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On Time-Adiabatic Theorems

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On Time-Adiabatic Theorems

THESIS

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On Time-Adiabatic Theorems

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Abstract

State preparation requires adiabaticity, the slow intrinsic time-scale of a quantum system. The 'folk' adiabatic theorem tells us how slowly we should interpolate a Hamiltonian to obtain a desired ground state. This thesis rigorously proves three time-adiabatic theorems that provide an upper bound on the adiabatic evolution of total evolved time τ of an isolated subset of the spectrum of a smooth gap-dependent Hamiltonian. It turns out that the upper bound for the state transition probability outside the subset is of order $1/\tau^2$. Moreover, the adiabatic and the ideal time evolution of the projection space associated with the isolated subset is of order $1/\tau$, and the adiabatic with the ideal unitary propagator also compare of order $1/\tau$. We provide explicit constants for the upper bounds.

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Introduction

The dynamics of physical systems unfolding within the quantum realm are governed by the Schrödinger equation, which given in reduced units reads

$$\partial_t \psi(t) = -iH(t)\psi(t), \quad (1.1)$$

with $\partial_t = \frac{d}{dt}$. Here H is a time-dependent Hermitian operator*, called the Hamiltonian of the quantum system, which determines the evolution of the state ψ . The Hamiltonian directly corresponds to the energy of the system through its real-valued spectrum.

Nature herself solves this differential equation, restricting us from impacting the real-time evolution of states only through the Hamiltonian, which we may alter via e.g. a variation of electric or magnetic fields. Our Universe favours lower energies over greater energies, and states generally evolve towards the ground state[†]. An (easily) prepared ground state is a ground state that can be experimentally obtained to great accuracy. An example of such an easily prepared ground state is a single-particle system with an upward or downward spin, where we measure the spin in a basis and flip it if necessary. In practise, we are usually interested in systems with Hamiltonians of which their ground states are not so easily accessible.

*An operator in quantum mechanics is a function over the space of states onto another space of states. These states, sometimes called state vectors, are configurations of the quantum system, expressible as a vector in some vector space.

[†]The ground state is the energetically preferred configuration of a system, i.e. an eigenvector associated with the lowest eigenvalue of the Hamiltonian.

Our strategy to approximate a difficult ground state (associated with a difficult Hamiltonian) is to start at an easily prepared ground state (associated with an easy Hamiltonian) and use an interpolating Hamiltonian to attempt to reach the desired ground state. A question that immediately surges is whether the final state is really the ground state of the difficult Hamiltonian. The time-adiabatic theorems, the central topic of this thesis, roughly state that if we start in a ground state of an easy Hamiltonian and we interpolate the Hamiltonian smoothly and gradually we will end up in the ground state of the difficult Hamiltonian upon a decreasing error depending on the evolved time.

For this reason, we will mostly be interested in Hamiltonians of the form $H(t/\tau)$, where τ is a time-scaling parameter representing the total evolved time, allowing us to finetune the evolution of the states. The associated Schrödinger equation is then given by

$$\partial_t \psi_\tau(t) = -iH(t/\tau)\psi_\tau(t),$$

where the states now depend on τ . Introducing the dimensionless time parameter $s = t/\tau$, sometimes called the adiabatic parameter, and defining $\tilde{\psi}_\tau(s) := \psi_\tau(\tau s)$ gives the Schrödinger equation

$$\partial_s \tilde{\psi}_\tau(s) = -i\tau H(s)\tilde{\psi}_\tau(s).$$

Note that $s \in [0, 1]$ since τ is the total evolved time and we take t positive without loss of generality. As will be shown, directly associated with the Hamiltonian H is a unitary operator U , which expresses a future state via an initial state, i.e. $\tilde{\psi}_\tau(s) = U_\tau(s, s_0)\tilde{\psi}_\tau(s_0)$ where $s_0 = t_0/\tau$. We permit all initial states to justify the omission of $\tilde{\psi}_\tau(s_0)$, and obtain the more conventional Schrödinger equation,

$$\partial_s U_\tau(s, s_0) = -i\tau H(s)U_\tau(s, s_0). \quad (1.2)$$

We can think of s as the slow or macroscopic time and similarly of t as the fast or microscopic time.[‡]

The interpolating Hamiltonians will then be of the form

$$H(s) = (1 - f(s))H_E(s) + f(s)H_P(s),$$

where H_E and H_P represent the easy and difficult Hamiltonian respectively. As for the interpolating function $f(s)$, we only require it to be

[‡]The terms micro- and macroscopic stem from the similarity of a parameter that considers spatial scales rather than temporal scales. [25]

smooth and monotone such that $f(0) = 0$ and $f(1) = 1$ to ensure that $H(0) = H_E(0)$ and $H(1) = H_P(1)$. Linear interpolation may often be the easiest choice, simply taking $f(s) = s$, since s runs from 0 to 1.

This thesis means to elaborately state and prove several gap-dependent time-adiabatic theorems, denoting steps and clarifying arguments which are often omitted in papers about time-adiabatic theorems, in such a way that the thesis is substantially self-contained. Moreover, it lays out a meticulous framework through its methods of proving, which can be extended to more general time-adiabatic theorems (e.g. those omitting the gap-dependence) or even to theorems concerning spatial adiabaticity. Several applications are given to enhance, through reasonable simplifications, the conceptual key insights of the time-adiabatic theorems and to provide a glimpse of the beauty embodied within the field of quantum adiabaticity.

The thesis sets off by establishing the preliminaries necessary to formulate the time-adiabatic theorems in Chapter 2, introducing among others the notions of Hilbert spaces, resolvents, Riesz projectors and unitary propagators. Equipped with these meticulous foundations, we venture into Chapter 3 which elaborates onto the concept of adiabaticity allowing us to formulate and supplement upon aforementioned theorems. In Chapter 4 we will be concerned with proving these theorems in a complete rigorous manner. Then, in Chapter 5, we provide applications of the theorems with a limited amount of eigenvalues, and finally in Chapter 6 we conclude our work and enlighten the reader with different views, physical applications and further works concerning adiabatic theorems.

Chapter 2

Preliminaries

This chapter serves the purpose of providing the reader with the necessary background on the material and introduces notations and terminology that may be uncommon in either fields of physics and mathematics. Many of the listed elementary definitions and lemmas will be familiar, yet are included to ensure self-containment. The advanced reader may decide to briefly scan the content and move on to the next chapter.

2.1 State vector spaces

2.1.1 Norms, inner products and Hilbert spaces

We assume familiarity to a reasonable degree with vector spaces and their properties; characteristics of norms and inner products; and topological concepts such as completeness, denseness and compactness. However, the notion of a Hilbert space might not be so elementary for some, and for that reason we will briefly show how to construct a Hilbert space from scratch. Hilbert spaces are important for they are the playground of the quantum states of a system, and the underpinning framework in which the axioms of quantum mechanics are established.

Overall, we will be concerned with vector spaces over \mathbb{C} , and therefore we will not generalise the forthcoming definitions.

We can equip a vector space with a norm map. The norm of vectors gives a sense of the magnitude or size of the vectors and allows for concepts such as continuity, boundedness and completeness.

Definition 2.1.1 (Norm map). Let \mathbb{F} be a vector space over \mathbb{C} . Then

$$\|\cdot\| : \mathbb{F} \rightarrow \mathbb{R}$$

is called a norm on \mathbb{F} if for all $x, y \in \mathbb{F}$ and $\lambda \in \mathbb{C}$ we have

- i. (positive definiteness) $\|x\| \geq 0$, and $\|x\| = 0$ if and only if $x = 0$;
- ii. (homogeneity) $\|\lambda x\| = |\lambda| \|x\|$;
- iii. (triangle inequality) $\|x + y\| \leq \|x\| + \|y\|$.

A vector space with a norm is called a normed vector space.

Using the norm we can introduce the concept of normalisation, which through probabilities quantum mechanics relies much upon. We say that vector $x \in \mathbb{F}$ is normalised if $\|x\| = 1$. For any vector $x \neq 0$, we can follow the procedure of normalisation defined by $x' = \|x\|^{-1}x$ where x' is now normalised.

For quantum systems, we will need to define geometric and algebraic properties such as angles, lengths and most importantly the notion of orthogonality; a vital requirement for the construction of projections. This is made formal with the inner product operation.

Definition 2.1.2 (Inner product). Let \mathbb{F} be a vector space over \mathbb{C} . Then the map

$$\langle \cdot, \cdot \rangle : \mathbb{F} \times \mathbb{F} \rightarrow \mathbb{C}$$

is an inner product if for all $x, y, z \in \mathbb{F}$ and $\lambda \in \mathbb{C}$ we have

- i. (positive definiteness) $\langle x, x \rangle \geq 0$, and $\langle x, x \rangle = 0$ if and only if $x = 0$;
- ii. (linear in first entry) $\langle \lambda x + y, z \rangle = \lambda \langle x, z \rangle + \langle y, z \rangle$;
- iii. (complex symmetric) $\langle x, y \rangle = \overline{\langle y, x \rangle}$.

The overline is used for complex conjugation. A vector space equipped with an inner product is called an inner product space.

Remark 2.1.1. The observant reader will note that we adopt the mathematical definition of the inner product. In the field of physics the inner product is usually antilinear with respect to the first component and linear with respect to the second component.

For an inner product space \mathbb{F} , we can combine the concepts of the norm and the inner product by defining $\|x\| := \sqrt{\langle x, x \rangle}$ for all $x \in \mathbb{F}$. The reader can confirm that this $\|\cdot\|$ is a norm on \mathbb{F} , commonly called the norm induced by the inner product. We are now able to define the Hilbert space.

Definition 2.1.3 (*Hilbert space*). A Hilbert space, denoted \mathcal{H} , is an inner product space that is complete in the norm induced by the inner product.

Recall that a metric space is complete if every Cauchy sequence converges to an element in the metric space, and that each Hilbert space is a Banach space equipped with an inner product.

2.1.2 Examples of Hilbert spaces

There are many Hilbert spaces, trivial examples being \mathbb{C} and \mathbb{C}^2 . The Hilbert space \mathbb{C}^2 , for example, is usually taken when we consider bits in the field of quantum information.

The Hilbert space that is usually required for physical quantum systems is constructed with square-integrable functions. A \mathbb{R}^3 -square-integrable function $f : \mathbb{R}^3 \rightarrow \mathbb{C}$ is a function f such that

$$\int_{-\infty}^{\infty} |f(x)|^2 d^3x < \infty.$$

The vector space of \mathbb{R}^3 -square-integrable functions, denoted by $L^2(\mathbb{R}^3)$ or simply L^2 , forms a Hilbert space with the inner product defined by

$$\langle f(x), g(x) \rangle = \int_{-\infty}^{\infty} f(x) \overline{g(x)} d^3x,$$

for all $f, g \in L^2$ [7]. We can estimate the inner product in terms of the norm by the Cauchy-Schwarz-Bunyakovsky inequality, $|\langle f, g \rangle| \leq \|f\| \|g\|$ holds for all $f, g \in L^2$.

The reason L^2 is complete and therefore a Hilbert space lies in its construction. Although we will not further investigate, the vector space of square-integrable functions is constructed as a completion of a normed vector space.

2.1.3 Time-dependence and smoothness

We refer to vectors in an arbitrary Hilbert space \mathcal{H} as state vectors (or simply states) and we usually use Greek symbols to denote them, i.e. φ, Ψ, ψ , etc. These states, however, are static agents living in the Hilbert space. The discussion in the introduction already assumed that the states would exhibit a time-dependent property, and we certainly require this to be able to talk about state evolution. Implementing a real parameter-dependence is

done by introducing a function $\psi(\cdot) : \mathbb{R} \rightarrow \mathcal{H}$. By varying the parameter s , the function $\psi(\cdot)$ captures some transformation of the state through the Hilbert space.

