^2} < 1. \end{aligned} \tag{5.5.11}$$

By [RS78], Lemma on p. 14, it follows that the two spectral projections on the left hand side of this inequality have equal dimension and hence the claim follows from the fact that

$$-\frac{1}{2\pi \mathrm{i}} \oint_\Gamma (H_{E_{*,s},s} - z)^{-1} dz = \left| \begin{matrix} v_{*,s} \\ 0 \end{matrix} \right\rangle \left\langle \begin{matrix} v_{*,s} \\ 0 \end{matrix} \right| + \left| \begin{matrix} 0 \\ v_{*,s} \end{matrix} \right\rangle \left\langle \begin{matrix} 0 \\ v_{*,s} \end{matrix} \right|.$$

is two-dimensional.

We may therefore write

$$P^d_{E,s} = \left| \begin{matrix} 0 \\ \psi_{E,s} \end{matrix} \right\rangle \left( \alpha_1 \left\langle \begin{matrix} \psi_{E,s} \\ 0 \end{matrix} \right| + \alpha_2 \left\langle \begin{matrix} 0 \\ \partial_E \psi_{E,s} \end{matrix} \right| \right) + \left| \begin{matrix} \partial_E \psi_{E,s} \\ 0 \end{matrix} \right\rangle \left( \beta_1 \left\langle \begin{matrix} \psi_{E,s} \\ 0 \end{matrix} \right| + \beta_2 \left\langle \begin{matrix} 0 \\ \partial_E \psi_{E,s} \end{matrix} \right| \right)$$

for some $\alpha_i, \beta_i \in \mathbb{C}$ to be determined. By

$$P^d_{E,s} \left| \begin{matrix} 0 \\ \psi_{E,s} \end{matrix} \right\rangle = \left| \begin{matrix} 0 \\ \psi_{E,s} \end{matrix} \right\rangle ,$$

$\beta_2 = 0$ and by

$$P^d_{E,s} \left| \begin{matrix} \partial_E \psi_{E,s} \\ 0 \end{matrix} \right\rangle = \left| \begin{matrix} \partial_E \psi_{E,s} \\ 0 \end{matrix} \right\rangle ,$$

$\alpha_1 = 0$. But then, by the same equations,

$$\alpha_2 = \beta_1 = \frac{1}{\langle \partial_E \psi_{E,s}, \psi_{E,s} \rangle} = \frac{2}{\partial_E \|\psi_{E,s}\|_2^2} ,$$

which proves the lemma. □

**Remark 5.8.** *We say that $\vec{\chi}_s$ belongs to the continuous subspace if $P^d_{E,s}\vec{\chi}_s = 0$ and we say that it belongs to the discrete subspace if $P^c_{E,s}\vec{\chi}_s := \vec{\chi}_s - P^d_{E,s}\vec{\chi}_s = 0$. That $P^c_{E,s}$ indeed corresponds to the continuous spectrum is true, however, this fact is not needed for the proof of Theorem 5.3 and hence we omit its proof. In that sense these expressions can be viewed as a handy terminology.*

## 5.6. Reformulation of Theorem 5.3

In the proof of the main theorem we shall make explicit use of dispersive estimates. For this, a slightly different decomposition than (5.5.1) turns out to be useful. It relies on the following lemma which can essentially be found in [YT02]. With this tool we will subsequently give a technically more convenient reformulation of Theorem 5.3.

**Lemma 5.9.** *For any $\phi$ with $\|\phi\|_2 \ll 1$ there exist parameters $\hat{E} = \hat{E}(E, s, \phi)$ and $\hat{\gamma} = \hat{\gamma}(E, s, \phi)$, with $\hat{E}(E, s, 0) = E$ and $\hat{\gamma}(E, s, 0) = 0$, such that*

$$\psi_{E,s} + \phi = \mathrm{e}^{i\hat{\gamma}} \left( \psi_{\hat{E},s} + \phi_{\hat{E},s} \right) ,$$

*where $\phi_{\hat{E},s}$ lies in the continuous subspace of $L_{\hat{E},s}$. The dependence of $\hat{E}$, $\hat{\gamma}$ on $E$, $\phi$ is smooth; the dependence on $s$ is $C^2$.*

PROOF. The proof is an application of the implicit function theorem. Recall the conditions for $\phi_{\hat{E},s}$ to be in the continuous subspace of $L_{\hat{E},s}$ (cf. Section 5.5): $\Re\phi_{\hat{E},s} \perp \psi_{\hat{E},s}$ and $\Im\phi_{\hat{E},s} \perp \partial_{\hat{E}}\psi_{\hat{E},s}$. Thus,

$$K_1(\hat{\gamma}, \hat{E}, E, s, \phi) := \langle \Re \left( \mathrm{e}^{-i\hat{\gamma}} \left( \psi_{E,s} + \phi \right) \right) - \psi_{\hat{E},s}, \psi_{\hat{E},s} \rangle = 0\,, \tag{5.6.1}$$

$$K_2(\hat{\gamma}, \hat{E}, E, s, \phi) := \langle \Im \left( \mathrm{e}^{-i\hat{\gamma}} \left( \psi_{E,s} + \phi \right) \right), \partial_{\hat{E}}\psi_{\hat{E},s} \rangle = 0\,. \tag{5.6.2}$$

Whenever $E$ is in a sufficiently small punctured neighborhood of $E_{*,s}$ and $\mathrm{sign}(E-E_*) = \mathrm{sign}(b)$ the function

$$K := (K_1, K_2)^\intercal : \mathbb{R}^4 \times L^2(\mathbb{R}^3) \to \mathbb{R}^2$$

is $C^2$ with respect to $s$ and smooth with respect to the other variables.

To verify the applicability of the implicit function theorem it is important to verify that $K = (K_1, K_2)^\intercal$ satisfies the conditions that

(i) $K(0, E, E, s, 0) = (0, 0)^\intercal$,

(ii) the matrix

$$\left. \begin{pmatrix} \frac{\partial K_1}{\partial \hat{\gamma}} & \frac{\partial K_1}{\partial \hat{E}} \\ \frac{\partial K_2}{\partial \hat{\gamma}} & \frac{\partial K_2}{\partial \hat{E}} \end{pmatrix} \right|_{(0,E,E,s,0)}$$

is invertible.

It is easy to see the first, for the second note that

$$\begin{aligned}
\frac{\partial K_1}{\partial \hat{\gamma}}|_{(0,E,E,s,0)} &= 0\,, \\
\frac{\partial K_1}{\partial \hat{E}}|_{(0,E,E,s,0)} &= -\langle \partial_E \psi_{E,s}, \psi_{E,s} \rangle \neq 0\,, \\
\frac{\partial K_2}{\partial \hat{\gamma}}|_{(0,E,E,s,0)} &= -\langle \psi_{E,s}, \partial_E \psi_{E,s} \rangle \neq 0\,, \\
\frac{\partial K_2}{\partial \hat{E}}|_{(0,E,E,s,0)} &= 0\,.
\end{aligned}$$

Hence there exist unique functions $\hat{E}(E, s, \phi)$ and $\hat{\gamma}(E, s, \phi)$ in a sufficiently small "punctured" neighborhood of $\{(E_{*,s}, s, 0) | s \in [0, 1]\}$ intersected with $\{(E, s, 0) | \mathrm{sign}(E - E_{*,s}) = \mathrm{sign}(b)\}$. $\hat{E}$ and $\hat{\gamma}$ satisfy Equations (5.6.1, 5.6.2) identically with the asserted regularity. □

In figurative language what the lemma says is the following: As long as $\varphi_s$ in Ansatz (5.5.1) is sufficiently small, then, at the cost of introducing an additional phase $\gamma_s^\varepsilon$, we can "shadow" $\psi_{E_s,s} \in \mathcal{M}$ by $\psi_{E_s^\varepsilon,s}$ such that

$$\Psi_s = e^{-\frac{i}{\varepsilon}(\int_0^s E_{s'}^\varepsilon ds' - \gamma_s^\varepsilon)} (\psi_{E_s^\varepsilon,s} + \phi_s) \tag{5.6.3}$$

with $P^d_{E_s^\varepsilon,s}\phi_s = 0$.

In the following we reformulate Theorem 5.3 in terms of estimates on various components of (5.6.3). Equation (5.5.5) is modified to (recall the convention (5.5.2))

$$\dot{\vec{\phi}}_s = \frac{1}{\varepsilon}L_s\vec{\phi}_s - \frac{1}{\varepsilon}\dot{\gamma}^\varepsilon_s J\vec{\phi}_s - \frac{d}{ds}\vec{\psi}_{E^\varepsilon_s,s} - \frac{1}{\varepsilon}\dot{\gamma}^\varepsilon_t J\vec{\psi}_{E^\varepsilon_s,s} - \frac{1}{\varepsilon}N(\vec{\psi}_{E^\varepsilon_s,s},\vec{\phi}_s)\,, \tag{5.6.4}$$

where $L_s := L_{E^\varepsilon_s,s}$ and, for later use, $P^d_s := P^d_{E^\varepsilon_s,s}$.

As a first consequence we derive equations for $\dot{E}^\varepsilon_s, \dot{\gamma}^\varepsilon_s$, the *modulation equations*. To that end recall the condition $P^d_s\vec{\phi}_s = 0$, which, by (5.5.7) amounts to

$$\left\langle \vec{\phi}_s \,\middle|\, \begin{matrix}\psi_{E,s}\\ 0\end{matrix} \right\rangle = \left\langle \vec{\phi}_s \,\middle|\, \begin{matrix}0\\ \partial_E\psi_{E,s}\end{matrix} \right\rangle = 0\,.$$

By this and Equation (5.6.4) we obtain

$$\begin{aligned}\dot{E}^\varepsilon_s(\langle\partial_E\psi_{E^\varepsilon_s,s},\phi_{1,s}\rangle - \langle\psi_{E^\varepsilon_s,s},\partial_E\psi_{E^\varepsilon_s,s}\rangle) + \frac{\dot{\gamma}^\varepsilon_s}{\varepsilon}\langle\psi_{E^\varepsilon_s,s},\phi_{2,s}\rangle &= -\langle\partial_s\psi_{E^\varepsilon_s,s},\phi_{1,s}\rangle + \langle\psi_{E^\varepsilon_s,s},\partial_s\psi_{E^\varepsilon_s,s}\rangle\\ &\quad + \frac{1}{\varepsilon}\langle\psi_{E^\varepsilon_s,s},N(\vec{\psi}_{E^\varepsilon_s,s},\vec{\phi}_s)\rangle,\end{aligned} \tag{5.6.5}$$

$$\begin{aligned}\dot{E}^\varepsilon_s\langle\partial^2_E\psi_{E^\varepsilon_s,s},\phi_{2,s}\rangle - \frac{\dot{\gamma}^\varepsilon_s}{\varepsilon}(\langle\partial_E\psi_{E^\varepsilon_s,s},\phi_{1,s}\rangle + \langle\partial_E\psi_{E^\varepsilon_s,s},\psi_{E^\varepsilon_s,s}\rangle) &= \frac{1}{\varepsilon}\langle\partial_E\psi_{E^\varepsilon_s,s},N(\vec{\psi}_{E^\varepsilon_s,s},\vec{\phi}_s)\rangle\\ &\quad - \langle\partial_s\partial_E\psi_{E^\varepsilon_s,s},\phi_{2,s}\rangle\,.\end{aligned} \tag{5.6.6}$$

Next, it turns out that we also need to establish a refined decomposition for the quantity $\vec{\phi}_s$ itself as follows

$$\vec{\phi}_s = \varepsilon L_s^{-1}P^c_s\frac{d}{ds}\vec{\psi}_{E^\varepsilon_s,s} + \vec{\tilde{\phi}}_s = \varepsilon L_s^{-1}P^c_s\partial_s\vec{\psi}_{E^\varepsilon_s,s} + \vec{\tilde{\phi}}_s\,. \tag{5.6.7}$$

By Lemma 5.7, $L_s^{-1} : P^c_s(L^2(\mathbb{R}^3)) \to P^c_s(L^2(\mathbb{R}^3))$ is a well-defined bounded operator. The second equality in (5.6.7) is a consequence of Equation (5.5.7). In particular, we obtain as initial data for Theorem 5.3

$$\vec{\tilde{\phi}}_0 = -\varepsilon L_0^{-1}P^c_0\partial_s\vec{\psi}_{E^\varepsilon_s,s}|_{t=0} = -\varepsilon L_0^{-1}P^c_0\partial_s\vec{\psi}_{E_s,s}|_{s=0}\,. \tag{5.6.8}$$

The proof of the following regularity lemma is given in Subsection 5.8.2.

