ECOLE POLYTECHNIQUE DE BRUXELLES

Alternative adiabatic quantum dynamics *with algorithmic applications*

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Chapter 0

Introduction and preliminaries

0.1 Introduction

Most objects we interact with everyday obey the laws of classical mechanics. The physics of very small objects is quite different and is better described by quantum mechanics. In quantum mechanics there are several effects, such as superposition and entanglement, that have no classical counterpart. The idea behind quantum algorithms is that maybe these effects can help to solve computational problems.

It turns out that they can. The most famous example being Shor's algorithm [3], an algorithm for finding the prime factors of an integer. Shor's algorithm can find a prime factor of a number N in $O\big(\log(N)^3\big)$ operations [4], which is exponentially faster than the best known classical algorithm. Shor's algorithm is based on the quantum Fourier transform introduced by Coppersmith [5]. There are a number of related algorithms, including algorithms for period-finding and discrete logarithms. When implemented in a quantum computer, these algorithms could break various forms of encryption, including RSA and Diffie-Hellman.

Another family of quantum algorithms were inspired by Grover's algorithm [6], which is an algorithm for brute-force search. Finding the correct element among N possibilities with classical brute-force search takes N tries in the worst case and $N/2$ tries in the average case. In both cases it is $O(N)$. Grover's algorithm takes $O(\sqrt{N})$ time, which is a polynomial speedup, not an exponential one. Grover's algorithm was generalised to a very useful quantum primitive called amplitude amplification in [7].

Subsequent research has considerably expanded these two families of quantum algorithms [8, 9, 10, 11].

Another source of inspiration for quantum algorithms comes from quantum mechanics itself. Being able to accurately simulate quantum mechanics would have many applications to materials science, chemistry and pharmacology, among many others. It turns out that simulating a quantum system on a classical computer is hard, which provided some of the earliest evidence that quantum computers could potentially be more powerful than classical computers [12].

Preparing ground states of systems is also of great interest. Besides the obvious applications to physics and chemistry, it turns out that many NP-hard problems, including various types of partitioning, covering, and satisfiability problems, can be mapped to the problem of finding the ground state of an Ising system [13].

In [14] a method for preparing ground states with a very physical intuition was proposed. A (pure) state of a quantum system is modelled as a vector $|\psi\rangle$ in a Hilbert space. The evolution of the state in time is determined by the Schrödinger equation[1]

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = -iH_t|\psi\rangle, \tag{1}$$

where H_t is a self-adjoint operator that may depend on time. If H is time-independent and the system is prepared in the ground state, then nothing will change except the rotation of the phase. Now suppose H is changed very slightly, then the state of the system will no longer be an eigenstate. It will still have a large overlap with the ground state, but will have many components, each with a phase rotating at different speeds. Whenever H changes, part of $|\psi\rangle$ migrates from the ground state to the excited subspace. If the changes in H are happening slowly enough, then large phase differences (due to time evolution) build up between the ground space and the excited space. This means that the part of the ground state that migrates to the excited space is essentially uncorrelated with what is already there and the net migration is suppressed. In other words: if $|\psi\rangle$ is initially in the ground state (or in fact any other eigenstate), and H_t changes slowly, then $|\psi\rangle$ is approximately in the ground state of H_t for all t. This fact is known as the adiabatic theorem.

The proposal of [14] is based on the observation that some ground states are easy to prepare, while others are very difficult. For example, in a strong uniform magnetic field a lattice of spins will all quickly align themselves in the direction of the field. On the other hand, one could consider a very intricate magnetic field B_1 that induces ferromagnetic coupling between some spins and antiferromagnetic coupling between others. Depending on the spatial configuration of these couplings, it might take a long time for the system to relax into its ground state, and it may not reach it in a practical time frame.

Suppose we really want to prepare the ground state of the system under the influence of B_1 (maybe because the couplings represent constraints in some constraint satisfaction problem we would like to solve), then we could prepare the system in the ground state induced by the strong uniform field and then slowly replace the strong uniform field with the more intricate field. The adiabatic theorem says that we will have (approximately) prepared the ground state corresponding to B_1 if the field was changed slowly enough. The big question is: how slow is slow enough? Several general answers to this question are given in chapter 1. Much of this material follows the orthodox presentation of adiabatic theorems, with minor improvements in presentation. There are also some new results, notably Theorem 1.28.

In practice it is usually quite difficult to get a system to evolve according to a prescribed time-dependent Hamiltonian H_t. When using a purpose-built quantum annealer, one is usually restricted to specific time-dependent Hamiltonians. It is also possible to simulate the continuous dynamics of (1) with a discrete procedure, but then one incurs an extra discretisation cost, which may be significant. See [15] for an in-depth analysis, but the problem can also be illustrated with the time-dependent Trotter product formula in Proposition C.13. Using the modulus of continuity ω_A proposed in Lemma C.11, we see that the discretisation error scales as the time complexity squared (this can presumably be reduced to $T^{1+k^{-1}}$ with k^{th}-order methods). The number of discrete operations necessary to implement the time-dependent dynamics with bounded error is therefore asymptotically larger than the time-complexity, which is the complexity we would like to match.

On the other hand, analysing discrete dynamics tends to be hard. The solution proposed in this thesis is to perform the discrete operations not according to a deterministic schedule, but rather according to a stochastic one. The average behaviour of the system will then satisfy a continuous differential equation, which is easier to analyse. This gives us the best of both

[1] In this thesis any factors of $\hbar$ will always be absorbed into the Hamiltonian H. In other words, the units are chosen such that $\hbar = 1$.

worlds: the operations are discrete, which makes it easy to implement, but the equations are continuous, which makes it easy to analyse.
The dynamics described by (1) are the unitary dynamics of a closed quantum system, which means that it is not possible to describe any (classical) randomness in this framework. In order to allow for classical randomness, we switch from pure states $|\psi\rangle$ to density matrices ρ (i.e. positive, trace-one operators on a Hilbert space). Now the time evolution is given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\rho = \mathcal{L}_t(\rho), \tag{2}$$

where $\mathcal{L}_t$ is the generator of the dynamics. If the generator is of the form $\mathcal{L}_t(\rho) = -i[H_t, \rho]$, then the dynamics are unitary and (2) is known as the Liouville-von Neumann equation.
In the second half of chapter 1 two other generators of physical processes derived from the time-dependent Hamiltonian H_t are proposed and corresponding adiabatic theorems are proved.
The use of the adiabatic theorem for computational means is called Adiabatic Quantum Computing (AQC). It is a framework for designing algorithms rather than an algorithm itself. In order to have an algorithm, one needs to supply a time-dependent Hamiltonian H_t and ideally have some knowledge of its spectrum. This is the focus of chapter 2. The analyses of Grover's algorithm and the Quantum Linear Systems of equations Problem (QLSP) are well-known. In section 2.3 the analysis of the Grover Hamiltonian is generalised to a large class of Hamiltonians that are diagonal in the computational basis. This is also the focus of [2].
The appendices contain supporting material. Some of this material just summarises well-known facts, but there are also a fair number of new results. In particular Appendix D develops a theory of integration in locally convex topological vector spaces which is substantially new. Its novelty is the reason it is included; for the purposes of the rest of the thesis Riemann integration in Banach spaces is enough.

0.2 A guide to this thesis

Adiabatic theorems are developed in chapter 1. In section 1.1 a well-trodden path to the development of adiabatic theorems is followed. Nonetheless, several improvements and new results are given. They are usually highlighted in the text. I would like to draw particular attention to Theorem 1.28, which is a new quantitative adiabatic theorem for unbounded operators.
Many adiabatic theorems are stated in the text. Many more are left implicit: the general approach will be (1) to write down an expression for a quantity that should be bounded (usually the difference between the time evolution and some idealised evolution) and (2) to bound each term and factor in this expression. Part (1) is performed in subsection 1.1.3; bounds for part (2) are developed in subsection 1.1.4.
Since the aim of subsection 1.1.4 is to present a broad range of bounding techniques, it may seem a little unfocused. The reader may want to skip parts that seem uninteresting. There is also some technical complexity: in order to deal with unbounded operators, new norms have to be introduced. The reader not intimately familiar with the graph norm may want to read subsection A.2.1, or just skip these results.
Finally a counterexample to a commonly cited informal result is presented in subsection 1.1.6.
In section 1.2, new dynamics and associated adiabatic theorems are developed. In particular, two new, Poisson-distributed, models are introduced that are based on existing deterministic procedures. The adiabatic theorems for these models are proved using a general framework that is slightly different from the setup for Hamiltonian evolution and will hopefully prove applicable to other situations.

Finally chapter 2 develops algorithms based on the various adiabatic theorems developed previously.
Appendix A is mostly a summary of well-known functional analysis, for reference and to fix notation. Much of it is just a sequence of results, with proofs if they are interesting. The subsection A.1.2 on functional calculi is much more informal than the rest and should give a relatively readable and motivated introduction to the topic.
Appendix B provides results that guarantee the existence of dynamics. On the one hand, it gives a reasonably complete development of the theory for bounded generators (this is often not given a lot of attention in textbooks, since they are more interested in the unbounded case).
On the other hand, a streamlined presentation of the unbounded case is given that is adapted to the present situation. Textbook presentations tend to focus on a more general setting that complicates the proof.
Appendix C gives some Trotter product results. The time-independent results are well-known. The time-dependent results are much less well-known and in particular there may be some novelty in the explicit bounds. The typical textbook result, see e.g. [16], does not give explicit bounds and indeed only proves strong convergence, not uniform convergence.
Appendix D develops an integral in locally convex topological spaces. It can be used as the integral in the rest of the thesis, but this is usually overkill: since the functions are usually continuous, a Riemann style integral usually suffices, although there is some complexity in the fact that the derivative of the schedule T may be discontinuous. In these cases it some kind of Bochner integral is necessary, but this will not be used in applications.

0.2.1 Levels of abstraction

Quantum algorithms usually live in finite-dimensional vector spaces. In finite dimensions there are not that many topological considerations: each space has a unique Hausdorff topology. Under this topology all linear operators are continuous (i.e. bounded) and all subspaces are closed. Consequently there are many interesting questions in infinite dimensions that become trivial in finite dimensions.
For most of the material in this thesis, this is not the case. The arguments are essentially the same in both the finite- and infinite-dimensional case. Accordingly, most result are stated without assuming anything about the dimension, except in chapter 2, where everything is finite-dimensional.
The one notable exception is when it comes to the existence of dynamics: in finite dimensions it is impossible to have an unbounded Hamiltonian. Thus the discussion on section B.3 is trivialised and reduces to the case discussed in section B.2. Consequently, there are some questions of continuity and domain in the first chapter. Any reader who is only interested in the finite-dimensional case may ignore questions of domain (i.e. the domain D is the whole Hilbert space $\mathcal{H}$) and questions of continuity (strong continuity and norm continuity may be considered as the same thing).

0.2.2 Notation

Straight brackets are used for the commutator: $[a, b] = ab - ba$. If a, b are real numbers such that $a \leq b$, then this notation refers to the closed interval.
The identity map is denoted $\mathbb{1}$. The statements $a \coloneqq b$ means a is defined as b. Brackets in a superscript mean taking a derivative: the expression $a^{(k)}$ means the k^{th} derivative of a.
The notation $\|H\|$ will always mean the operator norm of H. Sometimes it will be necessary to clarify which spaces H is supposed to map between. In these cases a subscript like $\|H\|_{V\to W}$

will be used, where V, W are normed spaces. Thus

$$\|H\|_{V\to W} \coloneqq \sup_{v\in V} \frac{\|Hv\|_W}{\|v\|_V}. \tag{3}$$

The set of linear functions H such that $\|H\|_{V\to W} < \infty$, i.e. the set of bounded operators, is denoted $\mathcal{B}(V, W)$, or $\mathcal{B}(V)$ if $V = W$.
I use the notation A^* for the adjoint of the operator A.[2] The domain of A is denoted $\mathrm{dom}(A)$.
Sometimes, mostly in the appendices, an arrow superscript will be used to denote the image function: if X, Y are sets, $A \subseteq X$ a subset and $f : X \to Y$ a function, then the image of A under f is

$$f^{\downarrow}(A) = \{f(x) \,|\, x \in A\}.$$

The notation $f : X \nrightarrow Y$ is used to denote a partial function from X to Y.
On occasion, constant functions will be denoted using an underline: $\underline{a}$ is the function that returns a for all inputs. For any proposition P, the Iverson bracket $[P]$ is 1 if the proposition is true and 0 otherwise.
Bachmann-Landau notation (also known as "big O" notation) is ubiquitous in computer science. In this thesis I make use of a non-standard variation of the notation.

Let P be an ordered set, X a normed space and $f, g : P \to X$ functions. Then

- $f = O_0(g)$ if $\|f(p)\| \leq \|g(p)\|$ for all $p \in P$;
- $f = O_1(g)$ if there exists $C \geq 0$ such that $\|f(p)\| \leq C\|g(p)\|$ for all $p \in P$;
- $f = O(g)$ if there exists $p_0 \in P$ and $C \geq 0$ such that $\|f(p)\| \leq C\|g(p)\|$ for all $p \in P$ such that $p_0 \leq p$.

This definition of O is essentially the usual one.

0.2.3 Resolvent and spectrum

The notions of spectrum and resolvent will be of central importance to this thesis. For this reason, the relevant concepts are introduced here.
The notion of spectrum is supposed to be a generalisation of the notion of eigenvalue. Indeed in finite dimensions the spectrum is just the set of eigenvalues. In infinite dimensions the situation is a little more subtle. Readers who are only interested in the finite-dimensional case should take note of the definition of the resolvent, $R_L(\lambda) \coloneqq (\lambda \mathbb{1} - L)^{-1}$, and its most important properties, Proposition 0.3. The rest may be skipped.
Let V be a normed space and L a linear operator on V. An eigenvalue of L is a number $\lambda \in \mathbb{C}$ such that there exists a non-zero vector $v \in V$ with $L(v) = \lambda v$. Or, equivalently, $(\lambda \mathbb{1} - L)v = 0$. Such a v exists if and only if $(\lambda \mathbb{1} - L)$ is not injective. In finite dimensions this is equivalent to $(\lambda \mathbb{1} - L)$ not being surjective. In fact the following three cases coincide:

1. $(\lambda \mathbb{1} - L)$ is injective;
2. $(\lambda \mathbb{1} - L)$ is surjective;
3. $(\lambda \mathbb{1} - L)$ has a bounded inverse.

[2] This is more in line with the mathematical literature than with the quantum information literature.

In infinite dimensions this equivalence no longer holds. In addition there is the question of domains. If L is unbounded, then it can often not be defined everywhere,[3] so $(\lambda \mathbb{1} - L)$ should be considered as a linear function from the domain $\operatorname{dom}(L)$ to V. Now λ is said to be an element of the spectrum of L, denoted $\sigma(L)$, if any of the following fail:

1. $(\lambda \mathbb{1} - L) : \operatorname{dom}(L) \to V$ is injective;
2. $(\lambda \mathbb{1} - L) : \operatorname{dom}(L) \to V$ is surjective;
3. $(\lambda \mathbb{1} - L) : \operatorname{dom}(L) \to V$ has a bounded inverse.

Any $\lambda \in \mathbb{C}$ that is not in the spectrum of L is said to be in the resolvent set of L, denoted $\rho(L)$. For any $\lambda \in \rho(L)$, the function $(\lambda \mathbb{1} - L) : \operatorname{dom}(L) \to V$ has a bounded inverse, by definition. This bounded inverse is called the resolvent of L at λ. It is denoted $R_L(\lambda)$ or $(\lambda \mathbb{1} - L)^{-1}$.[4]
It turns out that spectral theory is only interesting for closed operators (in finite dimensions all operators are closed).

Proposition 0.1. *Let V be a normed space and $L : \operatorname{dom}(L) \subseteq V \to V$ a linear operator. If L is not closed, then $\sigma(L) = \mathbb{C}$.*

Proof. Suppose, towards a contradiction, that there exists $\lambda \in \rho(L)$. Then $R_L(\lambda) = (\lambda \mathbb{1} - L)^{-1}$ is bounded and, a fortiori, closed. Inverting and adding a multiple of the identity preserves closedness, so this would mean that L was closed. □

When dealing with closed operators on a Banach space, point (3) above is not independent from the other two:

Proposition 0.2. *Let V be a Banach space and $L : \operatorname{dom}(L) \subseteq V \to V$ a closed linear operator. Then $\lambda \in \rho(L)$ if and only if $(\lambda \mathbb{1} - L)$ is bijective.*

Proof. This is an application of the closed graph theorem, Theorem A.48. □

For closed operators, the spectrum is conventionally split into three parts:

- The point spectrum $\sigma_{\mathrm{p}}(L)$ contains the values of λ where $\lambda \mathbb{1}_V - L$ fails to be injective, so the resolvent fails to exist. These values are called the eigenvalues of L.

  We call

  - $E_\lambda \coloneqq \ker(\lambda \mathbb{1} - L)$ the multiplicity space or geometric eigenspace of λ; and
  - $\dim \ker(\lambda \mathbb{1} - L)$ the (geometric) multiplicity of λ.

- The continuous spectrum $\sigma_{\mathrm{c}}(L)$ is the set of all $\lambda \in \mathbb{C}$ such that $(\lambda \mathbb{1} - L)$ is injective and its range is dense in V, but is not all of V.

- The residual spectrum $\sigma_{\mathrm{r}}(L)$ is the set of all $\lambda \in \mathbb{C}$ such that $(\lambda \mathbb{1} - L)$ is injective, but its range is not dense in V.

Next recall the (very important) resolvent identities:

[3] Any symmetric operator on a Hilbert space that is defined everywhere is bounded. This observation is known as the Hellinger-Toeplitz theorem, Theorem A.92. The same is true for any closed operator on a Banach space, see Theorem A.48. All operators in this thesis will be closed, since operators that generate semigroups are closed, see Theorem B.3.

[4] Sometimes the resolvent is defined as $(L - \lambda \mathbb{1})^{-1}$ rather than $(\lambda \mathbb{1} - L)^{-1}$, which can lead to sign differences. In particular the convention in this thesis is opposite to the one in [17].

Proposition 0.3 (First and second resolvent identities)**.** *Let V be a Banach space and $S, T : V \nrightarrow V$. Then*

1. $R_T(\lambda) - R_T(\mu) = (\mu - \lambda) R_T(\lambda) R_T(\mu)$ *for all* $\lambda, \mu \in \rho(T)$*;*
2. *if* $\operatorname{dom}(S) \subseteq \operatorname{dom}(T)$*, then* $R_T(\lambda)\big(T - S\big)R_S(\lambda) = R_T(\lambda) - R_S(\lambda)$ *for all* $\lambda \in \rho(S) \cap \rho(T)$*.*

The formal manipulations are straightforward. A little care is needed when dealing with the domains.

Proof. (1) We have

$$\begin{aligned} R_T(\lambda) - R_T(\mu) &= R_T(\lambda)(\mu - T)R_T(\mu) - R_T(\lambda)(\lambda - T)R_T(\mu) \\ &= \mu R_T(\lambda)R_T(\mu) - R_T(\lambda)TR_T(\mu) - \lambda R_T(\lambda)R_T(\mu) + R_T(\lambda)TR_T(\mu) \\ &= \mu R_T(\lambda)R_T(\mu) - \cancel{R_T(\lambda)TR_T(\mu)} - \lambda R_T(\lambda)R_T(\mu) + \cancel{R_T(\lambda)TR_T(\mu)} \\ &= (\mu - \lambda)R_T(\lambda)R_T(\mu). \end{aligned}$$

(2) We have $\operatorname{dom}(T - S) = \operatorname{dom}(S)$, so $R_T(\lambda)\big(T - S\big)R_S(\lambda)$ is well-defined and

$$\begin{aligned} R_T(\lambda)\big(T - S\big)R_S(\lambda) &= R_T(\lambda)\big(\lambda\mathbb{1} - S - (\lambda\mathbb{1} - T)\big)R_S(\lambda) \\ &= R_T(\lambda)(\lambda\mathbb{1} - S)R_S(\lambda) - R_T(\lambda)(\lambda\mathbb{1} - T)R_S(\lambda) \\ &= R_T(\lambda)\,\mathbb{1}_V - \mathbb{1}_{\operatorname{dom}(T)}\,R_S(\lambda) \\ &= R_T(\lambda) - R_S(\lambda). \end{aligned}$$

□

Another fact that will be very useful is the following:

Proposition 0.4. *Let L be a linear operator on a Banach space V. The spectrum $\sigma(L)$ is closed.*

Finally an elementary lemma that is sometimes useful.

Lemma 0.5. *Let T be a linear operator on a Banach space V and $\lambda \in \rho(T)$. Then*

$$TR_T(\lambda) = \lambda R_T(\lambda) - \mathbb{1}\,.$$

Note in particular that $TR_T(\lambda)$ is bounded and defined everywhere.

Proof. We have $\mathbb{1} = (\lambda\mathbb{1} - T)R_T(\lambda) = \lambda R_T(\lambda) - TR_T(\lambda)$. □

0.3 Acknowledgements

First and foremost I would like to thank Jérémie. In March of 2021 I cold emailed the group looking for a PhD position. At the time I thought I wanted to do a PhD, but I did not really know what in. I had heard a little bit about "quantum information" and it sounded interesting. Jérémie took a chance on me and I had no idea what I was getting myself into. As it turns out, I was very lucky: I could hardly have hoped for a better supervisor. Jérémie was always supportive, patient in his explanations and meticulous in his checking of my work. Thank you for supporting me and believing in me.

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0.4 List of papers

This thesis is based on the following papers:

[1] Joseph Cunningham and Jérémie Roland. "Eigenpath Traversal by Poisson-Distributed Phase Randomisation". In: *19th Conference on the Theory of Quantum Computation, Communication and Cryptography (TQC 2024)*. Ed. by Frédéric Magniez and Alex Bredariol Grilo. Vol. 310. Leibniz International Proceedings in Informatics (LIPIcs). Dagstuhl, Germany: Schloss Dagstuhl – Leibniz-Zentrum für Informatik, 2024, 7:1–7:20. DOI: 10.4230/LIPIcs.TQC.2024.7.

[2] Arthur Braida, Shantanav Chakraborty, Alapan Chaudhuri, Joseph Cunningham, Rutvij Menavlikar, Leonardo Novo, and Jérémie Roland. "Unstructured Adiabatic Quantum Optimization: Optimality with Limitations". In: *Quantum* 9 (July 2025), p. 1790. DOI: 10.22331/q-2025-07-11-1790.

Chapter 1

Adiabatic theorems

1.1 Adiabatic theorems for unitary dynamics

The adiabatic theorem has a long and storied history with many people contributing and the result has been taken in many directions. Here I will develop a version that is particularly suited for adiabatic applications.

The idea of a quantum adiabatic theorem originates with Ehrenfest [18, 19].[1] He formulated it in what will come to be known as the "old quantum mechanics". In [26], Born and Fock update it to the "new quantum mechanics" and make the result more rigorous, but their result is restricted to matrices.

Kato gives an operator-theoretic treatment in [27] and introduces many features of the theory in its modern form, in particular the idea of comparing the evolution to an ideal adiabatic evolution (Proposition 1.8) and the solution to the operator equation in Lemma 1.3.

Avron, Seiler and Yaffe take these ideas further [28]. They introduce the solution to the operator equation in Lemma 1.4 and prove many of the results reproduced here, but do not give explicit bounds on the error.

Fahri, Goldstone, Gutmann and Sipser realised that the adiabatic theorem could be used to design algorithms [14], but they quote an incorrect version of the adiabatic theorem. A counter-example to their version is presented in subsection 1.1.6.

More rigorous bounds are proved in [17] by extracting quantitative results from the methods of [28]. This brief history has left out many important and interesting results. We will meet some of them as we develop the theory.

1.1.1 Assumptions on the Hamiltonian

The adiabatic theorem describes a feature of evolution under a time-dependent Hamiltonian H_t. We will need to make two kinds of assumptions on H_t. On the one hand, H_t needs to be regular enough that it actually generates a unitary evolution, i.e. the Schrödinger equation should have a solution.

On the other hand, the aim of the adiabatic theorem is to track some eigenspace. We need some definitions and assumptions to make it clear what this means.

[1] Some papers on adiabatic quantum computing [20, 21, 22] attribute the adiabatic hypothesis to Einstein, based on [23]. This is a historical inaccuracy; Einstein refers to "Ehrenfest's adiabatic hypothesis" in this work. (It does seem to be the first time the phrase "adiabatic hypothesis" is used in print, which may be the source of the confusion). Ironically, Einstein's application of the adiabatic hypothesis is incorrect. See [24, 25] for the early history of the adiabatic theorem and its role in the formulation of quantum mechanics.

1.1.1.1 Assumptions guaranteeing existence of dynamics

To make sure the dynamics exist, the results of Appendix B are used. If the Hamiltonian is bounded, it is enough to assume H_t is continuous in t (although most of the adiabatic theorems will require something stronger, usually at least that H_t is twice continuously differentiable in t).
In more generality, H_t may be unbounded. The following assumption is then made:

Assumption 1. *Let $\mathcal{H}$ be a Hilbert space. Then H_t is assumed to be a (densely defined)*[2] *self-adjoint operator on $\mathcal{H}$, for all $t \in \mathbb{R}^+$, such that*

- *the domain of H_t is the same for all t, let it be denoted D;*
- *for all $x \in D$, the function $t \mapsto H_t x$ is continuously differentiable.*

This is sometimes summarised by saying that H_t is "strongly $\mathcal{C}^1$". If $t \mapsto H_t x$ is k times continuously differentiable, then we will also say that H_t is "strongly $\mathcal{C}^k$".
If H_t is a bounded operator for all t, then it must necessarily be true that $D = \mathcal{H}$, since self-adjoint operators are closed. In addition, these hypotheses force $t \mapsto H_t$ to be norm-continuous, see Corollary B.13.
These assumptions are enough to guarantee existence and uniqueness of the dynamics, Theorem B.16.

1.1.1.2 Defining the spectral region of interest and the gap

An adiabatic theorem gives a guarantee that a time-evolved vector will stay (approximately) in a "good" subspace, i.e. a subspace of particular interest. These subspaces will always correspond to a certain region of the spectrum. More exactly, they will always correspond to the part of the spectrum that lies in some interval. In addition, this interval should not vary too wildly in time: its bounds are taken to be continuous functions. This gives us the following assumption:

Assumption 2. *Assume there exist two continuous functions $b_0, b_1 : \mathbb{R} \to \mathbb{R}$ such that*

- *$b_0(t), b_1(t) \notin \sigma(H_t)$, for all t; and*
- *$b_0 \leq b_1$ pointwise.*

Let $P(t)$ be the spectral projector associated with $\sigma(H_t) \cap [b_0(t), b_1(t)]$.

We also define $Q(t) \coloneqq \mathbb{1} - P(t)$. Any bounded operator $X \in \mathcal{B}(\mathcal{H})$ such that

$$X = P(t)XQ(t) + Q(t)XP(t) \tag{1.1}$$

is called off-diagonal at t.
Now the (spectral) gap g can be defined[3] as $g(t) \coloneqq \min\{g_{b_0}(t), g_{b_1}(t)\}$, where

$$g_{b_0}(t) \coloneqq \min_{x \in \sigma(H_t) \cap [-\infty, b_0(t)]} |x - b_0(t)| + \min_{x \in \sigma(H_t) \cap [b_0(t), +\infty]} |x - b_0(t)| \tag{1.2}$$

and

$$g_{b_1}(t) \coloneqq \min_{x \in \sigma(H_t) \cap [-\infty, b_1(t)]} |x - b_1(t)| + \min_{x \in \sigma(H_t) \cap [b_1(t), +\infty]} |x - b_1(t)|. \tag{1.3}$$

[2] If H_t does not have a dense domain, then its adjoint is not an operator and, in particular, it cannot be self-adjoint.

[3] This definition is well-defined, i.e. the minimum exists, because the spectrum is closed.

The minimum of this function (minimised over t) will be denoted $g_m := \min_t g(t)$. If t is restricted to a finite interval, then it is a consequence of Assumption 2 that $g_m > 0$. [4]
Since the spectrum is closed, there exist neighbourhoods of $b_0(t), b_1(t)$ that are disjoint from it. Now the spectral projector can be written in its Riesz form as

$$P(t) = \frac{1}{2\pi i} \oint_\Gamma R_{H_t}(z) \, \mathrm{d}z, \tag{1.4}$$

where Γ is some simple curve in the complex plane that crosses the real line twice, once within a distance $g(t)$ of $b_0(t)$ and once within a distance $g(t)$ of $b_1(t)$, and otherwise stays at a distance of at least $g(t)$ from $\sigma(H_t)$.[5]

Lemma 1.1. *Suppose H_t is a time-dependent Hamiltonian satisfying the stated assumptions. Then*

1. *$P(t)$ is norm-continuous;*
2. *the linear operator*
$$P'(t) : \mathcal{H} \to \mathcal{H} : |\psi\rangle \mapsto \frac{\mathrm{d}P(t)|\psi\rangle}{\mathrm{d}t} \tag{1.5}$$
is well-defined and bounded;
3. *the function $t \mapsto P'(t)$ is strongly continuous.*

In general, if H_t is strongly $\mathcal{C}^k$, then $P(t)$ is strongly $\mathcal{C}^k$ and norm-$\mathcal{C}^{k-1}$.

Proof. (1) Fix t_0. Then there exists a neighbourhood of t_0 and a fixed curve Γ such that Γ can be used in the definition of the Riesz projector (1.4) for t in the neighbourhood of t_0. Now continuity follows from Corollary B.13 and the fact that taking the inverse is a continuous operation.
(2,3) The existence and strong continuity of P' are due to the equation

$$\frac{\mathrm{d}}{\mathrm{d}t} R_{H_t}(z) = R_{H_t}(z) \Big(\frac{\mathrm{d}H_t}{\mathrm{d}t} \Big) R_{H_t}(z). \tag{1.6}$$

Its boundedness is due to Corollary A.44. □

Lemma 1.2. *The operator $P'(t)$ is off-diagonal, for all t.*

Proof. It follows from $P' = (PP)' = P'P + PP'$ that $PP'P = 0$. Then it also follows that

$$P' = P'P + PP' = (P+Q)P'P + PP'(P+Q) = QP'P + PP'Q. \tag{1.7}$$

□

[4] There are also versions of the adiabatic theorem with weaker assumptions such that $g_m = 0$ is allowed, [29, 30, 31], but these lack quantitative error bounds and need to make separate assumptions for the existence and continuity of the spectral projections P.
[5] We want $\|R_{H_t}(z)\|$ to be bounded along the curve.

1.1.2 Solving an important operator equation

The proofs of the adiabatic theorem that will be developed here rely on finding a solution Y to the operator equation

$$[H_t, Y] = [P(t), X], \tag{1.8}$$

where X is some operator defined on D, the domain of H_t. The range of the operator Y should be a subset of D; the operator equation is only expected to hold on D. This equation will later allow us to replace factors of $P(t)$ by H_t, which combine with the evolution operator to give derivatives. This allows integration by parts.
The first solution to (1.8) that will be discussed is applicable only when P is the spectral projector associated to a single point ω_0. Due to Assumption 2, ω_0 is an isolated point in the spectrum. Now Corollary A.17 gives that ω_0 is an eigenvalue.

Lemma 1.3. *Let $\mathcal{H}$ be a Hilbert space, H a self-adjoint operator on $\mathcal{H}$ and P the spectral projector on some eigenvalue ω_0. For any X defined on D, the operator equation (1.8) has a solution*

$$Y = (\omega_0 \mathbb{1} - H)^+ XP + PX(\omega_0 \mathbb{1} - H)^+, \tag{1.9}$$

which is off-diagonal.

The plus in superscript denotes the pseudoinverse.[6]
This solution only works if P projects onto the eigenspace of a single eigenvalue. This eigenspace may be degenerate.

Proof. With functional calculus, Theorem A.16, it is straightforward to see that both $(\omega_0 \mathbb{1} - H)^+$ and $H(\omega_0 \mathbb{1} - H)^+$ are bounded operators, which means that the range of Y is indeed a subset of D. The proof is then a straightforward verification of the proposed solution:

$$[H, Y] = H(\omega_0 \mathbb{1} - H)^+ XP + HPX(\omega_0 \mathbb{1} - H)^+ - (\omega_0 \mathbb{1} - H)^+ XPH - PX(\omega_0 \mathbb{1} - H)^+ H \tag{1.11}$$

$$= H(\omega_0 \mathbb{1} - H)^+ XP + \omega_0 PX(\omega_0 \mathbb{1} - H)^+ - \omega_0(\omega_0 \mathbb{1} - H)^+ XP - PX(\omega_0 \mathbb{1} - H)^+ H \tag{1.12}$$

$$= PX\Big((\omega_0 \mathbb{1} - H)^+ \omega_0 - (\omega_0 \mathbb{1} - H)^+ H\Big) - \Big(\omega_0(\omega_0 \mathbb{1} - H)^+ - H(\omega_0 \mathbb{1} - H)^+\Big)XP \tag{1.13}$$

$$= PX(\omega_0 \mathbb{1} - H)^+(\omega_0 \mathbb{1} - H) - (\omega_0 \mathbb{1} - H)^+(\omega_0 \mathbb{1} - H)XP \tag{1.14}$$

$$= PXQ - QXP \tag{1.15}$$

$$= PXQ + PXP - QXP - PXP = [P, X], \tag{1.16}$$

where $Q = \mathbb{1} - P$. □

[6] There are many equivalent ways of understanding the pseudoinverse. The theory is especially well-known in the matrix case. Some elements in a C^*-algebra have a pseudoinverse [32, 33]. For our purposes the most convenient way of understanding the pseudoinverse X^+ is as $f(X)$, where

$$f : \mathbb{R} \to \mathbb{R} : x \mapsto \begin{cases} 0 & (x = 0) \\ x^{-1} & (\text{otherwise}). \end{cases} \tag{1.10}$$

This requires X to be normal. Note in particular that $X^+ X = XX^+$ is the projector on the space orthogonal to the kernel of X.

Lemma 1.4. *Let $\mathcal{H}$ be a Hilbert space, H a self-adjoint operator and Γ a closed simple curve in the complex plane that is disjoint from the spectrum $\sigma(H)$. Let P the spectral projector on the part of the spectrum that lies inside Γ. For any $X \in \mathcal{B}(D, \mathcal{H})$, the operator equation (1.8) has a solution*

$$Y = \frac{1}{2\pi i} \oint_\Gamma R_H(z) X R_H(z) \, \mathrm{d}z, \tag{1.17}$$

which is off-diagonal.

If P is the projector on a single eigenvalue, then this solution is actually the same as the one in Lemma 1.3, except there is the additional boundedness assumption on X (which is enough to guarantee the existence of the integral, see Proposition A.41).
The contents of this lemma is well-established, [28, 17], but I have not seen the construction in Figure 1.1 anywhere else and I think this is quite a nice way to obtain the proof.

Proof. The proof starts with a straightforward verification of the proposed solution:

$$\begin{aligned} [H, Y] &= \frac{1}{2\pi i} \oint_\Gamma \big[H, R_H(z) X R_H(z)\big] \, \mathrm{d}z & (1.18)\\ &= \frac{1}{2\pi i} \oint_\Gamma \big[R_H(z) X R_H(z), z\mathbb{1} - H\big] \, \mathrm{d}z & (1.19)\\ &= \frac{1}{2\pi i} \oint_\Gamma \big(R_H(z) X - X R_H(z)\big) \, \mathrm{d}z & (1.20)\\ &= \Big(\frac{1}{2\pi i} \oint_\Gamma R_H(z) \, \mathrm{d}z\Big) X - X \Big(\frac{1}{2\pi i} \oint_\Gamma R_H(z) \, \mathrm{d}z\Big) & (1.21)\\ &= PX - XP = [P, X]. & (1.22) \end{aligned}$$

Next we show that this Y is off-diagonal. Since the spectrum $\sigma(H)$ is closed, the curve Γ can be enlarged slightly without intersecting any of the spectrum. Call this new curve Γ_1. For any $z \in \Gamma$, consider the integral $\frac{1}{2\pi i} \oint_{\Gamma_1} \frac{R_H(w)}{w-z} \, \mathrm{d}w$. In order to calculate this integral, we can deform Γ_1 such that it splits into two parts: one curve Γ_2 that lies inside Γ, but contains the same part of $\sigma(H)$ and another Γ_3 that is a small circle around z. See Figure 1.1. Now using Cauchy's theorem on the one hand, and holomorphic functional calculus, Theorem A.21, on the other,

$$\begin{aligned} \frac{1}{2\pi i} \oint_{\Gamma_1} \frac{R_H(w)}{w - z} \, \mathrm{d}w &= \frac{1}{2\pi i} \oint_{\Gamma_3} \frac{R_H(w)}{w - z} \, \mathrm{d}w + \frac{1}{2\pi i} \oint_{\Gamma_2} \frac{R_H(w)}{w - z} \, \mathrm{d}w & (1.23)\\ &= R_H(z) - P R_H(z) = Q R_H(z). & (1.24) \end{aligned}$$

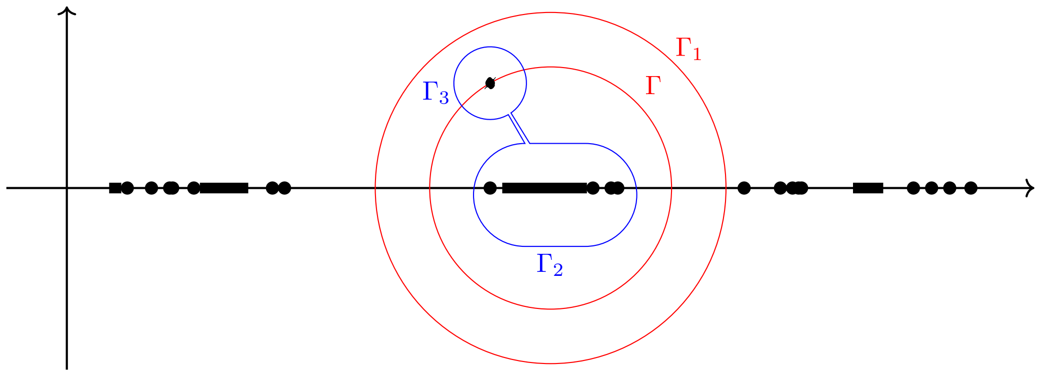


Figure 1.1: An illustration of the integration contours used in the proof of Lemma 1.4.

This result can also be obtained without deforming curves, using the resolvent identity.[7] Then

$$\begin{aligned}
YQ &= \frac{1}{2\pi i}\oint_\Gamma R_H(z)XR_H(z)Q\,\mathrm{d}z && (1.29)\\
&= \frac{1}{(2\pi i)^2}\oint_\Gamma R_H(z)X\oint_{\Gamma_1}\frac{R_H(w)}{w-z}\,\mathrm{d}w\,\mathrm{d}z && (1.30)\\
&= \frac{1}{(2\pi i)^2}\oint_{\Gamma_1}\Big(\oint_\Gamma \frac{R_H(z)}{w-z}\,\mathrm{d}z\Big)XR_H(w)\,\mathrm{d}w && (1.31)\\
&= \frac{1}{(2\pi i)^2}\oint_{\Gamma_1}\Big(\oint_\Gamma \frac{R_H(z)-R_H(w)}{w-z}\,\mathrm{d}z\Big)XR_H(w)\,\mathrm{d}w && (1.32)\\
&= \frac{1}{(2\pi i)^2}\oint_{\Gamma_1}\Big(\oint_\Gamma R_H(w)R_H(z)\,\mathrm{d}z\Big)XR_H(w)\,\mathrm{d}w && (1.33)\\
&= \frac{1}{(2\pi i)^2}\Big(\oint_\Gamma R_H(z)\,\mathrm{d}z\Big)\oint_{\Gamma_1} R_H(w)XR_H(w)\,\mathrm{d}w && (1.34)\\
&= PY, && (1.35)
\end{aligned}$$

where the first resolvent identity has been used, as well as the fact that

$$\oint_\Gamma \frac{R_H(w)}{w-z}\,\mathrm{d}z = 0, \qquad (1.36)$$

since the function is analytic inside Γ.

[7] Cauchy's theorem and the Riesz form of the projector give

$$Q = \mathbb{1} - P = \frac{1}{2\pi i}\oint_{\Gamma_1}\Big(\frac{\mathbb{1}}{w-z} - R_H(w)\Big)\,\mathrm{d}w, \qquad (1.25)$$

so

$$\begin{aligned}
QR_H(z) &= \frac{1}{2\pi i}\oint_{\Gamma_1}\Big(\frac{R_H(z)}{w-z} - R_H(w)R_H(z)\Big)\,\mathrm{d}w && (1.26)\\
&= \frac{1}{2\pi i}\oint_{\Gamma_1}\Big(\frac{R_H(z)}{w-z} - \frac{R_H(z)-R_H(w)}{w-z}\Big)\,\mathrm{d}w && (1.27)\\
&= \frac{1}{2\pi i}\oint_{\Gamma_1}\frac{R_H(w)}{w-z}\,\mathrm{d}w. && (1.28)
\end{aligned}$$

Finally, we check that the range of Y is a subset of D. For all $|\psi\rangle \in \mathcal{H}$, the integral

$$\frac{1}{2\pi i}\oint_\Gamma R_H(z)XR_H(z)|\psi\rangle \,\mathrm{d}z \tag{1.37}$$

Since $z \mapsto R_H(z)XR_H(z)|\psi\rangle$ is continuous along Γ as a function to D equipped with the graph norm, the integral exists in D, see Corollary D.19. □

We have now considered two solutions to the operator equation (1.8). The solution in Lemma 1.4 is more general, but it will prove easier to compute reasonable bounds for Lemma 1.3. When both solutions are applicable, it turns out they coincide.

Lemma 1.5. *Let $\mathcal{H}$ be a Hilbert space, H a self-adjoint operator on $\mathcal{H}$, P the spectral projector on some isolated eigenvalue ω_0, Γ a simple curve that contains ω_0, but no other part of the spectrum and $X \in \mathcal{B}(\mathcal{H})$. Then*

$$\frac{1}{2\pi i}\oint_\Gamma R_H(z)XR_H(z)\,\mathrm{d}z = (\omega_0 \mathbb{1} - H)^+XP + PX(\omega_0 \mathbb{1} - H)^+. \tag{1.38}$$

Proof. Set $\widetilde{X} = \frac{1}{2\pi i}\oint_\Gamma R_H(z)XR_H(z)\,\mathrm{d}z$. Now

$$\begin{aligned} PXQ &= P[P,X]Q && (1.39)\\ &= P[H,\widetilde{X}]Q && (1.40)\\ &= \omega_0 P\widetilde{X}Q - P\widetilde{X}QH && (1.41)\\ &= P\widetilde{X}Q(\omega_0 \mathbb{1} - H). && (1.42)\end{aligned}$$

Multiplying both sides by $(\omega_0 \mathbb{1} - H)^+$ on the right give $PX(\omega_0 \mathbb{1} - H)^+ = P\widetilde{X}Q$. Similarly $Q\widetilde{X}Q = (\omega_0 \mathbb{1} - H)^+XP$. Since we also know that $\widetilde{X}$ is off-diagonal, we are done. □

It is possible to push the equivalence slightly further.

Corollary 1.6. *Let $\mathcal{H}$ be a Hilbert space, H a self-adjoint operator on $\mathcal{H}$, P the spectral projector on a set of m isolated eigenvalues $\{\omega_0, \ldots, \omega_{m-1}\}$, Γ a simple curve that contains $\omega_0, \ldots, \omega_{m-1}$, but no other part of the spectrum and $X \in \mathcal{B}(\mathcal{H})$. Then*

$$\frac{1}{2\pi i}\oint_\Gamma R_H(z)XR_H(z)\,\mathrm{d}z = \sum_{k=0}^{m-1}(\omega_k \mathbb{1} - H)^+QXP_k + P_kXQ(\omega_k \mathbb{1} - H)^+, \tag{1.43}$$

where P_k projects onto the eigenspace associated by ω_k.

Proof. Deform Γ such that it breaks into m separate curves, each circling one ω_k. See Figure 1.2. This deformation does not change the result, but does mean it can be written as the sum of m simpler terms. Each one can be computed using Lemma 1.5. Finally, the factors of Q can be added, since we know the operator is off-diagonal. □

The equality of the solutions in Lemma 1.3 and Lemma 1.4 is not a coincidence.