The parameter s will be interpreted as (macroscopic) time, thus we require the state variations to exhibit a reasonable and predictable behaviour, so that small changes in time directly correspond to small changes in the states. Specifically, we require $\psi(\cdot) \in C^k(\mathbb{R}, \mathcal{H})$ for some positive integer $k \in \mathbb{Z}_{\geq 1}$, where $C^k(\mathbb{R}, \mathcal{H})$ denotes the set of k -smooth* functions from \mathbb{R} to \mathcal{H} .† The smoothness of an operator in the operator space $\mathcal{L}(\mathcal{H})$ of the Hilbert space \mathcal{H} can be defined in a similar manner. We say that for some $k \in \mathbb{Z}_{\geq 1}$ a function $X(\cdot) \in C^k(\mathbb{R}, \mathcal{L}(\mathcal{H}))$ is called a k -smooth family of time-dependent operators.

In the beginning we will stress this time implementation by explicitly denoting the time dependence of states and operators (e.g. $\psi(s)$, $\psi(0)$ or $H(s)$), but eventually, and primarily in proofs, it will be in the interest of clarity of presentation that we drop this parameter dependence. From the context, it will always be clear whether said state or operator exhibits time-dependent behaviour.

2.2 Operators

2.2.1 Properties of operators

Operators, such as the Hamiltonian from the introduction, are linear maps between states and play an important part in their evolution. As briefly mentioned in the previous paragraph, the space of these operators on the Hilbert space is denoted as $\mathcal{L}(\mathcal{H}, \mathcal{H})$ or $\mathcal{L}(\mathcal{H})$. Some operators must represent quantities of the physical system (the energy must be a real-valued eigenvalue of a Hamiltonian). This is mathematically implemented via certain properties of the operators (the Hamiltonian must be Hermitian). We will, without elaborating, present five of the most useful properties.

Definition 2.2.1. *A bounded operator $X : \mathcal{H} \rightarrow \mathcal{H}$ is an operator X such that there exists a strictly positive $M \in \mathbb{R}$ so that for all $\psi \in \mathcal{H}$ we have $\|X\psi\| \leq M\|\psi\|$. We denote $\mathcal{B}(\mathcal{H}, \mathcal{H})$ or $\mathcal{B}(\mathcal{H})$ for the set of bounded operators from \mathcal{H} to \mathcal{H} .*

*The term k -smoothness is a shorthand way of saying that we require the function to be continuously differentiable up to the k -th order.

†The smoothness of states emerges naturally from the smoothness of the Hamiltonian operator, as will be demonstrated in Lemma 2.2.4.

Definition 2.2.2. An invertible operator $X : \mathcal{H} \rightarrow \mathcal{H}$ is an operator X such that there exists an $X^{-1} \in \mathcal{B}(\mathcal{H})$ such that $X^{-1}X = XX^{-1} = I$.

Definition 2.2.3. The adjoint of an operator $X : \mathcal{H} \rightarrow \mathcal{H}$ is an operator $X^\dagger : \mathcal{H} \rightarrow \mathcal{H}$ such that $\langle Xv, w \rangle = \langle v, X^\dagger w \rangle$ for all $v, w \in \mathcal{H}$.

Definition 2.2.4. A unitary operator $X : \mathcal{H} \rightarrow \mathcal{H}$ is an operator X such that $X \in \mathcal{B}(\mathcal{H})$ and $XX^\dagger = X^\dagger X = I$. We denote the set of unitary operators on \mathcal{H} as $\mathcal{U}(\mathcal{H}) \subset \mathcal{B}(\mathcal{H})$.

Definition 2.2.5. A Hermitian operator $X : \mathcal{H} \rightarrow \mathcal{H}$ is an operator X such that $X \in \mathcal{B}(\mathcal{H})$ and it is self-adjoint, i.e. $X^\dagger = X$.

We define the norm of an operator $X : \mathcal{H} \rightarrow \mathcal{H}$ by

$$\|X\| := \sup \{ \|X\psi\| : \psi \in \mathcal{H}, \|\psi\| = 1 \}, \quad (2.1)$$

which is rather unsurprisingly called the operator norm. Using this norm, it follows that $\mathcal{B}(\mathcal{H})$, through the completeness of \mathcal{H} , becomes a Banach space [13]. This motivates us to use the operator norm in our further considerations. Moreover, the operator norm has some convenient properties for unitary and Hermitian operators. For a unitary operator $U \in \mathcal{U}(\mathcal{H})$ and an operator $X \in \mathcal{L}(\mathcal{H})$ it holds that $\|U\| = 1$ and $\|UX\| = \|X\|$. For a bounded operator $X \in \mathcal{B}(\mathcal{H})$ we have that $\|X^\dagger\| = \|X\|$. Additionally, for two operators $X, Y \in \mathcal{L}(\mathcal{H})$ submultiplicativity holds, i.e. $\|XY\| \leq \|X\|\|Y\|$. For the proofs of these properties the reader is referred to Bhatia (1997) [4].

2.2.2 The resolvent

For an operator $X : \mathcal{H} \rightarrow \mathcal{H}$ and a complex number $\lambda \in \mathbb{C}$, consider the operator $X - \lambda I$, also commonly written as $X - \lambda$. We examine the invertibility of this operator.

Definition 2.2.6. Let $X : \mathcal{H} \rightarrow \mathcal{H}$ be an operator.

- i. The set of the $\lambda \in \mathbb{C}$ for which $X - \lambda$ is not invertible is called the spectrum of X , denoted by $\sigma(X)$.
- ii. The set of the $\lambda \in \mathbb{C}$ for which $X - \lambda$ is invertible is called the resolvent set of X , denoted by $\rho(X)$.

For an $\lambda \in \rho(X)$, the inverse of $X - \lambda$ is called the resolvent, denoted by $R(\lambda; X) = (X - \lambda)^{-1}$.

This definition ensures that all the eigenvalues of an operator $X : \mathcal{H} \rightarrow \mathcal{H}$ are contained in $\sigma(X)$, since $\lambda \in \mathbb{C}$ is an eigenvalue of X if and only if we have for some nonzero eigenvector $v \in \mathcal{H}$ that $Xv = \lambda v$, i.e. $(X - \lambda)v = 0$, such that $X - \lambda$ is not invertible. The spectrum and the resolvent set are by definition a disjoint decomposition of \mathbb{C} . Moreover, the resolvent $R(\lambda; X)$ is analytic in the resolvent set $\rho(X)$ [26], which means that it is well-defined and holomorphic on $\rho(X)$ [12] and bounded over \mathcal{H} .

By distributing the identities $(X - \lambda)R(\lambda; X) = 1 = R(\lambda; X)(X - \lambda)$ we obtain

$$XR(\lambda; X) = 1 + \lambda R(\lambda; X) = R(\lambda; X)X. \quad (2.2)$$

Moreover, since X commutes with itself, we find

$$(X - \lambda)(X - \mu) = (X - \mu)(X - \lambda), \quad (2.3)$$

whence the resolvents mutually commute,

$$R(\lambda; X)R(\mu; X) = R(\mu; X)R(\lambda; X).$$

We follow with a lemma known as the first resolvent identity.

Lemma 2.2.1 (*First resolvent identity*). For an operator $X : \mathcal{H} \rightarrow \mathcal{H}$ the expression

$$R(\lambda; X) - R(\mu; X) = (\lambda - \mu)R(\lambda; X)R(\mu; X) \quad (2.4)$$

holds for all $\lambda, \mu \in \rho(X)$.

Proof. By definition of the resolvent, and Eq. (2.2) and Eq. (2.3) we have

$$\begin{aligned} (X - \mu)(X - \lambda)[R(\lambda; X) - R(\mu; X)] &= (X - \mu) - (X - \lambda) \\ &= (\lambda - \mu). \end{aligned}$$

Left-multiplying by $R(\lambda; X)R(\mu; X)$ gives the desired result. \square

Remark 2.2.1. *The second resolvent identity is, for two operators $X, Y : \mathcal{H} \rightarrow \mathcal{H}$, given by*

$$R(\lambda; X) - R(\lambda; Y) = R(\lambda; X)(X - Y)R(\lambda; Y), \quad (2.5)$$

for all $\lambda \in \rho(X) \cap \rho(Y)$. Though we will not need this identity, it is included for the sake of completeness. We refer the interested reader to mentioned sources for its proof and implications. [12, 13]

Remark 2.2.2. For a time-dependent operator $X(\cdot) \in C^k(\mathbb{R}, \mathcal{L}(\mathcal{H}))$, the spectrum and the resolvent set of $X(s)$ will generally depend on time. For convenience we write $\sigma(X)$ and $\rho(X)$ for $\sigma(X(s))$ and $\rho(X(s))$. Likewise, we write the time-dependent resolvent $R(\lambda; X(s))$ as $R(\lambda; X)$.

Analyticity of the resolvent $R(\lambda; X)$ for an smooth family of operators $X(\cdot) \in C^1(\mathbb{R}, \mathcal{L}(\mathcal{H}))$ allows for the differentiation of the identity $1 = (X - \lambda)R(\lambda; X)$ which, using the product rule, yields

$$\dot{R}(\lambda; X) = -R(\lambda; X)\dot{X}(s)R(\lambda; X), \quad (2.6)$$

where $\dot{Y}(s) = \partial_s Y(s)$.

Remark 2.2.3. Smoothness of the resolvent also follows from the second resolvent identity. Let $Z(\cdot) \in C^k(\mathbb{R}, \mathcal{L}(\mathcal{H}))$ and the associated resolvents $R(\lambda; Z(s)) \in \mathcal{B}(\mathcal{H})$ for all $s \in \mathbb{R}$. The second resolvent identity Eq. (2.5) defining $X = Z(s)$ and $Y = Z(t)$ tells us that since $Z(\cdot) \in C^1(\mathbb{R}, \mathcal{L}(\mathcal{H}))$ we have $R(\lambda; Z(\cdot)) \in C^1(\mathbb{R}, \mathcal{L}(\mathcal{H}))$. This allows us to obtain Eq. (2.6), which together with $Z(\cdot) \in C^k(\mathbb{R}, \mathcal{L}(\mathcal{H}))$ implies that $R(\lambda; Z(\cdot)) \in C^k(\mathbb{R}, \mathcal{L}(\mathcal{H}))$. [23]

2.2.3 Orthogonal projections

A special type of operators are projections. As the name suggests, the projection projects states onto a subspace of the Hilbert space. They find their importance in quantum mechanics in representing and manipulating quantum states.

Definition 2.2.7. An operator $P : \mathcal{H} \rightarrow \mathcal{H}$ is called a projection if it is idempotent, i.e. $P^2 = P$. Additionally, if P is self-adjoint, i.e. $P^\dagger = P$, then it is called an orthogonal projection.

For an orthogonal projection P , we define the operator $Q : \mathcal{H} \rightarrow \mathcal{H}$ by $Q = 1 - P$ as the orthogonal projection on the complement. To see that Q is an orthogonal projection, note

$$\begin{aligned} Q^2 &= (1 - P)^2 = 1 - 2P + P^2 = 1 - P = Q; \\ Q^\dagger &= 1 - P^\dagger = 1 - P = Q. \end{aligned}$$

The reason for labelling Q the projection on the *complement* can be justified by the following observation,

$$QP = (1 - P)P = P - P^2 = 0 = P - P^2 = P(1 - P) = PQ.$$

Moreover, it follows that an orthogonal operator P is bounded by the Cauchy-Schwarz-Bunyakovsky inequality,

$$\|P\psi\|^2 = |\langle P\psi, P\psi \rangle| = |\langle P\psi, \psi \rangle| \leq \|P\psi\| \|\psi\|,$$

hence $\|P\psi\| \leq \|\psi\|$. From now onwards, whenever a projection is mentioned we always mean an orthogonal projection unless otherwise stated.

Lemma 2.2.2. For a smooth family of projections $P(\cdot) \in C^k(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ and the associated projections on complement $Q(\cdot) = 1 - P(\cdot) \in C^k(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ the following identity holds

$$\dot{P}(s) = P(s)\dot{P}(s)Q(s) + Q(s)\dot{P}(s)P(s). \quad (2.7)$$

Using $Q(s)P(s) = 0$ it immediately follows that

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

Operators with this property are sometimes referred to as "off-diagonal".