**Lemma 5.10.** *For* $(E,s)$ *sufficiently close to* $(E_{*,s},s)$ *and* $\operatorname{sign}(E-E_{*,s}) = \operatorname{sign}(b)$ *the map*

$$\begin{aligned}\Phi : \mathbb{R}^2 &\to H^{2,\sigma}(\mathbb{R}^3)\\ (E,s) &\mapsto L^{-1}_{E,s}P^c_s\partial_s\vec{\psi}_{E,s}\end{aligned}$$

*is well-defined and continuously differentiable.*

To complement the modulation equations we may now continue the analysis of Equation (5.6.4) in the range of $P^c_s$. Plugging the Decomposition (5.6.7) into (5.6.4) yields the equation for $\vec{\tilde{\phi}}_s$,

$$\begin{aligned}\dot{\vec{\tilde{\phi}}}_s = \frac{1}{\varepsilon}L_s\vec{\tilde{\phi}}_s - \frac{\dot{\gamma}^\varepsilon_s}{\varepsilon}J\vec{\tilde{\phi}}_s - \dot{\gamma}^\varepsilon_s JL_s^{-1}P^c_s\partial_s\vec{\psi}_{E^\varepsilon_s,s} - P^d_s\frac{d}{ds}\vec{\psi}_{E^\varepsilon_s,s} - \frac{\dot{\gamma}^\varepsilon_s}{\varepsilon}J\vec{\psi}_{E^\varepsilon_s,s} - \varepsilon\frac{d}{ds}(L_s^{-1}P^c_s\partial_s\vec{\psi}_{E^\varepsilon_s,s})\\ - \frac{1}{\varepsilon}N(\vec{\psi}_{E^\varepsilon_s,s},\varepsilon L_s^{-1}P^c_s\partial_s\vec{\psi}_{E^\varepsilon_s,s} + \vec{\tilde{\phi}}_s)\,.\end{aligned}$$

We put $P_s^c$ on both sides and use $\dot{\tilde{\vec{\phi}}}_s = \dot{P}_s^c\tilde{\vec{\phi}}_s + P_s^c\dot{\tilde{\vec{\phi}}}_s = -\dot{P}_s^d\tilde{\vec{\phi}}_s + P_s^c\dot{\tilde{\vec{\phi}}}_s$ in order to obtain

$$\dot{\tilde{\vec{\phi}}}_s = \frac{1}{\varepsilon}L_s\tilde{\vec{\phi}}_s - \frac{\dot{\gamma}_s^\varepsilon}{\varepsilon}P_s^c J\tilde{\vec{\phi}}_s - \dot{P}_s^d\tilde{\vec{\phi}}_s - \dot{\gamma}_s^\varepsilon P_s^c J L_s^{-1}P_s^c\partial_s\vec{\psi}_{E_s^\varepsilon,s} - \frac{\dot{\gamma}_s^\varepsilon}{\varepsilon}\underbrace{P_s^c J\vec{\psi}_{E_s^\varepsilon,s}}_{=0} - \varepsilon P_s^c\frac{d}{ds}(L_s^{-1}P_s^c\partial_s\vec{\psi}_{E_s^\varepsilon,s})$$
$$-\frac{1}{\varepsilon}P_s^c N(\vec{\psi}_{E_s^\varepsilon,s}, \varepsilon L_s^{-1}P_s^c\partial_s\vec{\psi}_{E_s^\varepsilon,s} + \tilde{\vec{\phi}}_s)\,. \tag{5.6.9}$$

The announced reformulation of Theorem 5.3 reads as follows:

**Theorem 5.11** (Reformulation of Theorem 5.3). *$\tilde{\vec{\phi}}_s, E_s^\varepsilon, \gamma_s^\varepsilon$ satisfy the following estimates:*

$$\sup_{0\le s\le 1}|E_s^\varepsilon - E_s| \lesssim \varepsilon\,, \tag{5.6.10}$$
$$\sup_{0\le s\le 1}|\dot{\gamma}_s^\varepsilon| \lesssim \varepsilon^2\,, \tag{5.6.11}$$
$$\sup_{0\le s\le 1}\|\tilde{\vec{\phi}}_s\|_{H^2} \lesssim \varepsilon\,. \tag{5.6.12}$$

Clearly, Theorem 5.11 implies Theorem 5.3: with $\xi_s^\varepsilon := \frac{1}{\varepsilon}\int_0^s \left(E_{s'}^\varepsilon - E_{s'}\right) ds'$ it follows that

$$\begin{aligned}\sup_{0\le s\le 1}\|\Psi_s - \mathrm{e}^{-\mathrm{i}(\xi_s^\varepsilon + \frac{1}{\varepsilon}\int_0^s E_{s'}ds')}\psi_{E_s,s}\|_{H^2} &= \sup_{0\le s\le 1}\|\mathrm{e}^{\mathrm{i}\frac{\gamma_s^\varepsilon}{\varepsilon}}(\psi_{E_s^\varepsilon,s} + \phi_s) - \psi_{E_s,s}\|_{H^2}\\ &\lesssim \sup_{0\le s\le 1}\|\psi_{E_s^\varepsilon,s} - \psi_{E_s,s}\|_{H^2} + \sup_{0\le s\le 1}\|\phi_s\|_{H^2} + \varepsilon\\ &\lesssim \varepsilon\,.\end{aligned}$$

The first inequality makes use of (5.6.11), the second of Proposition 5.2 in combination with (5.6.10) as well as (5.6.12).

## 5.7. Proof of Theorem 5.11

In this section we prove Theorem 5.11. We begin with presenting the main ideas. The core of the proof is a bootstrap argument. Specifically: Recall that $\sigma > 2$. Define a locally controlling function $M_s^{(l)}$ as

$$M_s^{(\mathrm{l})} := \sup_{0\le s'\le s}\|\tilde{\vec{\phi}}_{s'}\|_{H^{2,-\sigma}}$$

and a globally controlling function $M_s^{(\mathrm{g})}$ as

$$M_s^{(\mathrm{g})} := \sup_{0\le s'\le s}\|\tilde{\vec{\phi}}_{s'}\|_{H^2}\,,$$

cf. Equation (5.6.7). We formulate the bootstrap assumptions

(B$_\mathrm{l}$) $\qquad M_s^{(\mathrm{l})} \le 2A\varepsilon\|L_0^{-1}P_0^c\partial_s\vec{\psi}_{E_s,s}|_{s=0}\|_{H^2\cap W^{2,1}}\quad,$

(B$_\mathrm{g}$) $\qquad M_s^{(\mathrm{g})} \le \varepsilon^{\frac{2}{3}}\quad,$

where $A$ is the constant in the dispersive Estimate (5.7.18) below. If $L_0^{-1}P_0^c\partial_s\vec{\psi}_{E_0,s}=0$ then $(\mathrm{B_l})$ is replaced by

$$(\mathrm{B_l'}) \qquad M_s^{(\mathrm{l})}\le\varepsilon\ .$$

Note that in view of Equation (5.6.7): $\|\vec{\phi}_{s'}\|_{H^{2,-\sigma}}\lesssim\varepsilon$ and $\|\vec{\phi}_{s'}\|_{H^{2,-\sigma}}\lesssim\varepsilon^{\frac{2}{3}}$ (both uniformly in $s'\le s\le 1$) under these assumptions.

We then first establish the assertion of Theorem 5.11 only for a small subinterval of positive length $[0,s_0]\subset[0,1]$. Here $s_0$ is independent of $\varepsilon$ if the latter is sufficiently small. We show that, given bootstrap assumption $(\mathrm{B_l})$, resp. $(\mathrm{B_l'})$ we can control the derivatives of the modulation parameters, $\dot{E}_s^\varepsilon$ and $\dot{\gamma}_s^\varepsilon$, given by (5.6.5, 5.6.6).

With this at hand we may turn to the analysis of $\tilde{\vec{\phi}}_s$ itself, which lies in the continuous subspace of the linear operator $L_s$. Here we make use of dispersive estimates for the propagator of a reference Hamiltonian $H_0$. This, together with bootstrap assumption $(\mathrm{B_g})$, will enable us to improve the estimates for $\tilde{\vec{\phi}}_s$ on the small interval $[0,s_0]$. The assertion then follows from a continuity argument.

In a second step, we extend the result to the whole interval $[0,1]$ using essentially the same reasoning.

### 5.7.1. Theorem 5.11 for small times

Mathematically, the main work for the proof of Theorem 5.11 lies in the demonstration of its validity on a small interval $[0,s_0]$ with $s_0$ being independent of $\varepsilon$.

The most important Estimate (5.6.12) of Theorem 5.11 is captured by the following proposition (the Estimates (5.6.10, 5.6.11) are treated in Subsection 5.7.2):

**Proposition 5.12** (Theorem 5.11 for small times). *There exists $s_0>0$ such that whenever $(\mathrm{B_l},\mathrm{B_g})$ resp. $(\mathrm{B_l'},\mathrm{B_g})$ hold for $s\le s_0$ then in fact the better estimates*

$$M_s^{(\mathrm{l})}\le\frac{5}{3}A\varepsilon\|L_0^{-1}P_0^c\partial_s\vec{\psi}_{E_0,s}|_{s=0}\|_{H^2\cap W^{2,1}}\ , \tag{5.7.1}$$

$$M_s^{(\mathrm{g})}\lesssim\varepsilon \tag{5.7.2}$$

*are true for all $\varepsilon\ll 1$. If $L_0^{-1}P_0^c\partial_s\vec{\psi}_{E_0,s}=0$ then (5.7.1) is replaced by*

$$M_s^{(l)}\lesssim\varepsilon^2\,. \tag{5.7.3}$$

*The implicit multiplicative constants in (5.7.2, 5.7.3) are uniform in $s\in[0,s_0]$. It follows that*

$$M_{s_0}^{(\mathrm{g})}\lesssim\varepsilon \tag{5.7.4}$$

*for all $\varepsilon\ll 1$.*

Clearly, Estimate (5.7.4) follows from (5.7.1, 5.7.2): By Proposition 5.5 and Lemma 5.10 $\|\tilde{\vec{\phi}}_s\|_{H^2}$ depends continuously on $s$ and hence so does $\|\tilde{\vec{\phi}}_s\|_{H^{2,-\sigma}}$. By (5.6.8) the initial data satisfies

$$\|\tilde{\vec{\phi}}_0\|_{H^{2,-\sigma}}\le A\varepsilon\|L_0^{-1}P_0^c\partial_s\vec{\psi}_{E_s,s}|_{s=0}\|_{H^2\cap W^{2,1}}\ ,$$

$$\|\tilde{\vec{\phi}}_0\|_{H^2}\le\varepsilon\|L_0^{-1}P_0^c\partial_s\vec{\psi}_{E_s,s}|_{s=0}\|_{H^2}\ ,$$

resp.

$$\vec{\tilde{\phi}}_0 = 0 \qquad \text{if } L_0^{-1} P_0^c \partial_s \vec{\psi}_{E_s,s} = 0\,.$$

Hence there is a maximal $0 < \tau \leq s_0$ such that ($\mathrm{B_l}$, $\mathrm{B_g}$) resp. ($\mathrm{B'_l}$, $\mathrm{B_g}$) are satisfied with $s = \tau$ as long as $\varepsilon \ll 1$. Note that *a priori* $\tau$ may depend on $\varepsilon$. But in fact, $\tau = s_0$: If we assume $\tau < s_0$, then by Estimates (5.7.1, 5.7.2) and continuity of the norms it follows that ($\mathrm{B_l}$, $\mathrm{B_g}$) resp. ($\mathrm{B'_l}$, $\mathrm{B_g}$) also hold on a slightly bigger interval than $[0, \tau]$. This contradicts the maximality of $\tau$.

In order to show Estimates (5.7.1, 5.7.2) we first establish controls for the modulation parameters. This will also yield the remaining assertions (Estimates (5.6.11, 5.6.12)) of Theorem 5.11 on $[0, s_0]$.

### 5.7.2. Control of modulation parameters

The two remaining Estimates (5.6.10, 5.6.11) of Theorem 5.11 are obtained by considering the modulation equations (5.6.5, 5.6.6): Since $\mathcal{M} \subset H^{2,l}(\mathbb{R}^3)$ for every $l \geq 0$ is a $C^2$-manifold it is immediate that every scalar product in (5.6.5) and (5.6.6) which involves $\phi_s$ is of order $\varepsilon$ whenever assumption ($\mathrm{B_l}$) resp. ($\mathrm{B'_l}$) holds. For $\varepsilon \ll 1$ it follows that

$$|\dot{E}_s^\varepsilon| \lesssim 1\,, \tag{5.7.5}$$

$$|\dot{\gamma}_s^\varepsilon| \lesssim \varepsilon^2\,, \tag{5.7.6}$$

both implicit relative constants being uniform in $s$. Furthermore the following holds:

**Lemma 5.13.** *If* ($\mathrm{B_l}$) *resp.* ($\mathrm{B'_l}$) *holds then*

$$|E_s^\varepsilon - E_s| \lesssim \varepsilon\,,$$

*uniformly in* $s$.

Proof. We apply a Grönwall-type argument. The function $f(E,s) := -\frac{\langle \psi_{E,s}, \partial_s \psi_{E,s}\rangle}{\langle \psi_{E,s}, \partial_E \psi_{E,s}\rangle}$ is $C^1$ in $s$ and smooth in $E$ by Proposition 5.2. By ($\mathrm{B_l}$) and (5.6.5)

$$\dot{E}_s^\varepsilon = f(E_s^\varepsilon, s) + O(\varepsilon)\,,$$

where $O(\varepsilon)$ is uniformly bounded in $s$. By constancy of $\langle \psi_{E_s,s}, \psi_{E_s,s}\rangle$ also

$$\dot{E}_s = f(E_s, s)\,.$$

Therefore the mean value theorem applied to $f$ yields

$$\begin{aligned} \dot{E}_s^\varepsilon - \dot{E}_s &= f(E_s, s) - f(E_s^\varepsilon, s) + O(\varepsilon) \\ &\leq C\,(|E_s^\varepsilon - E_s| + \varepsilon)\,, \end{aligned} \tag{5.7.7}$$

with an $s$-independent constant $C$ and thus, using $E_0^\varepsilon = E_0$ (see Theorem 5.3)

$$|E_s^\varepsilon - E_s| \leq C\varepsilon s + C \int_0^s |E_{s'}^\varepsilon - E_{s'}| ds'\,.$$

This last inequality yields for $x(s) := \mathrm{e}^{-Cs} \int_0^s ds'\, |E_{s'}^\varepsilon - E_{s'}|$

$$\dot{x}(s) \leq C\varepsilon s \mathrm{e}^{-Cs}$$

which, after integration, implies the claim. □

### 5.7.3. Proof of Proposition 5.12

We now turn to the proof of the remaining Estimates (5.7.1, 5.7.2) in Proposition 5.12. Our starting point is the following refinement of Equation (5.6.9)

$$\dot{\tilde{\vec{\phi}}}_s = -\frac{1}{\varepsilon}J(H_{E_s^\varepsilon,u} + \dot\gamma_s^\varepsilon)\tilde{\vec{\phi}}_s + \frac{1}{\varepsilon}(L_s + JH_{E_s^\varepsilon,u})\tilde{\vec{\phi}}_s + \frac{\dot\gamma_s^\varepsilon}{\varepsilon}P_s^d J\tilde{\vec{\phi}}_s - P_s^d\dot P_s^d\tilde{\vec{\phi}}_s - \dot\gamma_s^\varepsilon P_s^c J L_s^{-1}P_s^c\partial_s\vec{\psi}_{E_s^\varepsilon,s}$$
$$- \varepsilon P_s^c\frac{d}{ds}(L_s^{-1}P_s^c\partial_s\vec{\psi}_{E_s^\varepsilon,s}) - \frac{1}{\varepsilon}P_s^c N(\vec{\psi}_{E_s^\varepsilon,s}, \varepsilon L_s^{-1}P_s^c\partial_s\vec{\psi}_{E_s^\varepsilon,s} + \tilde{\vec{\phi}}_s)\,. \tag{5.7.8}$$

Here we made use of

$$\dot P_s^d\tilde{\vec{\phi}}_s = \dot P_s^d P_s^c\tilde{\vec{\phi}}_s = -P_s^d\dot P_s^c\tilde{\vec{\phi}}_s = P_s^d\dot P_s^d\tilde{\vec{\phi}}_s\,.$$

The fact that the linear operator $L_s$ is time-dependent complicates the analysis and we find it convenient to introduce the reference Hamiltonian

$$H_{E_s^\varepsilon,u} := \begin{pmatrix} -\Delta + V_u - E_s^\varepsilon & 0 \\ 0 & -\Delta + V_u - E_s^\varepsilon \end{pmatrix}, \qquad (0 \le u \le 1)\,. \tag{5.7.9}$$