Proposition 1.7. *Let $\mathcal{H}$ be a Hilbert space, H a self-adjoint operator and Γ a closed simple curve in the complex plane that is disjoint from the spectrum $\sigma(H)$. Let P the spectral projector on the part of the spectrum that lies inside Γ and $X \in \mathcal{B}(D, \mathcal{H})$. Then*

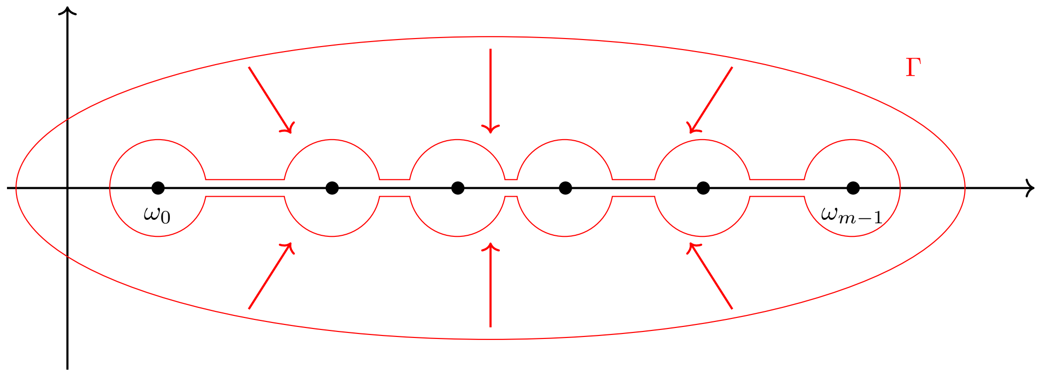


Figure 1.2: An illustration of the proof of Corollary 1.6.

1. *for any solution Y of the operator equation (1.8), the off-diagonal operator $PYQ+QYP$ is also a solution;*

2. *the off-diagonal solution is unique.*

Proof. (1) This is straightforward verification:

$$\begin{aligned}
[H, PYQ + QYP] &= P[H,Y]Q + Q[H,Y]P && (1.44)\\
&= P[P,X]Q + Q[P,X]P && (1.45)\\
&= P[P,X]Q + Q[P,X]P + P[P,X]P + Q[P,X]Q && (1.46)\\
&= [P,X]. && (1.47)
\end{aligned}$$

(2) Taking the off-diagonal components of operator equation (1.8) gives two new equations:

$$PH(PYQ) - (PYQ)HQ = P[P,X]Q = PXQ \tag{1.48}$$

and

$$QH(QYP) - (QYP)HP = Q[P,X]P = -QXP. \tag{1.49}$$

Since $\sigma(PH)$ and $\sigma(QH)$ are disjoint, uniqueness follows from Proposition A.22 if H is bounded. It is possible, but somewhat technical, to extend this result to the unbounded case. Instead, we extend the method of Proposition A.25 to show that solutions of (1.48) and (1.49) must be of a certain form. The claim is that

$$PYQ = \frac{1}{2\pi i}\oint_\Gamma R_{PH}(z)(PXQ)R_{QH}(z)\,\mathrm{d}z, \tag{1.50}$$

which uniquely determines PYQ. This follows by straightforward verification

$$\begin{aligned}
&\frac{1}{2\pi i}\oint_\Gamma R_{PH}(z)(PXQ)R_{QH}(z)\,\mathrm{d}z && (1.51)\\
&\qquad = \frac{1}{2\pi i}\oint_\Gamma R_{PH}(z)\Big(PH(PYQ)-(PYQ)HQ\Big)R_{QH}(z)\,\mathrm{d}z && (1.52)\\
&\qquad = \frac{1}{2\pi i}\oint_\Gamma \Big(\cancel{zR_{PH}(z)(PYQ)R_{QH}(z)}-(PYQ)R_{QH}(z) && (1.53)\\
&\qquad\qquad -\cancel{zR_{PH}(z)(PYQ)R_{QH}(z)}+R_{PH}(z)(PYQ)\Big)\,\mathrm{d}z\\
&\qquad = \Big(\frac{1}{2\pi i}\oint_\Gamma R_{PH}(z)\,\mathrm{d}z\Big)(PYQ)-(PYQ)\Big(\frac{1}{2\pi i}\oint_\Gamma R_{QH}(z)\,\mathrm{d}z\Big) && (1.54)\\
&\qquad = (PYQ), && (1.55)
\end{aligned}$$

where we have used Lemma 0.5, the Riesz form of the projector and the fact that the spectrum of QH lies outside Γ.
The formula

$$QYP = \frac{1}{2\pi i}\oint_\Gamma R_{QH}(z)(QXP)R_{PH}(z)\,\mathrm{d}z \tag{1.56}$$

can be proved in a similar fashion. □

1.1.3 Adiabatic evolution

In this section adiabatic theorems will be derived by comparing the evolution of the system to an idealised evolution, so our first task will be to define this idealised evolution. This is the content of Proposition 1.8.
The adiabatic theorem says that the evolution keeps the system close to the instantaneous ground state, if the Hamiltonian changes slowly enough. Proving this is easiest if we have some way of "slowing down" the evolution. To that end, we reparametrise time: rather than letting the dynamics be generated by H_t for $t \in [0,T]$, we now consider a "reduced time parameter" $s \in [0,1]$ and let the dynamics $U(s_1,s_0)$ be generated by $-iTH_s$, in the sense of Theorem B.16. All derivatives are with respect to the parameter s. Assumption 1 and Assumption 2 are in effect. The starting points of all evolution operators are fixed to 0: $U(s)$ is used to mean $U(s,0)$. Often s-dependence will be suppressed, especially inside integrals.
As a technical tool, we define new dynamics $U_A(s)$ that are supposed to represent an idealised adiabatic evolution. The existence and main property of these dynamics are proved in Proposition 1.8.

Proposition 1.8. *Let H_s be a time-dependent Hamiltonians. Let $U(s)$ be generated by $-iTH_s$ and $U_A(s)$ by $-iTH_s + [P'(s), P(s)]$. Then*

1. *$U_A(s)$ exists and is unitary;*
2. *$U_A(s)P(0) = P(s)U_A(s)$.*

Point (2) is sometimes referred to as the "intertwining property". It implies that vectors in the range of $P(0)$ are mapped to the range of $P(s)$.

Proof. (1) Computing the adjoint gives

$$\big(-iTH_s + [P',P]\big)^* = iTH_s + [P,P'] = iTH_s - [P',P], \tag{1.57}$$

so the generator is skew-adjoint. It is a bounded perturbation of H_s, so the existence of $U_A(s)$ follows in the same way as the existence of $U(s)$ from Theorem B.16.
(2) We have

$$
\begin{aligned}
U_A(s)^* P(s) U_A(s) &= P(0) + \int_0^s \frac{\mathrm{d}}{\mathrm{d}r} \big(U_A(r)^* P(r) U_A(r)\big)\,\mathrm{d}r && (1.58)\\
&= P(0) + \int_0^s \Big(U_A^*\big(\cancel{iTH} - [P',P]\big)PU_A + U_A^* P' U_A + U_A^* P\big(\cancel{-iTH} + [P',P]\big)U_A\Big)\,\mathrm{d}r && (1.59)\\
&= P(0) + \int_0^s \big(U_A^*(PP'P - P'P)U_A + U_A^* P' U_A + U_A^*(PP'P - PP')U_A\big)\,\mathrm{d}r && (1.60)\\
&= P(0) + \int_0^s \big(U_A^* P' U_A - U_A^* P' U_A\big)\,\mathrm{d}r = P(0), && (1.61)
\end{aligned}
$$

where we have used $PP'P = 0$ and $P'P + PP' = P'$. If the domain D is not the whole of $\mathcal{H}$, then the equality holds pointwise on D. Since D is dense, we conclude by continuity. □

It turns out that the easiest way to compare the unitaries $U(s)$ and $U_A(s)$ is by considering $\Omega(s) \coloneqq U(s)^* U_A(s)$, which is known as the wave operator. We have $U \approx U_A$ if and only if $\Omega \approx \mathbb{1}$.

Proposition 1.9. *Let H_s be a time-dependent Hamiltonian. Let $U(s)$ be generated by $-iTH_s$ and $U_A(s)$ by $-iTH_s + [P', P]$. Suppose $T(s)^{-1}$ is absolutely continuous. Set $\Omega(s) \coloneqq U(s)^* U_A(s)$. For all X, let $\widetilde{X}$ be a solution of the operator equation (1.8). Then*

$$
\Omega(1) = \mathbb{1} + \Big[\frac{i}{T} U^* \widetilde{P'} U \Omega\Big]_0^1 - \int_0^1 \frac{i}{T} U^* \big(\widetilde{P'}[P', P] + \widetilde{P'}'\big) U \Omega \,\mathrm{d}s + \int_0^1 \frac{iT'}{T^2} U^* \widetilde{P'} U \Omega \,\mathrm{d}s. \qquad (1.62)
$$

There are two peculiarities of this result, compared to similar treatments (e.g. [28, 17]). Firstly T is allowed to be time-dependent, which gives an extra term containing T'. This is particularly convenient for algorithmic purposes because it makes it easier to consider schedules that are adapted to the gap.
Secondly, Ω is defined as $U^* U_A$, not $U_A^* U$. This makes the calculations slightly cleaner, in my opinion.

Proof. We calculate

$$\Omega(t) = \mathbb{1} + \int_0^1 \frac{\mathrm{d}}{\mathrm{d}s}\,\Omega(s)\,\mathrm{d}s \tag{1.63}$$

$$= \mathbb{1} + \int_0^1 U^*[P', P]U_A\,\mathrm{d}s \tag{1.64}$$

$$= \mathbb{1} + \int_0^1 U^*[P', P]U\Omega\,\mathrm{d}s \tag{1.65}$$

$$= \mathbb{1} + \int_0^1 U^*[\widetilde{P'}, H]U\Omega\,\mathrm{d}s \tag{1.66}$$

$$= \mathbb{1} + \int_0^1 \frac{i}{T}\big(U^*\widetilde{P'}U' + U'^*\widetilde{P'}U\big)\Omega\,\mathrm{d}s \tag{1.67}$$

$$= \mathbb{1} + \int_0^1 \frac{i}{T}\Big(\big(U^*\widetilde{P'}U\big)' - U^*\widetilde{P'}'U\Big)\Omega\,\mathrm{d}s \tag{1.68}$$

$$= \mathbb{1} + \Big[\frac{i}{T}U^*\widetilde{P'}U\Omega\Big]_0^1 - \int_0^1 \frac{i}{T}U^*\widetilde{P'}U\Omega'\,\mathrm{d}s - \int_0^1 \Big(\frac{i}{T}\Big)'U^*\widetilde{P'}U\Omega\,\mathrm{d}s - \int_0^1 \frac{i}{T}U^*\widetilde{P'}'U\Omega\,\mathrm{d}s \tag{1.69}$$

$$= \mathbb{1} + \Big[\frac{i}{T}U^*\widetilde{P'}U\Omega\Big]_0^1 - \int_0^1 \frac{i}{T}U^*\widetilde{P'}[P', P]U\Omega\,\mathrm{d}s + \int_0^1 \frac{iT'}{T^2}U^*\widetilde{P'}U\Omega\,\mathrm{d}s - \int_0^t \frac{i}{T}U^*\widetilde{P'}'U\Omega\,\mathrm{d}s \tag{1.70}$$

$$= \mathbb{1} + \Big[\frac{i}{T}U^*\widetilde{P'}U\Omega\Big]_0^1 - \int_0^1 \frac{i}{T}U^*\big(\widetilde{P'}[P', P] + \widetilde{P'}'\big)U\Omega\,\mathrm{d}s + \int_0^1 \frac{iT'}{T^2}U^*\widetilde{P'}U\Omega\,\mathrm{d}s. \tag{1.71}$$

Integration by parts has been used. To make this rigorous when T is not constant, Proposition D.34 can be used.
If the Hamiltonian is unbounded, we can use the same trick as before: first observe the equality on the domain D and then extend to the whole of $\mathcal{H}$ using continuity. □

1.1.4 Some norm bounds

In order to get a useful quantitative bound, it is necessary to estimate the terms in Proposition 1.9. In this section an array of techniques will be developed that can be applied to this problem. Not all the techniques in this section will be used in the proof of an adiabatic theorem in this thesis, but they all could be. The aim is to develop a broad arsenal for attacking adiabatic bounds. In particular, various assumptions on the spectrum and spectral region of interest can lead to many (non-trivially) different adiabatic theorems, each derived using a suitable combination of bounds from this section. A selection will be explored in the following section.
This section can safely be skimmed (and returned to when later results refer to it).

Proposition 1.10. *Let $\mathcal{H}$ be a Hilbert space, P an orthogonal projector, $Q = \mathbb{1} - P$ and $X \in \mathcal{B}(\mathcal{H})$ a bounded operator. If*

$$X = PX_{0,0}P + PX_{0,1}Q + QX_{1,0}P + QX_{1,1}Q, \tag{1.72}$$

then

$$\|X\| \leq \left\| \begin{pmatrix} \|X_{0,0}\| & \|X_{0,1}\| \\ \|X_{1,0}\| & \|X_{1,1}\| \end{pmatrix} \right\|. \tag{1.73}$$

Proof. Take an arbitrary unit vector $|\psi\rangle \in \mathcal{H}$. Using the Pythagorean theorem gives

$$\begin{aligned}
\|X|\psi\rangle\|^2 &= \|PX_{0,0}P|\psi\rangle + PX_{0,1}Q|\psi\rangle\|^2 + \|QX_{1,0}P|\psi\rangle + QX_{1,1}Q|\psi\rangle\|^2 && (1.74)\\
&\le \big(\|X_{0,0}\|\|P|\psi\rangle\| + \|X_{0,1}\|\|Q|\psi\rangle\|\big)^2 + \big(\|X_{1,0}\|\|P|\psi\rangle\| + \|X_{1,1}\|\|Q|\psi\rangle\|\big)^2 && (1.75)\\
&= \left\| \begin{pmatrix} \|X_{0,0}\|\|P|\psi\rangle\| + \|X_{0,1}\|\|Q|\psi\rangle\| \\ \|X_{1,0}\|\|P|\psi\rangle\| + \|X_{1,1}\|\|Q|\psi\rangle\| \end{pmatrix} \right\|^2 && (1.76)\\
&= \left\| \begin{pmatrix} \|X_{0,0}\| & \|X_{0,1}\| \\ \|X_{1,0}\| & \|X_{1,1}\| \end{pmatrix} \begin{pmatrix} \|P|\psi\rangle\| \\ \|Q|\psi\rangle\| \end{pmatrix} \right\|^2 \le \left\| \begin{pmatrix} \|X_{0,0}\| & \|X_{0,1}\| \\ \|X_{1,0}\| & \|X_{1,1}\| \end{pmatrix} \right\|. && (1.77)
\end{aligned}$$

The final inequality is due to the fact that the column vector is a unit vector. Since this bound holds for all unit vectors $|\psi\rangle$, the norm bound holds. □

Corollary 1.11.

1. *If* $X_{0,1} = 0 = X_{1,0}$*, then*
$$\|X\| \le \max\{\|X_{0,0}\|, \|X_{1,1}\|\}. \tag{1.78}$$
2. *If* $X_{0,0} = 0 = X_{1,1}$*, then*
$$\|X\| \le \max\{\|X_{0,1}\|, \|X_{0,1}\|\}. \tag{1.79}$$
3. *If* $X_{0,0} = 0 = X_{1,0}$*, then*
$$\|X\| \le \sqrt{\|X_{0,1}\|^2 + \|X_{1,1}\|^2}. \tag{1.80}$$
4. *If* $\|X_{0,1}\| = \|X_{1,0}\|$*, then*
$$\|X\| \le \frac{\|X_{0,0}\| + \|X_{1,1}\|}{2} + \frac{1}{2}\sqrt{\big(\|X_{0,0}\| - \|X_{1,1}\|\big)^2 + 4\|X_{0,1}\|^2}. \tag{1.81}$$
5. *If* $X_{0,0} = 0$ *and* $\|X_{0,1}\| = \|X_{1,0}\|$*, then*
$$\|X\| \le \frac{\|X_{1,1}\|}{2} + \sqrt{\frac{\|X_{1,1}\|^2}{4} + \|X_{0,1}\|^2}. \tag{1.82}$$

1.1.4.1 Properties of the pseudoinverse

Proposition 1.12. *Let $H(s)$ be a normal operator with a dependence on s such that it is differentiable. Let $P(s)$ be the spectral projector on $\{0\}$ and $Q(s) = \mathbb{1} - P(s)$. Assume $P(s)$ is also differentiable. Then*

$$(H^+)' = -H^+H'H^+ - P'H^+ - H^+P'. \tag{1.83}$$

I have deliberately been vague about the type of differentiability. By inspecting the proof one sees that various choices are possible. In particular "differentiability" may be read as "norm differentiability" or "pointwise differentiability on D".

This result seems to be new.[8]

Proof. We calculate

$$(H^+)' = \lim_{h\to 0} \frac{H^+(s+h) - H^+(s)}{h} \tag{1.86}$$

$$= \lim_{h\to 0} \frac{Q(s)H^+(s+h) - H^+(s)Q(s+h)}{h} + \frac{P(s)H^+(s+h) - H^+(s)P(s+h)}{h}. \tag{1.87}$$

We first develop the second part, using the fact that $H^+(s)P(s) = 0 = P(s+h)H^+(s+h)$:

$$\begin{aligned}\lim_{h\to 0} &\frac{P(s)H^+(s+h) - H^+(s)P(s+h)}{h} \\ &= \lim_{h\to 0} \frac{P(s)H^+(s+h) - P(s+h)H^+(s+h) - H^+(s)P(s+h) + H^+(s)P(s)}{h} \\ &= -\lim_{h\to 0} \frac{P(s+h) - P(s)}{h} H^+(s+h) - H^+(s)\frac{P(s+h) - P(s)}{h}. \end{aligned}\tag{1.88}$$

Taking the limit gives $-P'H^+ - H^+P'$. For the first part, we calculate

$$\lim_{h\to 0} \frac{Q(s)H^+(s+h) - H^+(s)Q(s+h)}{h} = \lim_{h\to 0} \frac{H^+(s)H(s)H^+(s+h) - H^+(s)H(s+h)H^+(s+h)}{h} \tag{1.89}$$

$$= \lim_{h\to 0} H^+(s)\frac{H(s) - H(s+h)}{h} H^+(s+h) \tag{1.90}$$

$$= \lim_{h\to 0} -H^+(s)\frac{H(s+h) - H(s)}{h} H^+(s+h) \tag{1.91}$$

$$= -H^+H'H^+. \tag{1.92}$$

□

Let H be a normal operator and ω_0 an isolated point of the spectrum. The spectral theorem, Theorem A.16, gives that $(\omega_0 \mathbb{1} - H)^+$ is bounded with $\left\|(\omega_0 \mathbb{1} - H)^+\right\| = \frac{1}{g}$, where g is the distance between ω_0 and the rest of the spectrum. In fact there is even a stronger result that is particularly useful if H is unbounded.

Proposition 1.13. *Let $\mathcal{H}$ be a Hilbert space, H a normal operator on $\mathcal{H}$, ω_0 an isolated point of the spectrum of H and g the distance between ω_0 and the rest of the spectrum. Then* $(\omega_0 \mathbb{1} - H)^+$

[8] It was slightly surprising to me that I was unable to find this result in the literature. The pseudoinverse (at least in the matrix setting) is well-studied. Indeed, there is a common formula for the derivative of the matrix pseudoinverse. In the current setting it can be stated as

$$(H^+)' = -H^+H'H^+ + H^+H^{+*}H^{*\prime}P + PH^{*\prime}H^{+*}H^+ \tag{1.84}$$

and seems to be originally due to [34]. (There is earlier work, e.g. [35], that gives more or less the same result, but phrased as a perturbation result rather than a derivative). There are a couple of explanations why (1.83) is less well-known than (1.84). Firstly it may be less useful in certain contexts, since it still depends on the derivative P'; secondly, when restricted to the matrix case, (1.84) can be stated more generally: it holds even if the matrices are not square and not normal.

Finally, note that (1.84) can be derived from (1.83) by substituting in the adjoint of

$$-PP'Q = PQ'Q = P(HH^+)'Q = PH'H^+Q \tag{1.85}$$

(where we have used $PH = 0$) and the corresponding formula for $-QP'P$.

is bounded as an operator from $\mathcal{H}$ to $\operatorname{dom}(H)$, when $\operatorname{dom}(H)$ is equipped with the graph norm of H. Also

$$\left\|(\omega_0 \mathbb{1} - H)^+\right\|_{\mathcal{H}\to\operatorname{dom}(H)} \leq 1 + \frac{1 + |\omega_0|}{g}. \tag{1.93}$$

Proof. Let $|\psi\rangle$ be a unit vector on $\mathcal{H}$. Then

$$H(\omega_0 \mathbb{1} - H)^+|\psi\rangle = \omega_0(\omega_0 \mathbb{1} - H)^+|\psi\rangle - (\omega_0 \mathbb{1} - H)(\omega_0 \mathbb{1} - H)^+|\psi\rangle, \tag{1.94}$$

so taking the norm gives

$$\left\|H(\omega_0 \mathbb{1} - H)^+|\psi\rangle\right\| \leq |\omega_0|\left\|(\omega_0 \mathbb{1} - H)^+\right\| + \left\|(\omega_0 \mathbb{1} - H)(\omega_0 \mathbb{1} - H)^+\right\| \tag{1.95}$$

$$\leq \frac{|\omega_0|}{g} + 1. \tag{1.96}$$

Now the graph norm can be computed

$$\left\|(\omega_0 \mathbb{1} - H)^+|\psi\rangle\right\|_H = \left\|H(\omega_0 \mathbb{1} - H)^+|\psi\rangle\right\| + \left\|(\omega_0 \mathbb{1} - H)^+|\psi\rangle\right\| \tag{1.97}$$

$$\leq 1 + \frac{|\omega_0|}{g} + \frac{1}{g}. \tag{1.98}$$

□

1.1.4.2 Bounding $\|\widetilde{X}\|$

From now on we will always assume $X \in \mathcal{B}(D, \mathcal{H})$. This is enough to ensure $\widetilde{X}$ is bounded as an operator on $\mathcal{H}$. (Compare Lemma 1.4 and Lemma 1.3 with Proposition A.40, Proposition 1.13 and Lemma 1.14).
It will also be convenient to assume that X is normal; it makes the unbounded case more tractable. For our applications this will pose no restriction. The first lemmas deal with some technical complexity on the unbounded case.

Lemma 1.14. *Let $\mathcal{H}$ be a Hilbert space, H a normal operator on $\mathcal{H}$, $b_0 \leq b_1$ and P the spectral projector associated to $\sigma(H) \cap [b_0, b_1]$. Then*

$$\|P\|_{\mathcal{H}\to\operatorname{dom}(H)} \leq \max\left\{|b_0|, |b_1|\right\} + 1. \tag{1.99}$$

Proof. Take an arbitrary unit vector $|\psi\rangle \in \mathcal{H}$. The graph norm can then be calculated as

$$\|P|\psi\rangle\|_H = \|HP|\psi\rangle\| + \|P|\psi\rangle\| \leq \max\left\{|b_0|, |b_1|\right\} + 1. \tag{1.100}$$

The bound on the norm $\|HP|\psi\rangle\|$ is due to the spectral theorem, Theorem A.16. □

Lemma 1.15. *Let $\mathcal{H}$ be a Hilbert space and X a normal operator on $\mathcal{H}$ such that $X \in \mathcal{B}(D, \mathcal{H})$. Then*

1. *$X^* \in \mathcal{B}(D, \mathcal{H})$;*
2. *QXP is a bounded operator on $\mathcal{H}$;*
3. *the closure of PXQ is a bounded operator on $\mathcal{H}$ and $\|PXQ\| = \|QX^*P\|$.*

Proof. (1) This follows from Proposition A.83.
(2) The operator QX^*P is bounded, since it is the composition of $P \in \mathcal{B}(\mathcal{H}, D)$ and $X^*Q \in \mathcal{B}(D, \mathcal{H})$. See Lemma 1.14 and point (1).
Next note that $PXQ \subseteq (QX^*P)^*$, from Proposition A.71. The latter is bounded due to Proposition A.78, which also gives the boundedness of $\overline{PXQ}$ and the equality of norms. □

Proposition 1.16. *Let $\mathcal{H}$ be a Hilbert space, H a Hamiltonian on $\mathcal{H}$ and P the spectral projector on a set of m isolated eigenvalues $\{\omega_0, \dots, \omega_{m-1}\}$. Let X be a normal operator on $\mathcal{H}$ such that $X \in \mathcal{B}(D, \mathcal{H})$ and $\widetilde{X}$ the solution of the operator equation from Corollary 1.6. Then*

$$\|\widetilde{X}\| \leq \sqrt{m}\frac{\max\{\|PXQ\|, \|QXP\|\}}{g}. \tag{1.101}$$

Note that the norms remain bounded, even if X is unbounded. See Lemma 1.15. This bound is independent of the degeneracy of any of the eigenvalues, but it does depend on the number of distinct eigenvalues.

Proof. We have $\|\widetilde{X}\|^2 = \|\widetilde{X}^*\widetilde{X}\|$ and

$$\widetilde{X}^*\widetilde{X} = \sum_{k=0}^{m-1}(\omega_k \mathbb{1} - H)^+QX^*P_kXQ(\omega_k \mathbb{1} - H)^+ + P_kX^*Q(\omega_k \mathbb{1} - H)^{+2}QXP_k. \tag{1.102}$$

Using Corollary 1.11, we see that it is enough to bound both terms separately. The spectral theorem, Theorem A.16, gives that $\|(\omega_k \mathbb{1} - H)^+Q\| \leq \frac{1}{g}$, so

$$\left\|\sum_{k=0}^{m-1}(\omega_k \mathbb{1} - H)^+QX^*P_kXQ(\omega_k \mathbb{1} - H)^+\right\| \leq \sum_{k=0}^{m-1}\frac{\|PXQ\|^2}{g^2} = m\frac{\|PXQ\|^2}{g^2}. \tag{1.103}$$

Here $\|QX^*P_k\|$ has been bounded by $\|PXQ\|$. This is justified by Proposition A.71 and Proposition A.78.
Observing a similar bound for the other term and taking the square root gives the result. □

Corollary 1.17. *Let $\mathcal{H}$ be a Hilbert space, H_s a time-dependent Hamiltonian on $\mathcal{H}$ and P the spectral projector on a set of m isolated eigenvalues $\{\omega_0, \dots, \omega_{m-1}\}$. Then*

$$\|P'\| = \|\widetilde{H'}\| \leq \sqrt{m}\frac{\|PH'Q\|}{g}. \tag{1.104}$$

Proof. This follows from the Riesz form of the projector, (1.4) and the identity (1.6). Also $\|PH'Q\| = \|QH'P\|$ from Lemma 1.15. □

Proposition 1.18. *Let $\mathcal{H}$ be a Hilbert space, H a Hamiltonian on $\mathcal{H}$ and P the spectral projector on a set of m isolated eigenvalues $\{\omega_0, \dots, \omega_{m-1}\} \subseteq [b_0, b_1]$. Let X be a normal operator on $\mathcal{H}$ such that $X \in \mathcal{B}(D, \mathcal{H})$ and $\widetilde{X}$ the solution of the operator equation from Corollary 1.6. Then*

1. $\|Q\widetilde{X}P\|_{\mathcal{H}\to D} \leq m\Big(1 + \dfrac{1 + \max\{|b_0|, |b_1|\}}{g}\Big)\|QXP\|$;
2. $\|P\widetilde{X}Q\|_{\mathcal{H}\to D} \leq m\dfrac{1 + \max\{|b_0|, |b_1|\}}{g}\|PXQ\|$;

3. $\|\widetilde{X}\|_{\mathcal{H}\to D} \le m\Big(1 + \dfrac{1+\max\{|b_0|,|b_1|\}}{g}\Big)\|QXP\| + m\dfrac{1+\max\{|b_0|,|b_1|\}}{g}\|PXQ\|.$

Proof. (1) The triangle inequality and Proposition 1.13 give

$$\|Q\widetilde{X}P\|_{\mathcal{H}\to D} \le \sum_{k=0}^{m-1} \|(\omega_k \mathbb{1} - H)^+ Q\|_{\mathcal{H}\to D}\|QXP\| \tag{1.105}$$

$$\le \sum_{k=0}^{m-1} \Big(1 + \frac{1+|\omega_k|}{g}\Big)\|QXP\| \tag{1.106}$$

$$\le m\Big(1 + \frac{1+\max\{|b_0|,|b_1|\}}{g}\Big)\|QXP\|. \tag{1.107}$$

(2) The triangle inequality and Lemma 1.14 give

$$\|P\widetilde{X}Q\|_{\mathcal{H}\to D} \le \sum_{k=0}^{m-1} \|P\|_{\mathcal{H}\to D}\|PXQ\|\|(\omega_k \mathbb{1} - H)^+ Q\| \tag{1.108}$$

$$\le \frac{1+|\omega_k|}{g}\|PXQ\| \tag{1.109}$$

$$\le m\frac{1+\max\{|b_0|,|b_1|\}}{g}\|PXQ\|. \tag{1.110}$$

(3) This follows because $\widetilde{X}$ is off-diagonal. □

It is also possible to give a bound on $\|\widetilde{X}\|$ taking into account the graph norm. In this case no assumption of normality is necessary. The result is stated for the case where P projects onto the eigenspace of a single eigenvalue, for simplicity. (Also because it is not clear it is particularly useful).

Lemma 1.19. *Let $\mathcal{H}$ be a Hilbert space, H a Hamiltonian on $\mathcal{H}$ and P the spectral projector on the eigenvalue ω_0. Let $X \in \mathcal{B}(D,\mathcal{H})$ be a relatively bounded operator and $\widetilde{X}$ the solution of the operator equation from Lemma 1.3. Then*

$$\|\widetilde{X}\| \le \max\Big\{\Big(1 + \frac{1+|\omega_0|}{g}\Big)\|PXQ\|_{D\to\mathcal{H}}, \frac{1+|\omega_0|}{g}\|QXP\|_{D\to\mathcal{H}}\Big\}. \tag{1.111}$$

Here D has been equipped with the graph norm of H. Later, when s-dependence is reintroduced, this will mean that the norms in the bound will be different for different s. For this reason, D is sometimes assumed to be equipped with the graph norm of H_0 (e.g. in section B.3). With a bit of luck it will be clear which norm D is equipped with, whenever this is relevant.[9]

Proof. Since $\widetilde{X}$ is off-diagonal, it is enough to bound each off-diagonal part separately. First,

$$\|P\widetilde{X}Q\| = \|PXQ(\omega_0 \mathbb{1} - H)^+\| \le \|PXQ\|_{D\to\mathcal{H}}\|(\omega_0 \mathbb{1} - H)^+\|_{\mathcal{H}\to D} \tag{1.112}$$

$$\le \Big(1 + \frac{1+|\omega_0|}{g}\Big)\|PXQ\|_{D\to\mathcal{H}}, \tag{1.113}$$

[9]The exact norm on D is not always relevant. It is relevant when stating quantitative bounds, but since all norms under consideration are equivalent, it is irrelevant when dealing with questions of continuity.

from Proposition 1.13. Next

$$\|Q\widetilde{X}P\| = \|(\omega_0 \mathbb{1} - H)^+ XP\| \leq \|(\omega_0 \mathbb{1} - H)^+\| \|QXP\|_{D\to\mathcal{H}} \|P\|_{\mathcal{H}\to D} \tag{1.114}$$

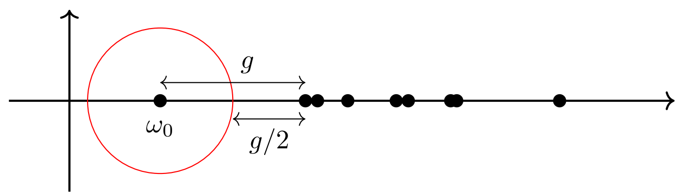
$$\leq \Big(\frac{1+|\omega_0|}{g}\Big) \|PXQ\|_{D\to\mathcal{H}}, \tag{1.115}$$

from Lemma 1.14. The result follows from Corollary 1.11. □

A couple of results have been presented that bound $\|\widetilde{X}\|$ when P is the spectral projection on a finite set of eigenvalues. There is a different general strategy that is applicable in more general situations: if $\widetilde{X}$ is the solution from Lemma 1.4, then we can bound

$$\|\widetilde{X}\| \leq \frac{1}{2\pi} \oint_\Gamma \|R_H(z)\| \|X\| \|R_H(z)\| \,\mathrm{d}z. \tag{1.116}$$

In the remainder of this section, we will first recover the results of Proposition 1.16 (in the special case of one eigenvalue) and Lemma 1.19 using this technique. Then this technique will be used to obtain a bound on $\|\widetilde{X}\|$ that is independent of the contents of the spectral region between b_0 and b_1 and will only depend on the distance $b_1 - b_0$, at the expense of a worse dependence on the gap.
Since $\|R_H(z)\|^{-1}$ is equal to the distance between z and the spectrum, the obvious path Γ is a circle around ω_0 with radius $g/2$.



The circumference of the path Γ is πg; the norm $\|R_H(z)\|$ is uniformly bounded by $2/g$. Filling this in (and assuming for a moment that X is bounded) gives $\|\widetilde{X}\| \leq 2\frac{\|X\|}{g}$. Compared to Proposition 1.16, we notice some inefficiencies: it depends on the full operator X, not just the off-diagonal components and there is an extra factor of 2.
Since $\widetilde{X}$ is off-diagonal (as was proved in Lemma 1.4), we can bound the off-diagonal components and use Corollary 1.11. First consider

$$\|P\widetilde{X}Q\| \leq \frac{1}{2\pi} \oint_\Gamma \|PR_H(z)\| \|PXQ\| \|QR_H(z)\| \,\mathrm{d}z. \tag{1.117}$$

Now $\|PR_H(z)\| = |\omega_0 - z|^{-1}$ and $\|QR_H(z)\|^{-1}$ is the distance between z and the spectrum excluding ω_0. In order to remove the factor of 2, we can now shrink the radius of Γ; let it be called ϵ. So the circumference of Γ is $2\pi\epsilon$, $\|PR_H(z)\| = \epsilon^{-1}$ and $\|QR_H(z)\| = (g-\epsilon)^{-1}$. Filling everything in gives

$$\|P\widetilde{X}Q\| \leq \frac{2\pi\epsilon}{2\pi} \frac{1}{\epsilon(g-\epsilon)} \|PXQ\| \to \frac{\|PXQ\|}{g}. \tag{1.118}$$

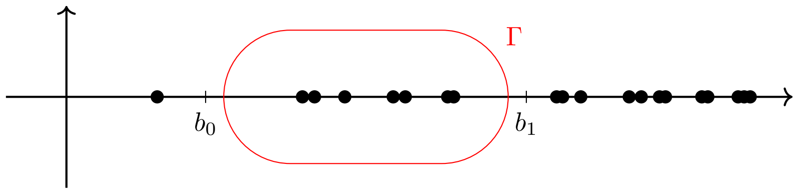
It was only possible to take this limit since we are dealing with the off-diagonal component. Now we can use Corollary 1.11 to get the same result as in Proposition 1.16.
Finally, in order to recover the result of Lemma 1.19, replace $\|PXQ\|$ by $\|PXQ\|_{D\to\mathcal{H}}$ and the right-hand resolvent bound by $\|QR_H(z)\|_{\mathcal{H}\to D}$. The latter can be bounded using Proposition A.40. Then

$$\|P\widetilde{X}Q\| \leq \frac{2\pi\epsilon}{2\pi}\frac{1}{\epsilon}\Big(1 + \frac{1+|\omega_0|+\epsilon}{g-\epsilon}\Big)\|PXQ\|_{D\to\mathcal{H}} \to \Big(1+\frac{1+|\omega_0|}{g}\Big)\|PXQ\|_{D\to\mathcal{H}} \tag{1.119}$$

and

$$\|Q\widetilde{X}P\| \leq \frac{2\pi\epsilon}{2\pi}\Big(1 + \frac{1+|\omega_0|+\epsilon}{\epsilon}\Big)\frac{1}{g-\epsilon}\|QXP\|_{D\to\mathcal{H}} \to \frac{1+|\omega_0|}{g}\|QXP\|_{D\to\mathcal{H}}. \tag{1.120}$$

We conclude with Corollary 1.11.
Finally, considering a path Γ of the following form:



immediately leads to the following result.

Lemma 1.20. *Let $\mathcal{H}$ be a Hilbert space, H a Hamiltonian on $\mathcal{H}$ and P the spectral projector on the part of the spectrum in $[b_0, b_1]$. Let X be a normal operator on $\mathcal{H}$ such that $X \in \mathcal{B}(D,\mathcal{H})$ and $\widetilde{X}$ the solution of the operator equation from Lemma 1.4. Then*

$$\|\widetilde{X}\| \leq \Big(\frac{2}{g} + \frac{4(b_1-b_0)}{\pi g^2}\Big)\max\big\{\|PXQ\|, \|QXP\|\big\}. \tag{1.121}$$

This result can almost certainly be improved.

1.1.4.3 Bounding $\|\widetilde{X}'\|$

In this section X_s is assumed to be an s-dependent normal operator that is defined and bounded on D. It is also assumed that $s \mapsto X_s|\psi\rangle$ is is continuously differentiable for all $|\psi\rangle \in D$. These assumptions are summarised by saying X_s is a time-dependent normal operator.

Lemma 1.21. *Let $\mathcal{H}$ be a Hilbert space, H a self-adjoint operator and Γ a closed simple curve in the complex plane that is disjoint from the spectrum $\sigma(H)$. Let P the spectral projector on the part of the spectrum that lies inside Γ and $X, Y \in \mathcal{B}(D,\mathcal{H})$. Then*

$$\frac{1}{2\pi i}\oint_\Gamma R_H(z)XR_H(z)YR_H(z)\,\mathrm{d}z = (Q-P)\big(\widetilde{X}\widetilde{Y} + \widetilde{X\widetilde{Y}} - \widetilde{\widetilde{X}Y}\big). \tag{1.122}$$

As before, the $\widetilde{\ }$ refers to the off-diagonal solution, Lemma 1.4.

The proof in [17] makes essential use of the assumption that P projects onto a finite set of eigenvalues. This new proof removes this assumption. Note also that there is a sign difference compared to [17], this is due to a sign difference in the definition of the resolvent.

Proof. For ease of notation, set $G(X,Y) \coloneqq \frac{1}{2\pi i}\oint_\Gamma R_H(z)XR_H(z)YR_H(z)\,\mathrm{d}z$. Now note that

$$\begin{aligned}
[H, G(X,Y)] &= \frac{1}{2\pi i}\oint_\Gamma \big[H, R_H(z)XR_H(z)YR_H(z)\big]\,\mathrm{d}z &(1.123)\\
&= -\frac{1}{2\pi i}\oint_\Gamma \big[z\,\mathbb{1} - H, R_H(z)XR_H(z)YR_H(z)\big]\,\mathrm{d}z &(1.124)\\
&= \frac{1}{2\pi i}\oint_\Gamma \big(R_H(z)XR_H(z)Y - XR_H(z)YR_H(z)\big)\,\mathrm{d}z &(1.125)\\
&= \widetilde{X}Y - X\widetilde{Y}. &(1.126)
\end{aligned}$$

Then

$$[H, PG(X,Y)Q] = P\big(\widetilde{X}Y - X\widetilde{Y}\big)Q = \big[P, P\big(\widetilde{X}Y - X\widetilde{Y}\big)Q\big], \tag{1.127}$$

so Proposition 1.7 gives

$$PG(X,Y)Q = P\big(\widetilde{\widetilde{X}Y} - \widetilde{X\widetilde{Y}}\big)Q. \tag{1.128}$$

Similarly, $[H, QG(X,Y)P] = -\big[P, Q\big(\widetilde{X}Y - X\widetilde{Y}\big)P\big]$, so

$$QG(X,Y)P = -Q\big(\widetilde{\widetilde{X}Y} - \widetilde{X\widetilde{Y}}\big)P. \tag{1.129}$$

With this we have derived the off-diagonal components of $G(X,Y)$. Now consider the diagonal components, starting with $QG(X,Y)Q$. The claim is that $QG(X,Y)Q = Q\widetilde{X}\widetilde{Y}Q$. This is verified by direct calculation. In the following, let Γ_1 be a curve that is slightly larger than Γ, but encircles the same spectral region, like in the proof of Lemma 1.4.

$$\begin{aligned}
Q\widetilde{X}\widetilde{Y}Q &= \frac{1}{(2\pi i)^2}\Big(\oint_\Gamma QR_H(z)XR_H(z)\,\mathrm{d}z\Big)\Big(\oint_{\Gamma_1} R_H(w)YQR_H(w)\,\mathrm{d}w\Big) && (1.130)\\
&= \frac{1}{(2\pi i)^2}\oint_{\Gamma_1}\oint_\Gamma QR_H(z)XR_H(z)R_H(w)YQR_H(w)\,\mathrm{d}z\,\mathrm{d}w && (1.131)\\
&= \frac{1}{(2\pi i)^2}\oint_{\Gamma_1}\oint_\Gamma QR_H(z)X\Big(\frac{R_H(z) - \cancel{R_H(w)}}{w-z}\Big)YQR_H(w)\,\mathrm{d}z\,\mathrm{d}w && (1.132)\\
&= \frac{1}{(2\pi i)^2}\oint_\Gamma QR_H(z)XR_H(z)YQ\Big(\oint_{\Gamma_1}\frac{QR_H(w)}{w-z}\,\mathrm{d}w\Big)\,\mathrm{d}z && (1.133)\\
&= \frac{1}{2\pi i}\oint_\Gamma QR_H(z)XR_H(z)YQR_H(z)\,\mathrm{d}z = QG(X,Y)Q. && (1.134)
\end{aligned}$$

The cancellation in (1.132) still needs to be justified. This is due to the fact that

$$\oint_\Gamma QR_H(z)X\frac{R_H(w)}{w-z}\,\mathrm{d}z = 0, \tag{1.135}$$

since the function in the integral is analytic (as a function of z) inside Γ: w lies on Γ_1, which is outside Γ and $QR_H(z)$ is only not analytic on the spectrum of QH, which also lies outside Γ. Also observe that $QR_H(w)$ is analytic inside Γ_1, so $\frac{1}{2\pi i}\oint_{\Gamma_1}\frac{QR_H(w)}{w-z}\,\mathrm{d}w = QR_H(z)$ follows from Cauchy's integral formula.

Finally $PG(X,Y)P$ is calculated in a similar fashion.

$$\begin{aligned}
P\widetilde{X}\widetilde{Y}P &= \frac{1}{(2\pi i)^2}\Big(\oint_\Gamma PR_H(z)XR_H(z)\,\mathrm{d}z\Big)\Big(\oint_{\Gamma_1} R_H(w)YPR_H(w)\,\mathrm{d}w\Big) && (1.136)\\
&= \frac{1}{(2\pi i)^2}\oint_{\Gamma_1}\oint_\Gamma PR_H(z)XR_H(z)R_H(w)YPR_H(w)\,\mathrm{d}z\,\mathrm{d}w && (1.137)\\
&= \frac{1}{(2\pi i)^2}\oint_{\Gamma_1}\oint_\Gamma PR_H(z)X\Big(\frac{\cancel{R_H(z)} - R_H(w)}{w-z}\Big)YPR_H(w)\,\mathrm{d}z\,\mathrm{d}w && (1.138)\\
&= -\frac{1}{(2\pi i)^2}\oint_{\Gamma_1}\Big(\oint_\Gamma\frac{PR_H(z)}{w-z}\,\mathrm{d}z\Big)XR_H(w)YQPR_H(w)\,\mathrm{d}w && (1.139)\\
&= -\frac{1}{2\pi i}\oint_{\Gamma_1} PR_H(w)XR_H(w)YPR_H(w)\,\mathrm{d}z = -PG(X,Y)P. && (1.140)
\end{aligned}$$

The cancellation in (1.138) is due to

$$\frac{1}{2\pi i}\oint_{\Gamma_1}\frac{PR_H(w)}{w-z}\,\mathrm{d}w = PQR_H(z) = 0, \tag{1.141}$$

from (1.24). Finally, we use the fact that all expressions under $\widetilde{\ }$ are off-diagonal to collect terms and obtain the final result. □

Corollary 1.22. *Let $\mathcal{H}$ be a Hilbert space, H_s a time-dependent Hamiltonian on $\mathcal{H}$ and P the spectral projector on $\sigma(H_s)\cap[b_0(s),b_1(s)]$. Let X_s be a time-dependent normal operator on $\mathcal{H}$ and $\widetilde{X}$ the solution of the operator equation from Lemma 1.4. Then*

$$(\widetilde{X})' = \widetilde{X'} + (Q-P)\big(P'\widetilde{X} + \widetilde{X}P' + \widetilde{[H',\widetilde{X}]} - \widetilde{[P',X]}\big). \tag{1.142}$$

Proof. Using (1.6), we have

$$(\widetilde{X})' = \widetilde{X'} + G(H',X) + G(X,H'). \tag{1.143}$$

The result follows with the observation that $\widetilde{H'} = P'$. □

Lemma 1.23. *Let X be a bounded operator that is twice continuously differentiable in s. Then*

1. $\|(\widetilde{X})'\| \le \frac{\sqrt{m}}{g}\|X'\| + 6m\frac{\|H'\|}{g^2}\|X\|$;
2. $\|\widetilde{X}''\| \le 64m\sqrt{m}\frac{\|H'\|^2}{g^3}\|X\| + 6m\frac{\|H''\|}{g^2}\|X\| + 12m\frac{\|H'\|}{g^2}\|X'\| + \frac{\sqrt{m}}{g}\|X''\|$.