Proof of Lemma 2.2.2. We drop the parameter dependence and differentiate $P = P^2$ using the product rule,

$$\dot{P} = \dot{P}P + P\dot{P}. \quad (2.8)$$

Multiplying P from both sides gives $P\dot{P}P = 2P\dot{P}P$, and hence $P\dot{P}P = 0$. We subtract this twice from Eq. (2.8) to obtain

$$\begin{aligned} \dot{P} &= \dot{P}P + P\dot{P} - 2P\dot{P}P \\ &= P\dot{P}(1 - P) + (1 - P)\dot{P}P, \end{aligned}$$

and Eq. (2.7) follows directly by definition of $Q = 1 - P$. \square

With Eq. (2.7) we can express the commutator of \dot{P} and P as

$$\begin{aligned} [\dot{P}, P] &:= \dot{P}P - P\dot{P} \\ &= (P\dot{P}Q + Q\dot{P}P)P - P(P\dot{P}Q + Q\dot{P}P) \\ &= Q\dot{P}P - P\dot{P}Q. \end{aligned} \quad (2.9)$$

Alternatively, using Eq. (2.8) and $\dot{P} = -\dot{Q}$, we can write

$$\begin{aligned} [\dot{P}, P] &= \dot{P}P - P\dot{P} \\ &= \dot{P}P + P\dot{P} - 2P\dot{P} \\ &= \dot{P} - 2P\dot{P} \\ &= -P\dot{P} + (1 - P)\dot{P} \\ &= -P\dot{P} - Q\dot{Q}. \end{aligned} \quad (2.10)$$

The commutator of the commutator evaluates to a surprisingly simple expression, where using Eq. (2.7) we find

$$[[\dot{P}, P], P] = [Q\dot{P}P - P\dot{P}Q, P] = Q\dot{P}P + P\dot{P}Q = \dot{P}. \quad (2.11)$$

2.2.4 Riesz projections

One recurring projection applicable to our purposes is the Riesz projector. This projection is directly associated with an isolated subset of the spectrum $\sigma(X)$. We will first define this notion of isolation on a subset of an operator's spectrum for which we need to quantify the amount of isolation

Definition 2.2.8. For two real subsets $X, Y \subset \mathbb{R}$, we define the distance between X and Y as

$$\text{dist}(X, Y) = \inf_{\substack{x \in X \\ y \in Y}} \|x - y\|.$$

Definition 2.2.9 (The gap condition). Consider some subset $\sigma^*(s) \subset \sigma(X)$ of the spectrum of a smooth family of Hermitian operators $X(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$. We say that $\sigma^*(s)$ is isolated with respect to $\sigma(X)$ if there exist smooth functions $f_1, f_2 \in C^1(\mathbb{R}, \mathbb{R})$ such that $\sigma^*(s) \subset I(s) = [f_1(s), f_2(s)]$ and there exists a strictly positive $d \in \mathbb{R}$ such that

$$\inf_{s \in \mathbb{R}} \text{dist}(I(s), \sigma(X) \setminus \sigma^*(s)) = d.$$

We say that $X(s)$ satisfies the gap condition for $\sigma^*(s)$ if $\sigma^*(s)$ is isolated with respect to $\sigma(X)$.

Loosely speaking, an operator that satisfies the gap condition has a spectrum with a subset of eigenvalues surrounded by two functions; it is isolated in the sense that the smallest distance between the functions and the spectrum without the subset is at least $d > 0$.

Definition 2.2.10. Let $X(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ be a smooth family of bounded operators that satisfies the gap condition for $\sigma^*(s) \subset \sigma(X)$. Let $\Gamma(s)$ be a time-dependent smooth closed curve[‡] in the resolvent set $\rho(X)$ that surrounds $\sigma^*(s)$

[‡]A smooth closed curve (or a smooth contour) is a concept from complex analysis or manifold courses we will not define here. The curve refers to a one-dimensional curved line in a higher dimensional space, where its starting point coincides with its ending point (hence: closed). The smoothness requirement ensures that the curve is continuous without sharp bends or irregularities.

and separates it from $\sigma(X)$. Then $P_{\sigma^*}(\cdot) : \mathbb{R} \rightarrow \mathcal{B}(\mathcal{H})$ given by

$$P_{\sigma^*}(s) = -\frac{1}{2\pi i} \oint_{\Gamma(s)} R(z; X) dz$$

is called the Riesz projector of $X(s)$ onto $\sigma^*(s)$.

The Riesz projector projects states onto the eigenspace spanned by the eigenvalues in $\sigma^*(s)$. If $R(z; X(\cdot)) \in C^k(\mathbb{R}, \mathcal{B}(\mathcal{H}))$, then we find that $P_{\sigma^*}(\cdot) \in C^k(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ [13]. Often we write P for P_{σ^*} if the subset σ^* is clear from the context. We will first confirm that the definition of the Riesz projector gives rise to a projection.

Lemma 2.2.3. The Riesz projector is an orthogonal projection.

Proof. To show this, we must prove that the Riesz projector P of X onto σ^* satisfies $P^2 = P$ and that P is self-adjoint. Let $\Gamma'(s)$ be a smooth contour contained within the area encircled by $\Gamma(s)$ such that $\Gamma'(s)$ still surrounds $\sigma^*(s)$. This $\Gamma'(s)$ exists since $X(s)$ satisfies the gap condition with infimum distance d strictly greater than 0. We find

$$\begin{aligned} P^2 &= \frac{1}{(2\pi i)^2} \oint_{\Gamma'(s)} R(z; X) dz \oint_{\Gamma(s)} R(w; X) dw \\ &= \frac{1}{(2\pi i)^2} \oint_{\Gamma'(s)} \oint_{\Gamma(s)} R(z; X) R(w; X) dwdz \\ &= \frac{1}{(2\pi i)^2} \oint_{\Gamma'(s)} \oint_{\Gamma(s)} \frac{R(z; X) - R(w; X)}{z - w} dwdz \\ &= \frac{1}{(2\pi i)^2} \left(\oint_{\Gamma'(s)} \oint_{\Gamma(s)} \frac{R(z; X)}{z - w} dwdz - \oint_{\Gamma'(s)} \oint_{\Gamma(s)} \frac{R(w; X)}{z - w} dwdz \right) \\ &= \frac{1}{(2\pi i)^2} \left(\oint_{\Gamma'(s)} R(z; X) \oint_{\Gamma(s)} \frac{dw}{z - w} dz - \oint_{\Gamma(s)} R(w; X) \oint_{\Gamma'(s)} \frac{dz}{z - w} dw \right) \\ &= -\frac{1}{2\pi i} \oint_{\Gamma'(s)} R(z; X) dz = P, \end{aligned}$$

where we used the first resolvent identity Eq. (2.4) in the third equality, and Cauchy's integral formula from complex analysis for the sixth equality: for the integral term $\oint_{\Gamma(s)} \frac{dw}{z-w}$ the contour $\Gamma(s)$ encloses the pole of $z = w$, evaluating this term to $-2\pi i$, whereas for the integral term $\oint_{\Gamma'(s)} \frac{dz}{z-w}$ this is not the case as w lies in the exterior of $\Gamma'(s)$, evaluating it to zero [23].

We will limit the proof that $P = P^\dagger$ to the special case when we only consider one eigenvalue; $\sigma^* = \{z_0(s)\}$. For multiple eigenvalues we will have to manually define a convenient smooth contour encircling the subset, which is a matter of strict bookkeeping. Note that for a self-adjoint operator $X : \mathcal{H} \rightarrow \mathcal{H}$, we have that

$$R(z; X)^\dagger = X^\dagger - \bar{z} = X - \bar{z} = R(\bar{z}; X).$$

Choose a strictly positive $r \in \mathbb{R}$ such that the circle $\Gamma(s) = \{z(s) \in \mathbb{R} : |z(s) - z_0(s)| = r\}$ satisfies the isolation requirements for a contour. (Again, this r exists because the subset is isolated.) Then for $z(s) = z_0(s) + re^{i\theta}$ the Riesz projector is given by

$$P_{z_0}(s) = -\frac{1}{2\pi} \int_{-\pi}^{\pi} R(z_0(s) + re^{i\theta}; X) r d\theta.$$

It follows that by taking the adjoint we obtain

$$P_{z_0}(s)^\dagger = -\frac{1}{2\pi} \int_{-\pi}^{\pi} R(z_0(s) + re^{-i\theta}; X) r d\theta,$$

which, upon the parameterisation with $\theta \rightarrow -\theta$, then yields $P_{z_0} = P_{z_0}^\dagger$. \square

Note that the Riesz projector $P_{\sigma^*}(s)$ commutes with $X(s)$, since $X(s)$ commutes with $R(z; X)$.

For an k -smooth family of operators $X(\cdot) \in C^k(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ that satisfies the gap condition for $\sigma^*(s)$, we will need the n -th time derivative (denoted by $\partial_s^n = \frac{d^n}{ds^n}$) of the associated Riesz projectors $P(\cdot) \in C^k(\mathbb{R}, \mathcal{B}(\mathcal{H}))$, where $n \leq k$. This time derivative is given by

$$\partial_s^n(P_{\sigma^*}(s)) = -\frac{1}{2\pi i} \oint_{\Gamma(s)} \partial_s^n R(z; X) dz. \quad (2.12)$$

2.2.5 Unitary propagators

Motivated by the discussion of the time evolution of states in the introduction, we construct the following, more general definition that captures the requirements for a family of the required unitary operators or shortly; a unitary propagator.

Definition 2.2.11. *A family of operators $U(\cdot, \cdot) : \mathbb{R}^2 \rightarrow \mathcal{B}(\mathcal{H})$ is called a unitary propagator if it satisfies the conditions*

- i. $U(\cdot, \cdot) \in C^1(\mathbb{R}^2, \mathcal{B}(\mathcal{H}))$;
- ii. $U(t, t) = 1$ for all $t \in \mathbb{R}$;
- iii. $U(r, s)U(s, t) = U(r, t)$ for all $r, s, t \in \mathbb{R}$.

By taking $r = t$ in the third condition, we find by the second condition that a unitary propagator $U(s, t)$ is unitary for all $s, t \in \mathbb{R}$, thus $U(\cdot, \cdot) \in C^1(\mathbb{R}^2, \mathcal{U}(\mathcal{H}))$. Its adjoint is given by $U(s, t)^\dagger = U(t, s)$.

Remark 2.2.4. *By the preceding discussion we are allowed to replace every adjoint of the unitary propagator by itself with parameters swapped. However, to avoid the unnecessary cluttering of equations, we will usually intentionally choose to use $U(s, t)^\dagger$ instead of $U(t, s)$ for the adjoint of $U(s, t)$.*

For a smooth family of time-dependent states $\psi(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ the unitary propagator $U(\cdot, \cdot) \in C^1(\mathbb{R}^2, \mathcal{U}(\mathcal{H}))$ will evolve the state at time $s_0 \in \mathbb{R}$ to the state at time $s \in \mathbb{R}$, i.e. $\psi(s) = U(s, s_0)\psi(s_0)$. In a similar way, time evolution for a smooth family of time-dependent operators $X(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ is given in the following way, $X(s) = U(s, s_0)X(s_0)U(s, s_0)^\dagger$. We will first give an existence lemma which relates the unitary propagators to the Schrödinger equation Eq. (1.2).

Lemma 2.2.4. Let $H(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ be a family of self-adjoint operators on some Hilbert space \mathcal{H} such that $H(s) \geq C$ for all $s \in \mathbb{R}$ and some finite $C \in \mathbb{R}$. Then there exists a unitary propagator U_τ such that for $s, s_0 \in \mathbb{R}$ and $\psi_0 \in \mathcal{H}$ we have a solution for the time-dependent Schrödinger equation

$$\partial_s \psi(s) = -i\tau H(s)\psi(s),$$

with initial value determined by $\psi(s_0) = \psi_0$. This solution is given by $\psi(s) = U_\tau(s, s_0)\psi_0$.

Proof. We omit the proof of this lemma, referring the reader to Reed and Simon (1975) [22]. □

In fact, we find that the unitary propagator as solution of the Schrödinger equation is uniquely determined [6, 22]. In case of a time-independent Hamiltonian we are able to deduce the unitary propagator without much effort, however, usually this deduction is not so straightforward and to approximate the unitary propagator we can resort to iteration methods such as the Dyson expansion [24].