Its difference to $L_s$,

$$L_s - \left(-JH_{E_s^\varepsilon,u}\right) = -J\begin{pmatrix} V_s - V_u + 3b\psi^2_{E_s^\varepsilon,s} & 0 \\ 0 & V_s - V_u + b\psi^2_{E_s^\varepsilon,s} \end{pmatrix}, \tag{5.7.10}$$

is small and decays at spatial infinity. More precisely: given $\delta > 0$ the first entry of this last matrix is estimated by

$$\|V_s - V_u + 3b\psi^2_{E_s^\varepsilon,s}\|_{H^{2,\sigma}} \le \delta\,, \tag{5.7.11}$$

and similarly for the second entry as long as $|s-u| \le \tau^* \ll 1$, $\eta \ll 1$ (recall Proposition 5.2 and ($\mathrm{H_d}$)). Duhamel's principle and application of $P^c_{H_0}$ yield for any $s \le s_0$

$$P^c_{H_0}\tilde{\vec{\phi}}_s = U_0(s,0)P^c_{H_0}\tilde{\vec{\phi}}_0 \tag{5.7.12}$$
$$+ \int_0^s ds'\; U_0(s,s')\Big(\frac{1}{\varepsilon}P^c_{H_0}(L_{s'} + JH_0)\tilde{\vec{\phi}}_{s'} + \frac{\dot\gamma^\varepsilon_{s'}}{\varepsilon}P^c_{H_0}P^d_{s'}J\tilde{\vec{\phi}}_{s'} - P^c_{H_0}P^d_{s'}\dot P^d_{s'}\tilde{\vec{\phi}}_{s'} \tag{5.7.13}$$
$$- \dot\gamma^\varepsilon_{s'}P^c_{H_0}P^c_{s'}JL^{-1}_{s'}P^c_{s'}\partial_{s'}\vec{\psi}_{E^\varepsilon_{s'},s'} - \varepsilon P^c_{H_0}P^c_{s'}\frac{d}{ds'}(L^{-1}_{s'}P^c_{s'}\partial_{s'}\vec{\psi}_{E^\varepsilon_{s'},s'}) \tag{5.7.14}$$
$$- \frac{1}{\varepsilon}P^c_{H_0}P^c_{s'}N(\vec{\psi}_{E^\varepsilon_{s'},s'}, \varepsilon L^{-1}_{s'}P^c_{s'}\partial_{s'}\vec{\psi}_{E^\varepsilon_{s'},s'} + \tilde{\vec{\phi}}_{s'})\Big)\,. \tag{5.7.15}$$

Here $U_u(s,s')$ is the propagator generated by $H_{E_s^\varepsilon,s'} + \dot\gamma_s^\varepsilon$, that is,

$$\varepsilon\partial_s U_u(s,s') = -J(H_{E_s^\varepsilon,u} + \dot\gamma_s^\varepsilon)U_u(s,s')\,.$$

Since $H_{E_s^\varepsilon,u}$ does – up to a multiple of the identity – not depend on $s$, it follows that also $U_u(s,s')$ satisfies the propagator estimates of Theorem 5.14 below for arbitrary $u \in [0,1]$. In addition this justifies the shorter notation $H_u := H_{E_s^\varepsilon,u}$. As before the projections onto the discrete and continuous subspace of $H_u$ are denoted by $P^d_{H_u}$ and $P^c_{H_u}$, respectively.

To estimate (5.7.12-5.7.15) we rely on appropriate propagator estimates:

**Theorem 5.14** (Goldberg). *Under conditions* $(\mathrm{H_r}, \mathrm{H_d})$ *it holds for arbitrary* $\tau \in [0,1]$ *and* $t \in \mathbb{R}$ *that*

$$\|\mathrm{e}^{-\mathrm{i}tH_\tau} P^c_{H_\tau}\|_{L^1 \to L^\infty} \lesssim |t|^{-\frac{3}{2}} \tag{5.7.16}$$

$$\|\mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}H_\tau} P^c_{H_\tau}\chi\|_{H^2} \simeq \|P^c_{H_\tau}\chi\|_{H^2} \lesssim \|\chi\|_{H^2}\,, \tag{5.7.17}$$

$$\|\mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}H_\tau} P^c_{H_\tau}\chi\|_{H^{2,-\sigma}} \le A\langle\frac{t}{\varepsilon}\rangle^{-\frac{3}{2}}\|\chi\|_{H^2\cap W^{2,1}}\,, \tag{5.7.18}$$

*where* $\|\chi\|_{H^2\cap W^{2,1}} := \|\chi\|_{H^2} + \|\chi\|_{W^{2,1}}$. *The constant* $A$ *and the multiplicative constant in (5.7.17) can be chosen independent of* $\tau$.

Estimate (5.7.16) can be found in [Gol06]; Estimates (5.7.17, 5.7.18) are easy consequences of it. For convenience we show this and the statement about $A$ in Subsection 5.8.2.

After these preparatory remarks we can proceed with our analysis of Equation (5.7.8). By the decay of $\vec{\psi}_{E^\varepsilon_s,s}$ and $v_{*,s}$, cf. (Sub)sections 5.2, 5.8.1, and by (5.7.11) the $H^2$-norm of every term in (5.7.13) can be estimated in terms of $\|\tilde{\vec{\phi}}_{s'}\|_{H^{2,-\sigma}}$. This motivates to consider such local estimates of $\tilde{\vec{\phi}}_{s'}$ first.

We start with the left hand side in Equation (5.7.12). The fact that the projection there can be neglected (and also in estimates with respect to $\|\cdot\|_{H^2}$) is the content of the following lemma whose proof is deferred to Subsection 5.8.2.

**Lemma 5.15.** *For sufficiently small* $s_0$, $\eta$ *the following holds: If* $0 \le s \le s_0$ *then for all* $\varepsilon \ll 1$

$$\|P^c_{H_0}\tilde{\vec{\phi}}_s\|_{H^2} \simeq \|\tilde{\vec{\phi}}_s\|_{H^2}\,,$$
$$\|P^c_{H_0}\tilde{\vec{\phi}}_s\|_{H^{2,-\sigma}} \simeq \|\tilde{\vec{\phi}}_s\|_{H^{2,-\sigma}}\,.$$

For the right hand side, the local estimates for (5.7.12-5.7.15) are collected in the following lemma. Its proof is provided in the next subsection.

**Lemma 5.16.** *Assume* $(\mathrm{B_l}, \mathrm{B_g})$ *resp.* $(\mathrm{B'_l}, \mathrm{B_g})$. *For any* $\delta > 0$ *there exists* $0 < s_0 \le 1$ *and* $\eta \ll 1$ *such that for* $s \le s_0$ *the following holds: For all* $\varepsilon \ll 1$ *we have*

$$\|(5.7.12)\|_{H^{2,-\sigma}} \le A\langle\frac{s}{\varepsilon}\rangle^{-\frac{3}{2}}\varepsilon\|L_0^{-1}P_0^c\partial_t\vec{\psi}_{E^\varepsilon_s,s}|_{t=0}\|_{H^2\cap W^{2,1}} \simeq \langle\frac{s}{\varepsilon}\rangle^{-\frac{3}{2}}\varepsilon\,,$$
$$\|(5.7.13)\|_{H^{2,-\sigma}} \lesssim \delta(\varepsilon\langle\frac{s}{\varepsilon}\rangle^{-\frac{3}{2}} + \varepsilon^2)M_s^{(\frac{3}{2},\mathrm{l})} + \varepsilon^2\,,$$
$$\|(5.7.14)\|_{H^{2,-\sigma}} \lesssim \varepsilon^2\,,$$
$$\|(5.7.15)\|_{H^{2,-\sigma}} \lesssim \varepsilon^2\,,$$

*where* $M_s^{(\frac{3}{2},\mathrm{l})} := \sup_{0\le s'\le s}(\varepsilon\langle\frac{s'}{\varepsilon}\rangle^{-\frac{3}{2}} + \varepsilon^2)^{-1}\|\tilde{\vec{\phi}}_{s'}\|_{H^{2,-\sigma}}$. *If* $L_0^{-1}P_0^c\partial_s\vec{\psi}_{E_0,s} = 0$ *then the first two estimates are replaced by*

$$\|(5.7.12)\|_{H^{2,-\sigma}} = 0\,,$$
$$\|(5.7.13)\|_{H^{2,-\sigma}} \lesssim \delta M_s^{(\mathrm{l})} + \varepsilon^2\,.$$

*All implicit multiplicative constants are uniform in* $s \in [0, s_0]$.

Given Lemma 5.16 we are ready to prove Proposition 5.12.

PROOF OF PROPOSITION 5.12. We discuss first the case where $L_0^{-1}P_0^c\partial_s\vec{\psi}_{E_0,s} \neq 0$. Given $\delta > 0$ we choose $s \leq s_0$ and $\eta$ accordingly so that the local estimates of Lemma 5.16 hold. Together with the results in Lemma 5.15 we obtain for all sufficiently small $\varepsilon$

$$\|\vec{\tilde{\phi}}_s\|_{H^{2,-\sigma}} \leq C_{s_0,A}\left(\varepsilon\langle\frac{s}{\varepsilon}\rangle^{-\frac{3}{2}} + \delta(\varepsilon\langle\frac{s}{\varepsilon}\rangle^{-\frac{3}{2}} + \varepsilon^2)M_s^{(\frac{3}{2},l)} + \varepsilon^2\right) . \tag{5.7.19}$$

Here we have made the multiplicative constant $C_{s_0,A}$ explicit in order to define our prescription for $\delta$: We choose

$$C_{s_0,A}\delta \leq 1/2 . \tag{5.7.20}$$

Consequently,

$$M_{s_0}^{(\frac{3}{2},l)} \leq 2C_{s_0,A} \tag{5.7.21}$$

and therefore

$$\|\vec{\tilde{\phi}}_s\|_{H^{2,-\sigma}} \leq 2C_{s_0,A}\left(\varepsilon\langle\frac{s}{\varepsilon}\rangle^{-\frac{3}{2}} + \varepsilon^2\right) . \tag{5.7.22}$$

This estimate has two important consequences. First, we obtain a $\vec{\tilde{\phi}}_s$-independent bound in the local estimates of (5.7.13) due to (5.7.21). That is, we have

$$\|\vec{\tilde{\phi}}_s\|_{H^{2,-\sigma}} \leq A\varepsilon\|L_0^{-1}P_0^c\partial_s\vec{\psi}_{E_0,s}|_{s=0}\|_{H^2\cap W^{2,1}} + \tilde{C}_{s_0,A}\left(\delta\varepsilon + \varepsilon^2\right) .$$

In addition to (5.7.20) we require that $\delta$ also satisfies $\delta \leq \frac{1}{2\tilde{C}_{s_0,A}}A\|L_0^{-1}P_0^c\partial_s\vec{\psi}_{E_0,s}|_{s=0}\|_{H^2\cap W^{2,1}}$. Accordingly, $s_0$ and $\eta$ can be chosen such that bootstrap assumption ($B_l$) is for $s \in [0, s_0]$ improved to

$$M_s^{(l)} \leq \frac{5}{3}A\varepsilon\|L_0^{-1}P_0^c\partial_s\vec{\psi}_{E_0,s}|_{s=0}\|_{H^2\cap W^{2,1}}$$

for all sufficiently small $\varepsilon$.

Second, by ($B_l$, $B_g$) and Lemma 5.13, for $s' \leq s_0$ it holds

$$\|N(\vec{\psi}_{E^\varepsilon_{s'},s'}, \vec{\phi}_{s'})\|_{H^2} \lesssim \varepsilon^2 .$$

Hence (5.7.12-5.7.15) as well as (5.7.22) yield

$$\begin{aligned}
\|\vec{\tilde{\phi}}_s\|_{H^2} \lesssim & \|\vec{\tilde{\phi}}_0\|_{H^2} + \int_0^s ds'\ \Big(\frac{1}{\varepsilon}\|\vec{\tilde{\phi}}_{s'}\|_{H^{2,-\sigma}} + \varepsilon^2\|L_{s'}^{-1}P_{s'}^c\partial_{s'}\vec{\psi}_{E^\varepsilon_{s'},s'}\|_{H^2} + \varepsilon\|\frac{d}{ds'}(L_{s'}^{-1}P_{s'}^c\partial_{s'}\vec{\psi}_{E^\varepsilon_{s'},s'})\|_{H^2} \\
& + \frac{1}{\varepsilon}\|N(\vec{\psi}_{E^\varepsilon_{s'},s'}, \varepsilon L_{s'}^{-1}P_{s'}^c\partial_{s'}\vec{\psi}_{E^\varepsilon_{s'},s'} + \vec{\tilde{\phi}}_{s'})\|_{H^2}\Big) \\
\lesssim & \ \varepsilon + \int_0^s ds'\ \left(\frac{1}{\varepsilon}(\varepsilon\langle\frac{s'}{\varepsilon}\rangle^{-\frac{3}{2}} + \varepsilon^2) + \varepsilon\right) \\
\lesssim & \ \varepsilon .
\end{aligned}$$

Note that the implicit multiplicative constant can be chosen to be uniform in $s \in [0, s_0]$.

The case $L_0^{-1}P_0^c\partial_s\vec{\psi}_{E_0,s} = 0$ is easier: Estimate (5.7.19) is then modified to

$$\|\vec{\tilde{\phi}}_s\|_{H^{2,-\sigma}} \leq C_{s_0,A}\left(\delta M_s^{(l)} + \varepsilon^2\right) . \tag{5.7.23}$$

With (5.7.20) one obtains

$$M_{s_0}^{(\mathrm{l})} \lesssim \varepsilon^2 \tag{5.7.24}$$

proving (5.7.3). Estimating (5.7.12-5.7.15) in $\|\cdot\|_{H^2}$ similarly as above yields

$$M_s^{(\mathrm{g})} \lesssim \varepsilon\,,$$

with an implicit multiplicative constant being uniform in $s \in [0, s_0]$. This proves Proposition 5.12. □

### 5.7.4. Proof of Lemma 5.16

This subsection will be devoted to the proof of Lemma 5.16 and we now estimate (5.7.12-5.7.15) in $H^{2,-\sigma}(\mathbb{R}^3)$ term by term.