Proof. (1) Straightforward from Corollary 1.22.
(2) We have

$$\begin{aligned}(\widetilde{X})'' = \widetilde{X'}' - P'\Big(P'\widetilde{X} + \widetilde{X}P' + \widetilde{[H',\widetilde{X}]} - \widetilde{[P',X]}\Big) \\ + (Q-P)\Big(P'\widetilde{X} + \widetilde{X}P' + \widetilde{[H',\widetilde{X}]} - \widetilde{[P',X]}\Big)'\end{aligned} \tag{1.144}$$

$$\begin{aligned}= \widetilde{X'}' - P'\Big(P'\widetilde{X} + \widetilde{X}P' + \widetilde{[H',\widetilde{X}]} - \widetilde{[P',X]}\Big) \\ + (Q-P)\Big(P''\widetilde{X} + \widetilde{X}P'' + P'\widetilde{X}' + \widetilde{X}'P' + \widetilde{[H',\widetilde{X}]}' - \widetilde{[P',X]}'\Big)\end{aligned} \tag{1.145}$$

Using (1), the norm of the first term of (1.145) can be bounded by

$$\|\widetilde{X'}'\| \le \frac{\sqrt{m}}{g}\|X''\| + 6m\frac{\|H'\|}{g^2}\|X'\|. \tag{1.146}$$

The norm of the second term can be bounded by

$$\Big\|P'\Big(P'\widetilde{X} + \widetilde{X}P' + \widetilde{[H',\widetilde{X}]} - \widetilde{[P',X]}\Big)\Big\| \le 6m\sqrt{m}\frac{\|H'\|^2}{g^3}\|X\|. \tag{1.147}$$

Now (1) can be used to bound

$$\Big\|\widetilde{[H',\widetilde{X}]}'\Big\| \le \frac{\sqrt{m}}{g}\big\|[H',\widetilde{X}]'\big\| + 6m\frac{\|H'\|}{g^2}\big\|[H',\widetilde{X}]\big\| \tag{1.148}$$

$$\le 24m\sqrt{m}\frac{\|H'\|^2}{g^3}\|X\| + 2m\frac{\|H''\|}{g^2}\|X\| + 2m\frac{\|H'\|}{g^2}\|X'\|. \tag{1.149}$$

Using

$$\|P''\| \le \frac{\sqrt{m}}{g}\|H''\| + 4m\frac{\|H'\|^2}{g^2}, \tag{1.150}$$

we also have

$$\left\|\widetilde{[P', X]}'\right\| \le 2\frac{\sqrt{m}}{g}\big(\|P''\|\|X\| + \|P'\|\|X'\|\big) + 6m\frac{\|H'\|}{g^2}\|P'\|\|X\| \tag{1.151}$$

$$\le 14m\sqrt{m}\frac{\|H'\|^2}{g^3}\|X\| + 2m\frac{\|H''\|}{g^2}\|X\| + 2m\frac{\|H'\|}{g^2}\|X'\|. \tag{1.152}$$

Also

$$2\|P''\|\|\widetilde{X}\| \le 8m\sqrt{m}\frac{\|H'\|^2}{g^3}\|X\| + 2m\frac{\|H''\|}{g^2}\|X\| \tag{1.153}$$

and

$$2\|P'\|\|\widetilde{X}'\| \le 12m\sqrt{m}\frac{\|H'\|^2}{g^3}\|X\| + 2m\frac{\|H'\|}{g^2}\|X'\|. \tag{1.154}$$

Finally, the third term of (1.145) can be bounded by combining the bounds (1.149), (1.152), (1.153) and (1.154):

$$58m\sqrt{m}\frac{\|H'\|^2}{g^3}\|X\| + 6m\frac{\|H''\|}{g^2}\|X\| + 6m\frac{\|H'\|}{g^2}\|X'\|. \tag{1.155}$$

Putting all these bounds together gives the result. □

1.1.5 Adiabatic theorems

We are now in a position to state some adiabatic theorems. For us the purpose of an adiabatic theorem will be to bound the difference between the time evolution and an ideal evolution. An evolution is ideal if it stays in the eigenspace. The degree of ideality can be expressed with the fidelity:

$$F \coloneqq \langle\psi(1)|P(1)|\psi(1)\rangle = \langle\psi|U(1)^* P(1)U(1)|\psi\rangle. \tag{1.156}$$

The aim will be to bound the infidelity $1 - F$.

Lemma 1.24. *Let H_s be a time-dependent Hamiltonian. Let $U(s)$ be generated by $-iTH_s$ and $U_A(s)$ by $-iTH_s + [P', P]$. Suppose $T(s)^{-1}$ is absolutely continuous. Set $\Omega(s) \coloneqq U(s)^* U_A(s)$. For all X, let $\widetilde{X}$ be a solution of the operator equation (1.8). Let $|\psi\rangle$ be a unit vector such that $P(0)|\psi\rangle = |\psi\rangle$. Then $\sqrt{1-F} \le \|P(0)\Omega(1)Q(0)\|$.*

Note that $1 - F \le \sqrt{1-F}$, so $\|P(0)\Omega(1)Q(0)\|$ also bounds the infidelity.

Proof. First, calculate

$$1 - F = \langle\psi|\psi\rangle - \langle\psi|U(1)^* P(1)U(1)|\psi\rangle \tag{1.157}$$

$$= \langle\psi|U(1)^* Q(1)U(1)|\psi\rangle \tag{1.158}$$

$$= \big\|Q(1)U(1)|\psi\rangle\big\|^2 \tag{1.159}$$

$$= \big\|Q(1)U(1)P(0)|\psi\rangle\big\|^2 \le \big\|Q(1)U(1)P(0)\big\|^2. \tag{1.160}$$

Next the intertwining property of Proposition 1.8 can be used to calculate

$$1 - F \leq \left\|Q(1)U(1)P(0)\right\|^2 = \left\|Q(1)U_A(1)\Omega(1)^*P(0)\right\|^2 \tag{1.161}$$
$$= \left\|U_A(1)Q(0)\Omega(1)^*P(0)\right\|^2 \tag{1.162}$$
$$= \left\|Q(0)\Omega(1)^*P(0)\right\|^2 = \left\|P(0)\Omega(1)Q(0)\right\|^2. \tag{1.163}$$

Taking the square root yields the result. □

1.1.5.1 Adiabatic theorems at first order

Recall the result of Proposition 1.9:

$$\Omega(1) = \mathbb{1} + \Big[\frac{i}{T}U^*\widetilde{P'}U\Omega\Big]_0^1 - \int_0^1 \frac{i}{T}U^*\big(\widetilde{P'}[P',P] + \widetilde{P'}'\big)U\Omega \, \mathrm{d}s + \int_0^1 \frac{iT'}{T^2}U^*\widetilde{P'}U\Omega \, \mathrm{d}s. \tag{1.164}$$

Our next step is to bound $\widetilde{P'}[P',P] + \widetilde{P'}'$.

Lemma 1.25. *Let $\mathcal{H}$ be a Hilbert space, H_s a time-dependent Hamiltonian on $\mathcal{H}$ and P the spectral projector on $\sigma(H_s)\cap[b_0(s),b_1(s)]$. Let X_s be a time-dependent normal operator on $\mathcal{H}$ and $\widetilde{X}$ the solution of the operator equation from Lemma 1.4. Then*

1. $\widetilde{P'}[P',P] + \widetilde{P'}' = \widetilde{P''} + (Q-P)\widetilde{[H',\widetilde{P'}]} + QP'\widetilde{P'}Q - PP'\widetilde{P'}P$;
2. $P'' = \widetilde{H''} + (Q-P)\big(2(P')^2 + \widetilde{[H',P']}\big)$;
3. $\widetilde{P''} = \widetilde{\widetilde{H''}} + (Q-P)\widetilde{\widetilde{[H',P']}}$.

Proof. (1) Corollary 1.22 gives the expansion

$$\widetilde{P'}' = \widetilde{P''} + (Q-P)\big(P'\widetilde{P'} + \widetilde{P'}P' + \widetilde{[H',\widetilde{P'}]}\big) \tag{1.165}$$
$$= \widetilde{P''} + (Q-P)\widetilde{[H',\widetilde{P'}]} + Q\big(P'\widetilde{P'} + \widetilde{P'}P'\big)Q - P\big(P'\widetilde{P'} + \widetilde{P'}P'\big)P, \tag{1.166}$$

which can be added to

$$\widetilde{P'}[P',P] = P\widetilde{P'}P'P - Q\widetilde{P'}P'Q. \tag{1.167}$$

to get the result.
(2) Since $P'' = \widetilde{H'}'$, the result follows from Corollary 1.22.
(3) This holds because $\widetilde{\ }$ kills the diagonal terms, is linear and commutes with multiplication by P and Q. □

Theorem 1.26. *Let H_s be a twice continuously differentiable time-dependent Hamiltonian. Let $U(s)$ be generated by $-iTH_s$, with T constant. Suppose H' is bounded and $\sigma(H_s)\cap[b_0(s),b_1(s)]$ consists of at most m points. Then*

$$\sqrt{1-F} \leq \frac{1}{T}\frac{m\|P(0)H'(0)Q(0)\|}{g(0)^2} + \frac{1}{T}\frac{m\|P(1)H'(1)Q(1)\|}{g(1)^2} + \frac{1}{T}\int_0^1 \Big(\frac{m\|PH''Q\|}{g^2} + 3m\sqrt{m}\frac{\|PH'Q\|^2}{g^3} + 2m\sqrt{m}\frac{\|PH'Q\|\|H'\|}{g^3}\Big)\,\mathrm{d}s. \tag{1.168}$$

The boundedness assumption on H' is only necessary to keep the factor $\|H'\|$ bounded in the last term. Later theorems will relax this assumption.

Proof. The bound is obtained by combining Lemma 1.24, Proposition 1.9 and Lemma 1.25. The norm bounds follow from Proposition 1.16 and Corollary 1.17. Corollary 1.11 gives $\|QP'\widetilde{P'}Q - PP'\widetilde{P'}P\| \leq \|P'\widetilde{P'}\|$.

The last term comes from the $[\widetilde{\widetilde{H', P'}}]$ in $\widetilde{P''}$. Bounding with Proposition 1.16 requires bounding a factor of the form $\|PP'H'Q\|$, which can naturally be bounded by $\|PH'Q\|\|H'\|$. □

Theorem 1.26 can be compared to theorem 3 of [17], which gives the bound

$$\sqrt{1-F} \;\leq\; \frac{1}{T}\frac{m\|H'(0)\|}{g(0)^2} \;+\; \frac{1}{T}\frac{m\|H'(1)\|}{g(1)^2} \;+\; \frac{1}{T}\int_0^1 \Big(\frac{m\|H''\|}{g^2} \;+\; 7m\sqrt{m}\frac{\|H'\|^2}{g^3}\Big)\,\mathrm{d}s. \quad (1.169)$$

There are two small improvements in Theorem 1.26: one the one hand the numerical constant is slightly better and on the other hand the bound mostly only depends on off-diagonal components, which, depending on the application, may be significantly smaller.
Restricting further to the case where P projects onto a single eigenvalue (i.e. $m = 1$) allows an even smaller numerical constant to be obtained.

Theorem 1.27. *Let H_s be a twice continuously differentiable time-dependent Hamiltonian. Let $U(s)$ be generated by $-iTH_s$, with T constant. Suppose H' is bounded and $\sigma(H_s) \cap [b_0(s), b_1(s)] = \{\omega_0(s)\}$. Then*

$$\sqrt{1-F} \leq \frac{1}{T}\frac{\|P(0)H'(0)Q(0)\|}{g(0)^2} + \frac{1}{T}\frac{\|P(1)H'(1)Q(1)\|}{g(1)^2} + \frac{1}{T}\int_0^1 \Big(\frac{\|PH''Q\|}{g^2} + \big(2\sqrt{2}+1\big)\frac{\|H'\|^2}{g^3}\Big)\,\mathrm{d}s. \quad (1.170)$$

The numerical constant has been reduced from 5 to less than 3.83, which is an improvement over the existing results in the literature. For simplicity, this result has not been optimised in the sense that some fraction of $\|H'\|$ may be replaced with $\|PH'Q\|$. The reader will hopefully not find it complicated to develop such a bound, if desired.

Proof. Set $R \coloneqq (\omega_0 \mathbb{1} - H)^+$. We have $\omega_0 P = PH$. Taking the derivative and multiplying by Q gives $\omega_0 P'Q = P'HQ + PH'Q$. Then $P'Q(\omega_0\mathbb{1} - H) = PH'Q$ and multiplying on the right by R gives $P'Q = PH'R$. Lemma 1.3 gives

$$\begin{aligned} P\big([H', \widetilde{P'}] + [\widetilde{H', P'}]\big)Q &= PH'P'R - P'RH'Q + PH'P'R - PP'H'R && (1.171)\\ &= 2PH'P'R - P'RH'Q - PP'H'R && (1.172)\\ &= 2PH'PH'R^2 - PH'R^2H'Q - PH'RH'R && (1.173)\\ &= PH'\big(2PH'R^2 - R^2H'Q - RH'R\big), && (1.174)\end{aligned}$$

where $P'Q = PH'R$ has been used to transform all P's into H's. Now Corollary 1.11 gives

$$\begin{aligned} \|2PH'R^2 - R^2H'Q - RH'R\| &\leq \sqrt{4\|PH'R^2\|^2 + \big(\|R^2H'Q\| + \|RH'R\|\big)^2} && (1.175)\\ &\leq 2\sqrt{2}\frac{\|H'\|}{g^2}. && (1.176)\end{aligned}$$

The rest of the bound can be completed as before. □

The adiabatic theorems in this section so far have only really been applicable to the bounded case, due to the appearance of $\|H'\|$ in the bound. We now state a truly unbounded theorem.

Theorem 1.28. *Let H_s be a twice continuously differentiable time-dependent Hamiltonian. Let $U(s)$ be generated by $-iTH_s$, with T constant. Suppose $\sigma(H_s) \cap [b_0(s), b_1(s)]$ consists of at most m points. Then*

$$\sqrt{1-F} \leq \frac{1}{T}\frac{m\|P(0)H'(0)Q(0)\|}{g(0)^2} + \frac{1}{T}\frac{m\|P(1)H'(1)Q(1)\|}{g(1)^2}$$
$$+\frac{1}{T}\int_0^1 \left(\frac{m\|PH''Q\|}{g^2} + 3m\sqrt{m}\frac{\|PH'Q\|^2}{g^3} + 4m^2\frac{\|PH'Q\|\|H'\|_{D\to\mathcal{H}}}{g^3}\Big(1+g+\max\{|b_0|,|b_1|\}\Big)\right) \mathrm{d}s. \tag{1.177}$$

Under Assumption 1 and Assumption 2, this bound is guaranteed to be finite, even for unbounded H.

Proof. The proof is very similar to that of Theorem 1.26, except the various permutation of $\|PP'H'Q\|$ will no longer be bounded by $\|PP'Q\|\|H'\|$, since $\|H'\|$ is potentially unbounded. Using Proposition 1.18, the problematic term can be bounded by

$$\begin{aligned}
\left\|\widetilde{\widetilde{[H', P']}}\right\| &\leq \frac{m}{g^2}\|Q[H', P']P\| && (1.178)\\
&\leq \frac{m}{g^2}\big(\|QH'P'P\| + \|QP'H'P\|\big) && (1.179)\\
&\leq 2m\frac{\|H'\|_{D\to\mathcal{H}}}{g^2}\|P'\|_{\mathcal{H}\to D} && (1.180)\\
&\leq 4m^2\frac{\|PH'Q\|\|H'\|_{D\to\mathcal{H}}}{g^3}\Big(1+g+\max\{|b_0|,|b_1|\}\Big). && (1.181)
\end{aligned}$$

□

To my knowledge Theorem 1.28 is the first quantitative adiabatic theorem for unbounded operators. I say quantitative because the fact that $\sqrt{1-F} = O_1(T^{-1})$ has been known for some time, at least since [28]. The closest result I am aware of is [22], but they do not claim to have established an adiabatic theorem for unbounded operators. Rather, they start with an unbounded Hamiltonian, project onto a finite-dimensional space with an energy cutoff and then argue that their bound is independent of the cutoff, in some cases.

So far all adiabatic theorems have assumed constant T. Using the same techniques, it is straightforward to derive theorems without this assumption. It may seem like the resulting bounds are worse, since they contain an extra term, but with the freedom to choose a variable T the other terms can be made significantly smaller. This variable T is known as a schedule and the fact that an adapted schedule can significantly improve performance was first reported in [36] and [37].

Theorem 1.29. *Let H_s be a twice continuously differentiable time-dependent Hamiltonian. Let $U(s)$ be generated by $-iT(s)H_s$, with $T(s)^{-1}$ absolutely continuous. Suppose H' is bounded and $\sigma(H_s) \cap [b_0(s), b_1(s)]$ consists of at most m points. Then*

$$\sqrt{1-F} \leq \frac{1}{T(0)}\frac{m\|P(0)H'(0)Q(0)\|}{g(0)^2} + \frac{1}{T(1)}\frac{m\|P(1)H'(1)Q(1)\|}{g(1)^2} + \int_0^1 \frac{|T'|}{T^2}m\frac{\|PH'Q\|}{g^2}\,\mathrm{d}s$$
$$+\int_0^1 \frac{1}{T}\Big(\frac{m\|PH''Q\|}{g^2} + 3m\sqrt{m}\frac{\|PH'Q\|^2}{g^3} + 2m\sqrt{m}\frac{\|PH'Q\|\|H'\|}{g^3}\Big)\,\mathrm{d}s. \tag{1.182}$$

Theorem 1.30. *Let H_s be a twice continuously differentiable time-dependent Hamiltonian. Let $U(s)$ be generated by $-iTH_s$, with $T(s)^{-1}$ absolutely continuous. Suppose H' is bounded and $\sigma(H_s) \cap [b_0(s), b_1(s)] = \{\omega_0(s)\}$. Then*

$$\sqrt{1-F} \leq \frac{1}{T(0)} \frac{\|P(0)H'(0)Q(0)\|}{g(0)^2} + \frac{1}{T(1)} \frac{\|P(1)H'(1)Q(1)\|}{g(1)^2} + \int_0^1 \frac{|T'|}{T^2} \frac{\|PH'Q\|}{g^2} \,\mathrm{d}s + \int_0^1 \frac{1}{T}\Big(\frac{\|PH''Q\|}{g^2} + \big(2\sqrt{2}+1\big) \frac{\|H'\|^2}{g^3} \Big) \,\mathrm{d}s. \quad (1.183)$$

Theorem 1.31. *Let H_s be a twice continuously differentiable time-dependent Hamiltonian. Let $U(s)$ be generated by $-iTH_s$, with $T(s)^{-1}$ absolutely continuous. Suppose $\sigma(H_s) \cap [b_0(s), b_1(s)]$ consists of at most m points. Then*

$$\sqrt{1-F} \leq \frac{1}{T(0)} \frac{m\|P(0)H'(0)Q(0)\|}{g(0)^2} + \frac{1}{T(1)} \frac{m\|P(1)H'(1)Q(1)\|}{g(1)^2} + \int_0^1 \frac{|T'|}{T^2} m \frac{\|PH'Q\|}{g^2} \,\mathrm{d}s + \int_0^1 \frac{1}{T}\Big(\frac{m\|PH''Q\|}{g^2} + 3m\sqrt{m} \frac{\|PH'Q\|^2}{g^3} + 4m^2 \frac{\|PH'Q\| \|H'\|_{D\to\mathcal{H}}}{g^3} \Big(1 + g + \max\{|b_0|, |b_1|\}\Big) \Big) \,\mathrm{d}s. \quad (1.184)$$

1.1.5.2 A quantum harmonic oscillator with varying frequency

As an application of the adiabatic theorem for unbounded Hamiltonians, Theorem 1.28, consider the following Hamiltonian:

$$H_s \coloneqq \frac{1}{2}\big(\hat{p}^2 + \omega(s)^2 \hat{x}^2\big), \quad (1.185)$$

where $\hat{p}$ is the momentum operator on $L^2(\mathbb{R})$, $\hat{x}$ is the position operator on $L^2(\mathbb{R})$ and $\omega(s)$ is some strictly positive function that is twice continuously differentiable. This is the Hamiltonian of the quantum harmonic oscillator with s-dependent frequency $\omega(s)$ and unit mass. Let the interval $[b_0, b_1]$ contain only the ground energy.

It is not hard to verify the assumptions in Assumption 1 and Assumption 2. In particular the domain of H_s is independent of s and the gap $g(s) = \omega(s)$.

In order to apply the theorem, the quantities in its bound need to be calculated. Clearly $H' = \omega'\omega\hat{x}^2$ and $H'' = \big(\omega''\omega + \omega'^2\big)\hat{x}^2$, so we need to bound $\|P\hat{x}^2 Q\|$ and $\|\hat{x}^2\|_{D\to\mathcal{H}}$. Let $|n\rangle$ be the n^{th} eigenstate, with energy $E_n = \omega(s)\big(n + \frac{1}{2}\big)$. The annihilation and creation operators are defined as

$$a \coloneqq \sqrt{\frac{\omega}{2}}\Big(\hat{x} + \frac{i\hat{p}}{\omega}\Big) \quad \text{and} \quad a^* \coloneqq \sqrt{\frac{\omega}{2}}\Big(\hat{x} - \frac{i\hat{p}}{\omega}\Big), \quad (1.186)$$

which have the property that $a^*|n\rangle = \sqrt{n+1}|n+1\rangle$ and $a|n\rangle = \sqrt{n}|n-1\rangle$. Then

$$2\omega\hat{x}^2 = (a^* + a)^2 = a^{*2} + a^2 + 2N + 1, \quad (1.187)$$

where N is the number operator a^*a. Now $\|\hat{x}^2 P\| = \|\hat{x}^2|0\rangle\|$ and

$$\hat{x}^2|0\rangle = \frac{1}{2\omega}\big(\sqrt{2}|2\rangle + |0\rangle\big), \quad (1.188)$$

so $\|\hat{x}^2 P\| = \frac{\sqrt{3}}{2\omega}$. Next, when calculating $\|\hat{x}^2\|_{D\to\mathcal{H}}$, it is enough to consider the states $|n\rangle$, since they span a dense subspace of D. In other words, $\operatorname{span}\{|n\rangle\}$ is a core of H. We have

$$2\omega\hat{x}^2|n\rangle = \sqrt{n+2}\sqrt{n+1}|n+2\rangle + \sqrt{n}\sqrt{n-1}|n-2\rangle + (2n+1)|n\rangle, \quad (1.189)$$

so $2\omega\|\hat{x}^2|n\rangle\|^2 = 6n^2+6n+3$. The graph norm of $|n\rangle$ is given by

$$\||n\rangle\|_D = \|H|n\rangle\| + \||n\rangle\| = \omega\Big(n+\frac{1}{2}\Big)+1 \tag{1.190}$$

and so the operator norm can be bounded by

$$\begin{aligned}
\|\hat{x}^2\|_{D\to\mathcal{H}} &= \sup_{n\in\mathbb{N}} \frac{\|\hat{x}^2|n\rangle\|}{\||n\rangle\|_D} &(1.191)\\
&= \sup_{n\in\mathbb{N}} \frac{1}{\sqrt{2\omega}} \frac{\sqrt{6n^2+6n+3}}{\omega\big(n+\frac{1}{2}\big)+1} &(1.192)\\
&\leq \sup_{n\in\mathbb{N}} \frac{1}{\omega\sqrt{2\omega}} \sqrt{\frac{6n^2+6n+3}{\big(n+\frac{1}{2}\big)^2}} &(1.193)\\
&= \sup_{n\in\mathbb{N}} \frac{1}{\omega\sqrt{2\omega}} \sqrt{6+\frac{3}{2\big(n+\frac{1}{2}\big)^2}} &(1.194)\\
&= \frac{\sqrt{6}}{\omega\sqrt{\omega}}. &(1.195)
\end{aligned}$$

Now that all the pieces of Theorem 1.28 have been assembled, the full bound is as follows:

$$\begin{aligned}
\sqrt{1-F} \leq \frac{1}{T}\Bigg(&\frac{\sqrt{3}}{2}\Big(\frac{\omega'(0)}{\omega(0)}+\frac{\omega'(1)}{\omega(1)}\Big)\\
&+\int_0^1 \bigg(\frac{\sqrt{3}}{2}\frac{|\omega''|}{\omega^2} + (\frac{9}{4}+\frac{\sqrt{3}}{2})\frac{\omega'^2}{\omega^3} + 3\sqrt{2}\frac{\omega'^2}{\omega^3\sqrt{\omega}}\big(1+2\omega\big)\bigg)\,\mathrm{d}s\Bigg).
\end{aligned} \tag{1.196}$$

Various observations can be deduced from this. For example, consider the regime where $\omega \gg 1$. The process can be made roughly adiabatic by taking

$$T = \Theta\Big(\frac{|\omega''|}{\omega^2}+\frac{\omega'^2}{\omega^{2.5}}\Big). \tag{1.197}$$

1.1.5.3 An adiabatic theorem with an adapted schedule

In this section an additional assumption will be introduced that will lead to better bounds in the first order adiabatic theorem, Theorem 1.29. The idea is to exploit the fact that the bound contains integrals. In general it is hard to bound the integrals by anything better than the maximum of the integrand, but in many cases the integral is actually a lot smaller. To that end the following assumption is made:

Assumption 3. *There exists an absolutely continuous function $g_0 : [0,1] \to \mathbb{R}$ such that*

- $0 < g_0(s) \leq g(s)$ *for all* $s \in [0,1]$*;*
- *there exists* $p \in [1,2]$ *and* $B_p, B_{3-p} \geq 0$ *such that*

$$\int_0^1 \frac{1}{g_0(s)^p}\,\mathrm{d}s \leq B_p g_{0m}^{1-p} \quad \textit{and} \quad \int_0^1 \frac{1}{g_0(s)^{3-p}}\,\mathrm{d}s \leq B_{3-p} g_{0m}^{p-2}, \tag{1.198}$$

where $g_{0m} = \min_{s\in[0,1]} g_0(s)$.

This assumption holds for many time-dependent Hamiltonians of interest. All Hamiltonians in chapter 2 satisfy this assumption. The following theorem shows how a good fidelity can be achieved while only evolving for a time proportional to the inverse minimal gap. This is much better than a naive application of Theorem 1.29.

Theorem 1.32. *Let H_s be a bounded twice continuously differentiable time-dependent Hamiltonian such that $\sigma(H_s) \cap [b_0(s), b_1(s)]$ contains at most m eigenvalues. Assume Assumption 3. Take $C \geq 0$ such that*

$$C \geq m \max_{s\in[0,1]} \Big(\big(2 + pB_{3-p}|g_0'|\big)\|PH'Q\| + \|PH''Q\| + 5\sqrt{m}B_{3-p}\|PH'Q\|\|H'\|\Big). \tag{1.199}$$

Fix $\epsilon > 0$ and set

$$T = \frac{1}{\sqrt{\epsilon}} \frac{C}{g_0(s)^p g_{0m}^{2-p}}. \tag{1.200}$$

Then the evolved state has fidelity $1 - F \leq \epsilon$. The total evolution time satisfies

$$\int_0^1 T \, \mathrm{d}s \leq \frac{1}{\sqrt{\epsilon}} \frac{CB_p}{g_{0m}}. \tag{1.201}$$

Proof. Two claims need to be proved: firstly that $1 - F \leq \epsilon$ and secondly that the total evolution time satisfies the bound (1.201).

For the first claim, Theorem 1.29 gives a bound on $1 - F$. This theorem can be applies since x^p is Lipschitz on $[g_{0m}, \max_s \|H_s\|]$, so T^{-1} is absolutely continuous. We just need to show that it evaluates to something smaller than ϵ in this case. First observe that

$$\frac{|T'|}{T^2} = \frac{\sqrt{\epsilon} g_{0m}^{2-p}}{C} p g_0^{p-1} |g_0'|. \tag{1.202}$$

Then the claim follows from the following calculation:

$$
\begin{aligned}
\sqrt{1-F} &\le \frac{1}{T(0)}\frac{m\|P(0)H'(0)Q(0)\|}{g(0)^2} + \frac{1}{T(1)}\frac{m\|P(1)H'(1)Q(1)\|}{g(1)^2} + \int_0^1 \frac{|T'|}{T^2} m \frac{\|PH'Q\|}{g^2}\,\mathrm{d}s \\
&\quad + \int_0^1 \frac{1}{T}\Big(\frac{m\|PH''Q\|}{g^2} + 3m\sqrt{m}\frac{\|PH'Q\|^2}{g^3} + 2m\sqrt{m}\frac{\|PH'Q\|\|H'\|}{g^3}\Big)\,\mathrm{d}s \qquad (1.203)\\
&\le \sqrt{\epsilon}C^{-1}\bigg(mg_0(0)^{p-2}g_{0m}^{2-p}\|P(0)H'(0)Q(0)\| + mg_0(1)^{p-2}g_{0m}^{2-p}\|P(1)H'(1)Q(1)\| \\
&\quad + mpg_{0m}^{2-p}\int_0^1 |g_0'|\frac{\|PH'Q\|}{g_0^{1-p}g^2}\,\mathrm{d}s + mg_{0m}^{2-p}\int_0^1 g_0(s)^p\frac{\|PH''Q\|}{g^2}\,\mathrm{d}s \\
&\quad + 3m\sqrt{m}g_{0m}^{2-p}\int_0^1 g_0(s)^p\frac{\|PH'Q\|^2}{g^3}\,\mathrm{d}s + 2m\sqrt{m}g_{0m}^{2-p}\int_0^1 g_0(s)^p\frac{\|PH'Q\|\|H'\|}{g^3}\,\mathrm{d}s\bigg) \qquad (1.204)\\
&\le \sqrt{\epsilon}C^{-1}\bigg(m\|P(0)H'(0)Q(0)\| + m\|P(1)H'(1)Q(1)\| \\
&\quad + mpg_{0m}^{2-p}\int_0^1 |g_0'|\frac{\|PH'Q\|}{g_0^{3-p}}\,\mathrm{d}s + mg_{0m}^{2-p}\int_0^1 \frac{\|PH''Q\|}{g_{0m}^{2-p}}\,\mathrm{d}s \\
&\quad + 3m\sqrt{m}g_{0m}^{2-p}\int_0^1 \frac{\|PH'Q\|^2}{g_0^{3-p}}\,\mathrm{d}s + 2m\sqrt{m}g_{0m}^{2-p}\int_0^1 \frac{\|PH'Q\|\|H'\|}{g_0^{3-p}}\,\mathrm{d}s\bigg) \qquad (1.205)\\
&\le \sqrt{\epsilon}C^{-1}\max_{s\in[0,1]}\bigg(2m\|PH'Q\| + mpB_{3-p}|g_0'|\|PH'Q\| \\
&\qquad\qquad + m\|PH''Q\| + 5m\sqrt{m}B_{3-p}\|PH'Q\|\|H'\|\bigg) \qquad (1.206)\\
&\le \sqrt{\epsilon}. \qquad (1.207)
\end{aligned}
$$

Finally, the total evolution time is given by

$$
\begin{aligned}
\int_0^1 T\,\mathrm{d}s &= \frac{C}{\sqrt{\epsilon}g_{0m}^{2-p}}\int_0^1 \frac{1}{g_0(s)^p}\,\mathrm{d}s \qquad (1.208)\\
&\le \frac{1}{\sqrt{\epsilon}}\frac{CB_p}{g_{0m}}. \qquad (1.209)
\end{aligned}
$$

□

If the eigenspace of interest consists of a single eigenvalue (that may be highly degenerate), then the constants can be slightly improved.

Theorem 1.33. *Let H_s be a bounded twice continuously differentiable time-dependent Hamiltonian such that $\sigma(H_s)\cap[b_0(s),b_1(s)] = \{\omega_0\}$. Assume Assumption 3. Take $C \ge 0$ such that*

$$C \ge \max_{s\in[0,1]}\Big(\big(2+p|g_0'|B_{3-p}\big)\|PH'Q\| + \|PH''Q\| + (2\sqrt{2}+1)B_{3-p}\|H'\|^2\,\mathrm{d}s\Big). \qquad (1.210)$$

Fix $\epsilon > 0$ and set

$$T = \frac{1}{\sqrt{\epsilon}}\frac{C}{g_0(s)^p g_{0m}^{2-p}}. \qquad (1.211)$$

Then the evolved state has fidelity $1-F \leq \epsilon$. The total evolution time satisfies

$$\int_0^1 T \,\mathrm{d}s \leq \frac{1}{\sqrt{\epsilon}} \frac{CB_p}{g_{0m}}. \tag{1.212}$$

The constant 5 in Theorem 1.32 has been replaced with $2\sqrt{2}+1 \approx 3.83$.

Proof. Two claims need to be proved: firstly that $1-F \leq \epsilon$ and secondly that the total evolution time satisfies the bound (1.212).
For the first claim, Theorem 1.30 gives a bound on $1-F$. This theorem can be applies since x^p is Lipschitz on $[g_{0m}, \max_s \|H_s\|]$, so T^{-1} is absolutely continuous. We just need to show that it evaluates to something smaller than ϵ in this case. First observe that

$$\frac{|T'|}{T^2} = \frac{\sqrt{\epsilon} g_{0m}^{2-p}}{C} p g_0^{p-1} |g_0'|. \tag{1.213}$$

Then the claim follows from the following calculation:

$$\begin{aligned}
\sqrt{1-F} &\leq \frac{\|PH'Q\|}{Tg^2}\Big|_{s=0} + \frac{\|PH'Q\|}{Tg^2}\Big|_{s=1} + \int_0^1 \frac{|T'|}{T^2}\frac{\|PH'Q\|}{g^2}\,\mathrm{d}s \\
&\quad + \int_0^1 \frac{1}{T}\Big(\frac{\|PH''Q\|}{g^2} + (2\sqrt{2}+1)\frac{\|H'\|^2}{g^3}\Big)\,\mathrm{d}s \qquad (1.214)\\
&\leq \frac{\sqrt{\epsilon}}{C}\Bigg(\frac{\|PH'Q\|}{g_{0m}^{p-2} g_0^{-p} g^2}\Big|_{s=0} + \frac{\|PH'Q\|}{g_{0m}^{p-2} g_0^{-p} g^2}\Big|_{s=1} + p g_{0m}^{2-p}\int_0^1 |g_0'|\frac{\|PH'Q\|}{g_0^{1-p} g^2}\,\mathrm{d}s \\
&\quad + \int_0^1 \frac{\|PH''Q\|}{g_{0m}^{p-2} g_0(s)^{-p} g^2}\,\mathrm{d}s + (2\sqrt{2}+1)\int_0^1 \frac{\|H'\|^2}{g_{0m}^{p-2} g_0^{-p} g^3}\,\mathrm{d}s\Bigg) \qquad (1.215)\\
&\leq \frac{\sqrt{\epsilon}}{C}\Bigg(\|PH'Q\|\Big|_{s=0} + \|PH'Q\|\Big|_{s=1} + p g_{0m}^{2-p}\int_0^1 |g_0'|\frac{\|PH'Q\|}{g_0^{3-p}}\,\mathrm{d}s \\
&\quad + \int_0^1 \|PH''Q\|\,\mathrm{d}s + (2\sqrt{2}+1) g_{0m}^{2-p}\int_0^1 \frac{\|H'\|^2}{g_0^{3-p}}\,\mathrm{d}s\Bigg) \qquad (1.216)\\
&\leq \frac{\sqrt{\epsilon}}{C}\max_{s\in[0,1]}\Big(\big(2 + p|g_0'|B_{3-p}\big)\|PH'Q\| + \|PH''Q\| + (2\sqrt{2}+1)B_{3-p}\|H'\|^2\,\mathrm{d}s\Big) \qquad (1.217)\\
&\leq \sqrt{\epsilon}. \qquad (1.218)
\end{aligned}$$

Finally, the total evolution time is given by

$$\begin{aligned}
\int_0^1 T\,\mathrm{d}s &= \frac{C}{\sqrt{\epsilon} g_{0m}^{2-p}}\int_0^1 \frac{1}{g_0(s)^p}\,\mathrm{d}s \qquad (1.219)\\
&\leq \frac{1}{\sqrt{\epsilon}}\frac{CB_p}{g_{0m}}. \qquad (1.220)
\end{aligned}$$

□

1.1.6 A counterexample to naive scaling

For a while the accepted wisdom was that the error in adiabatic quantum computing scaled as $O(\|H'\|/g^2)$. This is what was stated in the original paper [14], based on a somewhat naive

reading of the adiabatic theorem. In this section, a counterexample to the naive scaling is presented. This presentation contains significant novelty, but the core idea has been known for a long time. The earliest version I know is from 1949, [38].
The counterexample has a nice physical interpretation: it is Rabi oscillation.

1.1.6.1 The Schrödinger equation in a rotating frame and averaging effects

We need two preliminary results before developing the counterexample. The first is an elementary result about the Schrödinger equation in a rotating frame. The second is an interesting bound due to [39].

Lemma 1.34. *Let $H(t)$ be a Hamiltonian of the form $Q(t)H_0(t)Q(t)^*$, where $H_0(t)$ is a continuous path of bounded Hamiltonians and $Q(t)$ is a continuously differentiable path of unitaries. Let $U(t)$ be the unitary generated by H and $U_R(t)$ the unitary generated by $H_0 - iQ^*Q'$. Then $U = QU_R$.*

The unitary U_R is the evolution in the rotating frame.

Proof. We calculate, using the fundamental theorem of calculus Corollary D.32,

$$U^*(t)Q(t)U_R(t) = \mathbf{1} + \int_0^t \frac{\mathrm{d}}{\mathrm{d}s} U^*QU_R \,\mathrm{d}s \tag{1.221}$$

$$= \mathbf{1} + \int_0^t \big(iU^*QH_0\cancel{Q^*Q}U_R + U^*Q'U_R + U^*Q(-iH_0 - Q^*Q')U_R\big)\,\mathrm{d}s = \mathbf{1}. \tag{1.222}$$

Multiplying on the left by U gives the result. □

Proposition 1.35. *Let $H_0(t), H_1(t)$ be two continuous, time-dependent Hamiltonians with associated evolution operators $U_0(t)$ and $U_1(t)$. Then*

$$\|U_1(t) - U_0(t)\| \leq \|S(t)\| + \int_0^t \|S(s)\|\big(\|H_0(s)\| + \|H_1(s)\|\big)\,\mathrm{d}s, \tag{1.223}$$

where $S(t) = \int_0^t \big(H_0(s) - H_1(s)\big)\,\mathrm{d}s$.

This is a simplified version of a key result in [39].

Proof. Consider the wave operator $\Omega(t) = U_0(t)^*U_1(t)$. Then

$$\Omega(t) = \mathbf{1} + \int_0^t \frac{\mathrm{d}}{\mathrm{d}s}\Omega(s)\,\mathrm{d}s \tag{1.224}$$

$$= \mathbf{1} + i\int_0^t U_0^*(H_0 - H_1)U_1\,\mathrm{d}s \tag{1.225}$$

$$= \mathbf{1} + i\int_0^t U_0^*S'U_1\,\mathrm{d}s \tag{1.226}$$

$$= \mathbf{1} + i\int_0^t \big((U_0^*SU_1)' - U_0^{*\prime}SU_1 - U_0^*SU_1'\big)\,\mathrm{d}s \tag{1.227}$$

$$= \mathbf{1} + iU_0^*(t)S(t)U_1(t) + \int_0^t U_0^*\big(H_0S - SH_1\big)U_1\,\mathrm{d}s. \tag{1.228}$$

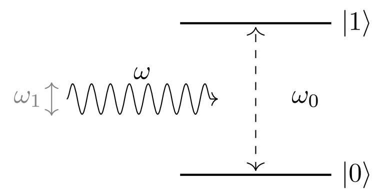
Multiplying by $U_0(t)$ and taking the norm gives the result. □

1.1.6.2 Rabi oscillation

Consider a spin-1/2 particle in a magnetic field. This can be modelled semi-classically by a qubit with a Hamiltonian given by

$$H = -\mu \mathbf{B} \cdot \boldsymbol{\sigma}, \tag{1.229}$$

where μ is the magnetic moment, $\mathbf{B}$ the magnetic field and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$. In order to distinguish the states $|0\rangle$ and $|1\rangle$, a static field is applied in the z-direction, which gives Zeeman splitting.
Next we would like a way to control the qubit. Applying a high-frequency magnetic field, with a frequency matched to the Zeeman energy induces a rotation, even if the amplitude of the control pulse is small.



In this case the Hamiltonian is

$$H_{\text{Rabi}}(s) = \frac{1}{2}\omega_0 \sigma_z + \omega_1 \cos(\omega s)\sigma_x. \tag{1.230}$$

Using $\cos(\omega s) = \frac{e^{i\omega s} + e^{-i\omega s}}{2}$, we have

$$H_{\text{Rabi}}(s) = \frac{1}{2}\begin{pmatrix} \omega_0 & \omega_1 e^{i\omega s} + \omega_1 e^{-i\omega s} \\ \omega_1 e^{i\omega s} + \omega_1 e^{-i\omega s} & -\omega_0 \end{pmatrix} \tag{1.231}$$

$$= \frac{1}{2}\begin{pmatrix} \omega_0 & \omega_1 e^{-i\omega s} \\ \omega_1 e^{i\omega s} & -\omega_0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 & \omega_1 e^{i\omega s} \\ \omega_1 e^{-i\omega s} & 0 \end{pmatrix} \tag{1.232}$$

Now it turns out that everything is much simpler if we only keep the first term and discard the second, i.e. we approximate $H_{\text{Rabi}}(s)$ by

$$H(s) \coloneqq \frac{1}{2}\begin{pmatrix} \omega_0 & \omega_1 e^{-i\omega s} \\ \omega_1 e^{i\omega s} & -\omega_0 \end{pmatrix}. \tag{1.233}$$

This is known as the "rotating wave approximation" (or RWA) and is a good approximation if $\omega \approx \omega_0$ and $\omega_1 \ll \omega_0$, i.e. if the frequency of the control pulse is close to the Zeeman energy and the amplitude is small compared to the static magnetic field.

Proposition 1.36. *Let U be the unitary generated by H and U_{Rabi} the unitary generated by H_{Rabi}. Then*

$$\|U(t) - U_{Rabi}(t)\| \leq \frac{\omega_1}{2\omega} + t\frac{\omega_1}{2\omega}\sqrt{(\omega_0 - \omega)^2 + 4\omega_1^2}, \tag{1.234}$$

for all $t \in \mathbb{R}^+$.

For more details, see [39].