Time-Adiabatic Theorems

This chapter will be dedicated to phrasing several time-adiabatic theorems and providing them with elaborate comments and perspectives. In order to do this, a new Hamiltonian must be constructed that considers adiabatic effects, permitting a comparison between the unitary propagators of the normal Hamiltonian and this adiabatic Hamiltonian.

3.1 Adiabatic operators

3.1.1 The adiabatic Hamiltonian

For a Hamiltonian $H(\cdot) \in C^2(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ that satisfies the gap condition with a Riesz projector $P(\cdot) \in C^2(\mathbb{R}, \mathcal{B}(\mathcal{H}))$, consider the *adiabatic Hamiltonian* $H_\tau^A(\cdot; P) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ defined by

$$H_\tau^A(s) := H_\tau^A(s; P) = H(s) + \frac{i}{\tau} [\dot{P}(s), P(s)] \quad (3.1a)$$

$$= H(s) - \frac{i}{\tau} P(s) \dot{P}(s) - \frac{i}{\tau} Q(s) \dot{Q}(s). \quad (3.1b)$$

The expression Eq. (3.1b), a direct consequence by virtue of Eq. (2.10), is included, since some literature adheres to this representation instead. Essentially, H_τ^A incorporates non-adiabatic effects via the additional commutator term $[\dot{P}(s), P(s)]$, this term represents the coupling between diabatic* and adiabatic dynamics, the prefactor i/τ capturing the relative strength

*Diabatic (sometimes just non-adiabatic) is used for the opposite of adiabatic.

of the diabatic effects. To see this, note that $\dot{P} \neq 0$ indicates that the eigenstates are changing over time. The system transitions between eigenvalues, a process that is usually diabatic. The approximation is mostly accurate for slow and smooth processes, i.e. $\tau \rightarrow \infty$ gives $H_\tau^A \rightarrow H$. Thus we can think of the adiabatic Hamiltonian H_τ^A as an ideal approximation of the physical evolution under these conditions.

The adiabatic Hamiltonian yields some immediate properties. Firstly, by symmetry of P and Q in Eq. (3.1b) it follows that $H_\tau^A(s; Q) = H_\tau^A(s, P)$. Secondly, we find that $H_\tau^A(s; I) = H(s) = H_\tau^A(s; 0)$ holds rather trivially. Additionally, where H would conveniently commute with P , the adiabatic Hamiltonian H^A does not commute with P as a consequence of Eq. (2.11). And lastly, H_τ^A is self-adjoint if H and P are self-adjoint; the minus sign of the i in Eq. (3.1) cancels against an additional minus sign from the adjoint of the commutator

$$[\dot{P}, P]^\dagger = (\dot{P}P - P\dot{P})^\dagger = P\dot{P} - \dot{P}P = -[\dot{P}, P].$$

The *adiabatic evolution* $U_\tau^A(\cdot, \cdot) \in C^1(\mathbb{R}^2, \mathcal{U}(\mathcal{H}))$ stemming from the adiabatic Hamiltonian H_τ^A is a unitary propagator by virtue of Lemma 2.2.4 and solves the Schrödinger equation of the adiabatic Hamiltonian,

$$\dot{U}_\tau^A(s, s_0) = -i\tau H_\tau^A(s)U_\tau^A(s, s_0). \quad (3.2)$$

3.1.2 The wave operator

We introduce the wave operator $\Omega_\tau(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ given by $\Omega_\tau(s) = U_\tau^A(s, 0)^\dagger U_\tau(s, 0)$, a useful tool from scattering theory to compare real-time evolution U_τ and adiabatic evolution U_τ^A . One can think of Ω_τ as an operator that relates an initial state of the adiabatic evolution with the obtained final state. It is entitled with information about the effects of adiabaticity on the system. The wave operator has a convenient integral expression.

Lemma 3.1.1. The wave operator $\Omega_\tau(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ satisfies the so-called Volterra integral equation,

$$\Omega_\tau(s) = 1 - \int_0^s K_\tau(s')\Omega_\tau(s')ds', \quad (3.3)$$

where $K_\tau(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ is called the kernel and is given by

$$K_\tau(s) = U_\tau^A(s, 0)^\dagger [\dot{P}(s), P(s)]U_\tau^A(s, 0). \quad (3.4)$$

Proof. Since $\Omega_\tau(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$, we are permitted to differentiate. With the (adjoint of) the Schrödinger equations Eq. (1.2) and Eq. (3.2), and the definition of the adiabatic Hamiltonian Eq. (3.1), we find

$$\begin{aligned}
\dot{\Omega}_\tau(s) &= \partial_s \left(U_\tau^A(s, 0)^\dagger U_\tau(s, 0) \right) \\
&= \dot{U}_\tau^A(s, 0)^\dagger U_\tau(s, 0) + U_\tau^A(s, 0) \dot{U}_\tau(s, 0) \\
&= i\tau U_\tau^A(s, 0)^\dagger H_\tau^A(s) U_\tau(s, 0) - i\tau U_\tau^A(s, 0) H(s) U_\tau(s, 0) \\
&= -U_\tau^A(s, 0)^\dagger [\dot{P}(s), P(s)] U_\tau(s, 0) \\
&= -U_\tau^A(s, 0)^\dagger [\dot{P}(s), P(s)] U_\tau^A(s, 0) \Omega_\tau(s) \\
&= -K_\tau(s) \Omega_\tau(s),
\end{aligned} \tag{3.5}$$

where K_τ is defined as in Eq. (3.4). We integrate both sides, and obtain

$$\Omega_\tau(s) - \Omega_\tau(0) = - \int_0^s K_\tau(s') \Omega_\tau(s') ds'.$$

Switching $\Omega_\tau(0) = 1$ from side gives the desired result. \square

We introduce a shorthand notation from Jansen et al. (2007) [14] for an operator surrounded by adiabatic evolution operators, which we will call the evolved operation.

Definition 3.1.1. For an operator $X(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ we define the evolved operator $X[\cdot] \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ by

$$X[s] := U_\tau^A(s, 0)^\dagger X(s) U_\tau^A(s, 0).$$

With the evolved operator we can write the kernel $K_\tau(s)$ of the Volterra integral equation as $K_\tau(s) = [\dot{P}(s), P(s)][s]$. We will derive the time derivative of the evolved operator, $\partial_s X[s]$.

Remark 3.1.1. We define exterior symbols on an operator to be evolved, e.g. the time derivative dot, to be considered before adjoining the adiabatic evolution operators, i.e. $\dot{X}[s]$ stands for $(\dot{X})[s] = U_\tau^A(s, 0)^\dagger \dot{X}(s) U_\tau^A(s, 0)$.

Lemma 3.1.2. For $X(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$, we have

$$\partial_s(X[s]) = i\tau[H_\tau^A, X][s] + \dot{X}[s]. \tag{3.6}$$

Proof. Using the adiabatic Schrödinger equation Eq. (3.2) and its adjoint, we find

$$\begin{aligned}
\partial_s(X[s]) &= \partial_s \left(U_\tau^A(s, 0)^\dagger X(s) U_\tau^A(s, 0) \right) \\
&= \dot{U}_\tau^A(s, 0)^\dagger X(s) U_\tau^A(s, 0) + U_\tau^A(s, 0)^\dagger \dot{X}(s) U_\tau^A(s, 0) \\
&\quad + U_\tau^A(s, 0)^\dagger X(s) \dot{U}_\tau^A(s, 0) \\
&= i\tau U_\tau^A(s, 0)^\dagger H_\tau^A(s) X(s) U_\tau^A(s, 0) + \dot{X}[s] \\
&\quad - i\tau U_\tau^A(s, 0)^\dagger X(s) H_\tau^A(s) U_\tau^A(s, 0) \\
&= i\tau U_\tau^A(s, 0)^\dagger (H_\tau^A(s) X(s) - X(s) H_\tau^A(s)) U_\tau^A(s, 0) + \dot{X}[s] \\
&= i\tau U_\tau^A(s, 0)^\dagger [H_\tau^A(s), X(s)] U_\tau^A(s, 0) + \dot{X}[s] \\
&= i\tau [H_\tau^A, X][s] + \dot{X}[s]. \quad \square
\end{aligned}$$

3.2 Time-adiabatic theorems

We are now in a position to formulate three time-adiabatic theorems. The theorems require certain smoothness conditions for the operators, self-adjointness for the Hamiltonian which satisfies the gap condition. We state these conditions in advance.

Assumption 3.2.1. Let the Hamiltonian $H(\cdot) \in C^k(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ be a k -smooth family of self-adjoint operators, let $\sigma^*(s)$ be an isolated subset of $\sigma(H)$ such that H satisfies the gap condition for σ^* and let $P(\cdot) \in C^k(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ be the associated k -smooth family of Riesz projectors.

Assumption 3.2.1 ensures that $R(z, H(\cdot)), H_\tau^A(\cdot) \in C^k(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ by Remark 2.2.3 and $U_\tau(\cdot, \cdot), U_\tau^A(\cdot, \cdot) \in C^k(\mathbb{R}^2, \mathcal{U}(\mathcal{H}))$ by Lemma 2.2.4.

The theorems are divided into two parts. Two of the theorems are called weak time-adiabatic, and these theorems consider the transition of states from the eigenspace spanned by the isolated eigenvalues to its complement. This is done by directly computing the norm of the complementary projection after applying the unitary propagator. Alternatively, we investigate on the difference between the projection and the time evolved projection, which also gives information about the transition out of the isolated subset. The third theorem is called the strong time-adiabatic theorem and considers the difference between the adiabatic and real-time unitary propagators. The theorem is stronger than the other two theorems in the sense that it also yields information about the time-evolution within the spanned

eigenspace. All three theorems will be supplemented with comprehensive comments. We begin with the weak time-adiabatic theorems.

3.2.1 The first weak time-adiabatic theorem

Theorem 3.2.1 (*First weak time-adiabatic theorem*). Assume that Assumption 3.2.1 holds for some Hamiltonian $H(\cdot) \in C^2(\mathbb{R}, \mathcal{B}(\mathcal{H}))$. Then there exist two constants $c, \tilde{c} \in \mathbb{R}$ such that

$$\|Q(0)\Omega_\tau(s)P(0)\| \leq \frac{c + \tilde{c}s}{\tau}. \quad (3.7)$$

The operator norm (recall: Eq. (2.1)) of $Q(0)\Omega_\tau(s)P(0)$ is an upper bound for the transition probability where we consider the transition from inside to outside the eigenspace spanned by the isolated eigenvalues, i.e.

$$U_\tau(s, 0)\psi(0) \rightarrow Q(s)U_\tau(s, 0)\psi(0)$$

for a state $\psi(0) \in P(0)$ starting in said eigenspace. To see this, notice that for such a state the transition probability is found to be

$$\begin{aligned} (U_\tau(s, 0)\psi, Q(s)U_\tau(s, 0)\psi) &= \|Q(s)U_\tau(s, 0)P(0)\psi(0)\|^2 \\ &= \|Q(s)U_\tau^A(s, 0)\Omega_\tau(s)P(0)\psi(0)\|^2 \\ &= \|U_\tau^A(s, 0)Q(0)\Omega_\tau(s)P(0)\psi(0)\|^2 \\ &\leq \|Q(0)\Omega_\tau(s)P(0)\|^2 \\ &\leq \frac{(c + \tilde{c}s)^2}{\tau^2}, \end{aligned}$$

where for the third equality we used the intertwining property which we will state and prove in Lemma 4.1.1, and in the inequality the fact that U_τ^A is unitary and that states are normalised, i.e. $\|\psi\|^2 = 1$. The transition probability is thus of order $1/\tau^2$.

3.2.2 The second weak time-adiabatic theorem

Theorem 3.2.2 (*Second weak time-adiabatic theorem*). Assume that Assumption 3.2.1 holds for some Hamiltonian $H(\cdot) \in C^2(\mathbb{R}, \mathcal{B}(\mathcal{H}))$. Then there exist two constants $c, \tilde{c} \in \mathbb{R}$ such that

$$\|P_\tau(s) - P(s)\| \leq \frac{c + \tilde{c}s}{\tau} \quad (3.9)$$

where $P_\tau(s) := U_\tau(s, 0)P(0)U_\tau(s, 0)^\dagger$ is the time-evolved projection.