*Local estimate for (5.7.12):* If $L_0^{-1}P_0^c\partial_s\vec{\psi}_{E_0,s} = 0$ there is nothing to do, otherwise: By

$$\|\langle x\rangle^{-\sigma}\langle x\rangle^{\sigma}L_s^{-1}P_s^c\partial_s\vec{\psi}_{E_s^\varepsilon,s}\|_{W^{2,1}} \lesssim \|\langle x\rangle^{-\sigma}\|_{H^2}\|L_s^{-1}P_s^c\partial_s\vec{\psi}_{E_s^\varepsilon,s}\|_{H^{2,\sigma}}\,,$$

and Theorem 5.14:

$$\|U_0(s,0)P_{H_0}^c\vec{\tilde{\phi}}_0\|_{H^{2,-\sigma}} \le A\langle\frac{s}{\varepsilon}\rangle^{-\frac{3}{2}}\varepsilon\|L_0^{-1}P_0^c\partial_s\vec{\psi}_{E_s^\varepsilon,s}|_{s=0}\|_{H^2\cap W^{2,1}} \simeq \langle\frac{s}{\varepsilon}\rangle^{-\frac{3}{2}}\varepsilon\,.$$

*Local estimate for (5.7.13):* To apply Theorem 5.14 we need bounds for the $\|\cdot\|_{H^2\cap W^{2,1}}$-norms of each term:

**Lemma 5.17.** *Given $\delta > 0$ there are (small) $s_0, \eta$ such that*

$$\|P_{H_0}^c(L_s + JH_0)\vec{\phi}_s\|_{H^2\cap W^{2,1}} \lesssim \delta\|\vec{\phi}_s\|_{H^{2,-\sigma}}\,, \tag{5.7.25}$$

$$\|P_{H_0}^c P_s^d J\vec{\phi}_s\|_{H^2\cap W^{2,1}} \lesssim \|\vec{\phi}_s\|_{H^{2,-\sigma}}\,, \tag{5.7.26}$$

$$\|P_{H_0}^c P_s^d \dot{P}_s^d\vec{\phi}_s\|_{H^2\cap W^{2,1}} \lesssim \|\vec{\phi}_s\|_{H^{2,-\sigma}}\,. \tag{5.7.27}$$

*All estimates are uniform in $s \in [0, s_0]$ and $\varepsilon$ as long as the latter is sufficiently small.*

A proof of this lemma is given in Subsection 5.8.2. Here we simply stress that it is in (5.7.25) where (5.7.11) enters.

First, we treat the case $L_0^{-1}P_0^c\partial_s\vec{\psi}_{E_0,s} \neq 0$. Lemma 5.17, Theorem 5.14, and Estimate (5.7.6) yield for $s \le s_0$ and $s_0, \eta, \varepsilon \ll 1$:

$$\begin{aligned}
&\Big\|\int_0^s ds'\; U_0(s,s')\left(\frac{1}{\varepsilon}P_{H_0}^c(L_{s'} + JH_0)\vec{\tilde{\phi}}_{s'} + \frac{\dot{\gamma}_{s'}^\varepsilon}{\varepsilon}P_{H_0}^c P_{s'}^d J\vec{\tilde{\phi}}_{s'} - P_{H_0}^c P_s^d \dot{P}_s^d\vec{\tilde{\phi}}_{s'}\right)\Big\|_{H^{2,-\sigma}} \\
&\quad\lesssim \int_0^s ds'\langle\frac{s-s'}{\varepsilon}\rangle^{-\frac{3}{2}}\Big(\frac{1}{\varepsilon}\|P_{H_0}^c(L_{s'} + JH_0)\vec{\tilde{\phi}}_{s'}\|_{H^2\cap W^{2,1}} + \varepsilon\|P_{H_0}^c P_{s'}^d J\vec{\tilde{\phi}}_{s'}\|_{H^2\cap W^{2,1}} \\
&\qquad\qquad + \|P_{H_0}^c P_{s'}^d \dot{P}_{s'}^d\vec{\tilde{\phi}}_{s'}\|_{H^2\cap W^{2,1}}\Big) \\
&\quad\lesssim \int_0^s ds'\langle\frac{s-s'}{\varepsilon}\rangle^{-\frac{3}{2}}\left((\varepsilon\langle\frac{s'}{\varepsilon}\rangle^{-\frac{3}{2}} + \varepsilon^2)(\varepsilon\langle\frac{s'}{\varepsilon}\rangle^{-\frac{3}{2}} + \varepsilon^2)^{-1}\frac{\delta}{\varepsilon}\|\vec{\tilde{\phi}}_{s'}\|_{H^{2,-\sigma}} + \|\vec{\tilde{\phi}}_{s'}\|_{H^{2,-\sigma}}\right) \\
&\quad\lesssim \delta(\varepsilon\langle\frac{s}{\varepsilon}\rangle^{-\frac{3}{2}} + \varepsilon^2)M_s^{(\frac{3}{2},\mathrm{l})} + \varepsilon^2\,,
\end{aligned}$$

with $M_s^{(\frac{3}{2},\mathrm{l})} = \sup_{0\le s'\le s}(\varepsilon\langle\frac{s'}{\varepsilon}\rangle^{-\frac{3}{2}}+\varepsilon^2)^{-1}\|\tilde{\vec{\phi}}_{s'}\|_{H^{2,-\sigma}}$. In the last inequality we applied ($\mathrm{B_l}$) as well as the following key observations:

**Lemma 5.18.**

$$\int_0^s ds'\langle\frac{s-s'}{\varepsilon}\rangle^{-\frac{3}{2}} \lesssim \varepsilon\,,$$
$$\int_0^s ds'\langle\frac{s-s'}{\varepsilon}\rangle^{-\frac{3}{2}}\langle\frac{s'}{\varepsilon}\rangle^{-\frac{3}{2}} \lesssim \varepsilon\langle\frac{s}{\varepsilon}\rangle^{-\frac{3}{2}}\,.$$

Proof. The first estimate follows immediately after a change of variables. For the second we divide the integral region into two parts $[0,s/2]$ and $[s/2,s]$ and obtain

$$\begin{aligned}\int_0^s ds'\langle\frac{s-s'}{\varepsilon}\rangle^{-\frac{3}{2}}\langle\frac{s'}{\varepsilon}\rangle^{-\frac{3}{2}} &= \int_0^{s/2} ds'\langle\frac{s-s'}{\varepsilon}\rangle^{-\frac{3}{2}}\langle\frac{s'}{\varepsilon}\rangle^{-\frac{3}{2}} + \int_{s/2}^s ds'\langle\frac{s-s'}{\varepsilon}\rangle^{-\frac{3}{2}}\langle\frac{s'}{\varepsilon}\rangle^{-\frac{3}{2}}\\ &\lesssim \langle\frac{s}{2\varepsilon}\rangle^{-\frac{3}{2}}\left(\int_0^{s/2} ds'\langle\frac{s'}{\varepsilon}\rangle^{-\frac{3}{2}} + \int_{s/2}^s ds'\langle\frac{s-s'}{\varepsilon}\rangle^{-\frac{3}{2}}\right)\\ &\lesssim \varepsilon\langle\frac{s}{\varepsilon}\rangle^{-\frac{3}{2}}\,.\end{aligned}$$

□

If $L_0^{-1}P_0^c\partial_s\vec{\psi}_{E_0,s}=0$ then the above estimates are simpler:

$$\begin{aligned}&\Big\|\int_0^s ds'\;U_0(s,s')\left(\frac{1}{\varepsilon}P^c_{H_0}(L_{s'}+JH_0)\tilde{\vec{\phi}}_{s'} + \frac{\dot{\gamma}^\varepsilon_{s'}}{\varepsilon}P^c_{H_0}P^d_{s'}J\tilde{\vec{\phi}}_{s'} - P^c_{H_0}P^d_s\dot{P}^d_s\tilde{\vec{\phi}}_{s'}\right)\Big\|_{H^{2,-\sigma}}\\ &\quad\lesssim \int_0^s ds'\langle\frac{s-s'}{\varepsilon}\rangle^{-\frac{3}{2}}\Big(\frac{1}{\varepsilon}\|P^c_{H_0}(L_{s'}+JH_0)\tilde{\vec{\phi}}_{s'}\|_{H^2\cap W^{2,1}} + \varepsilon\|P^c_{H_0}P^d_{s'}J\tilde{\vec{\phi}}_{s'}\|_{H^2\cap W^{2,1}}\\ &\qquad\qquad + \|P^c_{H_0}P^d_{s'}\dot{P}^d_{s'}\tilde{\vec{\phi}}_{s'}\|_{H^2\cap W^{2,1}}\Big)\\ &\quad\lesssim \int_0^s ds'\langle\frac{s-s'}{\varepsilon}\rangle^{-\frac{3}{2}}\left(\frac{\delta}{\varepsilon}\|\tilde{\vec{\phi}}_{s'}\|_{H^{2,-\sigma}} + \|\tilde{\vec{\phi}}_{s'}\|_{H^{2,-\sigma}}\right)\\ &\quad\lesssim \delta M_s^{(\mathrm{l})} + \varepsilon^2\,.\end{aligned}$$

*Local estimate for (5.7.14):*

$$\begin{aligned}&\|\int_0^s ds'\;U_0(s,s')\left(-\dot{\gamma}^\varepsilon_{s'}P^c_{H_0}P^c_{s'}JL^{-1}_{s'}P^c_{s'}\partial_{s'}\vec{\psi}_{E^\varepsilon_{s'},s'} - \varepsilon P^c_{H_0}P^c_{s'}\frac{d}{ds'}(L^{-1}_{s'}P^c_{s'}\partial_{s'}\vec{\psi}_{E^\varepsilon_{s'},s'})\right)\|_{H^{2,-\sigma}}\\ &\quad\lesssim \int_0^s ds'\;\langle\frac{s-s'}{\varepsilon}\rangle^{-\frac{3}{2}}\varepsilon\left(\|L^{-1}_{s'}P^c_{s'}\partial_{s'}\vec{\psi}_{E^\varepsilon_{s'},s'}\|_{H^2\cap W^{2,1}} + \|\frac{d}{ds'}(L^{-1}_{s'}P^c_{s'}\partial_{s'}\vec{\psi}_{E^\varepsilon_{s'},s'})\|_{H^2\cap W^{2,1}}\right)\\ &\quad\lesssim \varepsilon^2.\end{aligned}$$

The first inequality results from Estimate (5.7.6) and the fact that $\|P^c_{H_0}P^c_s\|_{H^2\cap W^{2,1}\to H^2\cap W^{2,1}}$ is uniformly bounded in $\varepsilon$. The second inequality follows from Lemmata 5.10, 5.18 and ($\mathrm{B_l}$) as well as $\|\cdot\|_{H^2\cap W^{2,1}} \lesssim \|\cdot\|_{H^{2,\sigma}}$.

*Local estimate for (5.7.15):* Instead of expanding $N(\vec{\psi}_{E^\varepsilon_{s'},s'}, \varepsilon L_{s'}^{-1} P^c_{s'} \partial_{s'} \vec{\psi}_{E^\varepsilon_{s'},s'} + \tilde{\vec{\phi}}_{s'})$ it is more convenient to consider $N(\vec{\psi}_{E^\varepsilon_{s'},s'}, \vec{\phi}_{s'})$. By Equation (5.5.5) we may conclude that

- terms which are quadratic in $\phi_{s'}$ come with a factor of $\psi_{E^\varepsilon_{s'},s'}$ which decays rapidly at spatial infinity. By ($B_l$)

$$\|\psi_{E^\varepsilon_{s'},s'} \phi^2_{s'}\|_{H^2 \cap W^{2,1}} = \|\langle x\rangle^{2\sigma} \psi_{E^\varepsilon_{s'},s'} \langle x\rangle^{-2\sigma} \phi^2_{s'}\|_{H^2\cap W^{2,1}} \lesssim \|\tilde{\vec{\phi}}_{s'}\|^2_{H^{2,-\sigma}} \lesssim \varepsilon^2 \,,$$

- terms which are cubic in $\phi_{s'}$ are estimated by

$$\||\phi_{s'}|^2 \phi_{s'}\|_{H^2\cap W^{2,1}} \lesssim \|\tilde{\vec{\phi}}_{s'}\|^3_{H^2} \lesssim \varepsilon^2 \,.$$

Here the bootstrap assumption ($B_g$) for the global norm $\|\tilde{\vec{\phi}}_s\|_{H^2}$ has been used.

Hence

$$\| \int_0^s ds'\ U_0(s,s') \frac{1}{\varepsilon} P^c_{H_0} P^c_{s'} N(\vec{\psi}_{E^\varepsilon_{s'},s'}, \vec{\phi}_{s'})\|_{H^{2,-\sigma}} \lesssim \int_0^s ds'\ \langle \frac{s-s'}{\varepsilon}\rangle^{-\frac{3}{2}} \frac{1}{\varepsilon} \cdot \varepsilon^2 \lesssim \varepsilon^2 \,.$$

This finishes the proof of Lemma 5.16. □

### 5.7.5. Proof of Theorem 5.11 for all $s \in [0,1]$

So far we have established Theorem 5.11 on the small interval $[0, s_0]$ only. Recall that $s_0$ does not depend on $\varepsilon$ if $\varepsilon \ll 1$. As announced in the beginning of this section the extension to all $s \in [0,1]$ is similar and we therefore give the proof in one step now.