Proof. The key idea is to move to the rotating frame determined by

$$Q = \begin{pmatrix} e^{-i\frac{\omega}{2}s} & 0 \\ 0 & e^{i\frac{\omega}{2}s} \end{pmatrix}. \tag{1.235}$$

Then

$$H = \frac{1}{2} Q \begin{pmatrix} \omega_0 & \omega_1 \\ \omega_1 & -\omega_0 \end{pmatrix} Q^* \quad \text{and} \quad H_{\text{Rabi}} = \frac{1}{2} Q \begin{pmatrix} \omega_0 & \omega_1 + \omega_1 e^{i2\omega s} \\ \omega_1 + \omega_1 e^{-i2\omega s} & -\omega_0 \end{pmatrix} Q^*. \tag{1.236}$$

Since

$$-iQ^* Q' = \frac{1}{2} \begin{pmatrix} -\omega & 0 \\ 0 & \omega \end{pmatrix}, \tag{1.237}$$

the evolutions in the rotating frame, cfr. Lemma 1.34, are given by

$$H_0 \coloneqq \frac{1}{2} \begin{pmatrix} \omega_0 - \omega & \omega_1 \\ \omega_1 & -(\omega_0 - \omega) \end{pmatrix} \quad \text{and} \quad H_1 \coloneqq \frac{1}{2} \begin{pmatrix} \omega_0 - \omega & \omega_1 + \omega_1 e^{i2\omega s} \\ \omega_1 + \omega_1 e^{-i2\omega s} & -(\omega_0 - \omega) \end{pmatrix}. \tag{1.238}$$

Let $U_0(t)$, resp. $U_1(t)$, be the unitary evolution generated by H_0, resp. H_1. The aim is now to use Proposition 1.35. Since

$$\begin{aligned} S(t) &= \int_0^1 \big(H_0(s) - H_1(s)\big) \, \mathrm{d}s \qquad (1.239) \\ &= \frac{1}{2} \int_0^1 \begin{pmatrix} 0 & -\omega_1 e^{i2\omega s} \\ -\omega_1 e^{-i2\omega s} & 0 \end{pmatrix} \mathrm{d}s \qquad (1.240) \\ &= \frac{\omega_1}{4\omega} \begin{pmatrix} 0 & -i(1 - e^{i2\omega t}) \\ i(1 - e^{-i2\omega t}) & 0 \end{pmatrix}. \qquad (1.241) \end{aligned}$$

Taking the norm gives $\|S(t)\| \leq \frac{\omega_1}{2\omega}$. Since H_0, H_1 are traceless 2×2 matrices, the norm is just the square root of the absolute value of the determinant, so

$$\|H_0(t)\| = \frac{1}{2} \sqrt{(\omega_0 - \omega)^2 + \omega_1^2} \tag{1.242}$$

and

$$\|H_1(t)\| = \frac{1}{2} \sqrt{(\omega_0 - \omega)^2 + \omega_1^2 |1 + e^{i2\omega s}|^2} \leq \sqrt{(\omega_0 - \omega)^2 + 4\omega_1^2}. \tag{1.243}$$

Plugging everything into the bound from Proposition 1.35 gives

$$\begin{aligned} \|U_1(t) - U_0(t)\| &\leq \frac{\omega_1}{2\omega} + t \frac{\omega_1}{4\omega} \left(\sqrt{(\omega_0 - \omega)^2 + \omega_1^2} + \sqrt{(\omega_0 - \omega)^2 + 4\omega_1^2} \right) \qquad (1.244) \\ &\leq \frac{\omega_1}{2\omega} + t \frac{\omega_1}{2\omega} \sqrt{(\omega_0 - \omega)^2 + 4\omega_1^2}. \qquad (1.245) \end{aligned}$$

Finally, we can revert back to the original frame

$$\|U(t) - U_{\text{Rabi}}(t)\| = \|Q(t)U_0(t) - Q(t)U_1(t)\| = \|U_1(t) - U_0(t)\|, \tag{1.246}$$

using Lemma 1.34. □

For our purposes, the fact that $H(s)$ is an approximation is essentially irrelevant: we are looking for a mathematical counter-example to the naive adiabatic theorem, not necessarily a physical system. It is nice, however, that the counter-example is physically motivated. The violation of the naive adiabatic theorem even happens in a regime where the rotating wave approximation is valid.

1.1.6.3 The contradiction

Proposition 1.37. *Consider the Hamiltonian* $H(s) \coloneqq \frac{1}{2}\begin{pmatrix} \omega_0 & \omega_1 e^{-i\omega s} \\ \omega_1 e^{i\omega s} & -\omega_0 \end{pmatrix}$*. Let* $|E_0(s)\rangle$ *be the instantaneous ground state of* $H(s)$*, set* $|E_0\rangle \coloneqq |E_0(0)\rangle$ *and let* $|\psi(s)\rangle = U(s)|E_0\rangle$ *be the evolved state. Then the fidelity* $F(s) = |\langle E_0(s)|\psi(s)\rangle|^2$ *is given by*

$$F(s) = \cos^2\left(\frac{\Omega}{2}s\right) + \frac{4\langle E_0|H_0|E_0\rangle^2}{\Omega^2}\sin^2\left(\frac{\Omega}{2}s\right), \tag{1.247}$$

where $\Omega \coloneqq \sqrt{(\omega_0-\omega)^2+\omega_1^2}$ *is the Rabi frequency.*

Proof. As before, it is easier if we work in the rotating frame. Recall Q, H_0, U_0 from the proof of Proposition 1.36.
Now $|E_0(s)\rangle = Q(s)|E_0\rangle$, so Lemma 1.34 gives

$$\begin{aligned} F(s) &= |\langle E_0(s)|\psi(s)\rangle|^2 && (1.248)\\ &= |\langle E_0|Q^*(s)U(s)|E_0\rangle|^2 && (1.249)\\ &= |\langle E_0|U_0(s)|E_0\rangle|^2 && (1.250)\\ &= |\langle E_0|e^{-isH_0}|E_0\rangle|^2. && (1.251)\end{aligned}$$

Calculating the matrix exponential of a 2×2 matrix is not too hard. In this case we have

$$e^{-isH_0} = -2i\frac{H_0}{\Omega}\sin\left(\frac{\Omega}{2}s\right) + \cos\left(\frac{\Omega}{2}s\right)\mathbf{1}. \tag{1.252}$$

Bracketing between $\langle E_0|\cdot|E_0\rangle$ and taking the modulus squared gives the result. ∎

First note that $\|H_0\| = \frac{\Omega}{2}$, so

$$\frac{4\langle E_0|H_0|E_0\rangle^2}{\Omega^2} \leq 1. \tag{1.253}$$

Next observe that bracketing with $\langle 1|\cdot|0\rangle$ gives the transition probability to go from $|0\rangle$ to $|1\rangle$. In this case we recover the usual Rabi formula

$$P_{0\to 1} = \frac{\omega_1^2}{\Omega^2}\sin^2\left(\frac{\Omega}{2}s\right). \tag{1.254}$$

The quantity $\langle E_0|H_0|E_0\rangle$ can be expressed in terms of the ωs, but this is somewhat involved. For reference, it is

$$\langle E_0|H_0|E_0\rangle = \frac{-\omega\omega_0^2 + \omega\omega_0\sqrt{\omega_0^2+\omega_1^2} + \omega_0^3 - \omega_0^2\sqrt{\omega_0^2+\omega_1^2} + \omega_0\omega_1^2 - \omega_1^2\sqrt{\omega_0^2+\omega_1^2}}{2\omega_0^2 - 2\omega_0\sqrt{\omega_0^2+\omega_1^2} + 2\omega_1^2}. \tag{1.255}$$

At resonance (i.e. $\omega = \omega_0$) this simplifies to

$$\langle E_0|H_0|E_0\rangle = \frac{\omega_0\omega_1^2 - \omega_1^2\sqrt{\omega_0^2+\omega_1^2}}{2\omega_0^2 - 2\omega_0\sqrt{\omega_0^2+\omega_1^2} + 2\omega_1^2}. \tag{1.256}$$

At resonance the prefactor only depends on $\frac{\omega_0}{\omega_1}$ and simplifies nicely. If $\omega_0 = a\omega_1$, then

$$\frac{4\langle E_0|H_0|E_0\rangle^2}{\Omega^2} = \frac{1}{a^2+1}. \tag{1.257}$$

Finally we are ready to consider the counterexample. Suppose there was a theorem of the following form: there exists $C_0 \geq 0$ such that if the evolution time is

$$T \geq C_0 \frac{\|H'\|}{g_m^2}, \tag{1.258}$$

then $1 - F(1) \leq 0.1$.
We now show that we can take $\omega_0, \omega_1, \omega$ such that this supposed theorem is rendered untrue. First observe

- $g = \sqrt{\omega_0^2 + \omega_1^2}$;
- $\|H'\| = \omega_1 \omega$;
- $\|H''\| = \omega_1 \omega^2$.

We set $\omega = \omega_0$, $\omega_1 = \pi$ and

$$\omega_0 = \max\{C_0, 1\}\omega_1. \tag{1.259}$$

Now

$$C_0 \frac{\|H'\|}{g_m^2} = C_0 \frac{\omega_0 \omega_1}{\omega_0^2 + \omega_1^2} \leq C_0 \frac{\omega_1}{\omega_0} \leq 1, \tag{1.260}$$

So evolving for time $T = 1$ should give a high fidelity, at least higher than 0.9, but if we compare with Proposition 1.37, we see that

$$F(1) = \cos^2\left(\frac{\pi}{2}\right) + \frac{4\langle E_0|H_0|E_0\rangle^2}{\Omega^2} \sin^2\left(\frac{\pi}{2}\right) = \frac{1}{\max\{C_0, 1\}^2 + 1} \leq \frac{1}{2} < 0.9, \tag{1.261}$$

where we have used that $\Omega = \omega_1$ at resonance. This is a contradiction.

1.2 Adiabatic theorems for dissipative dynamics

In this section some adiabatic theorems will be discussed that can be applied to dynamics that are not unitary. This means that states are no longer represented by unit vectors $|\psi\rangle$, but by positive trace-one matrices, i.e. density matrices ρ.
The evolutions are no longer unitary operators, but rather positive trace-preserving operators.[10]

1.2.1 Some motivating examples

The primitive operation in adiabatic quantum computing is time-dependent Hamiltonian evolution. Ideally the cost of the operation is given by the total time spent evolving the system.
Of course, we cannot hope to be able to evolve under all time-dependent Hamiltonians with this cost: one could then scale down the cost arbitrarily much by scaling up the Hamiltonian. Instead, let us assume we can evolve under all time-dependent Hamiltonians H_t that satisfy $\|H_t\| \leq 1$.
Is this a reasonable assumption? It would seem not: as discussed in the introduction, building a device that can implement any possible time-dependent Hamiltonian is an infeasible engineering

[10] Often complete positivity, rather than just positivity, is imposed. It is not imposed here because it is not necessary and so relaxing this requirement makes the proofs more general. In particular, the adiabatic theorems can then also be applied to certain approximations of physical evolutions, which have no reason to be completely positive. In addition, there is some debate about the necessity of complete positivity in physical systems, see e.g. [40].

challenge and simulating such a device on a conventional gate-based quantum computer leads to overhead due to discretisation.
On the other hand, there exist problems with natural time-dependent Hamiltonians such that the evolution time required by the adiabatic theorem matches the expected complexity of the problem. For example, see section 2.1 and section 2.2.
This suggests there may exist a procedure based on the time-independent Hamiltonian H_s that can be performed in the same time as it would take to do the time-dependent Hamiltonian evolution and is dephasing[11] enough for there to be an associated adiabatic theorem that guarantees the same fidelity as the usual adiabatic theorem does for time-dependent Hamiltonian evolution. In this thesis two such procedures are proposed. Both can be implemented straightforwardly on a conventional gate-based quantum computer with classical control.

1.2.1.1 Poisson-distributed phase randomisation

The first procedure is based on performing time-independent Hamiltonian evolution for random amounts of time.
The idea to use randomised time-independent Hamiltonian evolution for dephasing has been around for some time [41]. The innovation here is to perform the dephasing operation according to a Poisson process. This will simplify the analysis, allowing an asymptotically better result to be obtained.
The dephasing property of randomised evolution is proved in the following result.

Proposition 1.38 (Phase randomisation)**.** *Let H be a Hamiltonian, ω_0 an isolated point in the spectrum, P the projector on the associated eigenspace and g_0 a lower bound on the spectral gap. Assume we can simulate e^{-itH} for any positive or negative time t at a cost of $|t|$. Then we can construct a stochastic variable τ such that for all states ρ,*

$$\langle e^{-i\tau H}\rho e^{i\tau H}\rangle = P\rho P + Q\langle e^{-i\tau H}\rho e^{i\tau H}\rangle Q, \tag{1.262}$$

with $\langle|\tau|\rangle = t_0/g_0$, where $t_0 = 2.32132$.

The angled brackets mean taking the average over τ. The result is originally from [41]. For simplicity, the Hilbert space is assumed finite-dimensional in this proof. The value for t_0 was obtained in [42].

Proof. We set $U(\tau) = e^{-i\tau H}$. In order to construct the stochastic variable τ, we start with a smooth[12] even function h_0 of compact support in $]-\frac{1}{2}, -\frac{1}{2}[$. Consider the convolution $h = \frac{h_0 * h_0}{(h_0*h_0)(0)}$, which is compactly supported in $]-1, 1[$. Next define the function h_{g_0} by $h_{g_0}(\omega) = h(\omega/g_0)$. Let f be the inverse Fourier transform of h and f_{g_0} the inverse Fourier transform of h_{g_0}. We have $f_{g_0}(t) = g_0 f(g_0 t)$. Since the inverse Fourier transform of h_0 is real, the function f_{g_0} is positive. By construction it is also normalised. Let τ be the stochastic variable with density f_{g_0}.
Now we show that $\langle U(\tau)P\rho Q U^*(\tau)\rangle = 0 = \langle U(\tau)Q\rho P U^*(\tau)\rangle$. We can write $Q = \sum_{i=1} Q_i$, where each Q_i is the projector on the eigenspace of energy ω_i. The projector P is associated to the eigenspace of energy ω_0. Since $\langle U(\tau)P\rho Q U^*(\tau)\rangle = \sum_{i=1}\langle U(\tau)P\rho Q_i U^*(\tau)\rangle$, it is enough

[11] I use dephasing here to mean the decoupling of the eigenspace of interest from the rest of the Hilbert space.
[12] Smoothness is only used to guarantee the inverse Fourier transform of h exists and is Fourier integrable. If this is satisfied, then we can drop the smoothness condition. For example, we can set h_0 to be a non-zero constant on $]-1/2, 1/2[$ and zero outside, then f is proportional to the sinc function squared.

to show that $\langle U(\tau)P\rho Q_i U^*(\tau)\rangle = 0$ for all i. Indeed,

$$\langle U(\tau)P\rho Q_i U^*(\tau)\rangle = \int_{-\infty}^{\infty} e^{-itH} P\rho Q_i e^{-itH} f_{g_0}(t)\,\mathrm{d}t \tag{1.263}$$

$$= \int_{-\infty}^{\infty} e^{-it\omega_0}\rho e^{-it\omega_i} f_{g_0}(t)\,\mathrm{d}t \tag{1.264}$$

$$= \rho \int_{-\infty}^{\infty} e^{it(\omega_i-\omega_0)} f_{g_0}(t)\,\mathrm{d}t \tag{1.265}$$

$$= \rho h_{g_0}(\omega_i - \omega_0) \tag{1.266}$$

$$= 0, \tag{1.267}$$

since $\omega_i - \omega_0 \geq g_0$ and h_{g_0} is supported in $]-g_0, g_0[$.
We also have $\langle U(\tau)P\rho PU^*(\tau)\rangle = \rho\int_{-\infty}^{\infty} e^{it(\omega_0-\omega_0)} f_{g_0}(t)\,\mathrm{d}t = \rho$. Putting everything together gives

$$\langle U(\tau)\rho U^*(\tau)\rangle = \langle U(\tau)P\rho PU^*(\tau)\rangle + \langle U(\tau)Q\rho QU^*(\tau)\rangle + \langle U(\tau)P\rho QU^*(\tau)\rangle + \langle U(\tau)Q\rho PU^*(\tau)\rangle \tag{1.268}$$

$$= P\rho P + Q\langle U(\tau)Q\rho U^*(\tau)\rangle Q. \tag{1.269}$$

Finally, we need to show that the cost scales as $\langle\tau\rangle = O(1/g_0)$. We calculate

$$\langle|\tau|\rangle = \int_{-\infty}^{\infty} |t| f_{g_0}(t)\,\mathrm{d}t \tag{1.270}$$

$$= \int_{-\infty}^{\infty} |t| g_0 f(g_0 t)\,\mathrm{d}t \tag{1.271}$$

$$= \frac{1}{g_0}\int_{-\infty}^{\infty} |u| f(u)\,\mathrm{d}u. \tag{1.272}$$

Now $t_0 \coloneqq \int_{-\infty}^{\infty} |u| f(u)\,\mathrm{d}u$ is just a constant that depends on the chosen h_0. It was shown in [42] that t_0 can be taken to be 2.32132. □

Now suppose we have a time-dependent Hamiltonian H_s. Choose some finite $\{s_0, \ldots, s_n\} \subseteq [0, 1]$. Take every s_k in order and apply $e^{-i\tau H}$ to the state, where τ is chosen randomly as in Proposition 1.38. This procedure prepares a state with good fidelity with the eigenprojector $P(1)$, if the subset $\{s_0, \ldots, s_n\}$ is chosen dense enough. The trick, as always, is to choose the subset dense enough, but not too dense (since this needlessly wastes time).
A first idea might be to let the s_k have uniform spacing. This yields a time-complexity of $T = O_1\big(\frac{\|H'\|}{g_m^3}\big)$ [41].[13] Typically better choices of s_k (better "schedules") are available, as was already noted in the original paper.
For example, for the quantum linear systems problem (see section 2.2 for more details), a better schedule was introduced in [43]. This schedule gives a complexity of $O\big(\kappa\log(\kappa)\big)$, which is slightly worse than the optimal $O(\kappa)$. It seems complicated to give a deterministic schedule that achieves optimal asymptotic scaling. Indeed the more recent [44] does not manage, despite significant effort to give tight bounds.[14]

[13] Note that this is significantly worse than the adiabatic Theorem 1.26, since $\int_0^1 \frac{\|H'\|}{g^3}\,\mathrm{d}s$ is in general much smaller than $\frac{\|H'\|}{g_m^3}$.

[14] The reference [44] is to an old version of the paper. The current version, [42], incorporates our suggestion for a randomised schedule, [1], and therefore achieves the same asymptotic scaling we do, which is optimal.

In [1] we propose randomising the schedule. This allows us to treat this setup as a dynamical system that is continuously evolving according to some differential equation. What is more, we can derive an adiabatic theorem that shares many features with the time-dephasing adiabatic theorems (like Theorem 1.29), so that it is not too hard to transfer result from usual adiabatic computing to this setting. In particular, we are able to show optimal asymptotic scaling for that quantum linear systems problem.

To be more concrete, we propose randomising the schedule according to a (variable-rate) Poisson process. Operationally, this amounts to algorithm 1.

Algorithm 1: Poisson-distributed phase randomisation.

1. Pick a Poisson process $N : [0,1] \times (\Omega, \mathcal{A}, P) \to \mathbb{N}$ with rate $\lambda(s)$;
2. At each jump point s of the Poisson process, pick an instance t of the random variable τ as defined in Proposition 1.38 and evolve the system under the Hamiltonian evolution e^{-itH_s};

The density matrix describing the system is a random variable that satisfies the stochastic differential equation $\mathrm{d}\rho = \left(e^{-i\tau(s)H_s}\rho e^{i\tau(s)H_s} - \rho\right)\mathrm{d}N$.

Marginalising over the Poisson process (i.e. forgetting which exact realisation of the Poisson process was picked) and over the stochastic variable τ, we get a new density matrix that is determined by the following differential equation:

$$\frac{\mathrm{d}\rho}{\mathrm{d}s} = \lambda\Big(P\rho P + \int Qe^{-i\tau H_s}\rho e^{i\tau H_s}Q\,\mathrm{d}\mu(\tau) - \rho\Big), \tag{1.273}$$

with probability distribution μ. This differential equation can be derived using the well-known heuristic that $\mathrm{d}N$ averages to $\lambda\,\mathrm{d}s$. The rigorous version of this statement is known as Campbell's theorem, at least in the case that the Poisson process is the only part that is stochastic. To derive (1.273), we actually need something slightly stronger since the operation performed at every jump point is itself stochastic. This stronger version of Campbell's theorem is proved in the appendix as Proposition D.37.

The total time taken by one run of the algorithm is a random variable T satisfying $\mathrm{d}T = \tau\,\mathrm{d}N$. In order to find the time complexity, we again marginalise over the Poisson realisations. This gives

$$\mathrm{d}T = g^{-1}\lambda\,\mathrm{d}s, \tag{1.274}$$

so $T = \int_0^1 \frac{\lambda}{g}\,\mathrm{d}s$.

The dynamics described by (1.273) constitute the first example for which we would like to find an adiabatic theorem.

1.2.1.2 Discrete adiabatic theorem

In the previous section, a differential equation was deduced by taking a discrete process (phase randomisation) and applying it randomly according to a Poisson process. In this section the same trick is applied, but now to the discrete adiabatic theorem.

The discrete adiabatic theorem is originally due to [45] and was extended and refined in [46]. The latter work also applies it in an algorithmic context, specifically to the quantum linear systems problem (see section 2.2). Let $U(s)$ be some unitary, parametrised by $s \in [0,1]$. The discrete adiabatic theorem states that the very application of $U(s)$ is dephasing: suppose $\{s_0, \ldots, s_m\} \subseteq [0,1]$ and we apply the unitary $U(s_k)$ to the system, for each s_k in order, then a

state will be produced that has high fidelity with the eigenspace of interest (i.e. corresponding to the one the state started in), so long as $\{s_0, \ldots, s_m\} \subseteq [0,1]$ is chosen dense enough.
As in the previous example, we propose to use a Poisson process. Operationally, the procedure becomes algorithm 2.

Algorithm 2: Poisson-distributed discrete adiabatic theorem.

1 Pick a Poisson process $N : [0,1] \times (\Omega, \mathcal{A}, P) \to \mathbb{N}$ with rate $\lambda(s)$;
2 At each jump point s of the Poisson process, apply $U(s)$;

Now the stochastic differential equation is $\mathrm{d}\rho = \big(U\rho U^* - \rho\big)\,\mathrm{d}N$. Marginalising over the realisations and applying Campbell's theorem gives the (non-stochastic) differential equation

$$\frac{\mathrm{d}\rho}{\mathrm{d}s} = \lambda\big(U\rho U^* - \rho\big). \tag{1.275}$$

The dynamics described by (1.275) seem like a prime candidate for an adiabatic theorem. Indeed, one will be derived for them. The link with the original adiabatic problem (determined by the time-dependent Hamiltonian) is slightly lost, however. In order the reintroduce H_s, a standard technique is used: qubitisation.

Qubitisation For any self-adjoint operator H such that $\|H\| \leq 1$, the following operator on $\mathbb{C}^2 \otimes \mathcal{H}$ can be constructed:

$$\begin{pmatrix} H & -\sqrt{\mathbb{1} - H^2} \\ \sqrt{\mathbb{1} - H^2} & H \end{pmatrix} \tag{1.276}$$

This operator goes by many names, including "elementary rotation", "Julia operator" [47] and "Halmos dilation" [48].[15] It is straightforward to see that (1.276) is unitary.[16] In addition, the spectrum of (1.276) can be derived from the spectrum of H.

Lemma 1.39. *Let H be a self-adjoint element of a unital C^*-algebra with $\|H\| \leq 1$. Then*

$$\sigma\begin{pmatrix} H & -\sqrt{\mathbb{1} - H^2} \\ \sqrt{\mathbb{1} - H^2} & H \end{pmatrix} = \big\{\omega \pm i\sqrt{1 - \omega^2} \,\big|\, \omega \in \sigma(H)\big\}. \tag{1.277}$$

In particular, this result applies to all bounded self-adjoint operators on (potentially infinite-dimensional) Hilbert spaces. In finite dimensions, the number of eigenvalues doubles. This is what we expect, since the dimension also doubles.

Proof. Consider the functional calculus $\Phi_H : \mathcal{C}(\sigma(H), \mathbb{C}) \to A$ from Theorem A.14. It is an isometry, which means that it is injective and (with the fact that $\mathcal{C}(\sigma(H), \mathbb{C})$ is complete) its

[15] Actually, these names typically refer to the operator $\begin{pmatrix} H & \sqrt{\mathbb{1} - H^2} \\ \sqrt{\mathbb{1} - H^2} & -H \end{pmatrix}$.

[16] At least, it is straightforward in this case, since H is self-adjoint. In more generality one can define $\begin{pmatrix} T & -\sqrt{\mathbb{1} - TT^*} \\ \sqrt{\mathbb{1} - T^*T} & T^* \end{pmatrix}$ for all bounded T such that $\|T\| \leq 1$. This operator is also always unitary, but proving this requires showing $T\sqrt{\mathbb{1} - T^*T} = \sqrt{\mathbb{1} - TT^*}T^*$, which is not entirely trivial. The original proof by Halmos uses the fact that $T\sqrt{\mathbb{1} - T^*T}^{2n} = \sqrt{\mathbb{1} - TT^*}^{2n}T^*$, for all $n \in \mathbb{N}$. By approximating the square root uniformly with polynomials, this can be used to recover $T\sqrt{\mathbb{1} - T^*T} = \sqrt{\mathbb{1} - TT^*}T^*$. There is also a more elementary proof [49].

image is closed. This allows us to conclude that $\Phi_H : \mathcal{C}(\sigma(H), \mathbb{C}) \to C^*(\mathbf{1}, H)$ is an isomorphism (of C^*-algebras), where $C^*(\mathbf{1}, H)$ is the C^*-algebra generated by $\{\mathbf{1}, H\}$.[17]
Let $M_2(B)$ denote the 2×2-matrix algebra of a C^*-algebra B. Then Φ_H readily extends to an isomorphism $M_2\big(C^*(\mathbf{1}, H)\big) \cong M_2\big(\mathcal{C}(\sigma(H), \mathbb{C})\big)$. There is also an obvious isomorphism $M_2\big(\mathcal{C}(\sigma(H), \mathbb{C})\big) \cong \mathcal{C}\left(\sigma(H), M_2(\mathbb{C})\right)$.
Composing these isomorphisms, we see that (1.276) gets mapped to the function

$$\sigma(H) \to M_2(\mathbb{C}) : \omega \mapsto \begin{pmatrix} \omega & -\sqrt{1-\omega^2} \\ \sqrt{1-\omega^2} & \omega \end{pmatrix}. \tag{1.278}$$

The spectrum of this function is clearly[18]

$$\bigcup_{t \in \sigma(H)} \sigma \begin{pmatrix} \omega & -\sqrt{1-\omega^2} \\ \sqrt{1-\omega^2} & \omega \end{pmatrix} = \big\{\omega \pm i\sqrt{1-\omega^2} \,\big|\, t \in \sigma(H)\big\}. \tag{1.279}$$

As a final note, one may be worried about the fact that we have calculated that spectrum of (1.276) as an element of $C^*(\mathbf{1}, H)$, not as an element of A. It is an important result about C^*-algebras that this gives the same result.[19] □

Corollary 1.40. *The gaps in* $\sigma \begin{pmatrix} H & -\sqrt{\mathbb{1} - H^2} \\ \sqrt{\mathbb{1} - H^2} & H \end{pmatrix}$ *are wider than in* $\sigma(H)$.

Note, however, that new gaps are formed at ± 1, which may be quite small! This is illustrated in Figure 1.3.

Proof. Consider $\omega_0, \omega_1 \in \sigma(H)$. Then

$$\left|(\omega_0 \pm i\sqrt{1-\omega_0^2}) - (\omega_1 \pm i\sqrt{1-\omega_1^2})\right| = \sqrt{\big(\omega_0 - \omega_2\big)^2 + \left(\sqrt{1-\omega_0^2} \pm \sqrt{1-\omega_1^2}\right)^2} \tag{1.280}$$

$$\geq |\omega_0 - \omega_1|. \tag{1.281}$$

□

Now, returning to the case where $H_s : \mathcal{H} \to \mathcal{H}$ is a self-adjoint operator with $\|H_s\| \leq 1$ for all. Each eigenvector $|\psi\rangle$ of H_s corresponds to two eigenvectors of (1.276):

$$\frac{1}{\sqrt{2}} \begin{pmatrix} |\psi\rangle \\ i|\psi\rangle \end{pmatrix}, \qquad \frac{1}{\sqrt{2}} \begin{pmatrix} |\psi\rangle \\ -i|\psi\rangle \end{pmatrix}. \tag{1.282}$$

Now the pieces have been assembled to apply algorithm 2 to the problem of tracking the eigenstate of a Hamiltonian (rather than a unitary). The result is algorithm 3.
The development so far has assumed that we can apply the unitary (1.276). Methods for implementing this operator will be considered in subsubsection 1.2.4.1.

[17] Of course this little argument is redundant, since this isomorphism is used to prove the continuous functional calculus in the first place! As only the statement of the continuous functional calculus is included in the appendices, it seemed reasonable to give this argument here.
[18] To calculate the spectrum of a function, note that a function is invertible if and only if it is invertible when evaluated at each point in its domain.
[19] This does not hold in general for Banach algebras.

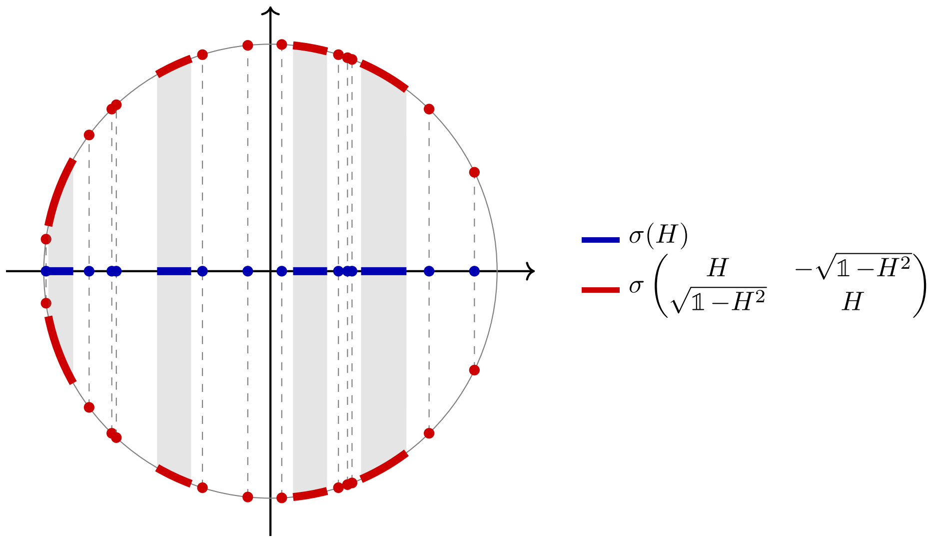


Figure 1.3: An illustration of Lemma 1.39.

Algorithm 3: Poisson-distributed qubitised unitaries.

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input: Time-dependent Hamiltonian H_s; an eigenvector $|\psi\rangle$ of H_0

Pick a Poisson process $N : [0,1] \times (\Omega, \mathcal{A}, P) \to \mathbb{N}$ with rate $\lambda(s)$;

Couple in an ancilla qubit in the $|0\rangle$ state and apply both a Hadamard and phase gate to obtain $\begin{pmatrix} |\psi\rangle \\ i|\psi\rangle \end{pmatrix}$;

At each jump point s of the Poisson process, apply $\begin{pmatrix} H_s & -\sqrt{\mathbb{1} - H_s^2} \\ \sqrt{\mathbb{1} - H_s^2} & H_s \end{pmatrix}$;

Trace out the ancilla qubit;

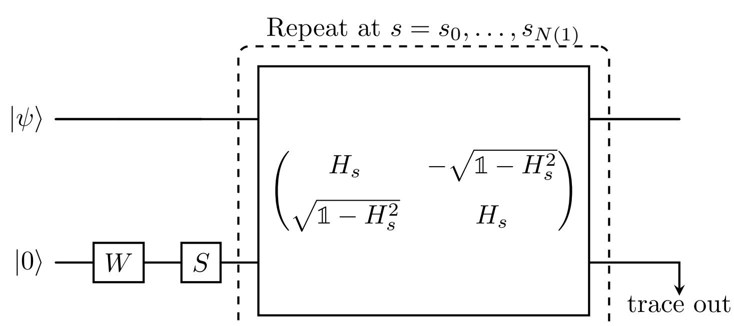


Figure 1.4: The quantum circuit implementing algorithm 3.

1.2.2 A general adiabatic theorem for dissipative dynamics

The current goal is to develop an adiabatic theorem that can be applied to the dynamics determined by (1.273) and (1.275).

In both cases the differential equation is of the form

$$\frac{\mathrm{d}\rho(s)}{\mathrm{d}s} = \lambda \mathcal{L}_s\big(\rho(s)\big). \tag{1.283}$$

For each s, $\mathcal{L}_s$ is a generator of a semigroup $\mathcal{E}_s(t)$ on the space of trace class operators, $\mathcal{B}_1(\mathcal{H})$, that is positive and trace-preserving. Then the adjoint semigroup $\mathcal{E}_s^*(t)$ is unital and positive, see Proposition A.111. This implies that $\|\mathcal{E}_s^*(t)\| \leq 1$ and so $\|\mathcal{E}_s(t)\| \leq 1$. In other words, $\mathcal{L}_s$ generates a contraction semigroup, for all s. Now the results about the existence of the dynamics as developed in Appendix B apply. We use $\mathcal{E}(s_1, s_0)$ to the denote the evolution operator that evolves the system from time s_0 to time s_1. Frequently $\mathcal{E}(s)$ will be used as a shorthand for $\mathcal{E}(s, 0)$.

1.2.2.1 A first attempt: adapting the previous results to the dissipative setting

The most obvious idea is to try to adapt the methods of section 1.1 to this more general setting. In principle this works. The ideal adiabatic evolution $\mathcal{E}_A(s)$ can be defined in complete analogy with $U_A(t)$. The self-adjointness of the generator is not really used, except (1) to bound the norm of evolution operator $U(s)$ and (2) to define the wave operator $\Omega(s) = U(s)^* U_A(s)$. For the first point, since the generators $\mathcal{L}_s$ generate contraction semigroups, the norm of the evolution operator is still bounded by one. The second point is slightly more tricky: in order to define the wave operator $\Omega(s) = \mathcal{E}(s)^{-1}\mathcal{E}_A(s)$, the evolution operator $\mathcal{E}(s)$ needs to be invertible. When restricted to the case where $\mathcal{L}_s$ is bounded, this is automatically true: replacing $\mathcal{L}_s$ by $-\mathcal{L}_s$ generates the inverse. The details in this case have been worked out in [21].

In the unbounded case progress can be made by replacing the wave operator development with the following method for bounding the difference between evolution operators:

$$\mathcal{E}(s) - \mathcal{E}_A(s) = \int_0^s \frac{\mathrm{d}}{\mathrm{d}r}\big(\mathcal{E}(s,r)\mathcal{E}_A(r,0)\big)\,\mathrm{d}r = \int_0^s \frac{i}{T}\mathcal{E}(s,r)[P', P]\mathcal{E}_A(r,0)\,\mathrm{d}s. \tag{1.284}$$

This idea has been developed, see e.g. [50] and [51].

These approaches work in the sense that they yield sensible adiabatic theorems, usually of the form "$\sqrt{1-F} \leq O_1(T^{-1})$". For our purposes it is important to be able to bound the constants involved, which will depend on the spectrum and in particular the gap. Here we encounter a problem: the spectrum of $\mathcal{L}_s$ is not the spectrum of H_s. For example, in the case of the Liouville-von Neumann equation, with $\mathcal{L}_s(\rho) = -i[H_s, \rho]$, the only obvious statement we can make is

$$\sigma(\mathcal{L}_s) \subseteq -i\big(\sigma(H_s) - \sigma(H_s)\big), \tag{1.285}$$

which is given by Corollary A.9. This is not great, because two highly exciting states whose energies are similar may yield a small gap, but this should not impact the fidelity of the actual evolution very much.

Equation 1.275 has a similar problem: with $\mathcal{L}_s$ defined by $\mathcal{L}_s(\rho) = U_t\rho U_t^* - \rho$, we have

$$\sigma(\mathcal{L}_s) \subseteq \sigma(U_s)\cdot\sigma(U_s)^{-1} - 1 \tag{1.286}$$

Determining the spectrum of the generator in (1.273) is even less clear. This problem is related to the fact that the adiabatic evolution, $\mathcal{E}_A(s)$, is defined by a spectral projector of $\mathcal{L}_s$. It is not entirely clear this is always the best definition; another is proposed in [52]. In our motivating examples there is a more precise subspace we want to track: the eigenspace of the underlying Hamiltonian H_s.

For these reasons a different strategy is pursued, inspired by the results in [53]. Instead of a bound on the gap of $\mathcal{L}_s$, the aim is now to bound the norm of the inverse of the generator.

1.2.2.2 The adiabatic theorem

In order to guarantee the existence of the dynamics, we adopt assumptions that are analogous to the ones in Assumption 1.

Assumption 4. *Let $\mathcal{H}$ be a Hilbert space. Suppose*

- $\mathcal{L}_s$ *generates a trace-preserving contraction semigroup on* $\mathcal{B}_1(\mathcal{H})$*, for all* $s \in [0,1]$*;*
- $\mathcal{L}_s$ *has the same domain* D *for all* $s \in [0,1]$*;*
- *the function* $[0,1] \to \mathcal{B}_1(\mathcal{H}) : s \mapsto \mathcal{L}_s(\rho)$ *is continuously differentiable for all* $\rho \in D$.

In addition, Assumption 2 on the time-dependent Hamiltonian H_s is still in force. When applying these results we will usually restrict ourselves to the case where $\mathcal{L}_s$ is bounded and norm-continuous in s, for simplicity.
The following theorem is heavily inspired by [53].

Theorem 1.41. *Let* $\rho(s)$ *be the solution of the differential equation*

$$\frac{\mathrm{d}\rho}{\mathrm{d}s} = \lambda \mathcal{L}_s(\rho). \tag{1.287}$$

Suppose

- $\mathrm{Tr}\big(P(0)\rho(0)\big) = 1$*;*
- $\mathrm{Tr}(P(s)Y) = 0$ *for all* $Y \in \mathrm{im}(\mathcal{L}_s)$ *and all* $s \in [0,1]$*;*
- *there exists* $X(s) \in \mathcal{B}(\mathcal{H})$ *such that* $P'(s) = \mathcal{L}_s^*\big(X(s)\big)$ *for all* $s \in [0,1]$*;*
- $[0,1] \to \mathcal{B}(\mathcal{H}) : s \mapsto X(s)$ *is differentiable and* λ^{-1} *is absolutely continuous.*

Then

$$1 - \mathrm{Tr}\big(P(1)\rho(1)\big) \leq \frac{\|X\|}{\lambda}\bigg|_{s=0} + \frac{\|X\|}{\lambda}\bigg|_{s=1} + \int_0^1 \Big(\frac{\|X'\|}{\lambda} + \Big|\Big(\frac{1}{\lambda}\Big)'\Big|\|X\|\Big)\,\mathrm{d}s. \tag{1.288}$$

Proof. The proof starts with a simple calculation:

$$\begin{aligned}
\mathrm{Tr}(P\rho)' &= \mathrm{Tr}(P'\rho) + \mathrm{Tr}(P\rho') && (1.289)\\
&= \mathrm{Tr}(P'\rho) + \lambda\,\mathrm{Tr}(P\mathcal{L}_s(\rho)) && (1.290)\\
&= \mathrm{Tr}(P'\rho) && (1.291)\\
&= \mathrm{Tr}\big(\mathcal{L}_s^*(X)\rho\big) && (1.292)\\
&= \mathrm{Tr}\big(X\mathcal{L}_s(\rho)\big) = \mathrm{Tr}(\lambda^{-1}X\rho'). && (1.293)
\end{aligned}$$

Next we integrate and integration by parts (see Proposition D.34) is used to calculate

$$\begin{aligned}
1 - \mathrm{Tr}\big(P(1)\rho(1)\big) = \mathrm{Tr}(P\rho)|_0^1 &= \int_0^1 \mathrm{Tr}(P\rho)'\,\mathrm{d}s && (1.294)\\
&= \int_0^1 \mathrm{Tr}(\lambda^{-1}X\rho')\,\mathrm{d}s && (1.295)\\
&= \lambda^{-1}\,\mathrm{Tr}(X\rho)|_0^1 - \int_0^1 \Big(\mathrm{Tr}(\lambda^{-1}X'\rho) + \Big(\frac{1}{\lambda}\Big)'\,\mathrm{Tr}(X\rho)\Big)\,\mathrm{d}s. && (1.296)
\end{aligned}$$

Finally we use $\mathrm{Tr}(\rho) = 1$ and Proposition A.106 to obtain

$$1 - \mathrm{Tr}\left(P(1)\rho(1)\right) \leq \|\frac{X}{\lambda}\|\Big|_{s=0} + \|\frac{X}{\lambda}\|\Big|_{s=1} + \int_0^1 \left(\frac{\|X'\|}{\lambda} + \Big|\left(\frac{1}{\lambda}\right)'\Big|\|X\|\right) \mathrm{d}s. \tag{1.297}$$

□

In the next sections this theorem is applied to the various examples.

1.2.3 Poisson-distributed phase randomisation

In this section the dynamics generated by

$$\frac{\mathrm{d}\rho}{\mathrm{d}s} = \lambda\mathcal{L}_s(\rho) := \lambda\Big(P\rho P + \int Qe^{-i\tau H_s}\rho e^{i\tau H_s}Q\,\mathrm{d}\mu(\tau) - \rho\Big), \tag{1.298}$$

are analysed.

Lemma 1.42. *Let H_s be a norm-continuous bounded time-dependent Hamiltonian that is twice continuously differentiable. The differential equation (1.298) satisfies the assumptions of Theorem 1.41 with*

$$X(s) = -P'(s) \tag{1.299}$$

Proof. First observe that any operator in the image of $\mathcal{L}_s$ is off-diagonal, so multiplying by P and taking the trace gives zero.
Let $\sigma \in \mathcal{B}_1(\mathcal{H})$ be an arbitrary trace class operator. We need to prove that $\mathrm{Tr}(X\mathcal{L}_s(\sigma)) = \mathrm{Tr}(P'\sigma)$. Since P' is off-diagonal, it is clear that

$$\mathrm{Tr}(P'\sigma) = -\,\mathrm{Tr}\left(P'\Big(P\rho P + \int Qe^{-i\tau H_s}\rho e^{i\tau H_s}Q\,\mathrm{d}\mu(\tau) - \sigma\Big)\right) \tag{1.300}$$

$$= \mathrm{Tr}\left((-P')\mathcal{L}_s(\sigma)\right). \tag{1.301}$$

□

Corollary 1.43. *Let H_s be a norm-continuous bounded time-dependent Hamiltonian that is twice continuously differentiable. Suppose $\sigma(H_s)\cap[b_0(s), b_1(s)]$ consists of at most m eigenvalues and λ^{-1} is absolutely continuous. The dynamics of (1.298) produces a state with infidelity bounded by*

$$1 - F \leq \big\|\lambda(0)^{-1}P'(0)\big\| + \big\|\lambda(1)^{-1}P'(1)\big\| + \int_0^1 \left(\Big\|\frac{P''}{\lambda}\Big\| + \Big|\left(\frac{1}{\lambda}\right)'\Big|\|P'\|\right)\mathrm{d}s \tag{1.302}$$

$$\leq \sqrt{m}\Big(\frac{\|P(0)H'(0)Q(0)\|}{\lambda(0)g(0)} + \frac{\|P(1)H'(1)Q(1)\|}{\lambda(1)g(1)}\Big) + \int_0^1 \left(\sqrt{m}\frac{\|PH''Q\|}{\lambda g} + 4m\frac{\|PH'Q\|\|H'\|}{\lambda g^2} + \sqrt{m}\Big|\left(\frac{1}{\lambda}\right)'\Big|\frac{\|PH'Q\|}{g}\right)\mathrm{d}s. \tag{1.303}$$

Proof. This is an immediate application of Theorem 1.41. The bounds on $\|P'\|$ and $\|P''\|$ are from Corollary 1.17, Lemma 1.25 and Proposition 1.16. □

With this result, specific performance guarantees of algorithm 1 can be given. Two cases will be analysed: one where λ is taken to be constant and one where λ is adapted to the gap in a manner similar to Theorem 1.32.