Using the intertwining property which we will state and prove in Lemma 4.1.1 we can rewrite $P(s) = U_\tau^A(s, 0)P(0)U_\tau^A(s, 0)^\dagger$, and with the norm of unitary propagators being unity, we find that it is directly related to Theorem 3.2.1,

$$\begin{aligned}
& \|P_\tau(s) - P(s)\| \\
&= \|U_\tau(s, 0)P(0)U_\tau(s, 0)^\dagger - U_\tau^A(s, 0)P(0)U_\tau^A(s, 0)^\dagger\| \\
&= \|U_\tau^A(s, 0)\Omega_\tau(s)P(0)U_\tau(s, 0)^\dagger - U_\tau^A(s, 0)P(0)\Omega_\tau(s)U_\tau(s, 0)^\dagger\| \\
&= \|U_\tau^A(s, 0)(\Omega_\tau(s)P(0) - P(0)\Omega_\tau(s))U_\tau(s, 0)^\dagger\| \\
&= \|\Omega_\tau(s)P(0) - P(0)\Omega_\tau(s)\| \\
&= \|\Omega_\tau(s)P(0) - P(0)\Omega_\tau(s) + P(0)\Omega_\tau(s)P(0) - P(0)\Omega_\tau(s)P(0)\| \\
&= \|(1 - P(0))\Omega_\tau(s)P(0) - P(0)\Omega_\tau(s)(1 - P(0))\| \\
&= \|Q(0)\Omega_\tau(s)P(0) - P(0)\Omega_\tau(s)Q(0)\| \\
&\leq \|Q(0)\Omega_\tau(s)P(0)\| + \|P(0)\Omega_\tau(s)Q(0)\|. \tag{3.10}
\end{aligned}$$

3.2.3 The strong time-adiabatic theorem

Theorem 3.2.3 (*Strong time-adiabatic theorem*). Assume that Assumption 3.2.1 holds for some Hamiltonian $H(\cdot) \in C^2(\mathbb{R}, \mathcal{B}(\mathcal{H}))$. Then there exist two constants $c, \tilde{c} \in \mathbb{R}$ such that

$$\|U_\tau(s, 0) - U_\tau^A(s, 0)\| \leq \frac{c + \tilde{c}s}{\tau}. \tag{3.11}$$

To estimate the norm of the difference between these evolution operators, we will rewrite the bound via an integral of their generators. We have

$$\begin{aligned}
& U_\tau(s, 0) - U_\tau^A(s, 0) \\
&= -U_\tau(s, 0) \left[U_\tau(s, 0)^\dagger U_\tau^A(s, 0) - 1 \right] \\
&= -U_\tau(s, 0) \left[U_\tau(s', 0)^\dagger U_\tau^A(s', 0) \right]_{s'=0}^s \\
&= -U_\tau(s, 0) \int_0^s \partial_{s'} \left(U_\tau(s', 0)^\dagger U_\tau^A(s', 0) \right) ds' \\
&= -i\tau U_\tau(s, 0) \int_0^s U_\tau(s', 0)^\dagger \left(H_\tau(s') - H_\tau^A(s') \right) U_\tau^A(s', 0) ds' \\
&= -U_\tau(s, 0) \int_0^s U_\tau(s', 0)^\dagger [\dot{P}(s'), P(s')] U_\tau^A(s', 0) ds'. \tag{3.12}
\end{aligned}$$

In the first equality we used $U(0, 0) = 1$ for both unitary propagators, and in the second equality we exploited the smoothness of said unitary propagators, i.e. $U_\tau(\cdot, \cdot), U_\tau^A(\cdot, \cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$. The fourth equality follows by

a similar calculation as in the proof of Lemma 3.1.2 and the last equality is by construction of the adiabatic Hamiltonian Eq. (3.1). As a result, to find the bound on the unitary propagators we need to find the bound on the integral of Eq. (3.12).

Remark 3.2.1. *For convenience purposes we considered the initial value $s_0 = 0$. However, without a specification of initial conditions one would obtain a more general bound given by*

$$\|U_\tau(s, s_0) - U_\tau^A(s, s_0)\| \leq \frac{c + \tilde{c}|s - s_0|}{\tau}$$

for Thm. 3.2.3.

Chapter 4

Proofs

This chapter serves the purpose of providing the proofs of the three theorems stated in the previous chapter. We adhere to two strategies; the proof for the weak time-adiabatic theorems is inspired by the approach from the Jansen et al. (2007) [14], and the proof for the strong time-adiabatic theorem is stimulated by Teufel (2003) [25] and Childs (2017) [8]. Aligned with the vision of this paper, every step will be meticulously justified to obtain complete understanding and rigour.

4.1 Intertwining, twiddles and integration

4.1.1 Intertwining property

An important reason for constructing the adiabatic Hamiltonian Eq. (3.1) is that its adiabatic evolution operator directly intertwines with the projection. We will show this in the following lemma, called the intertwining lemma. The intertwining lemma finds its purpose in eliminating time dependence of projections, simplifying time derivatives and integrals.

Lemma 4.1.1 (*Intertwining lemma*). Assume that Assumption 3.2.1 holds for some Hamiltonian $H(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ that satisfies the gap condition for $\sigma^*(s)$. Then the following expression

$$U_\tau^A(s, 0)P(0) = P(s)U_\tau^A(s, 0) \quad (4.1)$$

holds for all $s \in \mathbb{R}$ and is called the intertwining property.

Corollary 4.1.1. By virtue of this intertwining property Eq. (4.1) we acquire as an immediate consequence the following expressions.

$$P(0)U_\tau^A(s,0)^\dagger = U_\tau^A(s,0)^\dagger P(s); \quad (4.2)$$

$$U_\tau^A(s,0)Q(0) = Q(s)U_\tau^A(s,0); \quad (4.3)$$

$$Q(0)U_\tau^A(s,0)^\dagger = U_\tau^A(s,0)^\dagger Q(s). \quad (4.4)$$

Proof. We obtain Eq. (4.2) by taking the adjoint of the intertwining property Eq. (4.1), using $(AB)^\dagger = B^\dagger A^\dagger$ and noticing that P is self-adjoint. The second equation Eq. (4.3) follows by definition of the complementary projection. Similarly, by self-adjointness of Q , taking the adjoint of Eq. (4.3) yields Eq. (4.4). \square

Proof of lemma 4.1.1. We show that the derivatives of both sides solve the same initial value problem, which by uniqueness proves that they are equal for all $s \in \mathbb{R}$. Note that the expression is trivially true for $s = 0$ since $U_\tau^A(0,0) = I$.

With the adiabatic Schrödinger equation Eq. (3.2), the left-hand side evaluates to

$$\dot{U}_\tau^A(s,0)P(0) = -i\tau H_\tau^A(s)U_\tau^A(s,0)P(0). \quad (4.5)$$

The right-hand side needs a bit more effort, we obtain

$$\begin{aligned} \partial_s(P(s)U_\tau^A(s,0)) &= P(s)\dot{U}_\tau^A(s,0) + \dot{P}(s)U_\tau^A(s,0) \\ &= -i\tau P(s)H_\tau^A(s)U_\tau^A(s,0) + \dot{P}(s)U_\tau^A(s,0) \\ &= (-i\tau P(s)H(s) + P(s)[\dot{P}(s), P(s)] + \dot{P}(s))U_\tau^A(s,0) \\ &= (-i\tau H(s)P(s) + [\dot{P}(s), P(s)]P(s))U_\tau^A(s,0) \\ &= -i(\tau H(s) + i[\dot{P}(s), P(s)])P(s)U_\tau^A(s,0) \\ &= -i\tau H_\tau^A(s)P(s)U_\tau^A(s,0), \end{aligned} \quad (4.6)$$

where we used the adiabatic Schrödinger equation Eq. (3.2) in the second equality. The definition of the adiabatic Hamiltonian Eq. (3.2) was needed in the third and last equality. In the fourth equality we used that P and H commute and Eq. (2.11). Then comparing Eq. (4.5) and Eq. (4.6) allows cancellation of the term $-i\tau H_\tau^A$, hence we obtain the desired $U_\tau^A(s,0)P(0) = P(s)U_\tau^A(s,0)$ for all $s \in \mathbb{R}$. \square

Remark 4.1.1. For the readers sceptical concerning the method of proving by solving the same initial value problem, which was introduced by Kato [15], one could also use a slightly different proof where it is shown that the time derivative of the expression $U_\tau^A(s,0)^\dagger P(s)U_\tau^A(s,0)$ vanishes[19]. This ultimately comes down to examining the term $\dot{P}(s) + i\tau[H_\tau^A(s), P(s)]$, which is 0 by virtue of Eq. (2.11).

Remark 4.1.2. The intertwining property holds only for the adiabatic propagator U_τ^A , not for its counterpart U_τ . We calculate

$$\begin{aligned} \partial_s(U_\tau(s,0)^\dagger P(s)U_\tau(s,0)) &= -i\tau U_\tau(s,0)^\dagger [H(s), P(s)]U_\tau(s,0) \\ &\quad + U_\tau(s,0)^\dagger \dot{P}(s)U_\tau(s,0) \\ &= U_\tau(s,0)^\dagger \dot{P}(s)U_\tau(s,0) \neq 0, \end{aligned}$$

where the first term vanishes since P and H commute. However, note that the expression holds for $\tau \rightarrow \infty$ (since $H_\tau^A \rightarrow H_\tau$), and for this reason the expression

$$\lim_{\tau \rightarrow \infty} \|U_\tau(s,0)P(0) - P(s)U_\tau(s,0)\| = 0$$

was taken as the adiabatic theorem by Nenciu back in 1979. [18]

Conceptually, the intertwining property tells us that it does not matter in which order we apply the adiabatic evolution operator and the projection. The projection P has been decoupled from its complement Q .

Before moving onto the next topic, recall the evolved operation for an operator $X(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ we defined in Definition 3.1.1. Using the intertwining property, we can conveniently toggle between $P(s)$ (or $Q(s)$) and $P(0)$ (or $Q(0)$), notice

$$\begin{aligned} (QXP)[s] &= U_\tau^A(s,0)^\dagger Q(s)X(s)P(s)U_\tau^A(s,0) \\ &= Q(0)U_\tau^A(s,0)^\dagger X(s)U_\tau^A(s,0)P(0) = Q(0)X[s]P(0), \end{aligned} \quad (4.7)$$

and a similar calculation for

$$(PXQ)[s] = P(0)X[s]Q(0). \quad (4.8)$$

4.1.2 The twiddle operation

Another property we will need, is the twiddle operation, explicitly introduced by Avron et al. (1987) [1]. The twiddle operator will be important to reduce the complexity of integrals, and additionally it has convenient commutator properties.

Definition 4.1.1 (*Twiddle operation*). Assume that Assumption 3.2.1 holds for some Hamiltonian $H(\cdot) \in C^2(\mathbb{R}, \mathcal{B}(\mathcal{H}))$. Let $X(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ be a smooth family of operators. The twiddle operation $\tilde{X}(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ is then defined by

$$\tilde{X}(s) := \frac{1}{2\pi i} \oint_{\Gamma} R(z; H) X(s) R(z; H) dz.$$

The twiddle operation is a special case of Friedrichs' Gamma operation [10]. We can think of the twiddle operation \tilde{X} as the partial inverse of the commutator map $X \mapsto [H, X]$, extracting the information that the eigenvalues that X and H share within the smooth contour. In particular, if X and H share all eigenvalues, i.e. H and X commute, $[H, X] = 0$, then X will commute with $R(z; H)$, allowing us to extract it completely from the integral. For X non-commuting with H , the twiddle operation \tilde{X} will extract the part of the information of the eigenvalues that X and H share within the smooth contour. We now prove some convenient twiddle properties.