**Proposition 5.19.** *For $\eta \ll 1$ there exists a small time $\tau^* > 0$ and constant $C_{\tau^*}$ with the following property: Whenever*

$$M^{(l)}_{s^*} \le C_{s^*} \varepsilon \left(\langle \frac{s}{\varepsilon}\rangle^{-\frac{3}{2}} + \varepsilon\right)$$
$$M^{(g)}_{s^*} \le C_{s^*} \varepsilon$$

*for $s^* \in [s_0, 1]$ then*

$$M^{(l)}_{s^*+\tau^*} \le C_{\tau^*} C_{s^*} \varepsilon \left(\langle \frac{s}{\varepsilon}\rangle^{-\frac{3}{2}} + \varepsilon\right) \tag{5.7.28}$$
$$M^{(g)}_{s^*+\tau^*} \le C_{\tau^*} C_{s^*} \varepsilon \tag{5.7.29}$$

*for all $\varepsilon \ll 1$.*

Proof of Theorem 5.11. Clearly the hypothesis of the proposition is satisfied at $s^* = s_0$. Estimate (5.6.12) follows by iteration. Estimates (5.6.10) and (5.6.11) are proven by the same techniques as before. □

PROOF OF PROPOSITION 5.19. We choose $s$ to satisfy

$$s^* \le s \le s^* + \tau^* \,, \tag{5.7.30}$$

where $\tau^*$ will be defined later. By Duhamel's principle,

$$\begin{aligned} P^c_{H_{s^*}} \vec{\tilde{\phi}}_s =& U_{s^*}(s,0) P^c_{H_{s^*}} \vec{\tilde{\phi}}_0 \qquad (5.7.31)\\ &+ \left( \int_0^{s^*} + \int_{s^*}^s \right) ds' \; U_{s^*}(s,s') \times \\ &\quad \times \Big( \frac{1}{\varepsilon} P^c_{H_{s^*}} (L_{s'} + JH_{s^*}) \vec{\tilde{\phi}}_{s'} + \frac{\dot{\gamma}^\varepsilon_{s'}}{\varepsilon} P^c_{H_{s^*}} P^d_{s'} J \vec{\tilde{\phi}}_{s'} - P^c_{H_{s^*}} P^d_{s'} \dot{P}^d_{s'} \vec{\tilde{\phi}}_{s'} \qquad (5.7.32)\\ &\quad - \dot{\gamma}^\varepsilon_{s'} P^c_{H_{s^*}} P^c_{s'} J L^{-1}_{s'} P^c_{s'} \partial_{s'} \vec{\psi}_{E^\varepsilon_{s'},s'} - \varepsilon P^c_{H_{s^*}} P^c_{s'} \frac{d}{ds'} (L^{-1}_{s'} P^c_{s'} \partial_{s'} \vec{\psi}_{E^\varepsilon_{s'},s'}) \qquad (5.7.33)\\ &\quad - \frac{1}{\varepsilon} P^c_{H_{s^*}} P^c_{s'} N(\vec{\psi}_{E^\varepsilon_{s'},s'}, \varepsilon L^{-1}_{s'} P^c_{s'} \partial_{s'} \vec{\psi}_{E^\varepsilon_{s'},s'} + \vec{\tilde{\phi}}_{s'}) \Big) \,. \qquad (5.7.34) \end{aligned}$$

In what follows we estimate (5.7.31-5.7.34) by *assuming* ($\mathrm{B_l}$, $\mathrm{B_g}$) resp. ($\mathrm{B'_l}$, $\mathrm{B_g}$) on $[s^*, s^* + \tau^*]$. In the end we will justify this and conclude the claim.

*Local estimate for (5.7.31):* By (5.7.30)

$$\| U_{s^*}(s,0) P^c_{H_{s^*}} \vec{\tilde{\phi}}_0 \|_{H^{2,-\sigma}} \le A \langle \frac{s}{\varepsilon} \rangle^{-\frac{3}{2}} \varepsilon \| L_0^{-1} P_0^c \partial_s \vec{\psi}_{E^\varepsilon_s,s}|_{s=0} \|_{H^2 \cap W^{2,1}} \lesssim \varepsilon^2 \,.$$

Here we used $s \ge s_0 > 0$.

*Local estimate for (5.7.32):* The integrals of the first summand $\frac{1}{\varepsilon} P^c_{H_{s^*}} (L_{s'} + JH_{s^*}) \vec{\tilde{\phi}}_{s'}$ dominate the others for $\varepsilon \ll 1$. By (5.7.22, 5.7.30) and Lemmata 5.17, 5.18

$$\begin{aligned} \| \frac{1}{\varepsilon} \int_0^{s^*} ds' \; U_{s^*}(s,s') P^c_{H_{s^*}} (L_{s'} + JH_{s^*}) \vec{\tilde{\phi}}_{s'} \|_{H^{2,-\sigma}} \le& \frac{C_{s^*} A}{\varepsilon} \int_0^{s^*} ds' \; \langle \frac{s-s'}{\varepsilon} \rangle^{-\frac{3}{2}} (\varepsilon \langle \frac{s'}{\varepsilon} \rangle^{-\frac{3}{2}} + \varepsilon^2) \\ \le& C_{s^*,A} \left( \varepsilon \langle \frac{s}{\varepsilon} \rangle^{-\frac{3}{2}} + \varepsilon^2 \right) \\ \le& C_{s^*,A} \varepsilon^2 \,, \end{aligned}$$

if $L_0^{-1} P_0^c \partial_s \vec{\psi}_{E_0,s} \ne 0$ and the same estimate holds if $L_0^{-1} P_0^c \partial_s \vec{\psi}_{E_0,s} = 0$.

Next, we use (5.7.25) in Lemma 5.17 with 0 replaced by $s_*$. Hence for given $\delta > 0$ we can choose $\eta$, $\tau^*$ sufficiently small such that the following holds: There exists a constant $C_1 = C_1(A) > 0$, so that for all $\varepsilon \ll 1$

$$\begin{aligned} \| \frac{1}{\varepsilon} \int_{s^*}^{s} ds' \; U_{s^*}(s,s') P^c_{H_{s^*}} (L_{s'} + JH_{s^*}) \vec{\tilde{\phi}}_{s'} \|_{H^{2,-\sigma}} \le& A \frac{\delta}{\varepsilon} \int_{s^*}^{s} ds' \; \langle \frac{s-s'}{\varepsilon} \rangle^{-\frac{3}{2}} \| \vec{\tilde{\phi}}_{s'} \|_{H^{2,-\sigma}} \\ \le& C_1 \delta \sup_{s^* \le s' \le s} \| \vec{\tilde{\phi}}_{s'} \|_{H^{2,-\sigma}} \,. \end{aligned}$$

Note that the choice of $\tau^*$, $\eta$ does not depend on $s^*$ due to the uniform continuity of the left hand side in 5.7.11.

*Local estimate for (5.7.33):* The integral of the second summand $\varepsilon P^c_{H_{s^*}} P^c_{s'} \frac{d}{ds'} (L^{-1}_{s'} P^c_{s'} \vec{\psi}_{E^\varepsilon_{s'},s'})$ dominates the other and

$$\varepsilon \| \int_0^s ds' \; U_{s^*}(s,s') P^c_{H_{s^*}} P^c_{s'} \frac{d}{ds'} (L^{-1}_{s'} P^c_{s'} \partial_{s'} \vec{\psi}_{E^\varepsilon_{s'},s'}) \|_{H^{2,-\sigma}} \lesssim C_{s^*} \varepsilon \int_0^s ds' \; \langle \frac{s-s'}{\varepsilon} \rangle^{-\frac{3}{2}} \lesssim \varepsilon^2 \,.$$

*Local estimate for (5.7.34):* By the same reasoning as in the local estimate for (5.7.15) we have

$$\| \int_0^s ds'\, U_{s^*}(s,s') \left( -\frac{1}{\varepsilon} P^c_{H_{s^*}} P^c_{s'} N(\vec{\psi}_{E^\varepsilon_{s'},s'}, \varepsilon L_s^{-1} P^c_s \partial_s \vec{\psi}_{E^\varepsilon_{s'},s'} + \tilde{\vec{\phi}}_s) \right) \|_{H^{2,-\sigma}} \lesssim C_{s^*}\varepsilon^2 \,.$$

Taking all local estimates into account, we conclude that there exists a constant $C_2 = C_2(C_{s^*}, A)$ such that for $s^* \le s \le s^* + \tau^*$

$$\|\tilde{\vec{\phi}}_s\|_{H^{2,-\sigma}} \le C_2\varepsilon^2 + C_1\delta \sup_{s^* \le s' \le s^*+\tau^*} \|\tilde{\vec{\phi}}_{s'}\|_{H^{2,-\sigma}}$$

for all $\varepsilon \ll 1$.

Now we fix $\delta$ (and with it $\tau^*$ and $\eta$) such that $C_1\delta \le 1/2$. It follows that

$$\sup_{s^* \le s' \le s^*+\tau^*} \|\tilde{\vec{\phi}}_{s'}\|_{H^{2,-\sigma}} \le 2C_2\varepsilon^2 \,. \tag{5.7.35}$$

Estimating (5.7.31-5.7.34) in $\|\cdot\|_{H^2}$ as in the proof of Proposition 5.12 yields with the help of (5.7.35)

$$\sup_{s^* \le s' \le s^*+\tau^*} \|\tilde{\vec{\phi}}_{s'}\|_{H^2} \lesssim C_{s^*}\varepsilon \,. \tag{5.7.36}$$

Estimates (5.7.35, 5.7.36) imply (5.7.28, 5.7.29). It remains to argue that the assumption of ($B_l$, $B_g$) resp. ($B_l'$, $B_g$) on $[s^*, s^*+\tau^*]$ was justified. But this is indeed the case: By Proposition 5.5 the bootstrap assumptions hold for a maximal subinterval $[s^*, s^*+\tau] \subset [s^*, s^*+\tau^*]$, where $\tau$ a priori depends on $\varepsilon$. However, $\tau = \tau^*$: If we assume $\tau < \tau^*$, then the better Estimates (5.7.35, 5.7.36) still hold (with $\tau^*$ replaced by $\tau$). But now Proposition 5.5 implies that the bootstrap assumptions also hold on a bigger interval (for $\varepsilon \ll 1$). This contradicts the maximality of $\tau$. □

## 5.8. Appendix

### 5.8.1. Ground state manifold: Proof of Proposition 5.2

In this section we provide a proof of Proposition 5.2. In the beginning we will concentrate on the situation where $V_s \in H^{2,\sigma}(\mathbb{R}^3)$ does not depend on time and hence the $s$-dependence will be suppressed, e.g. $V_s \to V$. In particular, we give the proof of Proposition 5.2 (i). The time-dependent case will then be discussed in a second step.

One possible approach to establish the existence of ground states relies on the calculus of variations using concentration compactness [RW88]. For our purposes however the following strategy is more convenient: We view Equation (5.1.2) as a bifurcation phenomenon arising from weakly perturbing the linear eigenvalue problem

$$Hv_* := (-\Delta + V)v_* = E_* v_* \,, \qquad \|v_*\|_{L^2} = 1 \,. \tag{5.8.1}$$

Our analysis is similar to [SW90, RW88]. Recall that the ground state $v_*$ is unique up to phase and can be chosen to be positive, see e.g. [Tes09], Theorem 10.12.

We need the following classical lemma due to Slaggie and Wichmann [SW62], see also [His00].

**Lemma 5.20.** *The eigenvector $v_*$ is continuous and satisfies for every $\lambda > 0$ the exponential decay estimates*

$$|v_*(x)| \lesssim \mathrm{e}^{-(\sqrt{|E|}-\lambda)|x|},$$
$$|\Delta v_*(x)| \lesssim \mathrm{e}^{-(\sqrt{|E|}-\lambda)|x|},$$

*and hence in particular $v_* \in H^{2,l}(\mathbb{R}^3)$ for all $l$.*

**Remark 5.21.** *Arbitrarily fast algebraic decay, which is enough for our purposes, can be achieved as a corollary of the proof of Lemma 5.23 below (set $b = 0$ there).*

Proof. We follow mostly the presentation in [His00]. Since $V \in L^\infty(\mathbb{R}^3)$ we have

$$-\Delta v_* = (E_* - V)v_* \in L^2(\mathbb{R}^3) \tag{5.8.2}$$

and therefore $v_* \in H^2(\mathbb{R}^3)$. By Sobolev's embedding theorem $v_*$ has a continuous representative in $L^\infty(\mathbb{R}^3)$. Thus it is meaningful to write for arbitrary $\lambda > 0$

$$\begin{aligned} v_*(x) &\leq \int_{\mathbb{R}^3} d^3x' \left| \left(\frac{1}{-\Delta - E_*}\right)(x,x')V(x')v_*(x')\right| \\ &\leq \int_{\mathbb{R}^3} d^3x' \frac{\mathrm{e}^{-\lambda|x-x'|}}{4\pi|x-x'|} C_V \langle x'\rangle^{-\sigma} \mathrm{e}^{-(\sqrt{|E_*|}-\lambda)|x-x'|} v_*(x') \\ &\leq C_V \left(\int_{\mathbb{R}^3} d^3x' \frac{\mathrm{e}^{-\lambda|x'|}}{4\pi|x'|}\langle x - x'\rangle^{-\sigma}\right) \sup_{x'\in\mathbb{R}^3} \mathrm{e}^{-(\sqrt{|E_*|}-\lambda)|x-x'|} v_*(x') \end{aligned}$$

The integral in the last line is a rotationally symmetric function in $x$ and by dominated convergence there exists $R > 0$ such that for every $x$ with $|x| > R$ it holds that

$$v_*(x) \leq \frac{1}{2} \sup_{x'\in\mathbb{R}^3} \mathrm{e}^{-(\sqrt{|E_*|}-\lambda)|x-x'|} v_*(x'). \tag{5.8.3}$$

By continuity the following manipulations are justified:

$$\begin{aligned} \sup_{\substack{x' \in \mathbb{R}^3 \\ |x'| > R}} \mathrm{e}^{-(\sqrt{|E_*|}-\lambda)|x-x'|} v_*(x') &< \sup_{\substack{x' \in \mathbb{R}^3 \\ |x'| > R}} \sup_{x''\in\mathbb{R}^3} \mathrm{e}^{-(\sqrt{|E_*|}-\lambda)(|x-x'|+|x''-x'|)} v_*(x'') \\ &\leq \sup_{x''\in\mathbb{R}^3} \sup_{x'\in\mathbb{R}^3} \mathrm{e}^{-(\sqrt{|E_*|}-\lambda)(|x-x'|+|x''-x'|)} v_*(x'') \\ &\leq \sup_{x''\in\mathbb{R}^3} \mathrm{e}^{-(\sqrt{|E_*|}-\lambda)(|x-x''|)} v_*(x'') \,. \end{aligned}$$

Hence for $|x| > R$ the supremum in (5.8.3) is assumed inside the ball of radius $R$ and hence we may conclude for those $x$ that

$$v_*(x) < \mathrm{e}^{-(\sqrt{|E_*|}-\lambda)|x|} \mathrm{e}^{(\sqrt{|E_*|}-\lambda)R} \sup_{\substack{x' \in \mathbb{R}^3 \\ |x'| \leq R}} v(x') \lesssim \mathrm{e}^{-(\sqrt{|E_*|}-\lambda)|x|},$$

by continuity of the eigenfunction $v_*(x)$. By (5.8.2) the same is true for $\Delta v_*(x)$. □

Next, we provide a crude, yet sufficient, control of the operator norm of $(-\Delta - z)^{-1}$ acting on the weighted space $L^{2,l}(\mathbb{R}^3) := \langle x\rangle^{-l} L^2(\mathbb{R}^3)$.