Theorem 1.44. *Let H_s be a norm-continuous bounded time-dependent Hamiltonian that is twice continuously differentiable. Suppose $\sigma(H_s) \cap [b_0(s), b_1(s)]$ consists of at most m eigenvalues. Suppose λ does not depend on s and fix $\epsilon > 0$. Then algorithm 1 produces a state with infidelity $1 - F$ less than ϵ if*

$$\frac{\sqrt{m}}{\epsilon}\left(\frac{\|PH'Q\|}{g}\Big|_{s=0} + \frac{\|PH'Q\|}{g}\Big|_{s=1} + \int_0^1 \Big(\frac{\|PH''Q\|}{g} + 4\sqrt{m}\frac{\|PH'Q\|\|H'\|}{g^2}\Big)\,\mathrm{d}s\right) \leq \lambda. \quad (1.304)$$

Suppose g_{0m} is constant that is a lower bound on the gap for all $s \in [0,1]$ and $\epsilon > 0$ is a target upper bound on the infidelity, then algorithm 1 can be executed with a time complexity less than

$$\frac{t_0\sqrt{m}}{\epsilon}\Big(2\frac{\|PH'Q\|}{g_{0m}^2} + \frac{\|PH''Q\|}{g_{0m}^2} + 4\sqrt{m}\frac{\|PH'Q\|\|H'\|}{g_{0m}^3}\Big). \quad (1.305)$$

The constant t_0 can be taken to be 2.33.

Proof. Equation 1.335 is an immediate consequence of Corollary 1.43. The second equation follows from the fact that the time complexity is given by $\lambda\int_0^1 \frac{1}{g_0}\,\mathrm{d}s$. □

The next theorem implements an adapted schedule, again using Assumption 3.

Theorem 1.45. *Let H_s be a norm-continuous bounded time-dependent Hamiltonian that is twice continuously differentiable. Suppose $\sigma(H_s) \cap [b_0(s), b_1(s)]$ consists of at most m eigenvalues and Assumption 3 holds. Take $C \geq 0$ such that*

$$C \geq \sqrt{m}\max_{s\in[0,1]}\Big(\big(2+(p-1)|g_0'|B_{3-p}\big)\|PH'Q\| + \|PH''Q\| + 4\sqrt{m}B_{3-p}\|PH'Q\|\|H'\|\Big). \quad (1.306)$$

Fix $\epsilon > 0$ and set

$$\lambda = \frac{1}{\epsilon}\frac{C}{g_0^{p-1}g_{0m}^{2-p}} \quad (1.307)$$

Then algorithm 1 produces a state with fidelity $F \geq 1 - \epsilon$ in a time bounded by

$$\frac{t_0}{\epsilon}\frac{CB_p}{g_{0m}}. \quad (1.308)$$

The constant t_0 can be taken to be 2.33.

Proof. Two claims need to be proved: firstly that $1 - F \leq \epsilon$ and secondly that the algorithm finishes in a time bounded by (1.308).
For the first claim, Corollary 1.43 gives a bound on $1 - F$. This theorem can be applies since x^p is Lipschitz on $[g_{0m}, \max_s \|H_s\|]$, so λ^{-1} is absolutely continuous. We just need to show that it evaluates to something smaller than ϵ in this case. First observe that

$$\Big|\Big(\frac{1}{\lambda}\Big)'\Big| = \frac{|\lambda'|}{\lambda^2} = \frac{\epsilon g_{0m}^{2-p}}{C}(p-1)g_0^{p-2}|g_0'|. \quad (1.309)$$

Then the claim follows from the following calculation:

$$
\begin{aligned}
1-F &\leq \sqrt{m}\Big(\frac{\|P(0)H'(0)Q(0)\|}{\lambda(0)g(0)} + \frac{\|P(1)H'(1)Q(1)\|}{\lambda(1)g(1)} \\
&\qquad + \int_0^1 \Big(\frac{\|PH''Q\|}{\lambda g} + 4\sqrt{m}\frac{\|PH'Q\|\|H'\|}{\lambda g^2} + \Big|\Big(\frac{1}{\lambda}\Big)'\Big|\frac{\|PH'Q\|}{g}\Big)\,\mathrm{d}s\Big) && (1.310)\\
&\leq \sqrt{m}\frac{\epsilon}{C}\Big(\frac{\|P(0)H'(0)Q(0)\|}{g_{0m}^{p-2}g_0^{1-p}(0)g(0)} + \frac{\|P(1)H'(1)Q(1)\|}{g_{0m}^{p-2}g_0^{1-p}(1)g(1)} \\
&\qquad + \int_0^1 \Big(\frac{\|PH''Q\|}{g_{0m}^{p-2}g_0^{1-p}g} + 4\sqrt{m}\frac{\|PH'Q\|\|H'\|}{g_{0m}^{p-2}g_0^{1-p}g^2} + g_{0m}^{2-p}(p-1)g_0^{p-2}|g_0'|\frac{\|PH'Q\|}{g}\Big)\,\mathrm{d}s\Big) && (1.311)\\
&\leq \sqrt{m}\frac{\epsilon}{C}\Big(\|P(0)H'(0)Q(0)\| + \|P(1)H'(1)Q(1)\| \\
&\qquad + \|PH''Q\| + 4\sqrt{m}\int_0^1 \frac{\|PH'Q\|\|H'\|}{g_{0m}^{p-2}g_0^{3-q}}\,\mathrm{d}s + \int_0^1 q|g_0'|\frac{\|PH'Q\|}{g_{0m}^{p-2}g_0^{3-p}}\,\mathrm{d}s\Big) && (1.312)\\
&\leq \sqrt{m}\frac{\epsilon}{C}\max_{s\in[0,1]}\Big(\big(2+(p-1)|g_0'|B_{3-p}\big)\|PH'Q\| + \|PH''Q\| + 4\sqrt{m}B_{3-p}\|PH'Q\|\|H'\|\Big) && (1.313)\\
&\leq \epsilon. && (1.314)
\end{aligned}
$$

Finally the time complexity of the algorithm is bounded by

$$
\begin{aligned}
\int_0^1 \frac{\lambda}{g_0}\,\mathrm{d}s &= \frac{C}{\epsilon}\int_0^1 \frac{1}{g_0^p g_{0m}^{2-p}}\,\mathrm{d}s && (1.315)\\
&\leq \frac{1}{\epsilon}\frac{CB_p}{g_{0m}}. && (1.316)
\end{aligned}
$$

□

Note that the time complexity is essentially the same as in the time-dephasing adiabatic case, Theorem 1.32. Since this is, operationally at least, a discrete procedure, the actual complexity[20] is much lower.

1.2.3.1 Eigenstate filtering

The use of eigenstate filtering was introduced in [54] to improve scaling in the error tolerance for algorithms based on adiabatic principles and the quantum Zeno effect, in particular with application to QLSP.
A similar technique was used in [46] to achieve optimal scaling, but using Linear Combinations of Unitaries (LCU) instead of Quantum Signal Processing (QSP). The aim of this section is to adapt the technique of [46], using time-independent Hamiltonian evolution as the primitive operation, rather than quantum gates.

Theorem 1.46. *Let H be a Hamiltonian with $\|H\| \leq 1$ and 0 in the spectrum of H, $\sigma(H)$. Suppose*

- $\Delta \geq 0$ *is such that* $[-\Delta, \Delta] \cap \sigma(H) = \{0\}$;

[20] In every sense of the word!

- *P is the orthogonal projector on the eigenspace associated to the eigenvalue* 0*, we set* $Q \coloneqq \mathbb{1} - P$*;*

- *ρ is a density matrix of the form* $P\rho_0 P + Q\rho_1 Q$ *with* $\mathrm{Tr}(P\rho_0) > 1/2$*, that we can prepare at cost* T_0*;*

- $\epsilon > 0$.

Further, suppose

- *we can adjoin two ancilla qubits to* ρ*;*

- *we can can measure and reprepare the ancilla qubits;*

- *we can evolve the system under* $H \otimes R$ *and* $\mathbb{1} \otimes R$ *for time* t *for all Hermitian operators* R *on* $\mathbb{C}^{2\times 2}$ *with* $\|R\| \leq 1$ *at a cost of* t*.*

Then we can prepare a state ρ_2 *such that* $\mathrm{Tr}(P\rho_2) \geq 1 - \epsilon$ *at a cost of* $O(T_0 + \Delta^{-1}\log(1/\epsilon))$*.*

The idea of the procedure is relatively simple. With these assumptions, we can apply controlled versions of the unitary e^{-itH}, i.e. $e^{itH\otimes\Pi}$ for some projector Π on $\mathbb{C}^{2\times 2}$. This means that we can apply linear combinations of $e^{itH\otimes\Pi}$ using the technique of linear combinations of unitaries, see Lemma 1.47 and Lemma 1.48. In particular we can apply a polynomial that has a large peak at 0 and is very small everywhere else. We use this to filter out the part of the state that we do not want.

Lemma 1.47 (LCU with arbitrarily large ancilla register)**.** *Let* $f(x) = \sum_{k=-n}^{n} a_k x^k$ *be a rational polynomial with complex coefficients such that* $\sum_{k=-n}^{n} |a_k|^2 = 1$*. Let* H *be a Hamiltonian and* ρ *the state of the system. Assume we have access to an ancilla register with orthonormal basis* $\{|k\rangle \mid k \in \mathbb{Z}\}$*. Then, at a cost of* $O(nt)$*, we can do an operation which either*

- *succeeds and applies* $\sum_{k=-n}^{n} |a_k|^2 e^{-itkH}$ *to the system,*

- *or fails, with a probability of* $1 - \mathrm{Tr}\left(\Big(\sum_{k=-n}^{n} |a_k|^2 e^{-itkH}\Big)\rho\Big(\sum_{k=-n}^{n} |a_k|^2 e^{itkH}\Big)\right)$*. We can see when this has happened thanks to the measured contents of the ancilla register.*

Proof. The procedure is as follows: we first prepare the ancilla in the state $|f\rangle \coloneqq \sum_{k=-n}^{n} a_k |k\rangle$, then apply $\sum_{k=-n}^{n} kH \otimes |k\rangle\langle k|$ for time t and finally measure the state $|f\rangle$. If we measure any other state than $|f\rangle$, the procedure fails.
The result then follows from the following identity:

$$\sum_{k,l=-n}^{n} \Big(\mathbb{1} \otimes a_k \langle k|\Big) e^{-it\sum_{m=-n}^{n} mH\otimes|m\rangle\langle m|} \Big(\mathbb{1} \otimes \overline{a_l}|l\rangle\Big) = \sum_m |a_m|^2 e^{-itmH}. \tag{1.317}$$

Defining

$$\Pi_m^0 = \mathbb{1} - \sum_{k=0}^{m} |k\rangle\langle k| \qquad \text{and} \qquad \Pi_m^1 = \mathbb{1} - \sum_{k=-m}^{0} |k\rangle\langle k|, \tag{1.318}$$

we can write $e^{-it\sum_{m=-n}^{n} mH\otimes|m\rangle\langle m|} = \prod_{m=0}^{n-1} e^{-itH\otimes\Pi_m^0} e^{itH\otimes\Pi_m^1}$, which we can clearly apply at a cost of $2nt$.
The cost of ancilla preparation depends on the admissible operations on the ancilla register, but in a worst-case scenario, each a_k needs to be set separately[21] which means that the cost is $O(n)$. The total cost is then still $O(nt)$. □

[21] This is the case for the procedure used in Lemma 1.48.

Lemma 1.48 (LCU with two ancilla qubits)**.** *We can achieve the results of Lemma 1.47 only using two ancilla qubits at a time.*

The construction is identical to the one in [46].

Proof of Theorem 1.46. Let $Q \coloneqq \mathbb{1} - P$ and write $Q = \sum_j Q_j$, where each Q_j is an eigenprojector of H associated to the eigenvalue ω_j. Now we observe

$$\Big(\sum_{k=-n}^{n} |a_k|^2 e^{-ikH}\Big)Q_j = \Big(\sum_{k=-n}^{n} |a_k|^2 e^{-ik\omega_j}\Big)Q_j = A(\omega_j)Q_j, \tag{1.319}$$

where $A(\omega)$ is the Fourier transform of the sequence $|a_k|^2$. Thus

$$\Big(\sum_{k=-n}^{n} |a_k|^2 e^{-ikH}\Big)Q\rho Q\Big(\sum_{k=-n}^{n} |a_k|^2 e^{ikH}\Big) = \sum_{j,l}\Big(\sum_{k=-n}^{n} |a_k|^2 e^{-ikH}\Big)Q_j\rho Q_l\Big(\sum_{k=-n}^{n} |a_k|^2 e^{ikH}\Big) \tag{1.320}$$

$$= \sum_{j,l} A(\omega_j)A(-\omega_l)Q_j\rho Q_l. \tag{1.321}$$

Taking the trace gives

$$\operatorname{Tr}\Big(\sum_{j,l} A(\omega_j)A(-\omega_l)Q_j\rho Q_l\Big) \le \max_{\omega\notin[-\Delta,\Delta]} A(\omega)^2 \operatorname{Tr}(Q\rho Q) \le \max_{\omega\notin[-\Delta,\Delta]} A(\omega)^2. \tag{1.322}$$

The goal then becomes to find a sequence and its Fourier transform such that $A(\omega_0) = 1$, $\max_{\omega\notin[-\Delta,\Delta]} A(\omega)^2 \le \epsilon$ and whose window n is as small as possible. The answer to this optimisation problem is well-known and is given by the Dolph-Chebyshev window [55]. In this case we need a window of[22]

$$n = \frac{\cosh^{-1}(1/\sqrt{\epsilon})}{\cosh^{-1}\big(\sec(\Delta)\big)} \le \frac{1}{2\Delta}\log\Big(\frac{4}{\epsilon}\Big). \tag{1.323}$$

By Lemma 1.47, we can implement this at a cost of $O(n)$. Note that this procedure terminates successfully with a probability of at least $\operatorname{Tr}(P\rho_0)$ (which is bounded below) and we can check to see whether the procedure failed. If it failed, we repeat. This requires we prepare a new copy of ρ. On average we need to repeat fewer than $\operatorname{Tr}(P\rho_0)^{-1}$ times, which is $O_1(1)$. □

1.2.4 Discrete adiabatic theorem

In this section the dynamics generated by

$$\frac{\mathrm{d}\rho}{\mathrm{d}s} = \lambda\mathcal{L}_s(\rho) \coloneqq \lambda\big(U\rho U^* - \rho\big), \tag{1.324}$$

are analysed, in complete analogy with the previous section.

Lemma 1.49. *Let U_s be a norm-continuous bounded time-dependent unitary that is twice continuously differentiable. Let μ be an eigenvalue of U and P the associated eigenprojector. The differential equation (1.298) satisfies the assumptions of Theorem 1.41 with*

$$X = P'(\mathbb{1} - \mu U^*)^+ + (\mathbb{1} - \overline{\mu}U)^+ P'. \tag{1.325}$$

[22] We note that we improve the scaling by a factor of two compared to [46]. This is because we are able to start from a state where $P\rho Q = 0 = Q\rho P$.

Proof. First observe that

$$\operatorname{Tr}\big(P(s)\mathcal{L}_s(\rho)\big) = \lambda \operatorname{Tr}\big(P(s)\big(\rho - U\rho U^*\big)\big) = 0. \tag{1.326}$$

for all $\rho \in \mathcal{B}_1(\mathcal{H})$.
Now let $\sigma \in \mathcal{B}_1(\mathcal{H})$ be an arbitrary trace class operator. We need to prove that $\operatorname{Tr}(X\mathcal{L}_s(\sigma)) = \operatorname{Tr}(P'\sigma)$. This follows from the following calculation:

$$\begin{aligned}
\operatorname{Tr}\big(X\mathcal{L}(\sigma)\big) &= \operatorname{Tr}\Big(\big((\mathbb{1}-\mu U^*)^+P' + P'(\mathbb{1}-\overline{\mu}U)^+\big)(\sigma - U\sigma U^*)\Big) && (1.327)\\
&= \operatorname{Tr}\big((\mathbb{1}-\mu U^*)^+P'\sigma\big) + \operatorname{Tr}\big(P'(\mathbb{1}-\overline{\mu}U)^+\sigma\big)\\
&\qquad - \operatorname{Tr}\big((\mathbb{1}-\mu U^*)^+P'U\sigma U^*\big) - \operatorname{Tr}\big(P'(\mathbb{1}-\overline{\mu}U)^+U\sigma U^*\big) && (1.328)\\
&= \operatorname{Tr}\big((\mathbb{1}-\mu U^*)^+P'\sigma\big) + \operatorname{Tr}\big(P'(\mathbb{1}-\overline{\mu}U)^+\sigma\big)\\
&\qquad - \operatorname{Tr}\big(\mu U^*(\mathbb{1}-\mu U^*)^+P'\sigma\big) - \operatorname{Tr}\big(P'(\mathbb{1}-\overline{\mu}U)^+\overline{\mu}U\sigma\big) && (1.329)\\
&= \operatorname{Tr}\big((\mathbb{1}-\mu U^*)(\mathbb{1}-\mu U^*)^+P'\sigma\big) + \operatorname{Tr}\big(P'(\mathbb{1}-\overline{\mu}U)^+(\mathbb{1}-\overline{\mu}U)\sigma\big) && (1.330)\\
&= \operatorname{Tr}(QP'\sigma) + \operatorname{Tr}(P'Q\sigma) = \operatorname{Tr}(P'\sigma). && (1.331)
\end{aligned}$$

□

Corollary 1.50. *Let U_s be a norm-continuous bounded time-dependent unitary that is twice continuously differentiable. Let μ be an eigenvalue of U and P the associated eigenprojector. Suppose λ^{-1} is absolutely continuous. The dynamics of (1.324) produces a state with infidelity bounded by*

$$1 - F \le \frac{\|P'\|}{\lambda g}\Big|_{s=0} + \frac{\|P'\|}{\lambda g}\Big|_{s=1} + 2\int_0^1 \left(\frac{\|P''\| + 2\|P'\|^2}{\lambda g} + 2\frac{\|U'\|\|P'\|}{\lambda g^2} + \left|\Big(\frac{1}{\lambda}\Big)'\right|\frac{\|P'\|}{g}\right)\mathrm{d}s \tag{1.332}$$

$$\le \frac{\|U'\|}{\lambda g^2}\Big|_{s=0} + \frac{\|U'\|}{\lambda g^2}\Big|_{s=1} + 2\int_0^1 \left(\frac{\|U''\|}{\lambda g^2} + 8\frac{\|U'\|^2}{\lambda g^3} + \left|\Big(\frac{1}{\lambda}\Big)'\right|\frac{\|U'\|}{g^2}\right)\mathrm{d}s. \tag{1.333}$$

Proof. The first inequality follows from Theorem 1.41, together with a series of norm bounds. The bound $\|(\mathbb{1}-\mu U^*)^+\| \le \frac{1}{g}$ can be seen as a consequence of Theorem A.14. Proposition 1.12 gives

$$(\mathbb{1}-\mu U^*)^{+\prime} = (\mathbb{1}-\mu U^*)^+\big(\mu' U^* + \mu U^{*\prime}\big)(\mathbb{1}-\mu U^*)^+ - P'(\mathbb{1}-\mu U^*)^+ - (\mathbb{1}-\mu U^*)^+P', \tag{1.334}$$

which can be bounded with the triangle inequality and the fact that $|\mu'| \le \|U'\|$, due to the Hellmann-Feynman theorem.
The second inequality follows by plugging in the bounds on $\|P'\|$ and $\|P''\|$ from Corollary 1.17, Lemma 1.25 and Proposition 1.16. □

Like in the last section, performance guarantees of algorithm 2 for two different choices of λ are now derived.

Theorem 1.51. *Let U_s be a norm-continuous bounded time-dependent unitary that is twice continuously differentiable. Let μ be an eigenvalue of U and P the associated eigenprojector. Suppose λ does not depend on s and fix $\epsilon > 0$. Then algorithm 2 produces a state with infidelity $1 - F$ less than ϵ if*

$$\frac{1}{\epsilon}\left(\frac{\|U'\|}{g^2}\Big|_{s=0} + \frac{\|U'\|}{g^2}\Big|_{s=1} + 2\int_0^1\left(\frac{\|U''\|}{g^2} + 8\frac{\|U'\|^2}{g^3}\right)\mathrm{d}s\right) \le \lambda. \tag{1.335}$$

Suppose g_{0m} is constant that is a lower bound on the gap for all $s \in [0,1]$ and $\epsilon > 0$ is a target upper bound on the infidelity, then algorithm 1 can be executed with a complexity less than

$$\frac{2}{\epsilon}\bigg(\frac{\|PH'Q\|}{g_{0m}^2} + \frac{\|U''\|}{g_{0m}^2} + 8\frac{\|U'\|^2}{g_{0m}^3}\bigg), \tag{1.336}$$

assuming U_s can be implemented at unit cost.

Proof. This is an immediate consequence of Corollary 1.50 and the fact that the complexity is simply given by λ. □

The next theorem implements an adapted schedule. In this case we can use the same hypothesis as for the time-dephasing adiabatic theorem, Assumption 3.

Theorem 1.52. *Let U_s be a norm-continuous bounded time-dependent unitary that is twice continuously differentiable. Let μ be an eigenvalue of U and P the associated eigenprojector. Suppose Assumption 3 holds. Take $C \geq 0$ such that*

$$C \geq 2\max_{s\in[0,1]}\Big(\big(1 + p|g_0'|B_{3-p}\big)\|U'\| + \|U''\| + 8B_{3-p}\|U'\|^2\Big). \tag{1.337}$$

Fix $\epsilon > 0$ and set

$$\lambda = \frac{1}{\epsilon}\frac{C}{g_0^p g_{0m}^{2-p}} \tag{1.338}$$

Then algorithm 2 produces a state with fidelity $F \geq 1-\epsilon$ in a time bounded by

$$\frac{1}{\epsilon}\frac{CB_p}{g_{0m}}. \tag{1.339}$$

Proof. Two claims need to be proved: firstly that $1-F \leq \epsilon$ and secondly that the algorithm finishes in a time bounded by (1.339).
For the first claim, Corollary 1.50 gives a bound on $1-F$. This theorem can be applies since x^p is Lipschitz on $[g_{0m}, \max_s \|H_s\|]$, so λ^{-1} is absolutely continuous. We just need to show that it evaluates to something smaller than ϵ in this case. First observe that

$$\Big|\Big(\frac{1}{\lambda}\Big)'\Big| = \frac{|\lambda'|}{\lambda^2} = \frac{\epsilon g_{0m}^{2-p}}{C}p g_0^{p-1}|g_0'|. \tag{1.340}$$

Then the claim follows from the following calculation:

$$\begin{aligned}
1-F &\leq \frac{\|U'\|}{\lambda g^2}\Big|_{s=0} + \frac{\|U'\|}{\lambda g^2}\Big|_{s=1} + 2\int_0^1\Big(\frac{\|U''\|}{\lambda g^2} + 8\frac{\|U'\|^2}{\lambda g^3} + \Big|\Big(\frac{1}{\lambda}\Big)'\Big|\frac{\|U'\|}{g^2}\Big)\,\mathrm{d}s & (1.341)\\
&\leq \frac{\epsilon}{C}\bigg(\frac{\|U'\|}{g_{0m}^{p-2}g_0^{-p}g^2}\Big|_{s=0} + \frac{\|U'\|}{g_{0m}^{p-2}g_0^{-p}g^2}\Big|_{s=1}\\
&\qquad + 2\int_0^1\Big(\frac{\|U''\|}{g_{0m}^{p-2}g_0^{-p}g^2} + 8\frac{\|U'\|^2}{g_{0m}^{p-2}g_0^{-p}g^3} + p|g_0'|g_{0m}^{2-p}g_0^{p-1}\frac{\|U'\|}{g^2}\Big)\,\mathrm{d}s\bigg) & (1.342)\\
&\leq \frac{\epsilon}{C}\bigg(\|U'\|\big|_{s=0} + \|U'\|\big|_{s=1} + 2\int_0^1\Big(\|U''\| + 8\frac{\|U'\|^2}{g_{0m}^{p-2}g_0^{3-p}} + p|g_0'|\frac{\|U'\|}{g_{0m}^{p-2}g_0^{3-p}}\Big)\,\mathrm{d}s\bigg) & (1.343)\\
&\leq \frac{2\epsilon}{C}\max_{s\in[0,1]}\Big(\big(1+p|g_0'|B_{3-p}\big)\|U'\| + \|U''\| + 8B_{3-p}\|U'\|^2\Big) & (1.344)\\
&\leq \epsilon. & (1.345)
\end{aligned}$$

Finally the cost of the algorithm is bounded by

$$\int_0^1 \lambda \, \mathrm{d}s = \frac{C}{\epsilon} \int_0^1 \frac{1}{g_0^p g_{0m}^{2-p}} \, \mathrm{d}s$$
$$\leq \frac{1}{\epsilon} \frac{C B_p}{g_{0m}}.$$

□

To compare the performance of this algorithm with Theorem 1.45 and Theorem 1.33, the gap g and the derivatives $\|U'\|, \|U''\|$ need to be compared with the Hamiltonian equivalents. The gaps were compared in Corollary 1.40. The derivatives should typically not impact the asymptotic complexity (so long as $\|H_s\|$ can be bounded away from 1). Nonetheless giving reasonable bounds on $\|U'\|, \|U''\|$ is an interesting endeavour that shall not be pursued further here. The following result could be useful:

Lemma 1.53. *Let T_s be a positive, bounded, differentiable time-dependent operator. Then $\sqrt{T_s}$ is differentiable and*

$$\frac{\mathrm{d}\sqrt{T_s}}{\mathrm{d}s} = \int_0^\infty e^{-r\sqrt{T_s}} \frac{\mathrm{d}T_s}{\mathrm{d}s} e^{-r\sqrt{T_s}} \, \mathrm{d}r.$$

There is a simple argument to show that $\frac{\mathrm{d}\sqrt{T_s}}{\mathrm{d}s}$ must have this form, if it exists: the Leibniz rule gives $T_s' = (\sqrt{T_s}^2)' = \sqrt{T_s}'\sqrt{T_s} + \sqrt{T_s}\sqrt{T_s}'$ and so the result follows from Proposition A.24.

1.2.4.1 Practical implementation of the qubitised Hamiltonian

In this section the construction of the unitary (1.276) is considered. In general we might have access to H via some arbitrary block encoding. A unitary $U : \mathcal{H} \oplus \mathcal{H}_a \to \mathcal{H} \oplus \mathcal{H}_a$, where $\mathcal{H}_a$ is some other Hilbert space, is called a block encoding of H if it is of the form

$$U = \begin{pmatrix} H & * \\ * & * \end{pmatrix}. \tag{1.346}$$

Now the idea, following [56], is to construct a new block encoding that operates on some subspace as (1.276). Indeed, it will turn out that any self-adjoint block encoding has this property. Such a block encoding is necessarily also self-inverse (i.e. $U^2 = \mathbb{1}$). If $\|H\| < 1$, then $U^{\downarrow}(\mathcal{H}) \cap \mathcal{H} = \{0\}$, so $\mathcal{H} \oplus U^{\downarrow}(\mathcal{H})$ is an invariant subspace for U, which means that U can be restricted to a unitary operating on a space isomorphic to $\mathbb{C}^2 \otimes \mathcal{H}$. This restricted unitary is essentially of the form we need.

Lemma 1.54. *Let H be a self-adjoint element of a unital C^*-algebra A such that $\|H\| < 1$. Suppose $X \in A^{2\times 2}$ is a self-adjoint block encoding of H. Then there exists a unitary $V \in A$ such that*

$$X = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & V \end{pmatrix} \begin{pmatrix} H & \sqrt{\mathbf{1} - H^2} \\ \sqrt{\mathbf{1} - H^2} & -H \end{pmatrix} \begin{pmatrix} \mathbf{1} & 0 \\ 0 & V \end{pmatrix}^*. \tag{1.347}$$

It is important that $\|H\|$ be strictly less than 1. Assuming only $\|H\| \leq 1$, the result is clearly false.[23] The result is essentially due to [56], but was only proved in the matrix case.

[23] For a simple counterexample, consider $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ as a block encoding of 1.

Proof. Define $X_{0,1}, X_{1,0}, X_{1,1}$ by $X = \begin{pmatrix} H & X_{0,1} \\ X_{1,0} & X_{1,1} \end{pmatrix}$. Since X is self-adjoint, $X_{0,1}^* = X_{1,0}$ Set $\Pi \coloneqq \begin{pmatrix} \mathbf{1} & 0 \\ 0 & 0 \end{pmatrix}$. Then

$$\begin{pmatrix} X_{1,0}^* X_{1,0} & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ X_{1,0} & 0 \end{pmatrix}^* \begin{pmatrix} 0 & 0 \\ X_{1,0} & 0 \end{pmatrix} \tag{1.348}$$

$$= \Pi X(\mathbf{1} - \Pi) X \Pi \tag{1.349}$$

$$= \Pi X^2 \Pi - (\Pi X \Pi)^2 \tag{1.350}$$

$$= \Pi - (\Pi X \Pi)^2 = \begin{pmatrix} \mathbf{1} - H^2 & 0 \\ 0 & 0 \end{pmatrix} \tag{1.351}$$

Because $\|H\| < 1$, $\sqrt{\mathbf{1} - H^2}$ is invertible, so we can set $V \coloneqq X_{1,0} \sqrt{\mathbf{1} - H^2}^{-1}$. Then

$$\begin{pmatrix} \mathbf{1} & 0 \\ 0 & V \end{pmatrix} \begin{pmatrix} H & \sqrt{\mathbf{1} - H^2} \\ \sqrt{\mathbf{1} - H^2} & -H \end{pmatrix} \begin{pmatrix} \mathbf{1} & 0 \\ 0 & V \end{pmatrix}^* = \begin{pmatrix} H & X_{1,0}^* \\ X_{1,0} & -VHV^* \end{pmatrix}. \tag{1.352}$$

Because X is unitary, we have $X_{0,1}^* H + X_{1,1} X_{1,0} = 0$. Multiplying on the right by $\sqrt{\mathbf{1} - H^2}^{-1}$ gives $VH + X_{1,1} V = 0$, or, $X_{1,1} = -VHV^*$. □

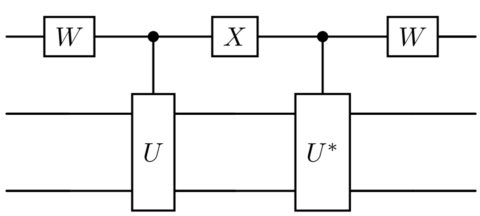
Corollary 1.55. *Let H be a self-adjoint element of a unital C^*-algebra A such that $\|H\| < 1$. Suppose $X \in A^{2\times 2}$ is a self-adjoint block encoding of H. Then there exists a unitary $V \in A$ such that*

$$X \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix} = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & V \end{pmatrix} \begin{pmatrix} H & -\sqrt{\mathbf{1} - H^2} \\ \sqrt{\mathbf{1} - H^2} & H \end{pmatrix} \begin{pmatrix} \mathbf{1} & 0 \\ 0 & V \end{pmatrix}^*. \tag{1.353}$$

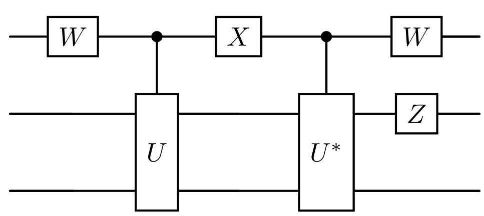
Now we just need to know that we can actually construct a self-adjoint block encoding, but this is not too complicated. Here is the one from [56]:

$$\frac{1}{2} \begin{pmatrix} U + U^* & U^* - U \\ U - U^* & -U - U^*. \end{pmatrix} \tag{1.354}$$

A circuit implementation is given in Figure 1.5.



(a) Self-inverse block encoding



(b) Elementary rotation

Figure 1.5: Given a block encoding U of H, (a) implements the self-inverse block encoding of H given by (1.354) and (b) implements an elementary rotation, in the sense of (1.276), up to a change of basis. The W represents the Hadamard gate.

There are two final points to consider:

- The subspace that we need to restrict the unitary to is, in general, s-dependent. So part of the state can leak out of the restricted subspace. The solution is to apply the adiabatic theorem to a slightly different, subunitary, operator: the unitary U is modified to send all vectors outside the intended domain to zero. It is not too hard to verify that the theorems in this setting as well. The performance of the actual procedure necessarily yields a higher fidelity than this modified (impractical) operation.
- The construction of the initial state is more complicated. Here knowledge of the original block encoding helps, but if necessary, the initial state can always be constructed using Linear Combinations of Unitaries (LCU).

1.2.5 Adiabatic eigenpath traversal

As a last application of Theorem 1.41, the usual time-dephasing adiabatic dynamics are discussed in this setting. The dynamics are generated by the Liouville-von Neumann equation

$$\frac{\mathrm{d}\rho}{\mathrm{d}s} = T\mathcal{L}_s(\rho) \coloneqq -iT[H_s, \rho] \tag{1.355}$$

Lemma 1.56. *Let H_s a bounded time-dependent Hamiltonian that is twice continuously differentiable.*
The differential equation (1.355) satisfies the assumptions of Theorem 1.41 with

$$X = -i\widetilde{[P, P']}. \tag{1.356}$$

The tilde refers to any solution of the operator equation (1.8).

Proof. Take arbitrary $\sigma \in \mathcal{B}_1(\mathcal{H})$. Then $\mathrm{Tr}\left(P[H_s, \sigma]\right) = \mathrm{Tr}\left([H_s, P\sigma]\right) = 0$.
Now we verify that the proposed X works. Let $\sigma \in \mathcal{B}_1(\mathcal{H})$ be an arbitrary trace class operator. We need to prove that $\mathrm{Tr}\left(X\mathcal{L}_s(\sigma)\right) = \mathrm{Tr}(P'\sigma)$. Indeed,

$$\begin{aligned} \mathrm{Tr}\left(X\mathcal{L}_s(\sigma)\right) &= -i\,\mathrm{Tr}\left(X[H_s, \sigma]\right) && (1.357)\\ &= -\mathrm{Tr}\left(\widetilde{[P, P']}[H_s, \sigma]\right) && (1.358)\\ &= \mathrm{Tr}\left(\left[H_s, \widetilde{[P, P']}\right]\sigma\right) && (1.359)\\ &= \mathrm{Tr}\left(\left[P, [P, P']\right]\sigma\right) = \mathrm{Tr}(P'\sigma). && (1.360) \end{aligned}$$

□

Corollary 1.57. *Let H_s be a norm-continuous bounded time-dependent Hamiltonian that is twice continuously differentiable. Suppose $\sigma(H_s) \cap [b_0(s), b_1(s)]$ consists of at most m eigenvalues and λ^{-1} is absolutely continuous. The state that has been evolved under (1.355) has an infidelity bounded by*

$$\begin{aligned} 1 - F \leq m\frac{\|PH'Q\|}{Tg^2}\Big|_{s=0} + m\frac{\|PH'Q\|}{Tg^2}\Big|_{s=1} + \int_0^1 \left|\left(\frac{1}{T}\right)'\right| m\frac{\|PH'Q\|}{g^2}\,\mathrm{d}s \\ + \int_0^1 \left(\frac{m}{Tg^2}\|PH''Q\| + 3\frac{m\sqrt{m}}{Tg^3}\|PH'Q\|\|H'\| + 2\frac{m\sqrt{m}}{Tg^3}\|PH'Q\|^2\right)\mathrm{d}s. \end{aligned} \tag{1.361}$$

This is essentially the same result as Theorem 1.29, except it bounds the infidelity, rather than the square root of the infidelity.

Proof. This is an application of Theorem 1.41. Proposition 1.16 gives

$$\|\widetilde{[P,P']}\| \le m\frac{\|PH'Q\|}{Tg^2}. \tag{1.362}$$

Next, Lemma 1.25 gives

$$\begin{aligned} [P,P']' &= \cancel{P'P'} + PP'' - P''P - \cancel{P'P'} && (1.363)\\ &= P\widetilde{H}'' - \cancel{2P(P')^2} - P\widetilde{[H',P']} - \widetilde{H}''P + \cancel{2(P')^2P} - \widetilde{[H',P']}P && (1.364)\\ &= P\widetilde{H}''Q - Q\widetilde{H}''P - \widetilde{[H',P']}. && (1.365)\end{aligned}$$

Also $\big[P',[P,P']\big]$ is diagonal, so $\widetilde{\big[P',[P,P']\big]} = 0$. Now we are ready to use Corollary 1.22:

$$\begin{aligned} \|\widetilde{[P,P']}'\| &\le \frac{\sqrt{m}}{g}\|[P,P']'\| + 2\frac{\sqrt{m}}{g}\|P'\|\|[P,P']\| + 2\frac{m}{g^2}\|H'\|\|[P,P']\| && (1.366)\\ &\le \frac{m}{g^2}\|PH''Q\| + 3\frac{m\sqrt{m}}{g^3}\|PH'Q\|\|H'\| + 2\frac{m\sqrt{m}}{g^3}\|PH'Q\|^2. && (1.367)\end{aligned}$$

Inserting these bounds into Theorem 1.41 gives the result. □

As before, bounds on the evolution time are developed, for two choices of T.

Theorem 1.58. *Let H_s be a norm-continuous bounded time-dependent Hamiltonian that is twice continuously differentiable. Suppose $\sigma(H_s) \cap [b_0(s), b_1(s)]$ consists of at most m eigenvalues. Suppose λ does not depend on s and fix $\epsilon > 0$. Then the infidelity $1 - F$ of the evolved state is bounded by ϵ if*

$$\begin{aligned} T \ge \frac{m}{\epsilon}\Bigg(&\frac{\|PH'Q\|}{Tg^2}\Big|_{s=0} + \frac{\|PH'Q\|}{Tg^2}\Big|_{s=1}\\ &+ \int_0^1 \Big(\frac{\|PH''Q\|}{g^2} + 3\sqrt{m}\frac{\|PH'Q\|\|H'\|}{g^3} + 2\sqrt{m}\frac{\|PH'Q\|^2}{g^3}\Big)\,\mathrm{d}s\Bigg). \end{aligned} \tag{1.368}$$

Proof. This is an immediate consequence of Corollary 1.57. □

The next theorem implements an adapted schedule. It is comparable to Theorem 1.32.

Theorem 1.59. *Let H_s be a norm-continuous bounded time-dependent Hamiltonian that is twice continuously differentiable. Suppose $\sigma(H_s) \cap [b_0(s), b_1(s)]$ consists of at most m eigenvalues and Assumption 3 holds. Take $C \ge 0$ such that*

$$C \ge m \max_{s\in[0,1]} \Big(\big(2 + p|g_0'|B_{3-p}\big)\|PH'Q\| + \|PH''Q\| + 5\sqrt{m}B_{3-p}\|PH'Q\|\|H'\|\Big). \tag{1.369}$$

Fix $\epsilon > 0$ and set

$$T = \frac{1}{\epsilon}\frac{C}{g_0^p g_{0m}^{2-p}} \tag{1.370}$$

Then the evolved statehas fidelity $F \ge 1 - \epsilon$. The total evolution time satisfies

$$\frac{1}{\epsilon}\frac{CB_p}{g_{0m}}. \tag{1.371}$$

Proof. Two claims need to be proved: firstly that $1 - F \leq \epsilon$ and secondly that the algorithm finishes in a time bounded by (1.371).
For the first claim, Corollary 1.57 gives a bound on $1-F$. This theorem can be applies since x^p is Lipschitz on $[g_{0m}, \max_s \|H_s\|]$, so T^{-1} is absolutely continuous. We just need to show that it evaluates to something smaller than ϵ in this case. First observe that

$$\left|\left(\frac{1}{T}\right)'\right| = \frac{|T'|}{T^2} = \frac{\epsilon g_{0m}^{2-p}}{C} p g_0^{p-1} |g_0'|. \tag{1.372}$$

Then the claim follows from the following calculation:

$$\begin{aligned}
1 - F &\leq m \frac{\|PH'Q\|}{Tg^2}\Big|_{s=0} + m\frac{\|PH'Q\|}{Tg^2}\Big|_{s=1} + \int_0^1 \left|\left(\frac{1}{T}\right)'\right| m \frac{\|PH'Q\|}{g^2}\,\mathrm{d}s \\
&\quad + \int_0^1 \left(\frac{m}{g^2}\|PH''Q\| + 3\frac{m\sqrt{m}}{g^3}\|PH'Q\|\|H'\| + 2\frac{m\sqrt{m}}{g^3}\|PH'Q\|^2\right)\mathrm{d}s && (1.373)\\
&\leq m\frac{\epsilon}{C}\Bigg(\frac{\|PH'Q\|}{g_{0m}^{p-2} g_0^{-p} g^2}\bigg|_{s=0} + \frac{\|PH'Q\|}{g_{0m}^{p-2} g_0^{-p} g^2}\bigg|_{s=1} + \int_0^1 p|g_0'| g_{0m}^{2-p} g_0^{p-1} \frac{\|PH'Q\|}{g^2}\,\mathrm{d}s \\
&\quad + \int_0^1 \left(\frac{\|PH''Q\|}{g_{0m}^{p-2} g_0^{-p} g^2} + 5\sqrt{m}\frac{\|PH'Q\|\|H'\|}{g_{0m}^{p-2} g_0^{-p} g^3}\right)\mathrm{d}s\Bigg) && (1.374)\\
&\leq m\frac{\epsilon}{C}\Bigg(\|PH'Q\|\Big|_{s=0} + \|PH'Q\|\Big|_{s=1} + \int_0^1 p|g_0'|\frac{\|PH'Q\|}{g_{0m}^{p-2} g_0^{3-p}}\,\mathrm{d}s \\
&\quad + \int_0^1 \left(\|PH''Q\| + 5\sqrt{m}\frac{\|PH'Q\|\|H'\|}{g_{0m}^{p-2} g_0^{3-p}}\right)\mathrm{d}s\Bigg) && (1.375)\\
&\leq m\frac{\epsilon}{C}\max_{s\in[0,1]}\Big(\big(2 + p|g_0'|B_{3-p}\big)\|PH'Q\| + \|PH''Q\| + 5\sqrt{m}B_{3-p}\|PH'Q\|\|H'\|\Big) \\
& && (1.376)\\
&\leq \epsilon. && (1.377)
\end{aligned}$$

Finally the time complexity of the algorithm is bounded by

$$\begin{aligned}
\int_0^1 T\,\mathrm{d}s &= \frac{C}{\epsilon g_{0m}^{2-p}}\int_0^1 \frac{1}{g_0^p}\,\mathrm{d}s \\
&\leq \frac{1}{\epsilon}\frac{CB_p}{g_{0m}}.
\end{aligned}$$

□

The only difference between this theorem and Theorem 1.32 is the fact that it bounds the infidelity, rather than the square root of the infidelity. This is not too much of a drawback, since in most cases the optimal strategy is probably to use adiabatic methods to obtain a state with constant overlap with the desired state and then to use something like eigenstate filtering [54] to improve the fidelity. This should yield a complexity that scales as $\log(\epsilon^{-1})$, rather than $1/\epsilon$ or $1/\sqrt{\epsilon}$. See also Theorem 1.46.

Chapter 2

Paths of Hamiltonians

In this chapter several time-dependent Hamiltonians are introduced to solve various algorithmic problems.

2.1 Adiabatic Grover

Problem

Suppose we have a set $\mathcal{N}$ of N items, some of which are marked. The marked items form a subset $\mathcal{M}$ of size M. Suppose we have an oracle that tells us whether an object is marked or not:

$$f : \mathcal{N} \to \{0,1\} : x \mapsto \begin{cases} 0 & (x \in \mathcal{M}) \\ 1 & (x \notin \mathcal{M}) \end{cases}$$

The problem is to find any marked item.

Classically we need to check $\Theta(N/M)$ items on average. Grover's algorithm allows this problem to be solved in a time that is $O(\sqrt{N/M})$. There are several variants of Grover's algorithm. The original [6] is circuit-based. There is also an analogue version [57]. Our focus here will be on the adiabatic version, first introduced in [14]. The initial proposal of the adiabatic version had a time complexity $O(N)$. It was realised in [36] and [37] that using an adapted schedule could improve the complexity to $O(\sqrt{N})$.