Lemma 4.1.2. Assume that Assumption 3.2.1 holds for some Hamiltonian $H(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ that satisfies the gap condition for $\sigma^*(s)$. Consider the twiddle operation $\tilde{X}(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ for a smooth family of operators $X(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ as defined in definition 4.1.1. Then the following relations hold

$$\tilde{X}(s)Q(s) = P(s)\tilde{X}(s)Q(s) = P(s)\tilde{X}(s) \quad (4.9)$$

$$[H(s), \tilde{X}(s)] = [P(s), X(s)]. \quad (4.10)$$

Corollary 4.1.2. As an immediate consequence of Eq. (4.9) and Eq. (4.10), we obtain the expressions

$$P(s)\tilde{X}(s)P(s) = Q(s)\tilde{X}(s)Q(s) = 0; \quad (4.11)$$

$$P(s)[H_{\tau}^A(s), \tilde{X}(s)]Q(s) = P(s)X(s)Q(s); \quad (4.12)$$

$$Q(s)[H_{\tau}^A(s), \tilde{X}(s)]P(s) = -Q(s)X(s)P(s). \quad (4.13)$$

Proof. We omit time dependence to avoid cluttering. The first expression Eq. (4.11) follows immediately by left-multiplication by Q or right-multiplication by P on Eq. (4.9). By definition of the adiabatic Hamiltonian and Eq. (4.10) we find

$$\begin{aligned} P[H_{\tau}^A, \tilde{X}]Q &= P[H + \frac{i}{\tau}[\dot{P}, P], \tilde{X}]Q = P[H, \tilde{X}]Q + \frac{i}{\tau}P[[\dot{P}, P], \tilde{X}]Q \\ &= P[P, X]Q + \frac{i}{\tau}P[\dot{P}, P]\tilde{X}Q - \frac{i}{\tau}P\tilde{X}[\dot{P}, P]Q. \end{aligned}$$

Notice that using Eq. (4.9), $P\dot{P}P = 0$ and orthogonality of the projections we find that the last two terms vanish.

- i. $P[\dot{P}, P]\tilde{X}Q = P[\dot{P}, P]P\tilde{X}Q = P(\dot{P}P - P\dot{P})P\tilde{X}Q = 0.$
- ii. $P\tilde{X}[\dot{P}, P]Q = P\tilde{X}Q[\dot{P}, P]Q = P\tilde{X}Q(\dot{P}P - P\dot{P})Q = 0.$

Thus we retrieve Eq. (4.12),

$$P[H_\tau^A, \tilde{X}]Q = P[P, X]Q = P(PX - XP)Q = PXQ.$$

In a similar manner, we find that Eq. (4.13) holds, the minus sign occurring as a consequence of the commutator.

$$\begin{aligned} Q[H_\tau^A, \tilde{X}]P &= Q[H + \frac{i}{\tau}[\dot{P}, P], \tilde{X}]P \\ &= Q[P, X]P + \frac{i}{\tau}Q[\dot{P}, P]\tilde{X}P - \frac{i}{\tau}Q\tilde{X}[\dot{P}, P]P \\ &= Q(PX - XP)P = -QXP. \end{aligned} \quad \square$$

Proof of Lemma 4.1.2. Take Γ' to be a contour in the resolvent set that surrounds Γ . We find by basic manipulation and the first resolvent identity Eq. (2.4) that

$$\begin{aligned} \tilde{X}Q &= \tilde{X}(1 - P) = \frac{1}{2\pi i} \oint_{\Gamma} R(z; H)XR(z; H)(1 - P)dz \\ &= \frac{1}{2\pi i} \oint_{\Gamma} R(z; H)XR(z; H)dz - \frac{1}{2\pi i} \oint_{\Gamma} R(z; H)XR(z; H)Pdz \\ &= \tilde{X} + \frac{1}{(2\pi i)^2} \oint_{\Gamma} R(z; H)XR(z; H) \oint_{\Gamma'} R(w; H)dw dz \\ &= \tilde{X} + \frac{1}{(2\pi i)^2} \oint_{\Gamma} \oint_{\Gamma'} R(z; H)XR(z; H)R(w; H)dw dz \\ &= \tilde{X} + \frac{1}{(2\pi i)^2} \oint_{\Gamma} \oint_{\Gamma'} \frac{1}{z - w} R(z; H)X(R(z; H) - R(w; H))dw dz. \end{aligned}$$

We distribute and investigate the integrals. With Cauchy's integral formula we find

$$\frac{1}{(2\pi i)^2} \oint_{\Gamma} \oint_{\Gamma'} \frac{1}{z - w} dw R(z; H)XR(z; H)dz = -\frac{1}{2\pi i} \oint_{\Gamma} R(z; H)XR(z; H),$$

which is simply $-\tilde{X}$ and cancels out against \tilde{X} . For the second contour

integral, we again need Cauchy's integral formula,

$$-\frac{1}{(2\pi i)^2} \oint_{\Gamma'} \oint_{\Gamma} \frac{1}{z-w} R(z; H) dz XR(w; H) dw = \frac{1}{2\pi i} \oint_{\Gamma'} PR(w; H) XR(w; H) dw,$$

which is simply $P\tilde{X}$. Hence $\tilde{X}Q = P\tilde{X}$. Then right-multiplication with Q or left-multiplication with P gives

$$\tilde{X}Q = P\tilde{X}Q = P\tilde{X}.$$

For the second equality, we find

$$\begin{aligned} [H, \tilde{X}] &= H\tilde{X} - \tilde{X}H - z\tilde{X} + \tilde{X}z = [H - z, \tilde{X}] \\ &= \frac{1}{2\pi i} \oint_{\Gamma} [H - z, R(z; H) XR(z; H)] dz \\ &= \frac{1}{2\pi i} \oint_{\Gamma} [XR(z; H) - R(z; H)X] dz \\ &= X \frac{1}{2\pi i} \oint_{\Gamma} R(z; H) dz - \frac{1}{2\pi i} \oint_{\Gamma} R(z; H) dz X \\ &= -XP + PX = [P, X]. \end{aligned} \quad \square$$

Note that the twiddle operation is off-diagonal by Eq. (4.9).

4.1.3 Integration by parts

We require one more lemma, which will simplify the Volterra integral equation using elementary integration by parts.

Lemma 4.1.3 (*Integration by parts*). Assume that Assumption 3.2.1 holds for some Hamiltonian $H(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$. Let $X(\cdot), Y(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ be two smooth families of operators. Then

$$\begin{aligned} \int_0^s Q(0)X[s']P(0)Y(s')ds' &= \frac{i}{\tau} \left(Q(0)\tilde{X}[s']P(0)Y(s') \Big|_{s'=0}^s \right. \\ &\quad - \int_0^s Q(0)\dot{\tilde{X}}[s']P(0)Y(s')ds' \\ &\quad \left. - \int_0^s Q(0)\tilde{X}[s']P(0)\dot{Y}(s')ds' \right), \end{aligned} \quad (4.14)$$

holds for all $s \in \mathbb{R}$.

Proof. As per usual for proofs concerning integration by parts, we start by differentiating the evaluated term. This yields

$$\partial_s (Q(0)\tilde{X}[s]P(0)Y(s)) = Q(0)\partial_s(\tilde{X}[s])P(0)Y(s) + Q(0)\tilde{X}[s]P(0)\dot{Y}(s) \quad (4.15)$$

We investigate the first term on the right-hand side. Using our earlier efforts from Eq. (3.6), the intertwining toggles Eq. (4.7) and Eq. (4.8) in both directions, and the twiddle commutator property Eq. (4.13), we find

$$\begin{aligned} Q(0)\partial_s(\tilde{X}[s])P(0) &= i\tau Q(0)[H_\tau^A, \tilde{X}][s]P(0) + Q(0)\dot{\tilde{X}}[s]P(0) \\ &= i\tau(Q[H_\tau^A, \tilde{X}]P)[s] + Q(0)\dot{\tilde{X}}[s]P(0) \\ &= -i\tau(QXP)[s] + Q(0)\dot{\tilde{X}}P(0) \\ &= -i\tau Q(0)X[s]P(0) + Q(0)\dot{\tilde{X}}[s]P(0). \end{aligned}$$

Returning to Eq. (4.15), we substitute our result and obtain

$$\begin{aligned} \partial_s (Q(0)\tilde{X}[s]P(0)Y(s)) &= -i\tau Q(0)X[s]P(0)Y(s) + Q(0)\dot{\tilde{X}}[s]P(0)Y(s) \\ &\quad + Q(0)\tilde{X}[s]P(0)\dot{Y}(s), \end{aligned}$$

which upon integration yields

$$\begin{aligned} Q(0)\tilde{X}[s']P(0)Y(s')\Big|_{s'=0}^s &= -i\tau \int_0^s Q(0)X[s']P(0)Y(s')ds' \\ &\quad + \int_0^s Q(0)\dot{\tilde{X}}[s']P(0)Y(s')ds' \\ &\quad + \int_0^s Q(0)\tilde{X}[s']P(0)\dot{Y}(s')ds'. \end{aligned}$$

Rearranging terms and dividing by $i\tau$ yields the desired equation. \square

Corollary 4.1.3. If instead we choose to investigate

$$\partial_s(P(0)\tilde{X}[s]Q(0)Y(s)),$$

we will find a similar result

$$\begin{aligned} \int_0^s P(0)X[s']Q(0)Y(s')ds' &= -\frac{i}{\tau} \left(P(0)\tilde{X}[s']Q(0)Y(s')\Big|_{s'=0}^s \right. \\ &\quad - \int_0^s Q(0)\dot{\tilde{X}}[s']Q(0)Y(s')ds' \\ &\quad \left. - \int_0^s P(0)\tilde{X}[s']Q(0)\dot{Y}(s')ds' \right). \quad (4.16) \end{aligned}$$

Proof. The proof is entirely similar to the proof of Lemma 4.1.3, except that we need to use the twiddle property Eq. (4.12) instead of Eq. (4.13), which introduces an additional minus sign. \square

4.2 Proofs of weak time-adiabatic theorems

We now prove the weak time-adiabatic theorems.

4.2.1 First weak time-adiabatic theorem

Proof of Theorem 3.2.1. We return to the kernel of the Volterra integral equation, $K_\tau(s) = [\dot{P}, P][s]$, which we evaluate using Eq. (2.9) and toggle with Eq. (4.7) and Eq. (4.8),

$$K_\tau(s) = [\dot{P}, P][s] = (Q\dot{P}P - P\dot{P}Q)[s] = Q(0)\dot{P}[s]P(0) - P(0)\dot{P}[s]Q(0).$$

Substituting this into the Volterra integral equation Eq. (3.3) gives

$$\Omega_\tau(s) = 1 - \int_0^s (Q(0)\dot{P}[s']P(0) - P(0)\dot{P}[s']Q(0))\Omega_\tau(s')ds'.$$

We rid the constant and one of the integral terms using the orthogonality of projections, we left-multiply by $Q(0)$ and right-multiply by $P(0)$,

$$Q(0)\Omega_\tau(s)P(0) = - \int_0^s Q(0)\dot{P}[s']P(0)\Omega_\tau(s')P(0)ds'. \quad (4.17)$$

By construction, this integral is of the form considered in the partial integration Lemma 4.1.3 where $X(s) = \dot{P}(s)$ and $Y(s) = \Omega_\tau(s)P(0)$. We have $\Omega_\tau(s)P(0) \in C^2(\mathbb{R}, \mathcal{B}(\mathcal{H}))$, and since $P(\cdot) \in C^2(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ we find $\dot{P}(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$. Thus we satisfy the conditions for integration by parts, and by Eq. (4.14) and Eq. (3.5) we obtain

$$\begin{aligned} Q(0)\Omega_\tau(s)P(0) &= -\frac{i}{\tau} \left(Q(0)\tilde{P}[s']P(0)\Omega_\tau(s')P(0) \Big|_{s'=0}^s \right. \\ &\quad - \int_0^s Q(0)\dot{\tilde{P}}[s']P(0)\Omega_\tau(s')P(0)ds' \\ &\quad \left. - \int_0^s Q(0)\tilde{P}[s']P(0)\dot{\Omega}_\tau(s')P(0)ds' \right), \end{aligned}$$