**Lemma 5.22.** *Let $z \in \mathbb{C}\backslash\mathbb{R}_{\geq 0}$. For arbitrary $l \in \mathbb{R}$ it holds that for every $\lambda$ with $|\Re\sqrt{-z}| > \lambda > 0$,*

$$\|(-\Delta - z)^{-1}\|_{L^{2,l}\to L^{2,l}} \leq C_l \frac{1}{|\Re\sqrt{-z}| - \lambda},$$

*where $\sqrt{\ }$ denotes the principle branch of the square root.*

Proof. For $f \in L^2(\mathbb{R}^3)$ we have almost everywhere

$$\begin{aligned} |\left(\langle x\rangle^l(-\Delta - z)^{-1}\langle x\rangle^{-l} f\right)(x)| &\lesssim \langle x\rangle^l \int_{\mathbb{R}^3} d^3x' \; \frac{\mathrm{e}^{-|\Re\sqrt{-z}||x-x'|}}{|x-x'|}\langle x'\rangle^{-l}|f(x')| \\ &\lesssim \int_{\mathbb{R}^3} d^3x' \; \frac{\mathrm{e}^{-|\Re\sqrt{-z}||x-x'|}}{|x-x'|}\frac{\langle x\rangle^l}{\langle x'\rangle^l}|f(x')| \\ &\lesssim \int_{\mathbb{R}^3} d^3x' \; \frac{\mathrm{e}^{-|\Re\sqrt{-z}||x-x'|}}{|x-x'|}\langle x-x'\rangle^l|f(x')| \\ &= \left(\frac{\mathrm{e}^{-|\Re\sqrt{-z}||\cdot|}}{|\cdot|}\langle\cdot\rangle^l * |f|\right)(x)\,, \end{aligned}$$

where in the third inequality we used

$$\frac{\langle x\rangle^2}{\langle x'\rangle^2} = \frac{1+|x|^2}{1+|x'|^2} \lesssim \frac{1+|x'|^2+|x-x'|^2}{1+|x'|^2} \lesssim 1 + |x-x'|^2 = \langle x-x'\rangle^2\,.$$

This implies the required result after applying Young's inequality for convolutions

$$\|\frac{\mathrm{e}^{-|\Re\sqrt{-z}||\cdot|}}{|\cdot|}\langle\cdot\rangle^l * |f|\|_2 \lesssim \|\frac{\mathrm{e}^{-|\Re\sqrt{-z}||\cdot|}}{|\cdot|}\langle\cdot\rangle^l\|_1\|f\|_2 \leq C_l\|\mathrm{e}^{-(|\Re\sqrt{-z}|-\lambda)|\cdot|}\|_1\|f\|_2\,,$$

and evaluating the integral on the right hand side. □

As a first application of Lemma 5.22 we note that for $H_E := -\Delta + V - E$ the following holds.

**Lemma 5.23.** *For $l \geq 0$,*

$$L^{2,l}(\mathbb{R}^3) = \mathrm{span}(v_*) \oplus \mathrm{ran}(H_{E_*} \restriction H^{2,l}(\mathbb{R}^3))\,.$$

Proof. It suffices to show that $\mathrm{ran}(H_{E_*} \restriction H^{2,l}(\mathbb{R}^3)) = \mathrm{ran}(H_{E_*}) \cap L^{2,l}(\mathbb{R}^3)$. The inclusion

$$\mathrm{ran}(H_{E_*} \restriction H^{2,l}(\mathbb{R}^3)) \subset \mathrm{ran}(H_{E_*}) \cap L^{2,l}(\mathbb{R}^3)$$

is immediate, for the converse let $H_{E_*}a = b \in L^{2,l}(\mathbb{R}^3)$ and note that for $m \leq m^* := \min\{\sigma, l\}$

$$\begin{aligned} \|\langle x\rangle^m a\|_2 &\lesssim \|\langle x\rangle^m(-\Delta - E_*)^{-1}b\|_2 + \|\langle x\rangle^m(-\Delta - E_*)^{-1}Va\|_2 \\ &\lesssim \|b\|_{L^{2,m^*}} + \|a\|_2 < \infty\,. \end{aligned}$$

Bootstrapping this inequality to $\|a\|_{L^{2,l}} < \infty$ for any $l \geq 0$ yields

$$\|\langle x\rangle^l\Delta a\|_2 \lesssim \|\langle x\rangle^l H_{E*}a\|_2 + \|a\|_{L^{2,l}} < \infty$$

which implies the claim. □

Proof of Proposition 5.2 (i). The proof is an application of the analytic implicit function theorem [Nir01]. It is convenient to introduce the notation $M_{\mathbb{R}} := \Re(M)$ for any space $M$ of complex valued functions. Then the map $F$ defined by

$$\begin{aligned} F : \mathbb{R} \times \mathbb{R} \times H^{2,l}_{\mathbb{R}}(\mathbb{R}^3) \cap \operatorname{ran}(H_{E_*}) &\to L^{2,l}_{\mathbb{R}}(\mathbb{R}^3) = \operatorname{span}_{\mathbb{R}}(v_*) \oplus \operatorname{ran}(H_{E_*} \restriction H^{2,l}_{\mathbb{R}}(\mathbb{R}^3)) \\ (E, \delta, w) &\mapsto H_E(\delta v_* + w) + b(\delta v_* + w)^3 . \end{aligned} \tag{5.8.4}$$

is differentiable as we will demonstrate below. It is useful to assume without loss of generality $l \geq 0$.

*Step 1: Continuous Fréchet differentiability of $F$:* We treat the partial derivatives separately and claim

$$\begin{aligned} \frac{\partial F}{\partial E}|_{(E,\delta,w)} &= -(\delta v_* + w) , \\ \frac{\partial F}{\partial \delta}|_{(E,\delta,w)} &= H_E v_* + 3b(\delta v_* + w)^2 v_* , \\ \frac{\partial F}{\partial w}|_{(E,\delta,w)} &= H_E + 3b(\delta v_* + w)^2 . \end{aligned}$$

The first two expressions follow in a straightforward manner, for the third, using Lemma 5.6, we compute for $u \in H^{2,l}_{\mathbb{R}}(\mathbb{R}^3) \cap \operatorname{ran}(H_{E_*})$.

$$\begin{aligned} \frac{\|F(E,\delta,w+u) - F(E,\delta,w) - (H_E + 3b(\delta v_* + w)^2)u\|_{L^{2,l}}}{\|u\|_{H^{2,l}}} &\lesssim \frac{\|3(\delta v_* + w)u^2 + u^3\|_{L^{2,l}}}{\|u\|_{H^{2,l}}} \\ &\lesssim \frac{(1 + \|w\|_{H^{2,l}})\|u\|^2_{H^{2,l}} + \|u\|^3_{H^{2,l}}}{\|u\|_{H^{2,l}}} , \end{aligned}$$

which vanishes for $\|u\|_{H^{2,l}} \to 0$. Since $H_E + 3b(\delta v_* + w)^2 : H^{2,l}(\mathbb{R}^3) \to L^{2,l}(\mathbb{R}^3)$ is bounded, all partial derivatives of $F$ exist. The continuity of the derivatives is simpler, exemplarily we show it for $\frac{\partial F}{\partial w}$,

$$\begin{aligned} &\left\| \left( \frac{\partial F}{\partial w}|_{(E_1,\delta_1,w_1)} - \frac{\partial F}{\partial w}|_{(E_2,\delta_2,w_2)} \right) v \right\|_{L^{2,l}} \\ &\quad \lesssim |E_1 - E_2| \|v\|_{L^{2,l}} + \|(\delta_1 v_* + w_1)^2 - (\delta_2 v_* + w_2)^2\|_\infty \|v\|_{L^{2,l}} \\ &\quad \lesssim (|E_1 - E_2| + \|(\delta_1 + \delta_2)v_* + w_1 + w_2\|_{H^{2,l}} \|(\delta_1 - \delta_2)v_* + w_1 - w_2\|_{H^{2,l}}) \|v\|_{H^{2,l}} . \end{aligned}$$

*Step 2: Analysis in $\operatorname{ran}(H_{E^*}) = \operatorname{ran}(P^c_H)$:* By the above arguments, after temporarily complexifying domain and target space in (5.8.4), we see that $F$ is an analytic function and furthermore

$$\frac{\partial F}{\partial w}|_{(E_*,0,0)} = H_{E_*} : H^{2,l}_{\mathbb{R}}(\mathbb{R}^3) \cap \operatorname{ran}(H_{E_*}) \to \operatorname{ran}(H_{E_*} \restriction H^{2,l}_{\mathbb{R}}(\mathbb{R}^3)) \subset L^{2,l}(\mathbb{R}^3)$$

is a linear isomorphism between Banach spaces. Thus by the analytic version of the implicit function theorem, for $|(E - E_*, \delta)|$ sufficiently small, there is a unique analytic map

$$w = w(E, \delta) : \mathbb{R}^2 \to H^{2,l}_{\mathbb{R}}(\mathbb{R}^3)$$

with $w(E_*, 0) = 0$ such that

$$P_H^c F(E, \delta, w(E, \delta)) = H_E w(E, \delta) + b P_H^c (\delta v_* + w(E, \delta))^3 \equiv 0. \tag{5.8.5}$$

It follows that $\|H_E w(E, \delta)\|_2 \lesssim (\delta + \|w(E, \delta)\|_{H^2})^3$ and since for $|E - E_*| \ll 1$, $\|H_E^{-1} P_H^c\|_{L^2 \to L^2}$ (like $\|H_{E_*}^{-1} P_H^c\|_{L^2 \to L^2}$) is of order one, we deduce

$$\|w(E, \delta)\|_2 + \|H_E w(E, \delta)\|_2 \simeq \|w(E, \delta)\|_{H^2} \lesssim (\delta + \|w(E, \delta)\|_{H^2})^3$$

which by continuity of $w(E, \delta)$ yields the bound

$$\|w(E, \delta)\|_{H^2} \lesssim \delta^3, \tag{5.8.6}$$

uniformly in $E$ in a neighborhood of $E_*$. The norm in this estimate can be improved to $\| \cdot \|_{H^{2,l}}$ as follows. By Equation (5.8.5) and Lemma 5.20 we get

$$\begin{aligned} \|\langle x \rangle^l H_E w(E, \delta)\|_2 &\lesssim \|\langle x \rangle^l (\delta v_* + w(E, \delta))^3\|_2 + \|\langle x \rangle^l \langle v_*, (\delta v_* + w(E, \delta))^3 \rangle v_*\|_2 \\ &\lesssim (\delta + \|w(E, \delta)\|_{H^{2,l}})^3 \end{aligned} \tag{5.8.7}$$

and furthermore by Lemma 5.22, Estimate (5.8.6) it holds for $l \leq \sigma$ that

$$\begin{aligned} \|\langle x \rangle^l w(E, \delta)\|_2 &\lesssim \|\langle x \rangle^l (-\Delta - E)^{-1} P_H^c (\delta v_* + w(E, \delta))^3\|_2 + \|\langle x \rangle^l (-\Delta - E)^{-1} V w(E, \delta)\|_2 \\ &\lesssim \|\langle x \rangle^l P_H^c (\delta v_* + w(E, \delta))^3\|_2 + \|\langle x \rangle^{l - \sigma} w(E, \delta)\|_2 \\ &\lesssim (\delta + \|w(E, \delta)\|_{H^{2,l}})^3 + \delta^3 \, . \end{aligned} \tag{5.8.8}$$

Estimates (5.8.7, 5.8.8) imply

$$\|w(E, \delta)\|_{H^{2,l}} \lesssim \delta^3 \tag{5.8.9}$$

uniformly in $E$ in a neighborhood of $E_*$. By induction on multiples of $\sigma$ we conclude that (5.8.9) holds for every $l \geq 0$ and hence in fact for any real $l$.

*Step 3: Analysis in* $\ker(H_{E_*}) = \operatorname{ran}(P_H^d)$*:* The equation for $P_H^d F(E, \delta, w(E, \delta))$ corresponds to

$$\begin{aligned} &\langle v_*, H_E(\delta v_* + w(E, \delta) + b(\delta v_* + w(E, \delta))^3 \rangle \\ &= \delta(E_* - E) + \langle v_*, b(\delta v_* + w(E, \delta))^3 \rangle \overset{!}{=} 0. \end{aligned} \tag{5.8.10}$$

which, for $\operatorname{sign}(b) = \operatorname{sign}(E - E_*)$ and $|E - E_*|$ sufficiently small, has a solution $\delta(E)$, unique up to sign, with $\delta(E_*) = 0$ as we shall see now. Define $a_* := \sqrt{\langle v_*^2, v_*^2 \rangle_{L^2}}$. If $\delta(\cdot)$ exists we infer from (5.8.10) the condition

$$\frac{\delta(E)^2}{E - E_*} \to \frac{1}{b a_*^2} \qquad \text{as } |E - E_*| \to 0 \, .$$

and hence $\operatorname{sign}(E - E_*) = \operatorname{sign}(b)$. Thus we choose the sign of $E$ accordingly and define $p := \sqrt{\frac{E - E_*}{b}}$. Furthermore, we introduce the quotient $q := \frac{\delta}{p}$ and consider an equation equivalent to (5.8.10) in these new variables:

$$G(p, q) := -q + \langle v_*, \left( q v_* + \frac{w(E_* + b p^2, pq)}{p} \right)^3 \rangle \overset{!}{=} 0 \, .$$

By analyticity of $w(\cdot,\cdot)$ and by (5.8.6) $G(p,q)$ is analytic for sufficiently small $p$. It possesses for $p=0$ two zeros $q=\pm\frac{1}{a_*}$ of which we choose the positive one since only this can lead to positive solutions for Equation (5.1.2). Observe that

$$\frac{\partial G}{\partial q}|_{(0,\frac{1}{a_*})}=2\,.$$

Thus there is a unique analytic map $q(p)$ with $q(0)=\frac{1}{a_*}$ satisfying

$$G(p,q(p))\equiv 0$$

for sufficiently small $p$ and hence

$$0\equiv bp^3G(p,q(p))=-q(p)p\cdot(E-E_*)+\langle v_*,b\,(q(p)pv_*+w(E,p(q)q))^3\rangle\,.$$

Therefore $\delta(E):=q(\sqrt{\frac{E-E_*}{b}})\sqrt{\frac{E-E_*}{b}}$ solves (5.8.10) with real analytic $q(\cdot)$ and $q(0)=\frac{1}{a^*}$. Positivity of $\psi_E$ follows from linear theory by considering the Hamiltonian $-\Delta+V+|\psi_E|^2$. □

From here on we allow the potential again to be time-dependent (in the sense of ($\mathrm{H_d}$)). Then in particular, $H_s=-\Delta+V_s$ is a $C^2$-family with values in $\mathcal{L}(H^2(\mathbb{R}^3),L^2(\mathbb{R}^3))$. As a consequence $P^d_{H_s}=|v_{*,s}\rangle\langle v_{*,s}|$ and $E_{*,s}=\mathrm{tr}\left(H_sP^d_{H_s}\right)$ are also $C^2$, see Lemma 2.14.