2.1.1 The time-dependent Hamiltonian

We assume the elements in $\mathcal{N}$ correspond to the elements of an orthonormal basis of some Hilbert space $\mathcal{H}$. Then the elements in $\mathcal{M}$ define a subspace. Let $|u\rangle \coloneqq \frac{1}{\sqrt{N}} \sum_{x\in\mathcal{N}} |n\rangle$ be the uniform superposition of all basis elements. Set

$$H_0 = \mathbb{1} - |u\rangle\langle u| \tag{2.1}$$

and

$$H_1 = \mathbb{1} - \sum_{m\in\mathcal{M}} |m\rangle\langle m| = \begin{pmatrix} 0 & 0 \\ 0 & \mathbb{1}_{N-M} \end{pmatrix}. \tag{2.2}$$

The time-dependent Hamiltonian that will be considered is the linear interpolation $H_s = (1 - s)H_0 + sH_1$. The ground state of H_0 is relatively easy to prepare: it is the uniform superposition.

The ground space of H_1 consists of superpositions of marked elements, which are what we want to find.
The next step is to investigate the spectrum, and in particular the spectral gap g. This quest is simplified by the matrix determinant lemma.

Lemma 2.1 (Matrix determinant lemma)**.** *Let A be an invertible matrix and $|\psi\rangle, |\varphi\rangle$ vectors. Then*

$$\det\big(A + |\psi\rangle\langle\varphi|\big) = \big(1 + \langle\varphi|A^{-1}|\psi\rangle\big)\det(A). \tag{2.3}$$

The Hamiltonian H_s can be rewritten as

$$H_s = (1-s)H_0 + sH_1 = \begin{pmatrix} (1-s)\mathbb{1}_M & 0 \\ 0 & \mathbb{1}_{N-M} \end{pmatrix} + (s-1)|u\rangle\langle u|. \tag{2.4}$$

Then, setting $A := \begin{pmatrix} (1-s-\lambda)\mathbb{1}_M & 0 \\ 0 & (1-\lambda)\mathbb{1}_{N-M} \end{pmatrix}$ for some $\lambda \in \mathbb{C}$, and using Lemma 2.1 gives

$$\begin{aligned} \det(H(s)-\lambda) &= \det(A)\Big(1 + (s-1)\langle u|A^{-1}|u\rangle\Big) && (2.5) \\ &= (1-s-\lambda)^M(1-\lambda)^{N-M}\Big(1 + \frac{M(s-1)}{(1-s-\lambda)N} + \frac{(N-M)(s-1)}{(1-\lambda)N}\Big) && (2.6) \\ &= (1-s-\lambda)^{M-1}(1-\lambda)^{N-M-1}\Big(\lambda^2 - \lambda + s(1-s)\frac{N-M}{N}\Big). && (2.7) \end{aligned}$$

It is now clear that there are four distinct eigenvalues (assuming $1 \neq M \neq N-1$; in these cases there are only three):

$$\begin{aligned} \lambda_{0,1} &= \frac{1}{2}\Bigg(1 \pm \sqrt{1 - 4\Big(1 - \frac{M}{N}\Big)s(1-s)}\Bigg) && \text{with multiplicity } 1 \\ \lambda_2 &= 1-s && \text{with multiplicity } M-1 \\ \lambda_3 &= 1 && \text{with multiplicity } N-M-1. \end{aligned}$$

These eigenvalues are plotted in Figure 2.1. The relevant spectral gap is

$$\begin{aligned} g(s) = \lambda_1(s) - \lambda_0(s) &= \sqrt{1 - 4\Big(1 - \frac{M}{N}\Big)s(1-s)} && (2.8) \\ &= \sqrt{\frac{M}{N} + 4\Big(1 - \frac{M}{N}\Big)\Big(\frac{1}{2} - s\Big)^2}. && (2.9) \end{aligned}$$

In principle one should be worried about the fact that the gap with λ_2 is very small, but actually the associated eigenspace is completely decoupled: the Hilbert space $\mathcal{H}$ can be written as a direct sum of the eigenspace of $\{\lambda_0, \lambda_1\}$ and $\{\lambda_2, \lambda_3\}$. Crucially this decomposition is s-independent! Therefore, if the initial state has no overlap with the eigenspace associated with $\{\lambda_2, \lambda_3\}$, then it will never evolve into this subspace. We may effectively ignore λ_2 and λ_3.
To see that the spaces decouple, let $|\psi\rangle$ be an eigenvector with eigenvalue $1-s$. Note that $|u\rangle\langle u||\psi\rangle$ is some multiple of $|u\rangle$, so all its components are the same. Considering the first component of $H_s|\psi\rangle$ (see (2.4)), we see that this multiple must be zero. This means that the eigenspace associated with $1-s$ is the corresponding eigenspace of

$$\begin{pmatrix} (1-s)\mathbb{1}_M & 0 \\ 0 & \mathbb{1}_{N-M} \end{pmatrix}, \tag{2.10}$$

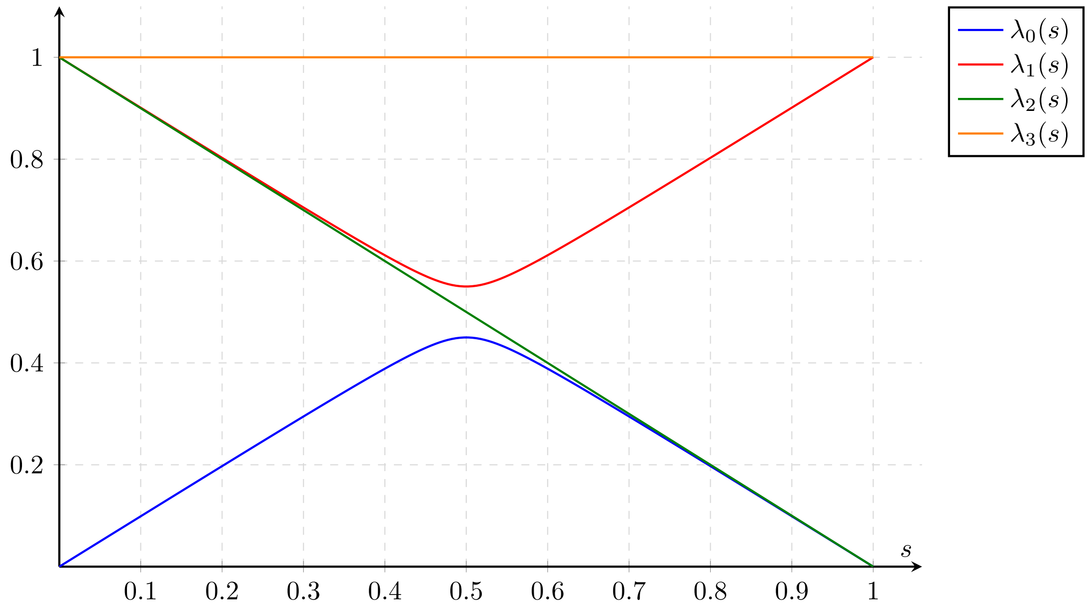


Figure 2.1: A plot of the spectrum of the time-dependent Hamiltonian H_s of (2.4).

with the additional requirement that $|u\rangle\langle u||\psi\rangle = 0$. This space is independent of s.
It is straightforward to see that $g_m = g(1/2) = \sqrt{M/N}$. We also show that this gap satisfies Assumption 3.

Lemma 2.2. *For all $p > 1$ and g given by (2.9), we have*

$$\int_0^1 \frac{1}{g(s)^p}\,\mathrm{d}s \leq \frac{6p-2}{3(p-1)}\sqrt{M/N}^{1-p} = O\big(g_m^{1-p}\big), \tag{2.11}$$

and, for $p = 1$,

$$\int_0^1 \frac{1}{g(s)}\,\mathrm{d}s \leq 2 + 2\ln(N/M) = O\big(\ln(g_m^{-1})\big). \tag{2.12}$$

Proof. If $\sqrt{M/N} \geq 1/2$, then

$$\int_0^1 \frac{1}{g(s)^p}\,\mathrm{d}s \leq \frac{1}{g_m^p} = \frac{1}{\sqrt{M/N}^p} \leq 2\sqrt{M/N}^{1-p} = 2g_m^{1-p}. \tag{2.13}$$

The result follows because

$$2 = \frac{6(p-1)}{3(p-1)} \leq \frac{6p-2}{3(p-1)}. \tag{2.14}$$

From now on suppose $\sqrt{M/N} \leq 1/2$. Note that $g(s)$ is symmetric about $s = 1/2$. It is also strictly decreasing on $[0, 1/2]$, going from 1 to a minimum of $\sqrt{M/N}$. This gives the decomposition

$$\int_0^1 \frac{1}{g(s)^p}\,\mathrm{d}s = 2\int_0^{1/2} \frac{1}{g(s)^p}\,\mathrm{d}s \tag{2.15}$$

$$= 2\Big(\int_0^{1/2-\sqrt{M/N}} \frac{1}{g(s)^p}\,\mathrm{d}s + \int_{1/2-\sqrt{M/N}}^{1/2} \frac{1}{g(s)^p}\,\mathrm{d}s\Big). \tag{2.16}$$

Since g has a minimum of $g_m = \sqrt{M/N}$, we can bound the second integral by

$$\int_{1/2-\sqrt{M/N}}^{1/2} \frac{1}{g(s)^p}\,\mathrm{d}s \le \sqrt{\frac{M}{N}}\frac{1}{g_m^p} = \frac{\sqrt{M/N}}{\sqrt{M/N}^p} = \sqrt{N/M}^{1-p}.$$

For the first integral, we write

$$\begin{aligned}\int_0^{1/2-\sqrt{M/N}} \frac{1}{g(s)^p}\,\mathrm{d}s &= \int_1^{g\left(1/2-\sqrt{M/N}\right)} \frac{1}{g^p}\frac{\mathrm{d}s}{\mathrm{d}g}\,\mathrm{d}g &(2.17)\\ &= \int_{g\left(1/2-\sqrt{M/N}\right)}^1 \frac{1}{g^p}\Big(-\frac{\mathrm{d}s}{\mathrm{d}g}\Big)\,\mathrm{d}g &(2.18)\\ &\le \int_{g_m}^1 \frac{1}{g^p}\Big(-\frac{\mathrm{d}s}{\mathrm{d}g}\Big)\,\mathrm{d}g. &(2.19)\end{aligned}$$

We can invert (2.9) to obtain $s = \frac{1}{2} - \frac{1}{2}\sqrt{1-\frac{1-g^2}{1-N/M}}$. Then

$$-\frac{\mathrm{d}s}{\mathrm{d}g} = \frac{g}{2\sqrt{(1-M/N)(g^2-M/N)}}. \tag{2.20}$$

and

$$\begin{aligned}\int_0^{1/2-\sqrt{M/N}} \frac{1}{g^p}\,\mathrm{d}s &\le \int_{\sqrt{\frac{M}{N}}}^1 \frac{1}{g^p}\Big(-\frac{\mathrm{d}s}{\mathrm{d}g}\Big)\,\mathrm{d}g &(2.21)\\ &= \int_{\sqrt{\frac{M}{N}}}^1 \frac{1}{g^p}\frac{g}{2\sqrt{(1-M/N)(g^2-M/N)}}\,\mathrm{d}g &(2.22)\\ &\le \int_{\sqrt{\frac{M}{N}}}^1 \frac{1}{g^p}\frac{g}{2\sqrt{(1-M/N)(g^2-g^2/4)}}\,\mathrm{d}g &(2.23)\\ &= \frac{1}{\sqrt{3(1-M/N)}}\int_{\sqrt{\frac{M}{N}}}^1 \frac{1}{g^p}\,\mathrm{d}g &(2.24)\\ &= \frac{2}{3}\int_{\sqrt{\frac{M}{N}}}^1 \frac{1}{g^p}\,\mathrm{d}g. &(2.25)\end{aligned}$$

If $p > 1$, then

$$\int_{\sqrt{\frac{M}{N}}}^1 \frac{1}{g^p}\,\mathrm{d}g = \frac{1}{p-1}\frac{1}{g^{p-1}}\bigg|_1^{\sqrt{M/N}} = \frac{1}{p-1}\bigg(\frac{1}{\sqrt{M/N}^{p-1}}-1\bigg) \le \frac{1}{p-1}\frac{1}{\sqrt{M/N}^{p-1}} \tag{2.26}$$

and the result follows.
If $p = 1$, then

$$\int_{\sqrt{\frac{M}{N}}}^1 \frac{1}{g^p}\,\mathrm{d}g = \ln(N/M) \tag{2.27}$$

and the result follows. □

Corollary 2.3. *The Hamiltonian* (2.4) *satisfies Assumption 3 for any* $p \in\,]1,2[$ *with*

$$B(p) = \frac{6p-2}{3(p-1)}. \tag{2.28}$$

In order to apply the procedures, a couple more quantities need to be bounded: $\|H_s'\| = \|H_1 - H_0\| \leq 2$, $\|H_s''\| = 0$ and

$$|g'| = \left| \frac{4(1-\frac{M}{N})(\frac{1}{2}-s)}{g} \right| \tag{2.29}$$

$$\leq 2\frac{\sqrt{4(1-\frac{M}{N})(\frac{1}{2}-s)^2}}{g} \tag{2.30}$$

$$\leq 2\frac{\sqrt{\frac{M}{N}+4(1-\frac{M}{N})(\frac{1}{2}-s)^2}}{g} = 2\frac{g}{g} = 2. \tag{2.31}$$

2.1.2 Algorithms derived from H_s

By direct application of the theorems, the following algorithms produce a state in the marked subspace with fidelity ϵ:

- Adiabatic evolution with a constant rate

$$T = \frac{1}{\sqrt{\epsilon}}\Big(\frac{64}{3}\sqrt{2}\frac{N}{M} + 4\Big). \tag{2.32}$$

  This is given by Theorem 1.27. Note that this requires an annealer that can implement H_s.

- Adiabatic evolution with an adapted rate

$$T = \frac{1}{\sqrt{\epsilon}}\left(4p - \frac{2}{3} + 16\sqrt{2} + \frac{\big(90+104\sqrt{2}\big)p - 128 - 104\sqrt{2}}{3(p-1)(2-p)}\right)\frac{\sqrt{N/M}^{2-p}}{g^p} \tag{2.33}$$

  which has time complexity

$$\int_0^1 T\,\mathrm{d}s \leq \frac{1}{\sqrt{\epsilon}}\left(4+8p+32\sqrt{2}\frac{176\big(1-\sqrt{2}\big) + \big(828+256\sqrt{2}\big)p - \big(500+432\sqrt{2}\big)p^2}{9(p-1)^2(q-2)}\right)\sqrt{N/M}. \tag{2.34}$$

  For example, setting $p = 3/2$ gives a rate of

$$T = \frac{1}{\sqrt{\epsilon}}\frac{152+112\sqrt{2}}{3}\frac{(N/M)^{1/4}}{g^{3/2}} \tag{2.35}$$

  and a time complexity of

$$\int_0^1 T\,\mathrm{d}s \leq \frac{1}{\sqrt{\epsilon}}\frac{2128+1568\sqrt{2}}{9}\sqrt{N/M}. \tag{2.36}$$

  This is given by Theorem 1.33 and also requires and annealer that can implement H_s.

- Poisson-distributed phase randomisation with a constant rate

$$\lambda = \frac{1}{\epsilon}\Big(4 + \frac{160}{3}\sqrt{N/M}\Big) \tag{2.37}$$

  has a time complexity of

$$t_0\lambda\int_0^1 \frac{1}{g}\,\mathrm{d}s \leq \frac{2.33}{\epsilon}\Big(4+\frac{160}{3}\sqrt{N/M}\Big)\Big(2+2\ln(N/M)\Big). \tag{2.38}$$

  This is given by Theorem 1.44.

- Poisson-distributed phase randomisation with an adapted rate

$$\lambda = \frac{1}{\epsilon}\Big(4p + \frac{58}{3} - \frac{208}{3(p-2)}\Big)\frac{\sqrt{N/M}^{2-p}}{g^{p-1}} \tag{2.39}$$

has a time complexity of

$$t_0 \int_0^1 \frac{\lambda}{g}\,\mathrm{d}s \leq \frac{2.33}{\epsilon}\Big(8p + 44 + \frac{144 + 968p}{9(p-1)(2-p)}\Big)\sqrt{N/M}. \tag{2.40}$$

For example, setting $p = 3/2$ gives a rate of

$$\lambda = \frac{88}{\epsilon}\frac{(N/M)^{1/4}}{\sqrt{g}} \tag{2.41}$$

and a time complexity of

$$t_0 \int_0^1 \frac{\lambda}{g}\,\mathrm{d}s \leq \frac{2.33}{\epsilon}\frac{1232}{3}\sqrt{N/M}. \tag{2.42}$$

This is given by Theorem 1.45.

In order to give a precise cost for the Poisson-distributed discrete adiabatic theorem, the cost of implementing the qubitised Hamiltonian should be bounded. In addition bounds on $\|U'\|$ and $\|U''\|$ should be developed. On the other hand, these can be taken to be constants, so asymptotic complexities can still be stated. With a constant rate, the asymptotic complexity is $O(N/M)$ and with an adapted rate the asymptotic complexity is $O(\sqrt{N/M})$. This follows from Theorem 1.51 and Theorem 1.52.
Notice that all the time complexities with adapted schedules are very similar. Of the variants with constant schedule, phase randomisation is asymptotically best. This is because the phase randomisation procedure is itself adapted to the size of the gap. If there is no knowledge of the gap at all, then it would have the same asymptotic complexity as the rest.

2.2 The linear systems of equations problem

The Quantum Linear Systems Problem (QLSP) was introduced in [58] and serves as a subroutine for many quantum algorithms.

Problem

Suppose A is an invertible $N \times N$ matrix $b \in \mathbb{C}^N$ a vector. The goal is to prepare the quantum state $\frac{A^{-1}|b\rangle}{\|A^{-1}|b\rangle\|}$.

The complexity of the algorithms will essentially depend on the condition number $\kappa = \|A\|\,\|A^{-1}\|$, which is always greater than one. The dependence on the dimension will be hidden by the assumption that we have access to a block encoding of A.
We may restrict ourselves to Hermitian matrices because we can use the following trick from [58]: If A is not Hermitian, we consider the matrix $\begin{pmatrix} 0 & A \\ A^* & 0 \end{pmatrix}$, which has the same condition number, and solve the equation $\begin{pmatrix} 0 & A \\ A^* & 0 \end{pmatrix}|y\rangle = \begin{pmatrix} |b\rangle \\ 0 \end{pmatrix}$.

First the matrix A is rescaled to $\frac{A}{\|A\|}$, which is necessary for there to be a block encoding of A. This has the effect of shifting the lowest singular value from $\frac{1}{\|A^{-1}\|}$ to $\frac{1}{\|A\|\|A^{-1}\|} = \kappa^{-1}$. Now we consider a path of Hamiltonians that was introduced in [43]. Define $A(s) \coloneqq (1-s)\sigma_z \otimes \mathbb{1} + s\sigma_x \otimes A$, $Q_{b,+} \coloneqq \mathbb{1} - \big(|+\rangle|b\rangle\big)\big(\langle+|\langle b|\big)$ and $\sigma_\pm \coloneqq \frac{1}{2}\big(\sigma_x \pm i\sigma_y\big)$. Set

$$H(s) = \sigma_+ \otimes \big(A(s)Q_{b,+}\big) + \sigma_- \otimes \big(Q_{b,+}A(s)\big). \tag{2.43}$$

This can be written as a linear interpolation $H(s) = (1-s)H_0 + sH_1$, where

$$H_0 \coloneqq \sigma_+ \otimes \big((\sigma_z \otimes \mathbb{1})Q_{b,+}\big) + \sigma_- \otimes \big(Q_{b,+}(\sigma_z \otimes \mathbb{1})\big) \tag{2.44}$$

$$H_1 \coloneqq \sigma_+ \otimes \big((\sigma_x \otimes A)Q_{b,+}\big) + \sigma_- \otimes \big(Q_{b,+}(\sigma_x \otimes A)\big). \tag{2.45}$$

Following the analysis of [43], we see that $H(s)$ has 0 as an eigenvalue for all $s \in [0,1]$. The corresponding eigenspace is spanned by $\{|0\rangle \otimes |x(s)\rangle, |1\rangle \otimes |+\rangle|b\rangle\}$, where $|x(s)\rangle \coloneqq \frac{A(s)^{-1}|b\rangle}{\|A(s)^{-1}|b\rangle\|}$. Since $H(s)$ does not allow transition between these states, we are sure to not prepare $|1\rangle \otimes |+\rangle|b\rangle$, so long as we start with $|0\rangle \otimes |x(0)\rangle$.
In [43] it was also shown that the eigenvalue zero is separated from the rest of the spectrum by a gap that is at least

$$g_0(s) = \sqrt{(1-s)^2 + \left(\frac{s}{\kappa}\right)^2}. \tag{2.46}$$

It is not hard to work out that this g_0 has a minimum $g_{0m} = \sqrt{\frac{1}{\kappa^2+1}}$ at $s = \frac{\kappa^2}{1+\kappa^2}$. Like in the Grover case, taking integrals reduces the order of the inverse gap.

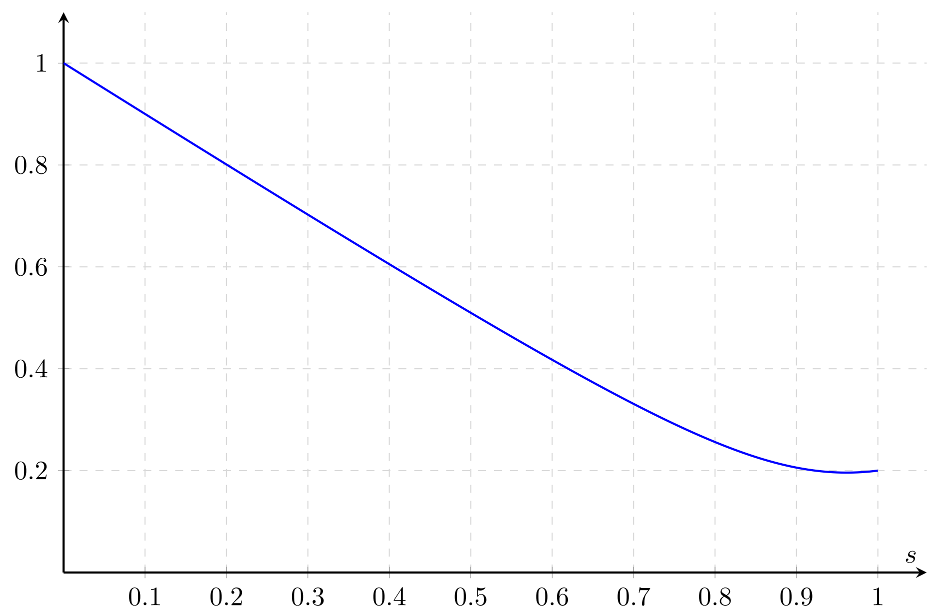


Figure 2.2: A plot of the bound on the gap in (2.46), with $\kappa = 5$.

Lemma 2.4. *For all $p > 1$ and g given by (2.46), we have*

$$\int_0^1 \frac{1}{g_0(s)^p}\,\mathrm{d}s \le (\sqrt{2}\kappa)^{p-2} + \frac{\sqrt{2}^{p-3}}{p-1}\kappa^{p-1} \tag{2.47}$$

$$= O\big(\kappa^{p-1}\big) = O\big(g_{0m}^{1-p}\big), \tag{2.48}$$

and, for $p = 1$,

$$\int_0^1 \frac{1}{g_0(s)}\,\mathrm{d}s \le \frac{1}{\sqrt{2}\kappa} + 12\ln(\kappa) \tag{2.49}$$

$$= O\big(\ln(\kappa)\big) = O\big(\ln(g_{0m}^{-1})\big). \tag{2.50}$$

Proof. We note that $g_0(s)$ is strictly decreasing on $\left[0, 1-\frac{1}{\kappa^2+1}\right]$, going from 1 to a minimum of $\sqrt{\frac{1}{\kappa^2+1}}$. So

$$\int_0^1 \frac{1}{g_0(s)^p}\,\mathrm{d}s = \int_0^{1-\frac{1}{\kappa^2+1}} \frac{1}{g_0(s)^p}\,\mathrm{d}s + \int_{1-\frac{1}{\kappa^2+1}}^1 \frac{1}{g_0(s)^p}\,\mathrm{d}s. \tag{2.51}$$

Since g_0 has a minimum of $\sqrt{\frac{1}{\kappa^2+1}}$, the second integral is bounded by

$$\int_{1-\frac{1}{\kappa^2+1}}^1 \frac{1}{g_0(s)^p}\,\mathrm{d}s \le \frac{1}{\kappa^2+1}\big(\kappa^2+1\big)^{p/2} = \big(\kappa^2+1\big)^{p/2-1} \le (\sqrt{2}\kappa)^{p-2}. \tag{2.52}$$

For the first integral, write

$$\int_0^{1-\frac{1}{\kappa^2+1}} \frac{1}{g_0^p}\,\mathrm{d}s = \int_1^{g_0\left(1-\frac{1}{\kappa^2+1}\right)} \frac{1}{g_0^p}\frac{\mathrm{d}s}{\mathrm{d}g_0}\,\mathrm{d}g_0 \tag{2.53}$$

$$= \int_{g_0\left(1-\frac{1}{\kappa^2+1}\right)}^1 \frac{1}{g_0^p}\Big(-\frac{\mathrm{d}s}{\mathrm{d}g_0}\Big)\,\mathrm{d}g_0 \tag{2.54}$$

$$= \int_{\sqrt{\frac{1}{\kappa^2+1}}}^1 \frac{1}{g_0^p}\Big(-\frac{\mathrm{d}s}{\mathrm{d}g_0}\Big)\,\mathrm{d}g_0. \tag{2.55}$$

We can invert (2.46) on $\left[0, 1-\frac{1}{\kappa^2+1}\right]$ to obtain $s = \frac{\kappa^2}{\kappa^2+1}(1-g_0)$. Then we have

$$-\frac{\mathrm{d}s}{\mathrm{d}g_0} = \frac{\kappa^2}{\kappa^2+1}, \tag{2.56}$$

so, if $p > 1$,

$$\int_0^{1-\frac{1}{\kappa^2+1}} \frac{1}{g_0^p}\,\mathrm{d}s = \int_{\sqrt{\frac{1}{\kappa^2+1}}}^1 \frac{1}{g_0^p}\frac{\kappa^2}{\kappa^2+1}\,\mathrm{d}g_0 \tag{2.57}$$

$$= \frac{\kappa^2}{\kappa^2+1}\Big(\frac{1}{(p-1)g_0^{p-1}}\Big)\Big|_{g_0=1}^{g_0=\sqrt{\frac{1}{\kappa^2+1}}} \tag{2.58}$$

$$= \frac{\kappa^2}{\kappa^2+1}\frac{1}{p-1}\big((\kappa^2+1)^{(p-1)/2} - 1\big) \tag{2.59}$$

$$\le \frac{\sqrt{2}^{p-3}}{p-1}\kappa^{p-1}. \tag{2.60}$$

If $p = 1$, then

$$\int_0^{1-\frac{1}{\kappa^2+1}} \frac{1}{g_0^p}\,\mathrm{d}s = \int_{\sqrt{\frac{1}{\kappa^2+1}}}^1 \frac{1}{g_0}\frac{\kappa^2}{\kappa^2+1}\,\mathrm{d}g_0 \tag{2.61}$$

$$= \frac{\kappa^2}{2(\kappa^2+1)}\ln\left(\kappa^2+1\right) \tag{2.62}$$

$$\leq 1 + 2\ln(\kappa) \tag{2.63}$$

Adding both contributions gives the result. □

If p is restricted to the interval $]1,2]$ (which it is in Assumption 3), then the bound can be simplified.

Corollary 2.5. *The Hamiltonian* (2.43) *satisfies Assumption 3 for any* $p \in]1,2[$ *with*

$$B(p) = \frac{p}{p-1}. \tag{2.64}$$

In order to apply the procedures, a couple more quantities need to be bounded: $\|H_s'\| = \|H_1 - H_0\| \leq 2$, $\|H_s''\| = 0$ and

$$|g_0'| = \left|\frac{s-1+s/\kappa^2}{g_0}\right| \tag{2.65}$$

$$= \frac{\sqrt{(s-1+s/\kappa^2)^2}}{g_0} \tag{2.66}$$

$$= \frac{\sqrt{(1+1/\kappa^2)^2 s^2 - (1+1/\kappa^2)2s + 1}}{g_0} \tag{2.67}$$

$$\leq \frac{\sqrt{(1+1/\kappa^2)^2 s^2 - (1+1/\kappa^2)2s + (1+1/\kappa^2)}}{g_0} \tag{2.68}$$

$$= \sqrt{1+1/\kappa^2}\,\frac{g_0}{g_0} = \sqrt{1+1/\kappa^2} \leq \sqrt{2}. \tag{2.69}$$

2.2.1 Algorithms derived from H_s

By direct application of the theorems, the following algorithms produce a state that solves the quantum linear systems problem with fidelity ϵ:

- Adiabatic evolution with a constant rate

$$T = \frac{1}{\sqrt{\epsilon}}\left(4 + 4(2\sqrt{2}+1)\sqrt{2}\kappa + (10+16\sqrt{2})\kappa^2\right). \tag{2.70}$$

  This is given by Theorem 1.27. Note that this requires an annealer that can implement H_s.

- Adiabatic evolution with an adapted rate

$$T = \frac{1}{\sqrt{\epsilon}}\left(8 + 6\sqrt{2} + 2\sqrt{2}p + \frac{4+12\sqrt{2}}{2-p}\right)\frac{(1+\kappa^2)^{1-p/2}}{g_0^p} \tag{2.71}$$

which has time complexity

$$\int_0^1 T\,\mathrm{d}s \leq \frac{\sqrt{1+\kappa^2}}{\sqrt{\epsilon}}\left(8(1+\sqrt{2})+2\sqrt{2}p+\frac{16(1+\sqrt{2})+4(1+\sqrt{2})p}{(p-1)(2-p)}\right). \tag{2.72}$$

For example, setting $p = 3/2$ gives a rate of

$$T = \frac{1}{\sqrt{\epsilon}}\big(16+33\sqrt{2}\big)\frac{(1+\kappa^2)^{1/4}}{g_0^{3/2}} \tag{2.73}$$

and a time complexity of

$$\int_0^1 T\,\mathrm{d}s \leq \frac{1}{\sqrt{\epsilon}}\big(48+99\sqrt{2}\big)\sqrt{1+\kappa^2}. \tag{2.74}$$

This is given by Theorem 1.33 and also requires and annealer that can implement H_s.

- Poisson-distributed phase randomisation with a constant rate

$$\lambda = \frac{1}{\epsilon}\Big(18+18\sqrt{2}\kappa\Big) \tag{2.75}$$

has a time complexity of

$$t_0\lambda\int_0^1 \frac{1}{g}\,\mathrm{d}s \leq \frac{2.33}{\epsilon}\Big(18+18\sqrt{2}\kappa\Big)\Big(\frac{1}{\sqrt{2}\kappa}+12\ln(\kappa)\Big). \tag{2.76}$$

This is given by Theorem 1.44.

- Poisson-distributed phase randomisation with an adapted rate

$$\lambda = \frac{1}{\epsilon}\Big(20-4\sqrt{2}+2\sqrt{2}p+\frac{16+2\sqrt{2}}{2-p}\Big)\frac{\sqrt{1+\kappa^2}^{2-p}}{g_0^{p-1}} \tag{2.77}$$

has a time complexity of

$$t_0\int_0^1 \frac{\lambda}{g_0}\,\mathrm{d}s \leq \frac{2.33}{\epsilon}\Big(20-2\sqrt{2}+2\sqrt{2}p+\frac{4(10-\sqrt{2})+4(\sqrt{2}-1)p}{(p-1)(2-p)}\Big)\sqrt{1+\kappa^2}. \tag{2.78}$$

For example, setting $p = 3/2$ gives a rate of

$$\lambda = \frac{1}{\epsilon}\big(52+3\sqrt{2}\big)\frac{(1+\kappa^2)^{1/4}}{\sqrt{g_0}} \tag{2.79}$$

and a time complexity of

$$t_0\int_0^1 \frac{\lambda}{g}\,\mathrm{d}s \leq \frac{2.33}{\epsilon}\big(156+96\sqrt{2}\big)\sqrt{1+\kappa^2} \leq \frac{2.33}{\epsilon}\big(192+156\sqrt{2}\big)\kappa. \tag{2.80}$$

This is given by Theorem 1.45.

The Poisson-distributed discrete adiabatic theorems Theorem 1.51 and Theorem 1.52 can also be used. They constitute a randomised version of the discrete adiabatic technique of [46], which was the first paper to obtain optimal asymptotic scaling for the QLSP of $O(\kappa\ln(\epsilon^{-1}))$.[1] The techniques are very similar; operationally the only difference is the use of a deterministic schedule, rather than a stochastic one. For this reason it seems reasonable to expect that the additional bounds necessary to give precise complexity bounds for the Poisson-distributed discrete adiabatic theorem can be readily derived, but this is left for subsequent work.
The result of this work should yield constant bounds on $\|U'\|$ and $\|U''\|$. Then Theorem 1.51 gives an asymptotic complexity of $O(\kappa^2/\epsilon)$ and Theorem 1.52 an asymptotic complexity of $O(\kappa/\epsilon)$. Then eigenstate filtering can be used the improve the ϵ-dependence to $O\big(\kappa^2+\kappa\ln(\epsilon^{-1})\big)$ and $O\big(\kappa\ln(\epsilon^{-1})\big)$, respectively.

2.3 Diagonal Hamiltonian starting from a uniform superposition

The aim of this section is to generalise the analysis of the Grover Hamiltonian (2.4). Its focus overlaps with the paper [2], but presents slightly improved methods that yield slightly stronger results.
The improved techniques are developed in subsection 2.3.1. They allow the use of a weaker assumption, Assumption 5, and give a tighter bound on the gap Proposition 2.9.
The initial Hamiltonian H_0 is like the projector on the uniform superposition $\mathbb{1} - |u\rangle\langle u|$, except the identity is omitted: $H_0 = -|u\rangle\langle u|$. The final Hamiltonian H_1 can now be any Hamiltonian that is diagonal in the basis of which $|u\rangle$ is the uniform superposition. Together this is

$$H_s = (s-1)|u\rangle\langle u| + sH_1. \tag{2.81}$$

The main technical content of this section is the derivation of a bound on the gap of H_s.
The prototypical example of such a Hamiltonian, and one that has many algorithmic applications, is the Ising Hamiltonian

$$H_1 = \sum_{i<j} J_{i,j}\sigma_z^{(i)}\sigma_z^{(j)} + \sum_i h_i\sigma_z^{(i)}, \tag{2.82}$$

where the indices i,j range over lattice sites and $\sigma_z^{(i)}$ is the Pauli-Z-matrix at the lattice site i. One additional technical assumption about H_1 is made.

Assumption 5. *Let $\{E_k\}$ be the eigenvalues of H_1, $\{P_k\}$ the eigenprojectors and d_k the dimension of the k^{th} eigenspace. Let N be the total dimension of the space. Set*

$$A_1 \coloneqq \sum_{k\neq 0}\frac{d_k}{N}\frac{1}{E_k - E_0} \quad \text{and} \quad A_2 \coloneqq \sum_{k\neq 0}\frac{d_k}{N}\frac{1}{(E_k-E_0)^2}. \tag{2.83}$$

Then the following inequality is assumed to hold:

$$\frac{\sqrt{A_2}}{A_1} \leq \big(2+\sqrt{2}\big)^{-1}\sqrt{\frac{N}{d_0}}. \tag{2.84}$$

[1] We note here that there is also a more elementary algorithm that achieves the same scaling, [59].

This assumption is used in the proof of Lemma 2.8. This typically holds for Ising type Hamiltonians: $\frac{\sqrt{A_2}}{A_1}$ scales polynomially in the number of qubits, while N scales exponentially. This is weaker than the assumption in [2],[2] which requires that

$$\sqrt{\frac{d_0}{A_2 N}} \leq 0.01(E_1 - E_0). \tag{2.85}$$

In fact, it is fairly close to not being an assumption at all: The inequality

$$\frac{\sqrt{A_2}}{A_1} \leq \sqrt{N} \tag{2.86}$$

holds unconditionally.

Lemma 2.6. *Let H_1 be any Hamiltonian. Then*

$$\sqrt{\frac{A_2}{N}} \leq A_1 \leq \sqrt{A_2}. \tag{2.87}$$

Proof. For this proof it will be convenient to consider the sequence of energies including degeneracy: let E'_j be the eigenvalues of H_1, where each E_k is listed d_k times, so j ranges from 0 to $N-1$ and

$$A_1 = \sum_{j=d_0}^{N-1} \frac{1}{N} \frac{1}{E'_j - E'_0} \quad \text{and} \quad A_2 = \sum_{j=d_0}^{N-1} \frac{1}{N} \frac{1}{(E'_j - E'_0)^2}. \tag{2.88}$$

For the first inequality, we have

$$\frac{A_2}{N} = \sum_{j=d_0}^{N-1} \Big(\frac{1}{N} \frac{1}{E'_j - E'_0}\Big)^2 \leq \Big(\sum_{j=d_0}^{N-1} \frac{1}{N} \frac{1}{E'_j - E'_0}\Big)^2 = A_1^2. \tag{2.89}$$

For the second, let $\mathbf{v}$ be the vector of length N with components E'_j. Let $\mathbf{w}$ be the vector of length N with all components equal to one. Then the Cauchy-Schwarz inequality gives

$$N A_1 = \langle \mathbf{w}, \mathbf{v} \rangle \leq \|\mathbf{w}\| \, \|\mathbf{v}\| = \sqrt{N}\sqrt{N A_2}, \tag{2.90}$$

from which the result follows. □

Lemma 2.7. *Let $\lambda \in \mathbb{C}$. Then λ is an eigenvalue of H_s from* (2.81) if and only if *one of the following holds:*

- *$\lambda = sE_k$ and $d_k \geq 2$; or*
- *λ is a solution to the following equation*

$$0 = F(\lambda) := 1 - (1-s) \sum_{k=0} \frac{d_k}{N} \frac{1}{sE_k - \lambda}. \tag{2.91}$$

This result has been around for a while [34]. The spectrum of an instance of H_s is plotted in Figure 2.3.

[2] To see this, just note that $A_2/A_1 \leq 1/(E_1 - E_0)$.

Proof. The argument is very similar to the Grover case. First suppose λ is not an eigenvalue of sH_1, so $\lambda \mathbb{1} - sH_1$ is invertible. Now λ is an eigenvalue of H_s if and only if

$$0 = \det(\lambda \mathbb{1} - H_s) = \det\left(\lambda \mathbb{1} - sH_1 + (1-s)|u\rangle\langle u|\right) \tag{2.92}$$

$$= \det\left(\lambda \mathbb{1} - sH_1\right)\left(1 + (1-s)\left\langle u \left| \left(\lambda \mathbb{1} - sH_1\right)^{-1} \right| u \right\rangle\right) \tag{2.93}$$

$$= \det\left(\lambda \mathbb{1} - sH_1\right)\left(1 + (1-s)\sum_k \frac{d_k}{N}\frac{1}{\lambda - sE_k}\right). \tag{2.94}$$

Here we have used that $|u\rangle$ has an overlap $\sqrt{N}^{-1}$ with all eigenvectors of H_1. Since $\lambda \mathbb{1} - sH_1$ was assumed invertible, $\det\left(\lambda \mathbb{1} - sH_1\right) \neq 0$ and dividing by this recovers the equation (2.91). This just leaves the question of whether the values sE_k are eigenvalues. Note that $P_k|u\rangle \neq 0$, for all k. On the other hand, any eigenvector with eigenvalue sE_k must have zero overlap with $|u\rangle$ (the reasoning is identical to the Grover case). We conclude that such an eigenvector exists if and only if the dimension of the eigenspace is strictly greater than 1, i.e. $d_k \geq 2$. □

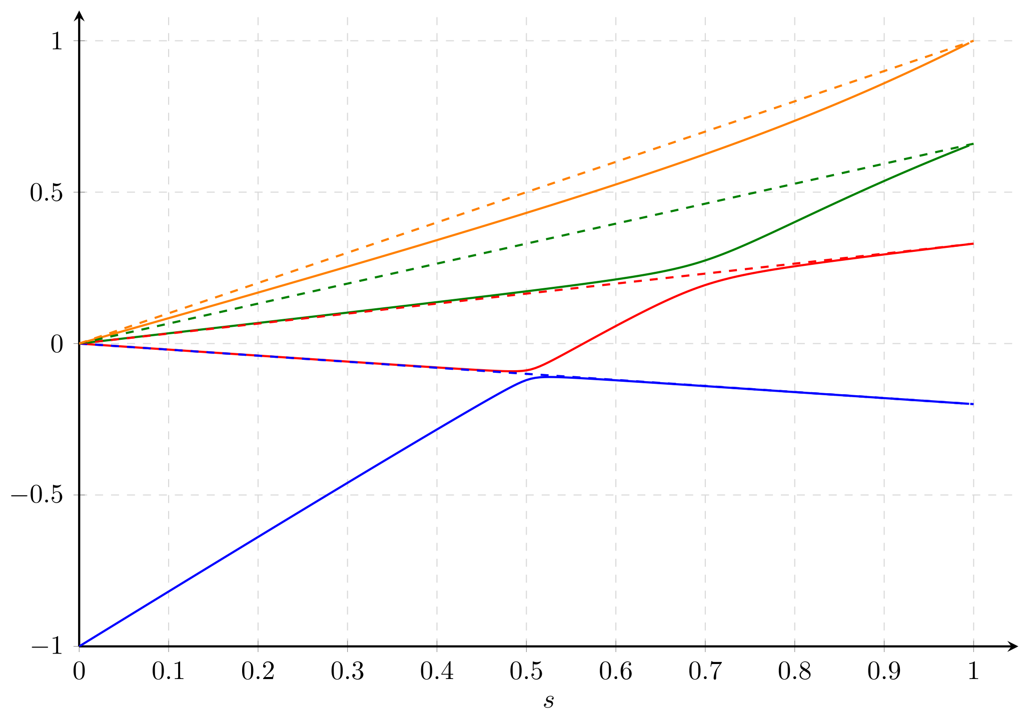


Figure 2.3: A plot of the spectrum of H_s from (2.81). The dashed lines represent the sE_k eigenvalues.

Equation 2.91 is usually not easy to solve in general, but we can learn some things about the solutions by studying the equation. Keeping a representative plot in mind, such as Figure 2.4a, will be helpful.

First note that F is a sum of decreasing functions, and so is decreasing. It has limits

$$\lim_{\lambda \to -\infty} F(\lambda) = 1 = \lim_{\lambda \to +\infty} F(\lambda) \tag{2.95}$$

and poles at sE_k, for all k. Consequently it must have the same number of solutions as H_1 has eigenvalues. The first solution lies to the left of sE_0 and the other solutions each lie in a different interval $[sE_k, sE_{k+1}]$. This can also be seen in Figure 2.3: each solid line lies inbetween two dashed lines.

Just like in the Grover case, we are not interested in the gap with the sE_k eigenvalues. Rather, we want to bound the distance between the smallest two solutions of (2.91); denote these roots λ_0 and λ_1. These lie either side of the line sE_0. In order to study these, it is convenient to make the substitution $\lambda = sE_0 + \delta$. Then the eigenvalue equation (2.91) becomes

$$\begin{aligned} F(\delta) &= 1 + (1-s)\frac{d_0}{N\delta} - (1-s)\sum_{k\neq 0}\frac{d_k}{N}\frac{1}{s(E_k - E_0) - \delta} && (2.96) \\ &= 1 + (1-s)\frac{d_0}{N\delta} - (1-s)\sum_{k\neq 0}\frac{d_k}{N}\Big(\frac{1}{s(E_k - E_0)} + \frac{\delta}{s(E_k - E_0)\big(s(E_k - E_0) - \delta\big)}\Big). && (2.97) \end{aligned}$$

Now the idea is to replace F with some other function that is easier to solve. If this new function (1) has a root left of sE_0 and (2) lies above F, then the root of the new function is an upper bound of λ_0. Similarly, if the new function (1) has a root between sE_0 and sE_1, and (2) lies below F, then the root of the new function is a lower bound of λ_1.

The details are developed in the next section.