Note that with submultiplicativity of the operator norm, $\|P\| \leq 1$ and $\|Q\| \leq 1$, and the unitary property of unitary propagators,

$$\|Q(0)\tilde{P}[s']P(0)\Omega_\tau(s')P(0)\| \leq \|\tilde{P}[s']\| \|\Omega_\tau(s')\| \leq \|\tilde{P}(s')\| \leq c_1,$$

where the last inequality follows since \tilde{P} is bounded. It remains to estimate the integrals, for which we use that $\|\int_0^s X(s')ds'\| \leq \int_0^s \|X(s')\|ds'$. Hence

$$\begin{aligned} \left\| \int_0^s Q(0)\dot{\tilde{P}}[s']P(0)\Omega_\tau(s')P(0)ds' \right\| &\leq \int_0^s \|Q(0)\dot{\tilde{P}}[s']P(0)\Omega_\tau(s')P(0)\|ds' \\ &\leq \int_0^s \|\dot{\tilde{P}}(s')\|ds' \\ &\leq s \sup_{m \in [0,s]} \|\dot{\tilde{P}}(m)\| \leq c_2s. \end{aligned}$$

In the last line we crudely estimated the integral by the greatest rectangle covering the integrand, which we can estimate with a constant $c_2 \in \mathbb{R}$ since $\dot{\tilde{P}}$ is bounded. Similarly, by Eq. (3.5) we find

$$\begin{aligned} \left\| \int_0^s Q(0)\tilde{P}[s']P(0)\dot{\Omega}_\tau(s')P(0)ds' \right\| &\leq \int_0^s \|\tilde{P}[s']\dot{\Omega}_\tau(s')\|ds' \\ &\leq \int_0^s \|\tilde{P}[s'][\dot{P}(s'), P(s')]\|ds' \\ &\leq 2s \sup_{m \in [0,s]} \|\tilde{P}(m)\| \|\dot{P}(m)\| \leq c_3s, \end{aligned}$$

using that \tilde{P} and \dot{P} are bounded. Altogether,

$$\|Q(0)\Omega_\tau(s)P(0)\| \leq \frac{c + \tilde{c}s}{\tau} \square$$

4.2.2 Second weak time-adiabatic theorem

Proof of Theorem 3.2.2. The terms that appear in the estimation of the projections in Eq. (3.10) should be familiar by now. We found the bound on $Q(0)\Omega_\tau(s)P(0)$ already, and the bound on $P(0)\Omega_\tau Q(0)$ is a consequence of Corollary 4.1.3, again taking $X(s) = \dot{P}(s)$ and $Y(s) = \Omega_\tau(s)P(0)$. Accordingly,

$$\|P_\tau(s) - P(s)\| \leq \frac{c_1 + \tilde{c}_1s}{\tau} + \frac{c_2 + \tilde{c}_2s}{\tau} = \frac{c + \tilde{c}s}{\tau}. \quad \square$$

4.3 Adiabatic connectivity

To prepare the proof of the bound on the unitary propagators we must specify and investigate a particular choice beyond the general twiddle formalism which permits investigation on the commutator $-[\dot{P}, P]$ from Eq. (3.12). Specifically, we wish to define a new commutator generator $F(s)$ such that we can express $[F(s), H(s)] = -[\dot{P}(s), P(s)]$.

Definition 4.3.1. Assume that Assumption 3.2.1 holds for some Hamiltonian $H(\cdot) \in C^2(\mathbb{R}, \mathcal{B}(\mathcal{H}))$. Define $G(\cdot) : \mathbb{R} \rightarrow \mathcal{B}(\mathcal{H})$ as

$$G(s) = -\frac{1}{2\pi i} \oint_{\Gamma(s)} Q(s)R(z; H)\dot{R}(z; H)dz. \quad (4.18)$$

Then the adiabatic connectivity $F(\cdot) : \mathbb{R} \rightarrow \mathcal{B}(\mathcal{H})$ is defined by $F(s) = G(s) + G(s)^\dagger$.

Notice that since $R(z; H(\cdot)), Q(\cdot) \in C^2(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ we have $G(\cdot), F(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$. One way to see the adiabatic connectivity F is that it encapsulates the transfer of information during an adiabatic process, where G considers the forward transformation and G^\dagger the backward transformation, and hence F connects both transformations. We will now prove that the commutator generator property holds.

Lemma 4.3.1. For $F(s)$ as defined in Lemma 4.3.1, we find that

$$[F(s), H(s)] = -[\dot{P}(s), P(s)]. \quad (4.19)$$

Proof. We drop parameter dependence. Then

$$\begin{aligned} [F, H] &= [G, H] + [G^\dagger, H] \\ &= -\frac{1}{2\pi i} \oint_{\Gamma} [QR\dot{R}, H]dz + \left[\left(-\frac{1}{2\pi i} \oint_{\Gamma} QR\dot{R}dz \right)^\dagger, H \right] \\ &= -\frac{1}{2\pi i} \oint_{\Gamma} (QR\dot{R}H - HQR\dot{R})dz - \left(\frac{1}{2\pi i} \oint_{\Gamma} [H, QR\dot{R}]dz \right)^\dagger \\ &= -\frac{1}{2\pi i} \oint_{\Gamma} Q(R\dot{R}H - HR\dot{R})dz - \left(\frac{1}{2\pi i} \oint_{\Gamma} Q(HR\dot{R} - R\dot{R}H)dz \right)^\dagger \\ &= -\frac{Q}{2\pi i} \oint_{\Gamma} (R\dot{R}H - (1+zR)\dot{R})dz - \left(\frac{Q}{2\pi i} \oint_{\Gamma} ((1+zR)\dot{R} - R\dot{R}H)dz \right)^\dagger \\ &= -\frac{Q}{2\pi i} \oint_{\Gamma} (R\dot{R}(H-z) - \dot{R})dz - \left(\frac{Q}{2\pi i} \oint_{\Gamma} (\dot{R} - R\dot{R}(H-z))dz \right)^\dagger \\ &= -Q\dot{P} + \frac{1}{2\pi i} \oint_{\Gamma} QR^2\dot{H}dz + \left(Q\dot{P} - \frac{1}{2\pi i} \oint_{\Gamma} QR^2\dot{H}dz \right)^\dagger \\ &= -Q\dot{P} + (Q\dot{P})^\dagger = -Q\dot{P} + \dot{P}Q = [\dot{P}, Q] = -[\dot{P}, P], \end{aligned}$$

where in the third equality we used that H is self-adjoint and thus $HA^\dagger = (AH)^\dagger$ and $A^\dagger H = (HA)^\dagger$, and in the fourth equality the commutativity of H and Q . Moreover, we used Eq. (2.2) in the fifth equality and for the

seventh equality we used Eq. (2.6) and the definition of \dot{P} from Eq. (2.12). Finally, we used that the map $z \mapsto QR^2H$ is holomorphic inside $\Gamma(s)$ [25], ensuring the integrals vanishes. \square

Definition 4.3.2. Assume that Assumption 3.2.1 holds for some Hamiltonian $H(\cdot) \in C^2(\mathbb{R}, \mathcal{B}(\mathcal{H}))$. Let $F(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ be the adiabatic connectivity. Then the scaled time-evolved adiabatic connectivity $A(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ is defined by

$$A(s) = -\frac{i}{\tau} U_\tau(s, 0)^\dagger F(s) U_\tau(s, 0). \quad (4.20)$$

Since $A(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ (which is a direct consequence of the smoothness of F and U_τ) we can differentiate Eq. (4.20) with respect to s . Using the strategy deployed in the proof of Lemma 3.1.2 and Eq. (4.19), we obtain

$$\begin{aligned} \dot{A}(s) &= U_\tau(s, 0)^\dagger [H(s), F(s)] U_\tau(s, 0) - \frac{i}{\tau} U_\tau(s, 0)^\dagger \dot{F}(s) U_\tau(s, 0) \\ &= U_\tau(s, 0)^\dagger [\dot{P}(s), P(s)] U_\tau(s, 0) - \frac{i}{\tau} U_\tau(s, 0)^\dagger \dot{F}(s) U_\tau(s, 0) \end{aligned} \quad (4.21)$$

4.4 Proof of strong time-adiabatic theorem

Proof of Theorem 3.2.3. We combine Eq. (3.12) with Eq. (4.21) and obtain

$$\begin{aligned} U_\tau(s, 0) - U_\tau^A(s, 0) &= -U_\tau(s, 0) \int_0^s U_\tau(s', 0)^\dagger [\dot{P}(s'), P(s')] U_\tau^A(s', 0) ds' \\ &= -U_\tau(s, 0) \int_0^s \dot{A}(s') U_\tau(s', 0)^\dagger U_\tau^A(s', 0) ds' \end{aligned} \quad (4.22a)$$

$$- \frac{i}{\tau} U_\tau(s, 0) \int_0^s U_\tau(s', 0)^\dagger \dot{F}(s') U_\tau^A(s', 0) ds'. \quad (4.22b)$$

Similarly to the proof for the weak time-adiabatic theorems, we can estimate the second term Eq. (4.22b) by

$$\begin{aligned} \left\| \frac{i}{\tau} U_\tau(s, 0) \int_0^s U_\tau(s', 0)^\dagger \dot{F}(s') U_\tau^A(s', 0) ds' \right\| &\leq \frac{s}{\tau} \sup_{m \in [0, s]} \|\dot{F}(m)\| \\ &\leq \frac{c_1 s}{\tau}. \end{aligned} \quad (4.23)$$

for some constant $c_1 \in \mathbb{R}$. The first term Eq. (4.22a) cannot be immediately deduced using this method, since we lack information about \dot{A} . We can integrate by parts,

$$\int_0^s \dot{A}(s') U_\tau(s', 0)^\dagger U_\tau^A(s', 0) ds' = A(s') U_\tau(s', 0)^\dagger U_\tau^A(s', 0) \Big|_{s'=0}^s - \int_0^s A(s') \partial_{s'} (U_\tau(s', 0)^\dagger U_\tau^A(s', 0)) ds',$$

where, using

$$\partial_s (U_\tau(s, 0)^\dagger U_\tau^A(s, 0)) = U_\tau(s, 0)^\dagger [\dot{P}(s), P(s)] U_\tau^A(s, 0)$$

and reverting A back to F with Eq. (4.20), we find that

$$\int_0^s \dot{A}(s') U_\tau(s', 0)^\dagger U_\tau^A(s', 0) ds' = \frac{1}{\tau} U_\tau(s', 0)^\dagger F(s') U_\tau^A(s', 0) \Big|_{s'=0}^s + \frac{1}{\tau} \int_0^s U_\tau(s', 0)^\dagger F(s') [\dot{P}(s'), P(s')] U_\tau^A(s', 0) ds'$$

Combining both results and using the fact that unitary propagators are unitary yields

$$\|U_\tau(s, 0) - U_\tau^A(s, 0)\| \leq \frac{1}{\tau} \left(\|F(0)\| + \|F(s)\| + \int_0^s (\|\dot{F}(s')\| + 2\|F(s')\| \|\dot{P}(s')\|) ds' \right). \quad (4.24)$$

Estimating the integral with

$$\int_0^s (\|\dot{F}(s')\| + 2\|F(s')\| \|\dot{P}(s')\|) ds' \leq s \sup_{m \in [0, s]} (\|\dot{F}(m)\| + 2\|F(m)\| \|\dot{P}(m)\|)$$

and using that F , \dot{F} and \dot{P} are bounded, we find

$$\|U_\tau(s, 0) - U_\tau^A(s, 0)\| \leq \frac{c + \tilde{c}s}{\tau},$$

for some constants $c, \tilde{c} \in \mathbb{R}$. □

Applications

In this chapter we will apply the time-adiabatic theorems in the special situations, where the spectrum subset contains only one or two eigenvalues, permitting the crossing of eigenvalues in the latter situation. These simplifications allows for the extraction of more information about the norms and specifically the quantities by which they are bounded.