Proof of Proposition 5.2 (ii) and (iii). For fixed $\tau\in[0,1]$ and $H_{E,s}:=-\Delta+V_s-E$ we generalize the Map (5.8.4) to

$$\begin{aligned}F_\tau:[0,1]\times\mathbb{R}\times\mathbb{R}\times H^{2,l}_{\mathbb{R}}(\mathbb{R}^3)\cap\mathrm{ran}(H_{E_{*,\tau},\tau})\to L^{2,l}_{\mathbb{R}}(\mathbb{R}^3)=\mathrm{span}_{\mathbb{R}}(v_{*,\tau})\oplus\mathrm{ran}(H_{E_{*,\tau},\tau}\restriction H^{2,l}_{\mathbb{R}}(\mathbb{R}^3))\\(s,E,\delta,w)\mapsto H_{E,s}(\delta v_{*,\tau}+w)+b(\delta v_{*,\tau}+w)^3\,.\end{aligned}$$

Since

$$\begin{aligned}\left\|\frac{F_\tau(s+\lambda,E,\delta,w)-F_\tau(s,E,\delta,w)}{\lambda}-\partial_sV_s(\delta v_{*,\tau}+w)\right\|_{L^{2,l}}\\\lesssim\left\|\frac{V_{s+\lambda}-V_s}{\lambda}-\partial_sV_s\right\|_\infty\|\delta v_{*,\tau}+w\|_{L^{2,l}}\,,\end{aligned}$$

and similarly for the second derivative, it follows that $F_\tau$ is $C^2$. By application of the implicit function theorem to $P^c_{H_\tau}F_\tau$ as in the proof of Proposition 5.2 (i), there is $w(s,E,\delta)$ which is $C^2$ with respect to time and $P^c_{H_\tau}F_\tau(s,E,\delta,w(s,E,\delta))\equiv 0$. Then, $P^d_{H_\tau}F_\tau(s,E,\delta,w(s,E,\delta))\equiv 0$ corresponds to

$$\begin{aligned}G_\tau(s,E,\delta):=&\delta(E_{*,\tau}-E)\\&+\langle v_{*,\tau},(V_s-V_\tau)(\delta v_{*,\tau}+w(s,E,\delta))\rangle+b\langle v_{*,\tau},(\delta v_{*,\tau}+w(s,E,\delta))^3\rangle\equiv 0\end{aligned}$$

and we have

$$\frac{\partial G_\tau}{\partial\delta}|_{(\tau,E,0)}=E_{*,\tau}-E\,,$$

see (5.8.9). For $E\neq E_{*,\tau}$ we obtain the desired regularity of the function $\delta(E,s)$ (whose existence is guaranteed by Proposition 5.2 (i)) with respect to $s$ near $s=\tau$, again by the implicit function theorem. Hence, since $\tau$ was arbitrary, a two-dimensional submanifold $\mathcal{M} \subset H^{2,l}(\mathbb{R}^3)$ of ground states with a single chart

$$\psi_{E,s} : \{(E,s)|0 < \frac{E - E_{*,s}}{b} \ll 1,\, s \in [0,1]\} \to \mathcal{M}$$

has been constructed. In particular, this proves (i).

Finally, we construct the submanifold of ground states with equal mass, (iii). By Proposition 5.2 (i) it holds for $|E - E_{*,s}|$ sufficiently small that

$$\frac{\partial \|\psi_{E,s}\|_2^2}{\partial E} = 2\langle \psi_{E,s}, \partial_E \psi_{E,s} \rangle > 0 \text{ on } \mathcal{M}\,, \tag{5.8.11}$$

in particular, $\|\psi_{E,s}\|_2$ is monotonic in $E$. Continuity of $(s,E) \mapsto \|\psi_{E,s}\|_2^2$ and compactness of $[0,1]$ yields the existence of $\eta_0 > 0$ such that $\|\psi_{E,s}\|_2^2 = \eta$ defines a nonempty subset $\mathcal{N}$ of $\mathcal{M}$ for each $0 < \eta \le \eta_0$. Moreover, by (5.8.11), $\eta$ is a regular value for

$$\begin{aligned} h : \mathcal{M} &\to \mathbb{R} \\ \psi_{E,s} &\mapsto \|\psi_{E,s}\|_2^2 \end{aligned}$$

and hence $\mathcal{N}$ is indeed a $C^2$-submanifold. □

### 5.8.2. Auxiliary results

This section presents the announced proofs of several lemmata needed before.

PROOF OF LEMMA 5.6. The first claim follows from Hölder's inequality and the triangle inequality,

$$\begin{aligned} \|\Delta\phi\|_2 + \|\phi\|_2 &\le \|(-\Delta + V)\phi\|_2 + \|V\phi\|_2 + \|\phi\|_2 \\ &\lesssim \|(-\Delta + V)\phi\|_2 + \|\phi\|_2 \\ &\lesssim \|\Delta\phi\|_2 + \|\phi\|_2\,. \end{aligned}$$

To prove the second claim we observe that

$$\Delta(\langle x\rangle^l \phi) - \langle x\rangle^l \Delta\phi = (\Delta\langle x\rangle^l)\phi + 2\nabla\langle x\rangle^l \cdot \nabla\phi\,.$$

The $L^2$-norm of the first term on the right hand side is estimated by $\|\langle x\rangle^l \phi\|_2$ whereas for the second term we compute

$$\begin{aligned} \|\nabla\langle x\rangle^l \cdot \nabla\phi\|_2^2 &= -\int_{\mathbb{R}^3} \mathrm{d}^3x\ \phi \nabla \cdot \left( \left( \nabla\langle x\rangle^l \cdot \nabla\overline{\phi} \right) \nabla\langle x\rangle^l \right) \\ &= -\int_{\mathbb{R}^3} \mathrm{d}^3x\ \phi \left( 2\Delta\langle x\rangle^l \nabla\overline{\phi} + \nabla\langle x\rangle^l \Delta\overline{\phi} \right) \cdot \nabla\langle x\rangle^l\,. \end{aligned}$$

Hölder's and Young's inequalities lead to

$$\left| \int_{\mathbb{R}^3} \mathrm{d}^3x\ \phi\Delta\overline{\phi} |\nabla\langle x\rangle^l|^2 \right| \lesssim (\|\langle x\rangle^l \phi\|_2 + \|\langle x\rangle^l \Delta\phi\|_2)^2\,,$$

and

$$\left|\int_{\mathbb{R}^3} \mathrm{d}^3x \; \phi\Delta\langle x\rangle^l \nabla\overline{\phi}\cdot\nabla\langle x\rangle^l\right| \lesssim \|\langle x\rangle^l\phi\|_2\|\nabla\langle x\rangle^l\cdot\nabla\phi\|_2 \,.$$

Hence we obtain

$$\|\phi\|_{H^{2,l}} \lesssim \|\langle x\rangle^l\phi\|_2 + \|\langle x\rangle^l\Delta\phi\|_2 \,.$$

To prove the converse inequality observe that

$$\|\nabla\langle x\rangle^l\cdot\nabla\phi\|_2 \lesssim \||\langle x\rangle^l\nabla\phi|\|_2 = \||\nabla(\langle x\rangle^l\phi) - (\nabla\langle x\rangle^l)\phi|\|_2 \lesssim \|\phi\|_{H^{2,l}}$$

by means of the equivalence

$$\|\cdot\|_2 + \|\Delta\cdot\|_2 \simeq \|\cdot\|_2 + \||\nabla\cdot|\|_2 + \|\Delta\cdot\|_2 \,. \tag{5.8.12}$$

To prove the product estimates for $\|\cdot\|_{W^{2,1}}$ note that

$$\int_{\mathbb{R}^3} \mathrm{d}^3x \; |\phi\chi| \lesssim \|\phi\|_2\|\chi\|_2$$

and

$$\begin{aligned}\int_{\mathbb{R}^3} \mathrm{d}^3x \; |\Delta(\phi\chi)| &\simeq \int_{\mathbb{R}^3} \mathrm{d}^3x \; |\nabla\cdot(\phi\nabla\chi + \chi\nabla\phi)\,| \\ &\lesssim \int_{\mathbb{R}^3} \mathrm{d}^3x \; |\nabla\phi\cdot\nabla\chi| + \int_{\mathbb{R}^3} \mathrm{d}^3x \; \left(|\phi\Delta\chi| + |\chi\Delta\phi|\right) \,.\end{aligned}$$

Hölder's inequality and (5.8.12) now yield (5.4.3). Estimate (5.4.4) is a consequence of a special case of Lemma A.8 in [Tao06], whose proof relies on Littlewood-Paley theory. We give a different proof in our setting: By the Sobolev embedding $H^2(\mathbb{R}^3) \hookrightarrow L^\infty(\mathbb{R}^3)$ we obtain

$$\|\phi\chi\|_2 \lesssim \|\phi\|_\infty\|\chi\|_2 \lesssim \|\phi\|_{H^2}\|\chi\|_2$$

and

$$\begin{aligned}\int_{\mathbb{R}^3} \mathrm{d}^3x \; |\Delta(\phi\chi)|^2 &\lesssim \int_{\mathbb{R}^3} \mathrm{d}^3x \; |\nabla\phi\cdot\nabla\chi|^2 + \int_{\mathbb{R}^3} \mathrm{d}^3x \; \left(|\phi\Delta\chi|^2 + |\chi\Delta\phi|^2\right) \\ &\lesssim \int_{\mathbb{R}^3} \mathrm{d}^3x \; |\nabla\phi|^2|\nabla\chi|^2 + \|\phi\|_{H^2}^2\|\chi\|_{H^2}^2 \,.\end{aligned}$$

Next, integration by parts and the Sobolev embedding $H^1(\mathbb{R}^3) \hookrightarrow L^4(\mathbb{R}^3)$ yield

$$\begin{aligned}\int_{\mathbb{R}^3} \mathrm{d}^3x \; |\nabla\phi|^2|\nabla\chi|^2 &= -\int_{\mathbb{R}^3} \mathrm{d}^3x \; \phi\Delta\overline{\phi}|\nabla\chi|^2 - 2\int_{\mathbb{R}^3} \mathrm{d}^3x \; \phi\nabla\overline{\phi}\cdot\Re\left(\nabla^2\chi\nabla\overline{\chi}\right) \\ &\lesssim \|\phi\|_\infty\|\Delta\phi\|_2\||\nabla\chi|\|_4^2 + \|\phi\|_\infty\|\chi\|_{H^2}\||\nabla\phi||\nabla\chi|\|_2 \\ &\lesssim \|\phi\|_{H^2}^2\|\chi\|_{H^2}^2 + \|\phi\|_{H^2}\|\chi\|_{H^2}\||\nabla\phi||\nabla\chi|\|_2\end{aligned}$$

and hence

$$\||\nabla\phi||\nabla\chi|\|_2 \lesssim \|\phi\|_{H^2}\|\chi\|_{H^2} \,,$$

implying (5.4.4). Ultimately, we note that for $l \geq 0$ applying (ii) and (5.4.4) leads to

$$\|\phi^2\|_{H^{2,l}} \lesssim \|\langle x\rangle^{2l}\phi^2\|_2 + \|\langle x\rangle^{2l}\Delta(\phi^2)\|_2 \simeq \|(\langle x\rangle^l\phi)^2\|_{H^2} \lesssim \|\phi\|_{H^{2,l}}^2 \,,$$

which proves (iii). □

Proof of Lemma 5.10. Continuous differentiability of $\partial_s \vec{\psi}_{E,s}$ has been established in Subsection 5.8.1 and hence it suffices to consider

$$P_s^c L_{E,s}^{-1} P_s^c : L^{2,\sigma}(\mathbb{R}^3) \to H^{2,\sigma}(\mathbb{R}^3)\,. \tag{5.8.13}$$

The Mapping (5.8.13) is well-defined: Note

$$\begin{aligned}\|P_s^c L_{E,s}^{-1} P_s^c \psi\|_{H^{2,\sigma}} &\simeq \|P_s^c L_{E,s}^{-1} P_s^c \psi\|_{L^{2,\sigma}} + \|L_{E,s} P_s^c L_{E,s}^{-1} P_s^c \psi\|_{L^{2,\sigma}} \\ &\lesssim \|P_s^c L_{E,s}^{-1} P_s^c\|_{L^{2,\sigma}\to L^{2,\sigma}} \|\psi\|_{L^{2,\sigma}}\,.\end{aligned}$$

By

$$P_s^c L_{E,s}^{-1} P_s^c = \frac{1}{2\pi \mathrm{i}} \int_\Gamma (L_{E,s} - z)^{-1} \frac{1}{z} dz\,, \tag{5.8.14}$$

for $\Gamma$ encircling 0 in counterclockwise direction at distance $G_0/2$, it suffices to estimate the norm of the resolvent $\|(L_{E,s} - z)^{-1}\|_{L^{2,\sigma}\to L^{2,\sigma}}$ for $|z| = G_0/2$. By the resolvent identity (5.5.9) we observe that all we need is a bound on $\|(H_{E_*,s,s} - z)^{-1}\|_{L^{2,\sigma}\to L^{2,\sigma}}$. However by Lemma 5.22, with $\lambda = \sqrt{G_0/8} > 0$,

$$\begin{aligned}\|(H_{E_*,s,s} - z)^{-1}\|_{L^{2,\sigma}\to L^{2,\sigma}} \le& \|(-\Delta - E_{*,s} - z)^{-1}\|_{L^{2,\sigma}\to L^{2,\sigma}} \\ &+ \|(-\Delta - E_{*,s} - z)^{-1} V_s (H_{E_*,s,s} - z)^{-1}\|_{L^{2,\sigma}\to L^{2,\sigma}} \\ \le& C_\sigma \frac{1}{\Re\sqrt{-E_{*,s} - z} - \lambda} \left(1 + \|\langle x\rangle^\sigma V_s (H_{E_*,s,s} - z)^{-1} \langle x\rangle^{-\sigma}\|_{L^2\to L^2}\right) \\ \le& C_{V,\sigma} \frac{1}{\Re\sqrt{-E_{*,s} - z} - \lambda} (1 + \frac{1}{|z|}) \\ \le& C_{V,\sigma} \frac{1}{2\sqrt{G_0}} (1 + \frac{1}{\sqrt{G_0/2}})\,.\end{aligned} \tag{5.8.15}$$

Therefore also $\|(L_{E,s} - z)^{-1}\|_{L^{2,\sigma}\to H^{2,\sigma}}$ is locally uniformly bounded. Differentiability of (5.8.13) with respect to $E$, $s$ follows from the first and second resolvent identity applied to Expression 5.8.14 and Hypothesis ($\mathrm{H_d}$), see also Lemma 2.14. □

Proof of Estimates (5.7.17, 5.7.18). The Estimate (5.7.17) follows from

$$\begin{aligned}\|\mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}H_\tau} P_{H_\tau}^c \chi\|_{H^2} &\simeq \|\mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}H_\tau} P_{H_\tau}^c \chi\|_2 + \|H_\tau \mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}H_\tau} P_{H_\tau}^c \chi\|_2 \\ &\simeq \|\mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}H_\tau} P_{H_\tau}^c \chi\|_2 + \|\mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}H_\tau} H_\tau P_{H_\tau}^c \chi\|_2 \\ &\simeq \|P_{H_\tau}^c \chi\|_2 + \|H_\tau P_{H_\tau}^c \chi\|_2 \\ &\simeq \|P_{H_\tau}^c \chi\|_{H^2} \\ &\simeq \|P_{H_\tau}^c \chi\|_2 + \|P_{H_\tau}^c H_\tau \chi\|_2 \lesssim \|\chi\|_{H^2}\,.\end{aligned} \tag{5.8.16}$$

By inspection we see that all multiplicative constants can be chosen to be independent of $\tau$ due to ($\mathrm{H_d}$).