2.3.1 Shifting F

First F is replaced by a new function F_0 such that $F_0 \leq F$ and F_0 has a root between sE_0 and sE_1. This corresponds to taking δ positive.

Next F is replaced by a function F_1 such that $F \leq F_1$ and F_1 has a root between $-\infty$ and sE_0. This corresponds to taking δ negative.

The functions F_0 and F_1 are illustrated in Figure 2.4.

2.3.1.1 Positive δ

Consider the function

$$F_0(\delta) \coloneqq 1 + (1-s)\frac{d_0}{N\delta} - (1-s)\Big(\frac{A_1}{s} + 2\frac{A_2\delta}{s^2}\Big). \tag{2.98}$$

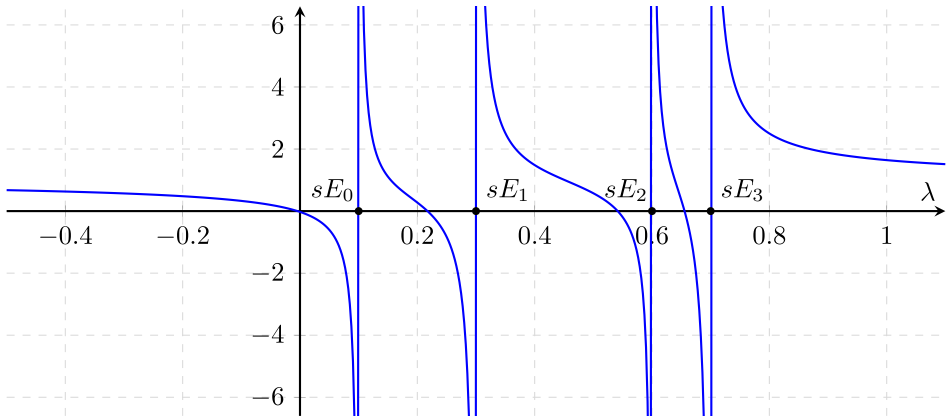
If $0 \leq \delta \leq s(E_1 - E_0)/2$, then $\delta \leq s(E_k - E_0)/2$ for all k. This implies $s(E_k - E_0) - \delta \geq s(E_k - E_0)/2$ and, comparing with (2.97), we see that $F_0(\delta) \leq F(\delta)$ for these values of δ.

Since $F_0(\delta) = 0$ is a quadratic equation, it has an explicit solution:

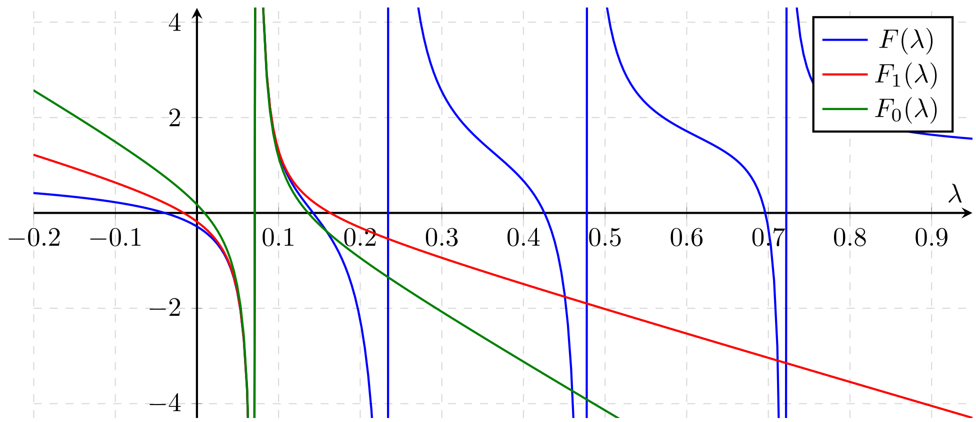
$$\delta = s\frac{\big(s - (1-s)A_1\big) \pm \sqrt{\big(s-(1-s)A_1\big)^2 + 8(1-s)^2A_2d_0/N}}{4(1-s)A_2}. \tag{2.99}$$

Only one of these solutions is positive; let it be denoted δ_0. Now two cases can be distinguished:

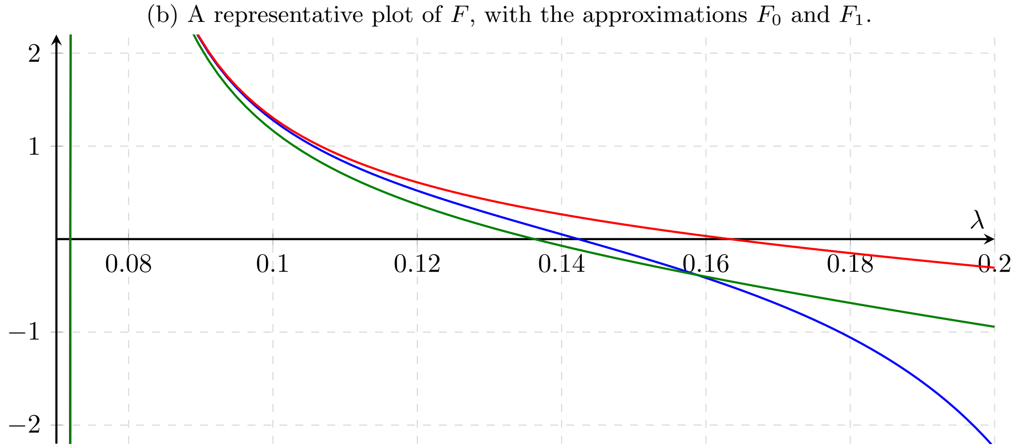
- if $\delta_0 \leq s(E_1 - E_0)/2$, then $0 = F_0(\delta_0) \leq F(\delta_0)$ and so $sE_0 + \delta_0$ is a lower bound of λ_1;
- if $\delta_0 \geq s(E_1 - E_0)/2$, then $F_0(\delta)$ is strictly positive on the interval $[0, s(E_1 - E_0)/2]$. Since $F(\delta) \geq F_0(\delta)$ on this interval, it must also be strictly positive. This implies that $\lambda_1 \geq s(E_1 - E_0)/2$.



(a) A representative plot of F, (2.91), with the poles sE_k marked.



(b) A representative plot of F, with the approximations F_0 and F_1.



(c) A close-up of figure (b).

Figure 2.4: Plots of F, F_0 and F_1

We conclude that $\lambda_1 \geq \min\{sE_0 + \delta_0, s(E_0 + E_1)/2\}$. This is illustrated in Figure 2.5.

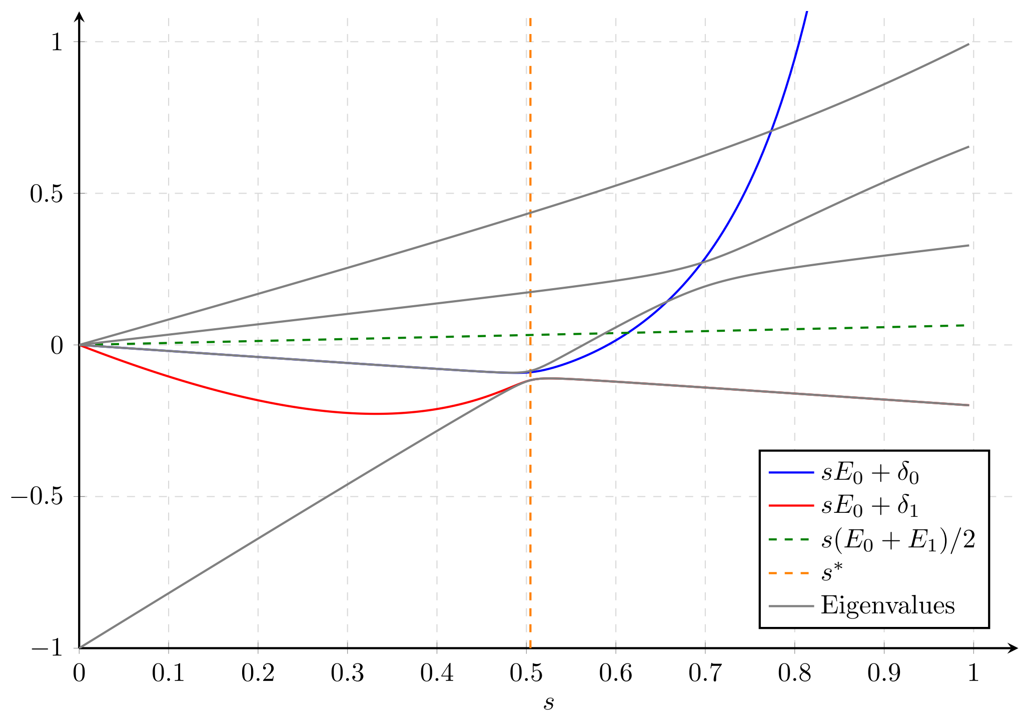


Figure 2.5: A plot of the bounds obtained by solving F_0 and F_1. The grey lines are the actual eigenvalues of H_s. The orange dashed line indicates $s = s^* := \frac{A_1}{1+A_1}$, which is the approximate location of the avoided crossing.

Note that δ_0 has a particularly simple form at $s = \frac{A_1}{1+A_1}$:

$$\delta_0\Big(\frac{A_1}{1+A_1}\Big) = \frac{A_1}{1+A_1}\sqrt{\frac{d_0}{2A_2N}}. \tag{2.100}$$

This location will be important in the analysis, so it is given a name: $s^* := \frac{A_1}{1+A_1}$. Next the derivative $\frac{\mathrm{d}\delta_0}{\mathrm{d}s}$ is computed using implicit differentiation:

$$\frac{\mathrm{d}\delta_0}{\mathrm{d}s} = -\frac{\partial_s F_0}{\partial_\delta F_0} \tag{2.101}$$

$$= \delta_0 \frac{A_1 N \delta_0 s^2 + 2A_2 N \delta_0^2 s + N(1-s)\delta_0(A_1 s + 4A_2\delta_0) - d_0 s^3}{s(1-s)(2A_2 N\delta_0^2 + d_0 s^2)}. \tag{2.102}$$

It will be useful to have a more convenient lower bound to the right of s^*. To derive this, note that $\delta_0(s) \geq s\sqrt{\frac{d_0}{2A_2N}}$ on this interval. This implies $d_0 s^3 \leq 2A_2N\delta_0^2 s$ and these two terms can be cancelled in the numerator. They can be combined in the denominator.

$$
\begin{aligned}
\frac{\mathrm{d}\delta_0}{\mathrm{d}s} &\geq \delta_0 \frac{A_1 N \delta_0 s^2 + N(1-s)\delta_0(A_1 s + 4A_2\delta_0)}{s(1-s)(2A_2 N\delta_0^2 + d_0 s^2)} && (2.103)\\
&\geq \delta_0 \frac{A_1 N \delta_0 s^2 + N(1-s)\delta_0(A_1 s + 4A_2\delta_0)}{4s(1-s)A_2 N\delta_0^2} && (2.104)\\
&= \frac{A_1 s^2 + (1-s)(A_1 s + 4A_2\delta_0)}{4s(1-s)A_2} && (2.105)\\
&= \frac{A_1 s}{4(1-s)A_2} + \frac{A_1}{4A_2} + \frac{\delta_0}{s} && (2.106)\\
&\geq \frac{A_1 s^*}{4(1-s^*)A_2} + \frac{A_1}{4A_2} && (2.107)\\
&= \frac{A_1(1+A_1)}{4A_2}. && (2.108)
\end{aligned}
$$

From this we see that δ_0 is strictly increasing on the interval $[s^*, 1]$ and also that

$$
\delta_0(s) \geq \frac{A_1}{1+A_1}\sqrt{\frac{d_0}{2A_2 N}} + \frac{A_1(1+A_1)}{4A_2}(s - s^*). \tag{2.109}
$$

This will be used to bound the gap.

2.3.1.2 Negative δ

Consider the function

$$
F_1(\delta) \coloneqq 1 + (1-s)\frac{d_0}{N\delta} - (1-s)\Big(\frac{A_1}{s} + \frac{A_2\delta}{s^2}\Big). \tag{2.110}
$$

When $\delta \leq 0$, we have $s(E_k - E_0) - \delta \geq s(E_k - E_0)$. This implies

$$
\frac{-\delta}{s(E_k - E_0)\big(s(E_k - E_0) - \delta\big)} \leq \frac{-\delta}{s^2(E_k - E_0)^2} \tag{2.111}
$$

and so $F(\delta) \leq F_1(\delta)$. Since $F_1(\delta) = 0$ is quadratic, it can be solved explicitly:

$$
\delta = s\frac{\big(s - (1-s)A_1\big) \pm \sqrt{\big(s - (1-s)A_1\big)^2 + 4(1-s)^2 A_2 d_0/N}}{2(1-s)A_2}. \tag{2.112}
$$

Clearly exactly one of these solutions is negative, so let δ_1 be the negative solution. Then $sE_0 + \delta_1$ is an upper bound of λ_0, which is illustrated in Figure 2.5.

Lemma 2.8. *Let H_s be a Hamiltonian of the form (2.81), that satisfies Assumption 5. Then*

$$
g(s) \geq \frac{A_1}{1+A_1}\sqrt{\frac{d_0}{2A_2 N}} \tag{2.113}
$$

for all $s^* - \frac{1}{(1+A_1)^2}\sqrt{\frac{A_2 d_0}{2N}} \leq s \leq s^*$.

Proof. The function $-\delta_1(s)$ lower bounds the gap in this interval. At $s = s^*$,

$$-\delta_1(s^*) = \frac{A_1}{1+A_1}\sqrt{\frac{d_0}{A_2 N}} \geq \frac{A_1}{1+A_1}\sqrt{\frac{d_0}{2A_2 N}}. \tag{2.114}$$

Now the proof is complete if we can show that $-\delta_1$ is decreasing on this interval or, equivalently, that δ_1 is increasing on this interval. To that end the derivative $\frac{\mathrm{d}\delta_1}{\mathrm{d}s}$ is computed using implicit differentiation:

$$\begin{aligned}
\frac{\mathrm{d}\delta_1}{\mathrm{d}s} &= -\frac{\partial_s F_1}{\partial_\delta F_1} && (2.115)\\
&= \delta_1 \frac{A_1 N \delta_1 s^2 + A_2 N \delta_1^2 s + N(1-s)\delta_1(A_1 s + 2A_2\delta_1) - d_0 s^3}{s(1-s)(A_2 N \delta_0^2 + d_0 s^2)} && (2.116)\\
&= |\delta_1| \frac{A_1 N|\delta_1|s^2 - A_2 N|\delta_1|^2 s + N(1-s)|\delta_1|(A_1 s - 2A_2|\delta_1|) + d_0 s^3}{s(1-s)(A_2 N|\delta_0|^2 + d_0 s^2)}. && (2.117)
\end{aligned}$$

We want to show that this quantity is positive, which will be accomplished by showing that $A_1 N|\delta_1|s^2 \geq A_2 N|\delta_1|^2 s$ and $A_1 s \geq 2A_2|\delta_1|$ (note that these inequalities are equivalent):

$$\begin{aligned}
2A_2\frac{|\delta_1(s)|}{s} &= \frac{\big((1-s)A_1 - s\big) + \sqrt{\big((1-s)A_1 - s\big)^2 + 4(1-s)^2 A_2 d_0/N}}{1-s}\\
&\leq 2\frac{(1-s)A_1 - s}{1-s} + 2\sqrt{A_2 d_0/N}\\
&\leq \frac{2}{1-s^*}\frac{(1+A_1)}{(1+A_1)^2}\sqrt{\frac{A_2 d_0}{2N}} + 2\sqrt{A_2 d_0/N}\\
&= (2+\sqrt{2})\sqrt{\frac{A_2 d_0}{N}} \leq A_1.
\end{aligned}$$

The Assumption 5 was used to obtain the last inequality. □

2.3.2 A bound using the variational principle

From Figure 2.5 we see that a reasonable bound on the gap can be constructed using a combination of $sE_0 + \delta_0$, $sE_0 + \delta_1$ and $s(E_0 + E_1)/2$ (i.e. the blue, red and green dashed lines) for all values of s in a neighbourhood of s^* (the orange dashed line) and above.

This just leaves an interval starting at $s = 0$. In this region a bound will be developed using the variational principle: $\langle\phi|H_s|\phi\rangle \geq \lambda_0$ for all unit vectors $|\phi\rangle$.

Consider the vector

$$|\phi\rangle = \frac{1}{\sqrt{A_2}}\sum_{k\neq 0}\frac{P_k|u\rangle}{E_k - E_0}. \tag{2.118}$$

Using $\langle u|P_k|u\rangle = \frac{d_k}{N}$, it is straightforward to see that it is a unit vector.

$$\lambda_0(s) \le \langle\phi|H_s|\phi\rangle = -(1-s)|\langle u|\phi\rangle|^2 + s\langle\phi|H_1|\phi\rangle \tag{2.119}$$

$$= -(1-s)\Big(\frac{A_1}{\sqrt{A_2}}\Big)^2 + sE_0 + s\langle\phi|(H_1 - E_0)|\phi\rangle \tag{2.120}$$

$$= -(1-s)\frac{A_1^2}{A_2} + sE_0 + s\frac{1}{A_2}\sum_{k\neq 0}\frac{(E_k - E_0)}{(E_k - E_0)^2}\langle u|P_k|u\rangle \tag{2.121}$$

$$= -(1-s)\frac{A_1^2}{A_2} + sE_0 + s\frac{A_1}{A_2} \tag{2.122}$$

$$= sE_0 - \frac{A_1}{A_2}\big(A_1 - s(1 + A_1)\big). \tag{2.123}$$

Since $\lambda_1 \ge sE_0$,

$$g(s) \ge sE_0 - \lambda_0(s) \ge \frac{A_1}{A_2}\big(A_1 - s(1 + A_1)\big). \tag{2.124}$$

This expression gives a positive bound on the gap, so long as $s \le \frac{A_1}{1+A_1}$. See Figure 2.6.

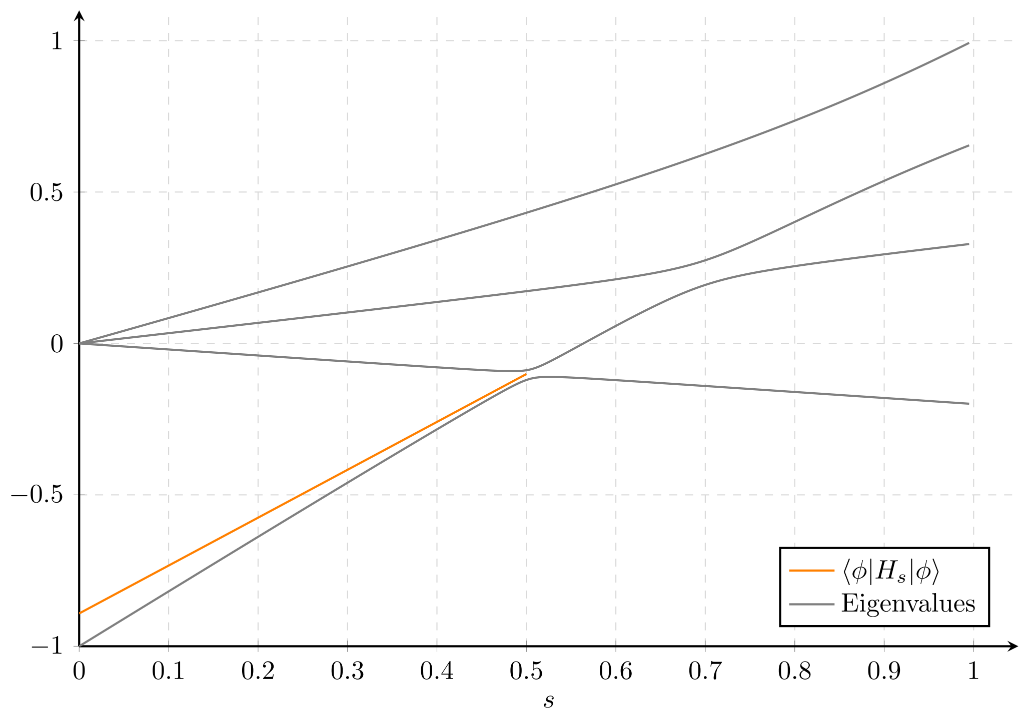


Figure 2.6: A bound on λ_0 using the variational principle.

For all $s \in \left[0, s^* - \frac{1}{(1+A_1)^2}\sqrt{\frac{A_2 d_0}{2N}}\right]$, we have

$$\begin{aligned} g(s) \geq sE_0 - \langle\phi|H_s|\phi\rangle &\geq \frac{A_1}{A_2}\Big(A_1 - s^*(1+A_1) + \frac{1}{(1+A_1)^2}\sqrt{\frac{A_2 d_0}{2N}}(1+A_1)\Big) \\ &= \frac{A_1}{1+A_1}\sqrt{\frac{d_0}{2A_2 N}} \end{aligned}$$

2.3.3 Bounding the gap

We are now ready to state and prove the bound g_0 on the gap. It is defined piecewise on four intervals:

- For $s \in \left[0, s^* - \frac{1}{(1+A_1)^2}\sqrt{\frac{A_2 d_0}{2N}}\right]$, we use the bound (2.124):

$$g_0(s) = \frac{A_1}{A_2}\big(A_1 - s(1+A_1)\big). \tag{2.125}$$

- For $s \in \left[s^* - \frac{1}{(1+A_1)^2}\sqrt{\frac{A_2 d_0}{2N}}, s^*\right]$, set

$$g_0(s) = \frac{A_1}{1+A_1}\sqrt{\frac{d_0}{2A_2 N}}. \tag{2.126}$$

- Let s^{**} be the point where $sE_0\delta_0$ crosses $s(E_0+E_1)/2$, i.e. the crossing of the blue and green dashed lines in Figure 2.5. On the interval $[s^*, s^{**}]$, $g(s)$ is lower bounded by $\delta_0(s)$, which in turn is lower bounded by

$$g_0(s) = \frac{A_1}{1+A_1}\sqrt{\frac{d_0}{2A_2 N}} + \frac{A_1(1+A_1)}{4A_2}(s - s^*). \tag{2.127}$$

- On the interval $[s^{**}, 1]$, set

$$g_0(s) = s\frac{E_1 - E_0}{2}. \tag{2.128}$$

In summary:

Proposition 2.9. *Let H_s be a Hamiltonian of the form (2.81), that satisfies Assumption 5. Then the function g_0 defined by*

$$g_0(s) = \begin{cases} \frac{A_1}{A_2}\big(A_1 - s(1+A_1)\big) & \Big(s \in \Big[0, s^* - \frac{1}{(1+A_1)^2}\sqrt{\frac{A_2 d_0}{2N}}\Big]\Big) \\ \frac{A_1}{1+A_1}\sqrt{\frac{d_0}{2A_2 N}} & \Big(s \in \Big[s^* - \frac{1}{(1+A_1)^2}\sqrt{\frac{A_2 d_0}{2N}}, s^*\Big]\Big) \\ \frac{A_1}{1+A_1}\sqrt{\frac{d_0}{2A_2 N}} + \frac{A_1(1+A_1)}{4A_2}(s - s^*) & \big(s \in [s^*, s^{**}]\big) \\ s\frac{E_1 - E_0}{2} & \big(s \in [s^{**}, 1]\big) \end{cases} \tag{2.129}$$

lower bounds the gap.

Proof. This follows from (2.124), Lemma 2.8 and (2.109). □

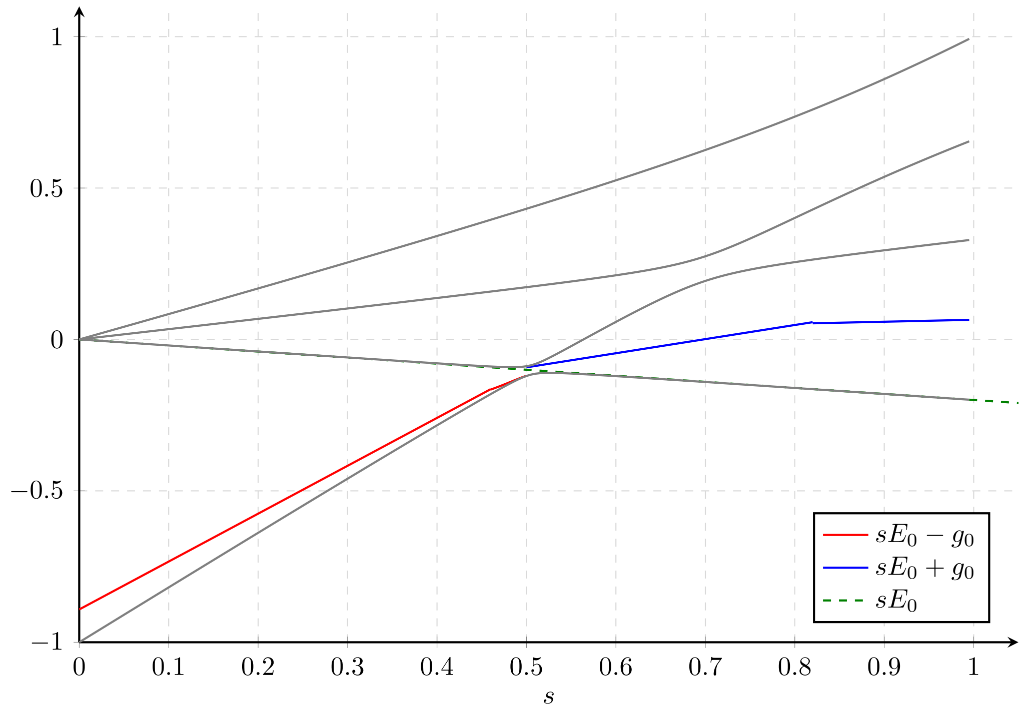


Figure 2.7: Left of s^*, the bound on the gap g_0 is the $\sqrt{2}^{-1}$ times the distance between the red line and sE_0. Right of s^*, g_0 is the distance between the red line and sE_0.

This bound is illustrated in Figure 2.7. Left of s^*, g_0 is $\sqrt{2}^{-1}$ times sE_0 minus the red line. Right of s^*, g_0 is sE_0 minus the blue line.

Proposition 2.10. *Let g_0 be as defined in* (2.129) *and $p > 1$. Then*

$$\int_0^1 \frac{1}{g_0(s)^p} \,\mathrm{d}s \leq \\ \left(\left(1 + \frac{5}{p-1}\right)\frac{A_2}{A_1(A_1+1)} + \left(\frac{2}{E_1 - E_0}\right)^p \frac{1}{p-1}\sqrt{\frac{d_0}{2A_2N}}^{p-1}\right)\left(\frac{A_1+1}{A_1}\sqrt{\frac{2A_2N}{d_0}}\right)^{p-1} \tag{2.130}$$

In typical applications the term $\left(\frac{2}{E_1-E_0}\right)^p \frac{1}{p-1}\sqrt{\frac{d_0}{2A_2N}}^{p-1}$ is exponentially small, since the total dimension is exponentially large, but $E_1 - E_0$ is only polynomially small.

Proof. The integral is split into the sum of four contributions:

$$\int_0^1 \frac{1}{g_0(s)^p} \,\mathrm{d}s = \\ \int_0^{s^* - \frac{1}{(1+A_1)^2}\sqrt{\frac{A_2 d_0}{2N}}} \frac{1}{g_0(s)^p}\,\mathrm{d}s + \int_{s^* - \frac{1}{(1+A_1)^2}\sqrt{\frac{A_2 d_0}{2N}}}^{s^*} \frac{1}{g_0(s)^p}\,\mathrm{d}s + \int_{s^*}^{s^{**}} \frac{1}{g_0(s)^p}\,\mathrm{d}s + \int_{s^{**}}^{1} \frac{1}{g_0(s)^p}\,\mathrm{d}s. \tag{2.131}$$

The first integral can be calculated as

$$\int_0^{s^*-\frac{1}{(1+A_1)^2}\sqrt{\frac{A_2 d_0}{2N}}} \frac{1}{g_0(s)^p}\,\mathrm{d}s = \Big(\frac{A_2}{A_1}\Big)^p \int_0^{s^*-\frac{1}{(1+A_1)^2}\sqrt{\frac{A_2 d_0}{2N}}} \big(A_1 - s(1+A_1)\big)^{-p}\,\mathrm{d}s \tag{2.132}$$

$$= \Big(\frac{A_2}{A_1}\Big)^p \left[\frac{\big(A_1 - s(1+A_1)\big)^{1-p}}{(p-1)(1+A_1)}\right]_0^{s^*-\frac{1}{(1+A_1)^2}\sqrt{\frac{A_2 d_0}{2N}}} \tag{2.133}$$

$$= \Big(\frac{A_2}{A_1}\Big)^p \frac{1}{(p-1)(1+A_1)} \left(\Big((1+A_1)\sqrt{\frac{2N}{A_2 d_0}}\Big)^{p-1} - \Big(\frac{1}{A_1}\Big)^{p-1}\right) \tag{2.134}$$

$$= \frac{A_2}{(p-1)A_1(A_1+1)}\Big(\frac{A_1+1}{A_1}\sqrt{\frac{2A_2N}{d_0}}\Big)^{p-1} - \Big(\frac{A_2}{A_1^2}\Big)^p \frac{A_1}{(1+A_1)(p-1)}. \tag{2.135}$$

The next integral gives

$$\int_{s^*-\frac{1}{(1+A_1)^2}\sqrt{\frac{A_2 d_0}{2N}}}^{s^*} \frac{1}{g_0(s)^p}\,\mathrm{d}s \le \frac{1}{(1+A_1)^2}\sqrt{\frac{A_2 d_0}{2N}}\Big(\frac{A_1+1}{A_1}\sqrt{\frac{2A_2N}{d_0}}\Big)^p \tag{2.136}$$

$$= \frac{A_2}{(1+A_1)A_1}\Big(\frac{A_1+1}{A_1}\sqrt{\frac{2A_2N}{d_0}}\Big)^{p-1} \tag{2.137}$$

$$\tag{2.138}$$

For the third integral, compare with (2.135). The dependence on s^{**} only shows up in the negative term, so we get an upper bound by ignoring it:

$$\int_{s^*}^{s^{**}} \frac{1}{g_0(s)^p}\,\mathrm{d}s \le \frac{4A_2}{(p-1)(1+A_1)A_1}\Big(\frac{A_1+1}{A_1}\sqrt{\frac{2A_2N}{d_0}}\Big)^{p-1}. \tag{2.139}$$

Finally, the last integral can be bounded by

$$\int_{s^{**}}^1 \frac{1}{g_0(s)^p}\,\mathrm{d}s \le \int_{s^*}^1 \Big(\frac{2}{s(E_1-E_0)}\Big)^p \mathrm{d}s \tag{2.140}$$

$$\le \Big(\frac{2}{E_1-E_0}\Big)^p \int_{s^*}^1 s^{-p}\,\mathrm{d}s \tag{2.141}$$

$$= \Big(\frac{2}{E_1-E_0}\Big)^p \frac{1}{p-1}\Big(\Big(\frac{1}{s^*}\Big)^{p-1} - 1\Big) \tag{2.142}$$

$$\le \Big(\frac{2}{E_1-E_0}\Big)^p \frac{1}{p-1}\sqrt{\frac{d_0}{2A_2N}}^{p-1}\Big(\frac{A_1+1}{A_1}\sqrt{\frac{2A_2N}{d_0}}\Big)^{p-1}. \tag{2.143}$$

Collecting all the positive terms, and ignoring the negative ones, gives the result. □

Corollary 2.11. *The Hamiltonian* (2.129) *satisfies Assumption 3 for any* $p \in \,]1,2[$ *with*

$$B(p) = \Big(1 + \frac{5}{p-1}\Big)\frac{A_2}{A_1(A_1+1)} + \Big(\frac{2}{E_1-E_0}\Big)^p \frac{1}{p-1}\sqrt{\frac{d_0}{2A_2N}}^{p-1}. \tag{2.144}$$

Next an assumption is introduced to capture the idea that $\left(\frac{2}{E_1-E_0}\right)^p \frac{1}{p-1}\sqrt{\frac{d_0}{2A_2N}}^{p-1}$ is much smaller than $\left(1+\frac{5}{p-1}\right)\frac{A_2}{A_1(A_1+1)}$. Again this is typically true for Ising Hamiltonians.

Assumption 6. *The following inequality is assumed to hold:*

$$\frac{d_0}{A_2N} \leq \frac{(E_1-E_0)^6}{32}. \tag{2.145}$$

Then the previous corollary can be simplified:

Corollary 2.12. *Suppose Assumption 6 holds. Then the Hamiltonian (2.129) satisfies Assumption 3 with $p = 3/2$ and*

$$B(3/2) = \frac{9}{2}\frac{A_2}{A_1(A_1+1)}. \tag{2.146}$$

2.3.4 Algorithms derived from H_s

The ground state of H_1 can be found by brute force search in time $O(N/d_0)$. This roughly corresponds to $O(1/g_{0m}^2)$. So, without an adapted schedule, none of the algorithmic frameworks give a speedup over classical brute force search.

Instead, we would like to use an adapted schedule based on the lower bound derived in Proposition 2.9. This can be done, assuming we know A_1, A_2 and d_0. Unfortunately calculating these quantities is typically quite hard. Various hardness results are presented in the paper [2].

If we are dealing with a problem where A_1, A_2 are not too hard to compute, then Theorem 1.33 and Theorem 1.45 can be applied. For simplicity, $\|H_1\| \leq 1$ and Assumption 6 are assumed to hold and only $p = 3/2$ is considered.

Since it is clear that $A_1/A_2 \leq E_1 - E_0$, the following bound holds almost everywhere:

$$|g_0'| \leq \frac{A_1(1+A_1)}{A_2}. \tag{2.147}$$

The following procedures prepare the ground state with fidelity greater than $1-\epsilon$:

- Adiabatic evolution with an adapted rate

$$T = \frac{1}{\sqrt{\epsilon}}\Big(\frac{35}{2} + 18\big(2\sqrt{2}+1\big)\frac{A_2}{A_1(A_1+1)}\Big)\sqrt{\frac{1+A_1}{A_1}}\Big(\frac{2A_2N}{d_0}\Big)^{1/4}\frac{1}{g_0^{3/2}} \tag{2.148}$$

  and a time complexity of

$$\int_0^1 T\,\mathrm{d}s \leq \frac{1}{\sqrt{\epsilon}}\left(\frac{315}{4}\frac{A_2}{A_1^2} + 81\big(2\sqrt{2}+1\big)\frac{A_2^2}{A_1^3(1+A_1)}\right)\sqrt{\frac{2A_2N}{d_0}}. \tag{2.149}$$

  This is given by Theorem 1.33 and also requires and annealer that can implement H_s.

- Poisson-distributed phase randomisation with an adapted rate

$$\lambda = \frac{1}{\epsilon}\Big(\frac{13}{2} + 72\frac{A_2}{A_1(1+A_1)}\Big)\sqrt{\frac{1+A_1}{A_1}}\left(\frac{2A_2N}{d_0}\right)^{1/4}\frac{1}{\sqrt{g_0}} \tag{2.150}$$

  has a time complexity of

$$t_0\int_0^1 \frac{\lambda}{g_0}\,\mathrm{d}s \leq \frac{2.33}{\epsilon}\left(\frac{117}{4}\frac{A_2}{A_1^2} + 324\frac{A_2^2}{A_1^3(1+A_1)}\right)\sqrt{\frac{2A_2N}{d_0}}. \tag{2.151}$$

  This is given by Theorem 1.45.

The time complexities, for fixed infidelity, given here are

$$O\left(\frac{A_2^2}{A_1^3(1+A_1)}\sqrt{\frac{A_2 N}{d_0}}\right), \tag{2.152}$$

which is asymptotically better than the time complexity reported in [2]:

$$O\left(\frac{1}{(E_1-E_0)^2 A_1(1+A_1)}\sqrt{\frac{A_2 N}{d_0}}\right). \tag{2.153}$$

This follows from the inequality $\frac{A_2}{A_1} \leq \frac{1}{E_1 - E_0}$.

2.3.5 NP-hardness

The aim of this section is to show that finding A_1, even up to relatively low precision, is NP-hard. This makes implementing the algorithms of the previous section potentially challenging to implement. The main idea is to exploit the sensitivity of A_1 to changes in the ground energy. As an initial idea, consider some NP-hard Boolean satisfiability problem, such as 3-SAT. Pick an instance and let the variable x range over all possible assignments and set $f(x) = 0$ if x is a satisfying assignment and $f(x) = 1$ otherwise. Consider the Hamiltonian

$$H_1 = \sum_x f(x)|x\rangle\langle x|. \tag{2.154}$$

If the instance is unsatisfiable, then $A_1 = 0$. Otherwise $A_1 \neq 0$. So, calculating A_1 allows us to solve the satisfiability problem!

There are a couple of problems with this approach; the main one is that this H_1 is highly non-local, so this is not the type of Hamiltonian one would want to use in adiabatic quantum computing anyway. Fortunately this idea can be modified to show that calculating A_1 of just 3-local Hamiltonians is NP-hard.

This is closely related to the *local Hamiltonian problem*, where the task is to determine if $E_0 = 0$ or $E_0 \geq \mu$. First it will be shown that knowledge of A_1 can be used to solve a version of this problem. Then the determination of A_1 will be shown to be NP-hard by a reduction of 3-SATto it.

Let A_1 of a Hamiltonian H be denoted $A_1(H)$.

Lemma 2.13. *Let $\epsilon,\ \mu_1, \mu_2 \in (0,1)$. Suppose there exists a classical procedure that accepts the description of a Hamiltonian H and outputs $\widetilde{A}_1(H)$ such that*

$$\left|\widetilde{A}_1(H) - A_1(H)\right| \leq \epsilon. \tag{2.155}$$

Now consider a positive n-qubit Hamiltonian H that is diagonal in the computational basis and has norm less than 1. Suppose that the ground energy E_0 of H satisfies the following: Either (i) $E_0 = 0$ or (ii) $0 \leq \mu_1 \leq E_0 \leq 1 - \mu_2 \leq 1$. Then, it is possible to decide whether (i) or (ii) holds, by making two calls to the classical procedure, provided

$$\epsilon < \frac{\mu_1}{6(1-\mu_1)} - \frac{d_0}{6\ 2^n} \cdot \frac{1}{\mu_1 \mu_2}. \tag{2.156}$$

Proof. The two calls to the classical procedure are to calculate $\widetilde{A}_1(H)$ and $\widetilde{A}_1(H')$, where

$$H' \coloneqq H \otimes \left(\frac{1+\sigma_z}{2}\right). \tag{2.157}$$

The aim is to disambiguate between $E_0 = 0$ and $\mu_1 \le E_0 \le 1 - \mu_2$. The two cases are considered separately.
When $\mathbf{E_0 = 0}$: In this case we have,

$$A_1(H) = \frac{1}{2^n} \sum_{k \neq 0} \frac{d_k}{E_k}. \tag{2.158}$$

Now, the ground energy of H' is zero, with degeneracy $d'_0 = d_0 + 2^n$, while for every other distinct eigenlevel has energy $E'_k = E_k$ with degeneracy d_k. So,

$$A_1(H') = \frac{1}{2^{n+1}} \sum_{k \neq 0} \frac{d_k}{E_k}. \tag{2.159}$$

This means that $A_1(H) - 2A_1(H') = 0$ and thus

$$\widetilde{A}_1(H) - 2\widetilde{A_1}(H') \le 3\varepsilon. \tag{2.160}$$

When $\mathbf{E_0 \neq 0}$: In this case the ground energy of H' is zero with degeneracy 2^n while every other distinct eigenlevel has energy $E'_k = E_{k-1}$ with degeneracy $d'_k = d_{k-1}$. Therefore,

$$A_1(H') = \frac{1}{2^{n+1}} \sum_{k} \frac{d_k}{E_k}. \tag{2.161}$$

Also,

$$\begin{aligned}
A_1(H) &= \frac{1}{2^n} \sum_{k=1}^{M-1} \frac{d_k}{E_k - E_0} && (2.162)\\
&= \frac{1}{2^n} \sum_{k=1}^{M-1} \frac{d_k}{E_k} + \frac{1}{2^n} \sum_{k=1}^{M-1} \frac{d_k E_0}{E_k(E_k - E_0)} && (2.163)\\
&= \frac{1}{2^n} \sum_{k=0}^{M-1} \frac{d_k}{E_k} - \frac{d_0}{2^n E_0} + \frac{1}{2^n} \sum_{k=1}^{M-1} \frac{d_k E_0}{E_k(E_k - E_0)} && (2.164)\\
&= 2A_1(H') - \frac{d_0}{2^n E_0} + \frac{1}{2^n} \sum_{k=1}^{M-1} \frac{d_k \; E_0}{E_k(E_k - E_0)} && (2.165)\\
&\ge 2A_1(H') - \frac{d_0}{2^n E_0} + \frac{1}{2^n} \sum_{k=1}^{M-1} \frac{d_k E_0}{1 - E_0} && (2.166)\\
&= 2A_1(H') - \frac{d_0}{2^n E_0} + \left(1 - \frac{d_0}{2^n}\right) \frac{E_0}{1 - E_0} && (2.167)\\
&= 2A_1(H') + \frac{E_0}{1 - E_0} - \frac{d_0}{2^n} \left(\frac{1 - E_0 + E_0^2}{E_0 - E_0^2}\right) && (2.168)\\
&\ge 2A_1(H') + \frac{\mu_1}{1 - \mu_1} - \frac{d_0}{2^n} \cdot \frac{1}{\mu_1 \mu_2} && (2.169)
\end{aligned}$$

Thus in this case,

$$A_1(H) - 2A_1(H') \ge \frac{\mu_1}{1 - \mu_1} - \frac{d_0}{2^n} \cdot \frac{1}{\mu_1 \mu_2}. \tag{2.170}$$

So

$$\widetilde{A}_1(H) - 2\widetilde{A}_1(H') \geq \frac{\mu_1}{1-\mu_1} - \frac{d_0}{2^n} \cdot \frac{1}{\mu_1\mu_2} - 3\epsilon. \tag{2.171}$$

In order to disambiguate between the two cases, we need

$$6\epsilon < \frac{\mu_1}{1-\mu_1} - \frac{d_0}{2^n} \cdot \frac{1}{\mu_1\mu_2}, \tag{2.172}$$

which completes the proof. □

Now Lemma 2.13 is used to prove a formal hardness result.

Theorem 2.14. *The problem of computing A_1 up to a precision*

$$\epsilon < \frac{1}{72} \cdot \frac{1}{n-1}, \tag{2.173}$$

for a 3-local Hamiltonian on n qubits is NP*-hard.*

Proof. We consider the 2-local version of 3-SAT, inspired by the reduction of 3-SAT to MAX-2-SAT (a variant of the 2-SATproblem which asks the maximum number satisfying clauses of a given Boolean formula) in [60]. Suppose $x_i \in \{0,1\}$ is a binary Boolean variable, and $\bar{x}_i$ be its negation. Consider that we are given some m clauses of the form $a_k \vee b_k \vee c_k$, where each a_k, b_k, c_k is either x_l or $\overline{x}_l$ with $0 \leq l \leq n-1$. A satisfying assignment makes

$$\bigwedge_{k=0}^{m-1} a_k \vee b_k \vee c_k$$

true. If $n+m < 15$, use brute-force search. Now assume $n+m \geq 15$. Set

$$P_{x_l} \coloneqq \frac{I - \sigma_z^{(l)}}{2}, \text{ and } P_{\overline{x}_l} \coloneqq \frac{I + \sigma_z^{(l)}}{2}.$$

For each $0 \leq k < m$, define the following Hamiltonian:

$$\begin{aligned} H_k \coloneqq\ & P_{\overline{a}_k} + P_{\overline{b}_k} + P_{\overline{c}_k} + P_{\overline{x}_{n+k}} \\ & + P_{a_k}P_{b_k} + P_{a_k}P_{c_k} + P_{b_k}P_{c_k} \\ & + P_{\overline{a}_k}P_{x_{n+k}} + P_{\overline{b}_k}P_{x_{n+k}} + P_{\overline{c}_k}P_{x_{n+k}}. \end{aligned}$$

If the k^{th} clause is satisfied, then the lowest eigenvalue of H_k is 3. Otherwise, it is 4. The largest possible eigenvalue of H_k is 6. Now consider the Hamiltonian, which acts on $2m+2n$ qubits,

$$H \coloneqq \frac{1}{6m}\sum_{k=0}^{m-1} H_k + \frac{1}{2n+2m}\sum_{k=n+m}^{2n+2m-1} P_{x_k} - \frac{1}{2}I. \tag{2.174}$$

Note that the eigenvalues of H lie between 0 and 1. We aim to disambiguate between $E_0 = 0$ and $E_0 \geq \frac{1}{6m}$ using Lemma 2.13. Since $d_0 \leq 2^{n+m}$ and we can take $\mu_1 = 1/6m$ and $\mu_2 = 1/2$. This requires,

$$\begin{aligned} \frac{1}{6} \cdot \frac{1}{6m-1} - \frac{d_0}{6 \cdot 2^{2n+2m}} \cdot 12m &= \frac{1}{6}\frac{1}{6m-1} - \frac{2\, d_0\, m}{2^{2n+2m}} && (2.175) \\ &\geq \frac{1}{36}\frac{1}{m+n-1} - \frac{2m}{2^{n+m}} && (2.176) \\ &\geq \frac{1}{72}\frac{1}{m+n-1} > \varepsilon. && (2.177) \end{aligned}$$

Here we have used $n + m \geq 15$ to bound

$$\frac{2m}{2^{n+m}} \leq \frac{1}{72} \cdot \frac{1}{m+n-1}. \tag{2.178}$$

□

From these reductions, we conclude that estimating the position of the avoided crossing to even a low precision is NP-hard.