5.1 One eigenvalue

For this paragraph, we are concerned with one non-degenerate isolated eigenvalue, i.e. $\sigma^*(s) = \{E(s)\}$. Assume that Assumption 3.2.1 holds for some Hamiltonian $H(\cdot) \in C^2(\mathbb{R}, \mathcal{B}(\mathcal{H}))$. We will investigate the bound on the unitary propagators as it is the strongest statement of the three theorems. The gap is expressed as

$$\Delta(s) = \text{dist}(E(s), \sigma(H) \setminus E(s)).$$

We assume that the resolvent $R(E; H)$ is a 2-smooth family of operators, i.e. $R(E(\cdot); H(\cdot)) \in C^2(\mathbb{R}, \mathcal{B}(\mathcal{H}))$, such that for a smooth family of states $v(\cdot) \in C^1(\mathbb{R}, \mathcal{H})$ we have

$$R(E; H)v = \begin{cases} 0 & \text{if } v(s) \in \text{Eig}_E(H(s)), \\ \left((H(s) - E(s))|_{\text{Eig}_E(H(s))} \right)^{-1} v(s) & \text{if } v(s) \perp \text{Eig}_E(H(s)), \end{cases}$$

where $\text{Eig}_E(H(\cdot))$ is the eigenspace spanned by the isolated eigenvalue E , the vertical line stands for the restriction to the eigenspace and \perp denotes

perpendicularity. This assumption turns out to be a reasonable assumption [8, 25]. By the operator norm we find that the resolvent is bounded by

$$\|R(E; H)\| \leq \frac{1}{\Delta(s)}. \quad (5.1)$$

Using this definition of the resolvent, the adiabatic connectivity $F(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ can be written as

$$F(s) = R(E; H)\dot{P}(s)P(s) + P(s)\dot{P}(s)R(E; H). \quad (5.2)$$

This choice of F provides a generator for the commutator $[\dot{P}, P]$, since, dropping parameter dependence,

$$\begin{aligned} [H, F] &= HR\dot{P}P + HP\dot{P}R - R\dot{P}PH - P\dot{P}RH \\ &= (1 + ER)\dot{P}P + EP\dot{P}R - ER\dot{P}P - P\dot{P}(1 + ER) \\ &= \dot{P}P - P\dot{P} = [\dot{P}, P], \end{aligned}$$

using Eq. (2.2) in the form $HR = 1 + ER = RH$, and $PH = HP = EP$ which holds since we only deal with one eigenvalue.

Recall that the operator norm of a bounded operator is equal to the operator norm of its adjoint, whence $\|F\| \leq 2\|R\dot{P}P\|$. Using the bound on the resolvent Eq. (5.1) and $\|P\| \leq 1$, we find

$$\|F\| \leq 2\|R\dot{P}P\| \leq 2\|R\|\|\dot{P}\|\|P\| \leq \frac{2\|\dot{P}\|}{\Delta(s)}. \quad (5.3)$$

Note that the adiabatic connectivity F is a 1-smooth family of operators, since $P(\cdot), R(E(\cdot), H(\cdot)) \in C^2(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ and thus $\dot{P}(\cdot) \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{H}))$. Differentiating then gives

$$\dot{F} = \dot{R}\dot{P}P + R\ddot{P}P + R\dot{P}^2 + \dot{P}^2R + P\ddot{P}R + P\dot{P}\dot{R}.$$

We only need to investigate on the first three terms, since the remaining three terms will follow using the operator norm of the adjoint. With Eq. (2.6) the first term gives

$$\|\dot{R}\dot{P}P\| = \|R\dot{H}RQ\dot{P}\| \leq \|R\|^2\|\dot{H}\|\|Q\|\|\dot{P}\| \leq \frac{\|\dot{H}\|\|\dot{P}\|}{\Delta(s)^2}.$$

The second term yields

$$\|R\ddot{P}P\| \leq \|R\|\|\ddot{P}\|\|P\| \leq \frac{\|\ddot{P}\|}{\Delta(s)},$$

and the third term gives

$$\|R\dot{P}^2\| \leq \|R\|\|\dot{P}\|^2 \leq \frac{\|\dot{P}\|^2}{\Delta(s)}.$$

Combining the three terms and accounting for their adjoints then gives

$$\|\dot{F}\| \leq 2 \left(\frac{\|\dot{H}\|\|\dot{P}\|}{\Delta(s)^2} + \frac{\|\ddot{P}\|}{\Delta(s)} + \frac{\|\dot{P}\|^2}{\Delta(s)} \right). \quad (5.4)$$

With the found bounds Eq. (5.3) and Eq. (5.4), and Eq. (4.24), we find an explicit expression that bounds the unitary propagators.

$$\begin{aligned} \|U_\tau(s,0) - U_\tau^A(s,0)\| &\leq \frac{2}{\tau} \left(\frac{\|\dot{P}(0)\|}{\Delta(0)} + \frac{\|\dot{P}(s)\|}{\Delta(s)} \right) \\ &+ \int_0^s \left(\frac{\|\dot{H}(s')\|\|\dot{P}(s')\|}{\Delta(s')^2} + \frac{\|\ddot{P}(s')\|}{\Delta(s')} + 3\frac{\|\dot{P}(s')\|^2}{\Delta(s')} \right) ds'. \end{aligned} \quad (5.5)$$

With perturbation theory we are able to specify the expression even further by finding relations between the norms of the time derivatives of the projection and the Hamiltonian. Using first order perturbation theory we can express the norm on \dot{P} in terms of \dot{H} [8],

$$\|\dot{P}(s)\| \leq C_1 \frac{\|\dot{H}(s)\|}{\Delta(s)}$$

for some constant $C_1 \in \mathbb{R}$, and similarly using second order perturbation theory we express \ddot{P} in terms of \dot{H} and \ddot{H} [8],

$$\|\ddot{P}(s)\| \leq C_2 \frac{\|\ddot{H}(s)\|}{\Delta(s)} + C_3 \frac{\|\dot{H}(s)\|^2}{\Delta(s)^2}$$

for some constants $C_2, C_3 \in \mathbb{R}$. Combining then yields

$$\begin{aligned} \|U_\tau(s,0) - U_\tau^A(s,0)\| &\leq \frac{2}{\tau} \left(C_1 \frac{\|\dot{H}(0)\|}{\Delta(0)^2} + C_1 \frac{\|\dot{H}(s)\|}{\Delta(s)^2} \right) \\ &+ \int_0^s \left((3C_1^2 + C_1 + C_3) \frac{\|\dot{H}(s')\|^2}{\Delta(s')^3} + C_2 \frac{\|\ddot{H}(s')\|}{\Delta(s')^2} \right) ds'. \end{aligned} \quad (5.6)$$

5.2 Two eigenvalues

We consider the situation where the isolated subset of the spectrum has two eigenvalues, i.e. $\sigma^*(s) = \{E_1(s), E_2(s)\}$. Assume that Assumption

3.2.1 holds for some Hamiltonian $H(\cdot) \in C^2(\mathbb{R}, \mathcal{B}(\mathcal{H}))$. Instead of the Riesz projector that associated with the entire isolated subset, let $P_1(\cdot) \in C^k(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ be the projection associated with eigenvalue E_1 and let $P_2(\cdot) \in C^k(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ be the projection associated with eigenvalue E_2 . The adiabatic Hamiltonian $H_\tau^A(\cdot) \in C^k(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ can then be written as

$$H_\tau^A(s) = H(s) - \frac{i}{\tau} P_1(s) \dot{P}_1(s) - \frac{i}{\tau} P_2(s) \dot{P}_2(s) - \frac{i}{\tau} Q(s) \dot{Q}(s),$$

where $Q(s) = 1 - P_1(s) - P_2(s)$.

Without loss of generality, we assume that there is exactly one crossing, i.e. $E_1(s) = E_2(s)$ if and only if $s = s_c \in \mathbb{R}$. Moreover, we require

$$\partial_s^n (E_1(s) - E_2(s))|_{s=s_c} \neq 0, \quad (5.7)$$

for some $n \in \{1, 2, \dots, n\}$. This conditions allows us to split the time interval near the crossing, which we can translate into a splitting of the unitary propagators. We find

$$\begin{aligned} \|U_\tau(s, 0) - U_\tau^A(s, 0)\| &\leq \|U_\tau(s_c - \tau^{-1/(2n)}, 0) - U_\tau^A(s_c - \tau^{-1/(2n)}, 0)\| \\ &+ \|U_\tau(s_c + \tau^{-1/(2n)}, s_c - \tau^{-1/(2n)}) - U_\tau^A(s_c + \tau^{-1/(2n)}, s_c - \tau^{-1/(2n)})\| \\ &+ \|U_\tau(s, s_c + \tau^{-1/(2n)}) - U_\tau^A(s, s_c + \tau^{-1/(2n)})\|. \end{aligned}$$

The first and last norms can be evaluated using the earlier findings when we considered one eigenvalue, which is Eq. (5.5) or Eq. (5.6) if we take perturbation theory in account. If we assume that the distance from the isolated subset to the rest of the spectrum is more than the distance between the two eigenvalues, then we can define the gap by

$$\Delta(s) = \text{dist}(E_1(s), E_2(s)). \quad (5.8)$$

It remains to evaluate the middle norm, for which we need to imitate the method adapted in Eq. (4.22). As it turns out, we have two constants $c, \tilde{c} \in \mathbb{R}$ such that [25]

$$\|U_\tau(s, 0) - U_\tau^A(s, 0)\| \leq \tau^{-1/(2n)} (c + \tilde{c}s).$$

Chapter 6

Discussion

In this thesis we provided bounds on three quantities that are related to the adiabatic evolution for a quantum system, where the evolution lasts for a total time τ . These bounds then hold if the Hamiltonian associated with the system exhibits smooth and gradual behaviour and possess an isolated subset contained within the spectrum of eigenvalues.

In the first bound we considered for states starting in the isolated subset the transition out of said subset. This transition has a probability of order of the reciprocal of the squared total evolved time, $1/\tau^2$. The second bound compared the real time evolution of the isolated subset with the ideal time evolution of said subset. This bound is of order of $1/\tau$. The third bound considered the comparison between the unitary propagators for the real and ideal time evolution, which is also of order of $1/\tau$.

The explicit constants which bound the three quantities have been determined, and can be expressed in the operator norm of certain bounded operators. Additionally, we supplied the theory with two examples that concern only a few eigenvalues.

The approach we adhered to used the intertwining property, the twiddle operation and the adiabatic connectivity. Other approaches to the time-adiabatic theorem include the formalism of section determinants of the Riesz projectors, using the innately related solutions of the Wiener-Hopf equations. [20]

With additional conditions the bounds can be narrowed down. If the Hamiltonian $H(\cdot)$ is a k -smooth family of operators, and $\dot{H}(\cdot)$ is compactly

supported, then the transition probability will be of order $1/\tau^{2(k-1)}$ and the bound on the difference between the real and ideal time evolution will be of order $1/\tau^{k-1}$. This follows from integrating iteratively, which pulls out additional factors of $1/\tau$. [14]

Moreover, developments by Avron et al. (1990) [3] and Avron and Elgart (1998) [2] have shown that the traditional time-adiabatic theorem can be extended to a formulation that forgoes the requirement the gap condition, merely requiring a smooth twice-differentiable finite spectral projection. The adiabatic theorem as formulated by Bornemann (1998) [6] also drops the gap dependence by considering density operators. These results are particularly interesting since the intrinsic time scale of fast and slow time is generally accepted to originate from the gap in the spectrum [5]. Finally, a paper by Mozgunov and Lidar (2022) [17] considers unbounded Hamiltonians with a cutoff through the considerations of the diabatic evolution.

Some of the most prominent applications of the time-adiabatic theorem in physical systems are related to the preparation of quantum states [11], to the Hall effect [1, 16], to the Stark effect [18], and to superconducting circuits [17, 19]. However, the theorems find their purpose outside traditional physics too, where they can be applied to solve optimisation problems in the field of combinatorics [8], or provide a supplementary foundation for quantum algorithms which can be used to solve certain satisfiability problems [9].

The formalism of the adiabatic connectivity can be extended to a formalism that considers a space-adiabatic evolution (or rather, the time-adiabatic theorem can be considered as a special case of the space-adiabatic theorem under certain conditions) [21, 25]. In the space-adiabatic theorem, one requires the potential energy landscape to change smoothly such that initial states remain localised. Similarly to its temporal counterpart, the theorem is conditioned by a space gap condition and requires smoothness of the energy landscape.

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