By $\|\langle x\rangle^{-\sigma}\chi\|_2 \leq \|\langle x\rangle^{-\sigma}\|_2\|\chi\|_\infty \lesssim \|\chi\|_\infty$ for any $\sigma > 2$ (recall ($\mathrm{H_d}$)) we obtain

$$\begin{aligned}
\|\mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}H_\tau}P^c_{H_\tau}\chi\|_{H^{2,-\sigma}} &\simeq \|\langle x\rangle^{-\sigma}\mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}H_\tau}P^c_{H_\tau}\chi\|_2 + \|\langle x\rangle^{-\sigma}H_\tau\mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}H_\tau}P^c_{H_\tau}\chi\|_2 \\
&\simeq \|\langle x\rangle^{-\sigma}\mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}H_\tau}P^c_{H_\tau}\chi\|_2 + \|\langle x\rangle^{-\sigma}\mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}H_\tau}P^c_{H_\tau}H_\tau\chi\|_2 \\
&\lesssim \|\mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}H_\tau}P^c_{H_\tau}\chi\|_\infty + \|\mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}H_\tau}P^c_{H_\tau}H_\tau\chi\|_\infty \\
&\lesssim \left|\frac{t}{\varepsilon}\right|^{-\frac{3}{2}}(\|\chi\|_1 + \|H_\tau\chi\|_1) \\
&\lesssim \left|\frac{t}{\varepsilon}\right|^{-\frac{3}{2}}\|\chi\|_{W^{2,1}}\,. \qquad (5.8.17)
\end{aligned}$$

This together with (5.8.16) yields the Estimate (5.7.18). □

The uniformity of the constant $A$ follows from compactness of $[0,1]$ and the following lemma.

**Lemma 5.24.** *Consider $H_0 = -\Delta + V_0$ with $V_0 \in H^{2,\sigma}(\mathbb{R}^3)$ admitting no zero energy resonance, thus*

$$\|\mathrm{e}^{-\mathrm{i}H_0t}P^c_{H_0}\phi\|_{H^{2,-\sigma}} \leq C_0\langle t\rangle^{-\frac{3}{2}}\|\phi\|_{H^2\cap W^{2,1}}.$$

*Then for $H = -\Delta + V$, $V \in H^{2,\sigma}(\mathbb{R}^3)$, $\|V - V_0\|_{H^{2,\sigma}}$ sufficiently small, it holds that*

$$\|\mathrm{e}^{-\mathrm{i}Ht}P^c_H\phi\|_{H^{2,-\sigma}} \leq C\langle t\rangle^{-\frac{3}{2}}\|\phi\|_{H^2\cap W^{2,1}},$$

*where $C$ can be chosen such that $C \to C_0$ as $\|V - V_0\|_{H^{2,\sigma}} \to 0$.*

Proof. To simplify the notation, $\delta > 0$ will denote a generic quantity which tends to zero as $\|V - V_0\|_{H^{2,\sigma}} \to 0$. By Duhamel's formula

$$\begin{aligned}
e^{-\mathrm{i}Ht}P^c_H\phi = e^{-\mathrm{i}P^c_HHP^c_Ht}P^c_H\phi =& e^{-\mathrm{i}P^c_HH_0P^c_Ht}P^c_H\phi \\
&- \mathrm{i}\int_0^t ds\; e^{-\mathrm{i}P^c_HH_0P^c_H(t-s)}P^c_H(V-V_0)P^c_He^{-\mathrm{i}P^c_HHP^c_Hs}P^c_H\phi\,.
\end{aligned} \qquad (5.8.18)$$

*Claim:* $\|\mathrm{e}^{-\mathrm{i}P^c_HH_0P^c_Ht}P^c_H\phi\|_{H^{2,-\sigma}} \leq \langle t\rangle^{-\frac{3}{2}}(C_0+\delta)\|\phi\|_{H^2\cap W^{2,1}}$.

We first show that the claim implies the lemma. With Lemma 5.6 we have

$$\|P^c_H(V-V_0)\langle x\rangle^{\sigma}\langle x\rangle^{-\sigma}P^c_He^{-\mathrm{i}P^c_HHP^c_Hs}P^c_H\phi\|_{H^2\cap W^{2,1}} \leq \delta\|e^{-\mathrm{i}P^c_HHP^c_Hs}P^c_H\phi\|_{H^{2,-\sigma}}$$

and thus estimating (5.8.18) for all $t \leq t^*$ we obtain

$$\begin{aligned}
\langle t\rangle^{\frac{3}{2}}\|\mathrm{e}^{-\mathrm{i}Ht}P^c_H\phi\|_{H^{2,-\sigma}} \leq (C_0+\delta)\|\phi\|_{H^2\cap W^{2,1}} + \delta\langle t\rangle^{\frac{3}{2}}\int_0^{t^*} ds(C_0+\delta)\langle t-s\rangle^{-\frac{3}{2}}\langle s\rangle^{-\frac{3}{2}}\times \\
\times \sup_{s\leq t^*}\langle s\rangle^{\frac{3}{2}}\|e^{-\mathrm{i}P^c_HHP^c_Hs}P^c_H\phi\|_{H^{2,-\sigma}}\,.
\end{aligned}$$

The lemma now follows from

$$\int_0^\infty ds\langle t-s\rangle^{-\frac{3}{2}}\langle s\rangle^{-\frac{3}{2}} \leq D\langle t\rangle^{-\frac{3}{2}}$$

for a numerical constant $D$. This is proved as in Lemma 5.18.

To prove the claim we define $\phi_t := \mathrm{e}^{-\mathrm{i}P_H^c H_0 P_H^c t} P_H^c \phi$ and apply Duhamel's formula again,

$$\phi_t = \mathrm{e}^{-\mathrm{i}H_0 t} P_H^c \phi + \mathrm{i} \int_0^t ds\ \mathrm{e}^{-\mathrm{i}H_0(t-s)} P_H^d H_0 P_H^c \phi_s$$

It holds that

$$\begin{aligned}\|\phi_t\|_{H^{2,-\sigma}} = \|P_H^c \phi_t\|_{H^{2,-\sigma}} \leq & \|(P_{H_0}^c - P_H^c)\phi_t\|_{H^{2,-\sigma}} + \|P_{H_0}^c \phi_t\|_{H^{2,-\sigma}} \\ \leq & \delta \|\phi_t\|_{H^{2,-\sigma}} + \|P_{H_0}^c \phi_t\|_{H^{2,-\sigma}}\,,\end{aligned}$$

and the same is true if $H^{2,-\sigma}(\mathbb{R}^3)$ is replaced by $H^2(\mathbb{R}^3) \cap W^{2,1}(\mathbb{R}^3)$. The second inequality can be proved with the Riesz formula and similar resolvent estimates as those in the proof of Lemma 5.10. It follows that it is sufficient to estimate

$$\begin{aligned}P_{H_0}^c \phi_t &= \mathrm{e}^{-\mathrm{i}H_0 t} P_{H_0}^c P_H^c \phi + \mathrm{i} \int_0^t ds\ \mathrm{e}^{-\mathrm{i}H_0(t-s)} P_{H_0}^c P_H^d H_0 P_H^c \phi_s \\ &= \mathrm{e}^{-\mathrm{i}H_0 t} P_{H_0}^c \phi + \mathrm{e}^{-\mathrm{i}H_0 t} P_{H_0}^c (P_H^c - P_{H_0}^c)\phi + \mathrm{i} \int_0^t ds\ \mathrm{e}^{-\mathrm{i}H_0(t-s)} P_{H_0}^c P_H^d (V_0 - V) P_H^c \phi_s\,.\end{aligned}$$

Hence for all $t \leq t^*$

$$\begin{aligned}\langle t\rangle^{\frac{3}{2}} \|\phi_t\|_{H^{2,-\sigma}} &\leq (1+\delta)\langle t\rangle^{\frac{3}{2}} \|P_{H_0}^c \phi_t\|_{H^{2,-\sigma}} \\ &\leq (C_0 + \delta)\|\phi\|_{H^2\cap W^{2,1}} \\ &\qquad + (1+\delta)\langle t\rangle^{\frac{3}{2}} \int_0^t ds \langle t-s\rangle^{-\frac{3}{2}} \langle s\rangle^{-\frac{3}{2}} \langle s\rangle^{\frac{3}{2}} \|(V_0 - V)\langle x\rangle^{\sigma}\langle x\rangle^{-\sigma} P_H^c \phi_s\|_{H^2\cap W^{2,1}} \\ &\leq (C_0 + \delta)\|\phi\|_{H^2\cap W^{2,1}} + \delta D \sup_{s\leq t^*} \langle s\rangle^{\frac{3}{2}} \|\phi_s\|_{H^{2,-\sigma}}\end{aligned}$$

This proves the claim. □

Proof of Lemma 5.15. Obviously, $\|P_{H_0}^c \tilde{\vec{\phi}}_s\|_2 \leq \|\tilde{\vec{\phi}}_s\|_2$ and $\|H_0 P_{H_0}^c \tilde{\vec{\phi}}_s\|_2 = \|P_{H_0}^c H_0 \tilde{\vec{\phi}}_s\|_2 \leq \|H_0 \tilde{\vec{\phi}}_s\|_2$ imply

$$\|P_{H_0}^c \tilde{\vec{\phi}}_s\|_2 + \|P_{H_0}^c H_0 \tilde{\vec{\phi}}_s\|_2 \simeq \|P_{H_0}^c \tilde{\vec{\phi}}_s\|_{H^2} \lesssim \|\tilde{\vec{\phi}}_s\|_{H^2}\,.$$

By Lemma 5.20

$$\|\langle x\rangle^{-\sigma} P_{H_0}^d \tilde{\vec{\phi}}_s\|_2 \lesssim \|\langle x\rangle^{-\sigma} \tilde{\vec{\phi}}_s\|_2\,,$$

and similarly,

$$\|\langle x\rangle^{-\sigma} H_0 P_{H_0}^d \tilde{\vec{\phi}}_s\|_2 = \|\langle x\rangle^{-\sigma} P_{H_0}^d H_0 \tilde{\vec{\phi}}_s\|_2 \lesssim \|\vec{\phi}_s\|_{H^{2,-\sigma}}\,,$$

whence $\|P_{H_0}^c \tilde{\vec{\phi}}_s\|_{H^{2,-\sigma}} \lesssim \|\tilde{\vec{\phi}}_s\|_{H^{2,-\sigma}}$. To show the converse inequalities note that for both norms

$$\|\tilde{\vec{\phi}}_s\| \leq \|P_{H_0}^c \tilde{\vec{\phi}}_s\| + \|\left(P_s - P_{H_0}^c\right) \tilde{\vec{\phi}}_s\|\,.$$

Therefore it suffices to show that $\|P_s - P^c_{H_0}\|_{H^2\to H^2}$ resp. $\|P_s - P^c_{H_0}\|_{H^{2,-\sigma}\to H^{2,-\sigma}}$ can be made arbitrarily small by choosing $s_0, \eta, \varepsilon$ suitably. By the second resolvent formula we obtain

$$\|P_s - P^c_{H_0}\| \lesssim \oint_\Gamma dz\ \|(JL_s - z)^{-1}\|\|JL_s - H_0\|\|(H_0 - z)^{-1}\|\,,$$

$\Gamma$ as above. Observe that for arbitrary $\delta > 0$ we can achieve

$$\|JL_s - H_0\| \lesssim \delta$$

in both operator norms as a consequence of (5.7.10) and (5.7.11). Furthermore it follows from a similar reasoning as for Estimate (5.8.15) that the norms of $(L_s - z)^{-1}$ and $(H_0 - z)^{-1}$ are both uniformly bounded on $H^{2,-\sigma}(\mathbb{R}^3)$ (the case $H^2(\mathbb{R}^3)$ is easier). This concludes the proof. □

PROOF OF LEMMA 5.17. By Lemma 5.15 $\|P^c_{H_0}(L_s + JH_0)\vec{\phi}_s\|_{H^2} \lesssim \|(L_s + JH_0)\vec{\phi}_s\|_{H^2}$ and by Lemma 5.20 also $\|P^c_{H_0}(L_s + JH_0)\vec{\phi}_s\|_{W^{2,1}} \lesssim \|(L_s + JH_0)\vec{\phi}_s\|_{W^{2,1}}$. Then, by means of Estimate (5.7.11)

$$\|(L_s + JH_0)\langle x\rangle^\sigma\langle x\rangle^{-\sigma}\vec{\phi}_s\|_{H^2} \lesssim \delta\|\vec{\phi}_s\|_{H^{2,-\sigma}}\,,$$
$$\|(L_s + JH_0)\langle x\rangle^\sigma\langle x\rangle^{-\sigma}\vec{\phi}_s\|_{W^{2,1}} \lesssim \delta\|\vec{\phi}_s\|_{H^{2,-\sigma}}\,.$$

The proof of (5.7.26) is follows from similar arguments using the explicit expression for $P^d_s$, Equation (5.5.7). Ultimately, to prove (5.7.27) we note that since
$\frac{d}{dt}\psi_{E^\varepsilon_s,s}, \frac{d}{dt}\partial_E\psi_{E^\varepsilon_s,s} \in H^{2,\sigma}(\mathbb{R}^3)$ it holds that

$$\|P^d_s\dot{P}^d_s\vec{\phi}_s\|_{H^2\cap W^{2,1}} \lesssim \|\dot{P}^d_s\vec{\phi}_s\|_{H^{2,-\sigma}} \lesssim \|\vec{\phi}_s\|_{H^{2,-\sigma}}\,.$$

□

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# Curriculum Vitae

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