Conclusion

The subject of this thesis was the formulation of new adiabatic theorems for new dynamics and their application to the design of algorithms.
The major novelty on the dynamics side was allowing discrete steps to be taken at random, according to a Poisson process. This has the advantage of being both relatively easy to implement: operationally all one has to do is perform a series of discrete operations, which is typically easier than trying to control something continuously in time.
It also has the advantage of being easy to analyse: on average the dynamics are continuous, which allows the development of adiabatic theorems in much the same way as in the context of continuous unitary evolution.
Concretely, two new dynamics were proposed: the first one uses time-independent Hamiltonian evolution for random amounts of time. It is the randomisation in time of a method known as "phase randomisation". The second considers applying general unitaries in a randomised fashion. In particular, these unitaries could be a block encoding of a Hamiltonian. All three dynamics (time-dependent Hamiltonian evolution, randomised time-independent Hamitonian evolution and randomised application of block-encodings) gives similar results. This is significant: it gives a way to match the asymptotic performance of adiabatic quantum computing without having to implement the time-dependent dynamics or incurring the discretisation cost, which can be significant.
As an application, this method was applied to the quantum linear systems of equations problem. It gave a straightforward way to achieve optimal scaling.
The second part of this thesis was concerned with the analysis of time-dependent Hamiltonians that have algorithmic potential. A fairly general family of Hamiltonians was proposed and their spectra were characterised. They offer an intuitive way to extend the adiabatic version of Grover's algorithm to a larger class of problems. A challenge remains, however, as obtaining optimal scaling requires knowing the location of the minimal gap. It was shown that in general this, in itself, is a hard problem.
Nonetheless some applications to the variable search problem were given. Comparing this to results for the circuit model leads me to suspect that the analysis is not quite as tight as it could be. This is one avenue for further work.
Another obvious question is whether there are problems for which finding the minimal gap is not hard. For these problems our work has in effect produced a novel quantum algorithm.
There are only relatively few time-dependent Hamiltonians for which we know how to perform the relevant spectral analysis. Having more results in this direction would be highly valuable.
There are also interesting open questions regarding the dissipative adiabatic theorems: are there other dynamics with algorithmic potential that can be analysed in this framework? Maybe tailored to quantum walks? Can the results be extended to unbounded generators?

Appendix A

Some functional analysis

Good references for this section are [61, 62]. Appendix A is for reference only. It contains essentially no new results or insights.

A.1 Banach algebras

A.1.1 Banach algebras

A normed algebra is an associative algebra A over $\mathbb{C}$ with norm $\|\cdot\|$ such that $(\mathbb{C}, A, +, \|\cdot\|)$ is a normed space and we have submultiplicativity, i.e.

$$\forall x, y \in A : \quad \|xy\| \leq \|x\|\|y\|. \tag{A.1}$$

We say A is unital if there exists a unit element $\mathbf{1} \in A$ such that

$$\forall x \in A : \mathbf{1} \cdot x = x = x \cdot \mathbf{1} \qquad \text{and} \qquad \|\mathbf{1}\| = 1. \tag{A.2}$$

A normed algebra is called a Banach algebra if it is complete.

Example

The most important example of a Banach algebra is the Banach algebra of bounded operators on a Banach space.

Lemma A.1. *Let A be a Banach algebra. The multiplication map $\cdot : A \times A \to A : (x, y) \mapsto xy$ is continuous.*

This is a straightforward consequence of submultiplicativity. Note that multiplication is continuous in both arguments simultaneously, which is a stronger statement than continuity in each argument separately.
The textbook [63] is a good reference for this section.

A.1.1.1 Neumann series

Proposition A.2 (Neumann series)**.** *Let A be a unital Banach algebra and $x \in A$. If $\|x\| < 1$, then $\mathbf{1} - x$ is invertible with inverse*

$$(\mathbf{1} - x)^{-1} = \sum_{n=0}^{\infty} x^n = \mathbf{1} + \sum_{n=1}^{\infty} x^n \qquad \textit{and} \qquad \|(\mathbf{1} - x)^{-1}\| \leq \frac{1}{1 - \|x\|}. \tag{A.3}$$

Equivalently, if $\|\mathbf{1} - x\| < 1$, then x is invertible with inverse

$$x^{-1} = \sum_{n=0}^{\infty} (\mathbf{1} - x)^n. \tag{A.4}$$

Proof. Since $\|x^n\| \leq \|x\|^n$ for all $n \geq 1$ and $\sum \|x\|^n$ is a convergent geometric series, the series $\sum x^n$ is absolutely convergent. Since A is complete, this implies that the series is convergent. Also

$$\|(\mathbf{1} - x)^{-1}\| = \left\| \sum_{i=0}^{\infty} x^i \right\| \leq \sum_{i=0}^{\infty} \|x\|^i = \frac{1}{1 - \|x\|}. \tag{A.5}$$

□

In fact the requirement of $\|x\| < 1$ can be weakened to $\exists k \in \mathbb{N} : \|x^k\| < 1$.
The Neumann series can be used to prove the following proposition:

Proposition A.3. *Let A be a unital Banach algebra. Then*

1. *the set of invertible elements is an open subset of A;*
2. *the function $^{-1} : \{$invertible elements of $A\} \to A : x \mapsto x^{-1}$ is continuous.*

A.1.1.2 The spectrum

Just as in the case of operators, the spectrum is a very important concept for Banach algebras. The definition is slightly easier since there is no concept of unboundedness.

Let A be a unital complex Banach algebra. The spectrum of an element $x \in A$ is defined as

$$\sigma(x) = \sigma_A(x) \coloneqq \{\lambda \in \mathbb{C} \mid \lambda \cdot \mathbf{1} - x \text{ is not invertible}\}. \tag{A.6}$$

The resolvent set and resolvent map are defined in complete analogy with the operator case.
The spectral radius of $x \in A$ is

$$\operatorname{spr}(x) = \sup\{|\lambda| \mid \lambda \in \sigma(x)\}. \tag{A.7}$$

The following proposition collects the most important facts about the spectrum. They will frequently be used without comment.

Proposition A.4. *Let A be a Banach algebra and $x \in A$. Then*

1. *$\sigma(x) \subseteq \{\lambda \in \mathbb{C} \mid |\lambda| \leq \|x\|\}$;*
2. *$\operatorname{spr}(x) \leq \|x\|$;*

3. *$\sigma(x)$ is compact;*

4. $\operatorname{spr}(x) = \max\{|\lambda| \mid \lambda \in \sigma(x)\}$*;*

5. $\operatorname{spr}(x) = \lim_{n\to\infty}\|x^n\|^{1/n} = \inf_{n\in\mathbb{N}}\|x^n\|^{1/n}$.

Proposition A.5 (Polynomial spectral mapping)**.** *Let A be a Banach algebra, $x \in A$ and p a complex polynomial with $p(0) = 0$. Then*

1. $p^{\downarrow}\big(\sigma(x)\big) = \sigma\big(p(x)\big)$*;*

2. *if x is invertible, then $\sigma(x^{-1}) = \sigma(x)^{-1}$.*

If A is unital, this holds for all p.

Lemma A.6. *Let A be a unital Banach algebra and $p \in A$ an idempotent element. Then $\sigma(p) \subseteq \{0, 1\}$.*

Proof. Take $\lambda \in \mathbb{C} \setminus \{0, 1\}$. Then $x - \lambda\mathbf{1}$ has an inverse given by $-\lambda^{-1} + (1-\lambda)^{-1}\lambda^{-1}x$, indeed

$$(x-\lambda)\left(-\frac{1}{\lambda} + \frac{x}{(1-\lambda)\lambda}\right) = \mathbf{1} - \frac{x}{\lambda} + \frac{x - x\lambda}{(1-\lambda)\lambda} = \mathbf{1} - \frac{x}{\lambda} + \frac{x}{\lambda} = \mathbf{1}. \tag{A.8}$$

The inverse is two-sided since it commutes. □

A.1.1.3 Calculating spectra

Proposition A.7. *Let A be a unital Banach algebra and $x, y \in A$ be commuting elements. Then*

1. $\sigma(x + y) \subseteq \sigma(x) + \sigma(y)$*;*

2. $\sigma(xy) \subseteq \sigma(x) \cdot \sigma(y)$*.*

Proposition A.8. *Let A be a Banach algebra and $a \in A$. Then*

$$\lambda_a : A \to A : x \mapsto ax \qquad \textit{and} \qquad \rho_a : A \to A : x \mapsto xa \tag{A.9}$$

are elements of $\mathcal{B}(A)$ such that

1. $\|\lambda_a\| \le \|a\|$ *and* $\|\rho_a\| \le \|a\|$*;*

2. $\sigma(\lambda_a) \subseteq \sigma(a)$ *and* $\sigma(\rho_a) \subseteq \sigma(a)$*;*

3. *if A is unital, then $\sigma(\lambda_a) = \sigma(a)$ and $\sigma(\rho_a) = \sigma(a)$.*

Proof. (1) For all $x \in A$, we have $\|\lambda_a(x)\| = \|ax\| \le \|a\|\,\|x\|$, so $\|\lambda_a\| \le \|a\|$ and thus $\lambda_a \in \mathcal{B}(A)$. The result for ρ_a is dual.
(2) Take $\mu \in \mathbb{C} \setminus \sigma(a)$. Then $(\mu \cdot \mathbf{1} - a)$ has an inverse in A if A is unital and in $A^\dagger$ otherwise. For all $x \in A$, we have

$$\Big(\lambda_{(\mu\cdot\mathbf{1}-a)^{-1}} \circ \big(\mu \cdot \mathbb{1} - \lambda_a\big)\Big)(x) = (\mu\cdot\mathbf{1} - a)^{-1}(\mu x - ax) \tag{A.10}$$

$$= (\mu\cdot\mathbf{1} - a)^{-1}(\mu\cdot\mathbf{1} - a)x = x. \tag{A.11}$$

Similarly

$$\Big((\mu\,\mathbb{1} - \lambda_a)\lambda_{(\mu\cdot\mathbf{1}-a)^{-1}}\Big)(x) = (\mu\cdot\mathbf{1} - a)^{-1}(\mu x - ax) \tag{A.12}$$

$$= (\mu\cdot\mathbf{1} - a)^{-1}(\mu\cdot\mathbf{1} - a)x = x. \tag{A.13}$$

Thus $\mu\,\mathbb{1} - \lambda_a$ has an inverse in $\mathcal{B}(A)$, namely $\lambda_{(\mu\cdot\mathbf{1}-a)^{-1}}$. If A is not unital, then $\lambda_{(\mu\cdot\mathbf{1}-a)^{-1}}$ is still an operator in $\mathcal{B}(A)$, since $A \subseteq A^\dagger$ is an idela. Then $\mu \notin \sigma(\lambda_a)$ and we conclude that $\sigma(\lambda_a) \subseteq \sigma(a)$ by contraposition.
The result for ρ_a is dual.
(3) Because of (2), it is enough to prove $\sigma(\lambda_a) \supseteq \sigma(a)$. Take $\mu \in \mathbb{C} \setminus \sigma(\lambda_a)$. Then $\mu\,\mathbb{1} - \lambda_a$ has an inverse $(\mu\,\mathbb{1} - \lambda_a)^{-1} \in \mathcal{B}(A)$. Set $b := (\mu\,\mathbb{1} - \lambda_a)^{-1}(\mathbf{1})$. Then

$$(\mu\mathbf{1} - a)b = (\mu\,\mathbb{1} - \lambda_a)(b) = (\mu\,\mathbb{1} - \lambda_a)(\mu\,\mathbb{1} - \lambda_a)^{-1}(\mathbf{1}) = \mathbf{1}, \tag{A.14}$$

so b is the right inverse of $(\mu\mathbf{1} - a)$. This implies that $\lambda_{\mu\mathbf{1}-a}\lambda_b = \lambda_{\mathbf{1}} = \mathbb{1}$, so $\lambda_b = \lambda_{\mu\mathbf{1}-a}^{-1}$, which is a two-sided inverse (by assumption). Thus

$$b(\mu\mathbf{1} - a) = (\lambda_b \circ \lambda_{\mu\mathbf{1}-a})(\mathbf{1}) = (\lambda_{\mu\mathbf{1}-a}^{-1} \circ \lambda_{\mu\mathbf{1}-a})(\mathbf{1}) = \mathbf{1} \tag{A.15}$$

and b is also the left inverse of $(\mu\mathbf{1} - a)$. We conclude that $\mu \notin \sigma(a)$. □

Corollary A.9. *Let A be a Banach algebra, $a \in A$ and $b \in A$ invertible. Then*

1. $\sigma\big([a, \_]\big) \subseteq \sigma(a) - \sigma(a)$;
2. $\sigma(b(\_)b) \subseteq \sigma(b)\sigma(b)^{-1}$.

Proof. Since

$$[a, \_] = \lambda_a - \rho_a \qquad \text{and} \qquad \mathrm{Ad}_b = \lambda_b \circ \rho_{b^{-1}}, \tag{A.16}$$

this follows from the proposition, Proposition A.7 (using the fact that the left- and right-multiplication commute) and Proposition A.5. □

A.1.1.4 Pseudoresolvents

Let A be a Banach algebra. A function $\mathcal{R} : \Lambda \subseteq \mathbb{C} \to A$ is called a pseudoresolvent if, for all $\lambda, \mu \in \Lambda$

$$\mathcal{R}(\lambda) - \mathcal{R}(\mu) = (\mu - \lambda)\mathcal{R}(\lambda)\mathcal{R}(\mu). \tag{A.17}$$

This equation is known as the (first) resolvent identity.

Note that if a pseudoresolvent $\mathcal{R}$ is zero anywhere, it is identically zero.

Lemma A.10. *Let $\mathcal{R} : \Lambda \subseteq \mathbb{C} \to A$ be a pseudoresolvent on a Banach algebra a and $\lambda, \mu \in \Lambda$. Then $\mathcal{R}(\lambda)\mathcal{R}(\mu) = \mathcal{R}(\mu)\mathcal{R}(\lambda)$.*

Proof. If $\lambda = \mu$, then the result is immediate. If $\lambda \neq \mu$, then

$$\mathcal{R}(\lambda)\mathcal{R}(\mu) = (\mu - \lambda)^{-1}\big(\mathcal{R}(\lambda) - \mathcal{R}(\mu)\big) = (\lambda - \mu)^{-1}\big(\mathcal{R}(\mu) - \mathcal{R}(\lambda)\big) = \mathcal{R}(\mu)\mathcal{R}(\lambda). \tag{A.18}$$

□

Proposition A.11. *Let A be a unital Banach algebra, $\mathcal{R} : \Lambda \subseteq \mathbb{C} \to A$ a pseudoresolvent, $\lambda_0 \in \Lambda$ and $\lambda \in \mathbb{C}$ such that $|\lambda - \lambda_0|\,\|\mathcal{R}(\lambda_0)\| < 1$. Then*

1. *if* $\lambda \in \Lambda$, *then* $\mathcal{R}(\lambda) = \sum_{n=0}^{\infty} (\lambda_0 - \lambda)^n \mathcal{R}(\lambda_0)^{n+1}$;
2. *if* $\lambda \notin \Lambda$, *this allows* $\mathcal{R}$ *to be extended to a pseudoresolvent on* $\Lambda \cup \{\lambda\}$;
3. $\|\mathcal{R}(\lambda)\| \leq \dfrac{1}{\|\mathcal{R}(\lambda_0)\|^{-1} - |\lambda_0 - \lambda|}$.

This implies $\mathcal{R}$ *can be extended as a pseudoresolvent to* $\Lambda \cup \mathrm{B}(\lambda_0, \|\mathcal{R}(\lambda_0)\|^{-1})$.

Proof. (1, 3) By assumption we have $(\lambda - \lambda_0)\mathcal{R}(\lambda_0)$ is a contraction, so $(\mathbf{1} - (\lambda - \lambda_0)\mathcal{R}(\lambda_0))^{-1}$ exists and has a Neumann series expansion by Proposition A.2. Then the resolvent identity gives

$$\mathcal{R}(\lambda)\big(\mathbf{1} - (\lambda_0 - \lambda)\mathcal{R}(\lambda_0)\big) = \mathcal{R}(\lambda_0), \tag{A.19}$$

so, using the Neumann series expansion,

$$\begin{aligned} \mathcal{R}(\lambda) &= \big(\mathbf{1} - (\lambda_0 - \lambda)\mathcal{R}(\lambda_0)\big)^{-1}\mathcal{R}(\lambda_0) && \text{(A.20)} \\ &= \sum_{n=0}^{\infty} (\lambda_0 - \lambda)^n \mathcal{R}(\lambda_0)^{n+1}. && \text{(A.21)} \end{aligned}$$

The norm bound in Proposition A.2 gives (3):

$$\begin{aligned} \|\mathcal{R}(\lambda)\| &= \Big\|\big(\mathbf{1} - (\lambda_0 - \lambda)\mathcal{R}(\lambda_0)\big)^{-1}\mathcal{R}(\lambda_0)\Big\| && \text{(A.22)} \\ &\leq \frac{\|\mathcal{R}(\lambda_0)\|}{1 - |\lambda_0 - \lambda|\|\mathcal{R}(\lambda_0)\|} && \text{(A.23)} \\ &= \frac{1}{\|\mathcal{R}(\lambda_0)\|^{-1} - |\lambda_0 - \lambda|}. && \text{(A.24)} \end{aligned}$$

(2) We need to check that the resolvent identity

$$\mathcal{R}(\lambda) - \mathcal{R}(\lambda_1) = (\lambda_1 - \lambda)\mathcal{R}(\lambda)\mathcal{R}(\lambda_1) \tag{A.25}$$

holds for all $\lambda_1 \in \Lambda$. We start from the resolvent identity for λ_0, λ_1:

$$\begin{aligned} \mathcal{R}(\lambda_0) - \mathcal{R}(\lambda_1) &= (\lambda_1 - \lambda_0)\mathcal{R}(\lambda_0)\mathcal{R}(\lambda_1) && \text{(A.26)} \\ &= (\lambda_1 - \lambda)\mathcal{R}(\lambda_0)\mathcal{R}(\lambda_1) - (\lambda_0 - \lambda)\mathcal{R}(\lambda_0)\mathcal{R}(\lambda_1). && \text{(A.27)} \end{aligned}$$

Then

$$\begin{aligned} (\lambda_1 - \lambda)\mathcal{R}(\lambda_0)\mathcal{R}(\lambda_1) &= \mathcal{R}(\lambda_0) - \mathcal{R}(\lambda_1) + (\lambda_0 - \lambda)\mathcal{R}(\lambda_0)\mathcal{R}(\lambda_1) && \text{(A.28)} \\ &= \mathcal{R}(\lambda_0) - \big(\mathbf{1} - (\lambda_0 - \lambda)\mathcal{R}(\lambda_0)\big)\mathcal{R}(\lambda_1). && \text{(A.29)} \end{aligned}$$

Multiplying both sides by $\big(\mathbf{1} - (\lambda_0 - \lambda)\mathcal{R}(\lambda_0)\big)^{-1}$ gives the result. □

Corollary A.12. *Let* $\mathcal{R} : \Lambda \subseteq \mathbb{C} \to A$ *be a pseudoresolvent. Then*

1. $\mathcal{R}$ *is continuous;*
2. $\mathcal{R}'(\lambda) = -\mathcal{R}(\lambda)^2$ *for all* $\lambda \in \Lambda$;
3. $\mathcal{R}^{(n)}(\lambda) = n!(-1)^n \mathcal{R}(\lambda)^{n+1}$ *for all* $n \in \mathbb{N}$.

In particular the map $\mathcal{R}$ *is holomorphic on its domain of definition.*

Proof. (1) Take $\lambda_0 \in \Lambda$ and $\epsilon > 0$. Set

$$\delta := \min\left\{\frac{1}{2\|\mathcal{R}(\lambda_0)\|}, \frac{\epsilon}{\|\mathcal{R}(\lambda_0)\|\big(\|\mathcal{R}(\lambda_0)\| + \epsilon\big)}\right\}. \tag{A.30}$$

Now take arbitrary $\lambda \in \Lambda$ such that $|\lambda_0 - \lambda| \leq \delta$. Then

$$|\lambda - \lambda_0| \, \|\mathcal{R}(\lambda_0)\| \leq \delta\|\mathcal{R}(\lambda_0)\| \leq \frac{1}{2} < 1, \tag{A.31}$$

so we can use the results of the proposition. Now

$$\begin{aligned}
\|\mathcal{R}(\lambda_0) - \mathcal{R}(\lambda)\| &\leq |\lambda_0 - \lambda|\|\mathcal{R}(\lambda_0)\|\|\mathcal{R}(\lambda)\| && \text{(A.32)}\\
&\leq \frac{|\lambda_0 - \lambda|\|\mathcal{R}(\lambda_0)\|^2}{1 - |\lambda_0 - \lambda|\|\mathcal{R}(\lambda_0)\|} && \text{(A.33)}\\
&\leq \frac{\delta\|\mathcal{R}(\lambda_0)\|^2}{1 - \delta\|\mathcal{R}(\lambda_0)\|} && \text{(A.34)}\\
&\leq \frac{\frac{\epsilon}{\|\mathcal{R}(\lambda_0)\|+\epsilon}\|\mathcal{R}(\lambda_0)\|}{1 - \frac{\epsilon}{\|\mathcal{R}(\lambda_0)\|+\epsilon}} = \frac{\epsilon\|\mathcal{R}(\lambda_0)\|}{\|\mathcal{R}(\lambda_0)\| + \epsilon - \epsilon} = \epsilon. && \text{(A.35)}
\end{aligned}$$

(2) We calculate

$$\begin{aligned}
\mathcal{R}'(\lambda) &= \lim_{\mu\to\lambda} \frac{\mathcal{R}(\mu) - \mathcal{R}(\lambda)}{\mu - \lambda} && \text{(A.36)}\\
&= \lim_{\mu\to\lambda} -\mathcal{R}(\lambda)\mathcal{R}(\mu) = -\mathcal{R}(\lambda)\lim_{\mu\to\lambda}\mathcal{R}(\mu) = -\mathcal{R}(\lambda)^2. && \text{(A.37)}
\end{aligned}$$

For the last equality we have used the fact that $\mathcal{R}$ is continuous, which is given by (1).
(3) By induction on n. □

A.1.2 Functional calculi

A functional calculus is a construction that allows (complex) functions to be applied to more abstract things. There are several different functional calculi, each allowing different sorts of functions to be evaluated at different sorts of objects.
As a first basic example, let A be an algebra and $a \in A$. Now $a^n \in A$ for all $n \in \mathbb{N}$ and we can also scalar multiples of elements in A (i.e. A is a vector space). Putting these facts together gives us a canonical way to understand $p(a)$ for any polynomial p such that $p(0) = 0$. Indeed if p is the polynomial

$$p : \mathbb{C} \to \mathbb{C} : z \mapsto \sum_{k=1}^{n} \alpha_k z^k, \tag{A.38}$$

then we can set $p(a) = \sum_{k=1}^{n} \alpha_k a^k$. The function Φ_a that maps a polynomial p to $p(a)$ is called the polynomial functional calculus of a. Already with this simple example we can illustrate some general features of functional calculi more general:

- If A is not unital, then there is no obvious meaning of $p(a)$ for any polynomial p that has a constant term. If A is unital, then this constant term is mapped to some multiple of the unit. In more general functional calculi, constant functions are mapped to multiples of the identity.

- Suppose p, q are two polynomials, then $(p \cdot q)(a) = p(a) \cdot q(a)$. This is the most important property of the functional calculus. It is alternatively expressed by requiring that Φ_a be an algebra homomorphism, where the multiplication in the space of polynomials is pointwise.
- The functional calculus has the spectral mapping property: Proposition A.5 can be rephrased as follows: $\sigma\big(\Phi_a(p)\big) = p^{\downarrow}\big(\sigma(a)\big)$.

Beyond polynomial functional calculus, there are essentially three major[1] types of functional calculus. For the first type, note that Φ_a is continuous when the space of polynomials is equipped with uniform convergence. We could hope to use this continuity to extend Φ_a to the closure of the space of polynomials. This does indeed work, but only if A is complete (otherwise the expected limit may fail to exist). In addition, the power of complex analysis and Cauchy's theorem give us a useful expression for the functional calculus. An immediate consequence of this form is that $\Phi_a(f)$ is independent of the values f takes outside the spectrum. In conclusion, this functional calculus allows the application of functions that are holomorphic on $\sigma(a)$.

Theorem A.13 (Holomorphic functional calculus)**.** *Let A be a unital Banach algebra and $x \in A$. Consider the function*

$$\Phi_x : \mathrm{Hol}(\sigma(x), \mathbb{C}) \to A : f \mapsto f(x) \coloneqq \frac{1}{2\pi i} \oint_{\Gamma} f(z) R_x(z) \, \mathrm{d}z. \tag{A.39}$$

Here Γ is any finite union of simple Jordan curves that contains $\sigma(x)$ such that f is holomorphic in a region that contains Γ and its interior. Then

1. *Φ_x is well-defined: it does not depend on the particular curve Γ;*
2. *Φ_x is an algebra homomorphism;*
3. *Φ_x is continuous if $\mathrm{Hol}(\sigma(x), \mathbb{C})$ is equipped with uniform convergence;*
4. *$\Phi_x(\mathbb{1}_{\mathbb{C}}) = x$ and $\Phi_x(\underline{1}) = \mathbf{1}$;*
5. *$\sigma(\Phi_x(f)) = f^{\downarrow}\big(\sigma(x)\big)$.*

In the transition from polynomial functional calculus to holomorphic functional calculus, the space of functions has been enlarged, at the cost of more assumptions on the algebra A. This trend continues. The following functional calculus is only applicable to C^*-algebras, indeed only normal elements of C^*-algebras (i.e. elements x such that $[x, x^*] = 0$), but does allow the application of all functions that are continuous on the spectrum.

Theorem A.14 (Continuous functional calculus)**.** *Let A be a C^*-algebra and $x \in A$ a normal element.*

1. *If A is unital, then there exists a unique $*$-homomorphism*

$$\Phi_x : \mathcal{C}(\sigma(x), \mathbb{C}) \to A \qquad \text{such that} \qquad \Phi_x(\mathbb{1}_{\sigma(x)}) = x \text{ and } \Phi_x(\underline{1}_{\sigma(x)}) = \mathbf{1}. \tag{A.40}$$

2. *If A is non-unital, then there exists a unique $*$-homomorphism*

$$\Phi_x : \{f \in \mathcal{C}\big(\sigma(x)\big) \mid f(0) = 0\} \to A \qquad \text{such that} \qquad \Phi_x(\mathbb{1}_{\sigma(x)}) = x. \tag{A.41}$$

[1] Of course there are many minor variations!

In both cases Φ_x is isometric (if the space of functions is equipped with the supremum norm) and $\sigma(f(x)) = f^{\downarrow}(\sigma(x))$.

Next a functional calculus that is applicable to all bounded Borel-measurable functions, but only works on von Neumann algebras. In this setting spectral mapping no longer holds in the same way as before;[2] there is a statement that exhibits $\sigma(f(x))$ as some sort of essential range, [61, 62]. For our purposes it is more useful to just note that spectral mapping holds for continuous functions: since every von Neumann algebra is a C^*-algebra, Theorem A.14 is applicable.

Theorem A.15 (Borel functional calculus)**.** *Let A be a unital von Neumann algebra and $x \in A$ a normal element. There exists an isometric $*$-homomorphism*

$$\Phi_x : L^\infty(\sigma(x), \mathbb{C}) \to A \qquad \text{such that} \qquad \Phi_x(\mathbb{1}_{\sigma(x)}) = x \text{ and } \Phi_x(\underline{1}_{\sigma(x)}) = \mathbf{1}. \tag{A.42}$$

Spectral mapping holds for continuous f.

So far all functional calculi have been defined for elements of an algebra. In fact all functional calculi are applicable to $\mathcal{B}(\mathcal{H})$, the algebra of bounded operators on a Hilbert space $\mathcal{H}$. There is a further possible generalisation: it would be nice to be able to have a functional calculus for unbounded normal operators on $\mathcal{H}$. One way to realise this is to reduce the problem to bounded normal operators with some sort of transform. If H is an unbounded normal operator, then $H\sqrt{\mathbb{1}+H^*H}^{-1}$ is bounded.[3] The result is the spectral theorem. Now Φ_H is defined via spectral integration. For details, see [61, 62].

Theorem A.16 (Spectral theorem for unbounded operators)**.** *Let $\mathcal{H}$ be a Hilbert space and H a normal operator on $\mathcal{H}$ (either bounded or unbounded). There exists a unique spectral measure E on $\sigma(H)$ such that*

$$H = \int_{\sigma(H)} z \, \mathrm{d}E(z). \tag{A.43}$$

For all measurable $f : \sigma(H) \to \mathbb{C}$, spectral integration gives

$$\Phi_H(f) \coloneqq \int_{\sigma(H)} f(z) \, \mathrm{d}E(z) \tag{A.44}$$

with the following properties:

1. $\mathrm{dom}(\Phi_H(f)) = \{|\psi\rangle \in \mathcal{H} \mid \int_{\sigma(H)} |f|^2 \, \mathrm{d}\langle\psi|E(z)|\psi\rangle < \infty\}$;
2. $\|\Phi_H(f)|\psi\rangle\|^2 = \int_{\sigma(H)} |f|^2 \, \mathrm{d}\langle\psi|E(z)|\psi\rangle$ *for all* $|\psi\rangle \in \mathrm{dom}(\Phi_H(f))$;
3. $\Phi_H(f)^* = \Phi_H(\overline{f})$;
4. $\Phi_H(f)\Phi_H(g) \subseteq \Phi_H(fg)$ *with* $\mathrm{dom}\big(\Phi_H(f)\Phi_H(g)\big) = \mathrm{dom}\big(\Phi_H(fg)\big) \cap \mathrm{dom}\big(\Phi_H(g)\big)$.

If f is continuous, then $\sigma\big(\Phi_H(f)\big) = \overline{f^{\downarrow}(\sigma(H))}$.

[2] Here is a way to see that $\sigma(f(x)) = f^{\downarrow}(\sigma(x))$ cannot hold for all Borel-measurable functions. If this were true, then the proof of Corollary A.17 would show that all elements of the spectrum were eigenvalue. This is of course not true.

[3] Of course I am simplifying and these hints of motivation should probably not be taken too seriously. The same can be said for the whole of this section.

The measure $\mathrm{d}\langle\psi|E(z)|\psi\rangle$ is a probability measure (i.e. integrates to one) whenever $|\psi\rangle$ is a unit vector, which gives us the very useful consequence that if f is bounded, then $\Phi_H(f)$ is bounded (and and $\mathrm{dom}(\Phi_H(f)) = \mathcal{H}$).
Note that Φ_H is no longer an algebra homomorphism, since the domain issues complicate things, but we do have $\Phi_H(f)\Phi_H(g) = \Phi_H(fg)$ if g is bounded.

Corollary A.17. *Let $\mathcal{H}$ be a Hilbert space and H a normal operator on $\mathcal{H}$. If ω_0 is an isolated point of $\sigma(H)$, then ω_0 is an eigenvalue.*

Proof. The function

$$f : \sigma(H) \to \mathbb{C} : x \mapsto \begin{cases} 1 & (x = \omega_0) \\ 0 & (\text{otherwise}) \end{cases} \tag{A.45}$$

is continuous. Spectral mapping gives that $\sigma\big(\Phi_H(f)\big) = \{0, 1\}$, which implies that $\Phi_H(f)$ is a non-zero orthogonal projector. The following calculation shows that it is the eigenprojector associated with the eigenvalue ω_0:

$$\begin{aligned} H\Phi_H(f) &= \Phi_H(\mathbb{1})\Phi_H(f) && \text{(A.46)} \\ &= \Phi_H(\mathbb{1} \cdot f) && \text{(A.47)} \\ &= \Phi_H(\omega_0 f) && \text{(A.48)} \\ &= \omega_0 \Phi_H(f). && \text{(A.49)} \end{aligned}$$

□

A.1.2.1 Holomorphic functional calculus

Let $U \subseteq \mathbb{C}$ be an open set, X a Banach space and $f : U \to X$ a function. Then

- f is called weakly holomorphic if $\rho \circ f : U \to \mathbb{C}$ is holomorphic for all $\rho \in X^*$;
- f is called strongly holomorphic if, for all $z_0 \in U$, the limit

$$\left.\frac{\mathrm{d}f}{\mathrm{d}z}\right|_{z_0} = \lim_{z \to z_0} \frac{f(z) - f(z_0)}{z - z_0} \tag{A.50}$$

  exists in the norm convergence.

Such functions are also called “weakly analytic”, resp. “strongly analytic”.

Lemma A.18. *Let $U \subseteq \mathbb{C}$ be an open set, X a Banach space and $f : U \to X$ a function. If f is strongly holomorphic, then f is continuous and weakly holomorphic.*

Proof. Suppose f is strongly holomorphic. Then

$$\lim_{z \to z_0} f(z) - f(z_0) = \lim_{z \to z_0} \frac{f(z) - f(z_0)}{z - z_0} \cdot (z - z_0) = \left.\frac{\mathrm{d}f}{\mathrm{d}z}\right|_{z_0} \big(\lim_{z \to z_0} z - z_0\big) = \left.\frac{\mathrm{d}f}{\mathrm{d}z}\right|_{z_0} \cdot 0 = 0, \tag{A.51}$$

so $\lim_{z \to z_0} f(z) = f(z_0)$, which means that f is continuous.

Take $\rho \in X^*$. Then

$$\frac{\mathrm{d}\rho \circ f}{\mathrm{d}z}\Big|_{z_0} = \lim_{z \to z_0} \frac{(\rho \circ f)(z) - (\rho \circ f)(z_0)}{z - z_0} \tag{A.52}$$

$$= \lim_{z \to z_0} \rho\Big(\frac{f(z) - f(z_0)}{z - z_0}\Big) \tag{A.53}$$

$$= \rho\Big(\lim_{z \to z_0} \frac{f(z) - f(z_0)}{z - z_0}\Big) \tag{A.54}$$

$$= \rho\Big(\frac{\mathrm{d}f}{\mathrm{d}z}\Big|_{z_0}\Big). \tag{A.55}$$

. □

Proposition A.19. *Let $U \subseteq \mathbb{C}$ be an open set, X a Banach space, $f : U \to X$ a weakly holomorphic function and Γ a Jordan curve in U whose interior is also in U. Then*

1. *f is continuous;*
2. *$\oint_\Gamma f(z)\,\mathrm{d}z = 0$ and $f(w) = \frac{1}{2\pi i}\oint_\Gamma \frac{f(z)}{z-w}\,\mathrm{d}z$ for all w in the interior of Γ;*
3. *f is strongly holomorphic.*

We are now free to refer to f as simply a holomorphic function, without specifying "weakly" or "strongly".

Proof. (1) Pick $z_0 \in U$ and $r > 0$ small enough such that the open ball $\mathrm{B}(z_0, r) \subseteq U$. Take arbitrary $\rho \in X^*$. Since $\rho \circ f$ is holomorphic, the function

$$z \mapsto \frac{(\rho \circ f)(z) - (\rho \circ f)(z_0)}{z - z_0} = \rho\Big(\frac{f(z) - f(z_0)}{z - z_0}\Big) \tag{A.56}$$

is continuous on $\mathrm{B}(z_0, r)$ and thus bounded on $\mathrm{B}(z_0, r)$ by the extreme value theorem. This means that the set

$$\Big\{\frac{f(z) - f(z_0)}{z - z_0}\ \Big|\ z \in \mathrm{B}(z_0, r)\Big\} \tag{A.57}$$

is weakly bounded, and thus bounded. There exists $M \geq 0$ such that

$$\|f(z) - f(z_0)\| \leq M(z - z_0) \tag{A.58}$$

for all $z \in \mathrm{B}(z_0, r)$. This implies that f is continuous at z_0.
(2) For all $\rho \in X^*$, we have

$$\rho\Big(\oint_\Gamma f\,\mathrm{d}z\Big) = \oint_\Gamma \rho \circ f\,\mathrm{d}z = 0, \tag{A.59}$$

by Proposition D.23 and Cauchy's theorem. By the Hahn-Banach theorem, Proposition A.54, we have $\oint_\Gamma f\,\mathrm{d}z = 0$.
Again, take arbitrary $\rho \in X^*$. Then

$$\rho\Big(f(w) - \frac{1}{2\pi i}\oint_\Gamma \frac{f(z)}{z - w}\,\mathrm{d}z\Big) = (\rho \circ f)(w) - \frac{1}{2\pi i}\oint_\Gamma \frac{(\rho \circ f)(z)}{z - w}\,\mathrm{d}z \tag{A.60}$$

$$= \frac{1}{2\pi i}\oint_\Gamma \frac{(\rho \circ f)(z)}{z - w}\,\mathrm{d}z - \frac{1}{2\pi i}\oint_\Gamma \frac{(\rho \circ f)(z)}{z - w}\,\mathrm{d}z = 0, \tag{A.61}$$

by Proposition D.23 and Cauchy's integral formula. By the Hahn-Banach theorem, Proposition A.54, we have $f(w) = \frac{1}{2\pi i}\oint_\Gamma \frac{f(z)}{z-w}\,\mathrm{d}z$.
(3) Take $z_0 \in U$ and $r > 0$ such that $\overline{\mathrm{B}}(z_0, r) \subseteq U$. Take $z \in \mathrm{B}(z_0, r)$. Then, using point (2) and the resolvent identity Proposition 0.3, we have

$$\begin{aligned}
\frac{f(z)-f(z_0)}{z-z_0} &= \frac{1}{2\pi i(z-z_0)}\Big(\oint_{|z'-z_0|=r}\frac{f(z')}{z'-z}\,\mathrm{d}z' - \oint_{|z'-z_0|=r}\frac{f(z')}{z'-z_0}\,\mathrm{d}z'\Big) && \text{(A.62)}\\
&= \frac{1}{2\pi i(z-z_0)}\oint_{|z'-z_0|=r} f(z')\Big(\frac{(z'-z)^{-1}-(z'-z_0)^{-1}}{z-z_0}\Big)\,\mathrm{d}z' && \text{(A.63)}\\
&= \frac{1}{2\pi i(z-z_0)}\oint_{|z'-z_0|=r} f(z')(z'-z)^{-1}(z'-z_0)^{-1}\,\mathrm{d}z' && \text{(A.64)}\\
&= \frac{1}{2\pi i}\oint_{|z'-z_0|=r} f(z')\Big(\frac{1}{(z'-z_0)^2}-\frac{1}{(z'-z_0)^2}+\frac{1}{(z'-z)(z'-z_0)}\Big)\,\mathrm{d}z' && \text{(A.65)}\\
&= \frac{1}{2\pi i}\oint_{|z'-z_0|=r} f(z')\Big(\frac{1}{(z'-z_0)^2}+\frac{(z'-z_0)-(z'-z)}{(z'-z_0)^2(z'-z)}\Big)\,\mathrm{d}z' && \text{(A.66)}\\
&= \frac{1}{2\pi i}\oint_{|z'-z_0|=r} f(z')\Big(\frac{1}{(z'-z_0)^2}+\frac{z-z_0}{(z'-z_0)^2(z'-z)}\Big)\,\mathrm{d}z' && \text{(A.67)}\\
&= \frac{1}{2\pi i}\oint_{|z'-z_0|=r}\frac{f(z')}{(z'-z_0)^2}\,\mathrm{d}z' + \frac{z-z_0}{2\pi i}\oint_{|z'-z_0|=r}\frac{f(z')}{(z'-z_0)^2(z'-z)}\,\mathrm{d}z'. && \text{(A.68)}
\end{aligned}$$

The first part is independent of z. For the second part, the integral is bounded as $z \to z_0$ (since z' stays r away from z_0 and z goes to z_0). Since the prefactor goes to 0, this means that the second term goes to zero. Thus the limit $\lim_{z\to z_0}\frac{f(z)-f(z_0)}{z-z_0}$ exists and is equal to $\frac{1}{2\pi i}\oint_{|z'-z_0|=r}\frac{f(z')}{(z'-z_0)^2}\,\mathrm{d}z'$. □

Corollary A.20. *Let $U \subseteq \mathbb{C}$ be an open set, X a Banach space, $f : U \to X$ a holomorphic function, Γ a Jordan curve in U whose interior is also in U and w an element of the interior of Γ. Then*

$$f^{(n)}(w) = \frac{n!}{2\pi i}\oint_\Gamma \frac{f(z)}{(z-w)^{n+1}}\,\mathrm{d}z. \tag{A.69}$$

The proof is the same as in the scalar case. It is included for completeness.

Proof. The proof is by induction on n. The base case $n = 0$ is given by the proposition.
For the induction step, assume that f has $n-1$ derivatives and the formula holds for $n-1$. Now the difference quotient can be expressed as

$$\frac{f^{(n-1)}(w+h)-f^{(n-1)}(w)}{h} = \frac{(n-1)!}{2\pi i}\oint_\Gamma \frac{f(z)}{h}\Big(\frac{1}{(z-w-h)^n}-\frac{1}{(z-w)^n}\Big). \tag{A.70}$$

Now using a telescoping sum, we can write

$$\frac{1}{h}\Big(\frac{1}{(z-w-h)^n}-\frac{1}{(z-w)^n}\Big) \tag{A.71}$$

$$= \frac{1}{h}\Bigg(\sum_{k=0}^{n-1}\frac{1}{(z-w-h)^{k+1}}\frac{1}{(z-w)^{n-k-1}} - \frac{1}{(z-w-h)^k}\frac{1}{(z-w)^{n-k}}\Bigg) \tag{A.72}$$

$$= \frac{1}{h}\Big(\frac{1}{z-w-h}-\frac{1}{z-w}\Big)\Bigg(\sum_{k=0}^{n-1}\frac{1}{(z-w-h)^k}\frac{1}{(z-w)^{n-k-1}}\Bigg) \tag{A.73}$$

$$= \frac{1}{(z-w-h)(z-w)}\Bigg(\sum_{k=0}^{n-1}\frac{1}{(z-w-h)^k}\frac{1}{(z-w)^{n-k-1}}\Bigg), \tag{A.74}$$

which converges to $\frac{n}{(z-w)^{n+1}}$ as $h \to 0$. This implies

$$f^{(n)}(w) = \lim_{h\to 0}\frac{f^{(n-1)}(w+h)-f^{(n-1)}(w)}{h} = \frac{n!}{2\pi i}\oint_\Gamma \frac{f(z)}{(z-w)^{n+1}}\,\mathrm{d}z. \tag{A.75}$$

□

Theorem A.21 (Holomorphic functional calculus). *Let A be a unital Banach algebra and $x \in A$. Consider the function*

$$\Phi_x : \mathrm{Hol}(\sigma(x),\mathbb{C}) \to A : f \mapsto f(x) \coloneqq \frac{1}{2\pi i}\oint_\Gamma f(z)R_x(z)\,\mathrm{d}z. \tag{A.76}$$

Here Γ is any finite union of simple Jordan curves that contains $\sigma(x)$ such that f is holomorphic in a region that contains Γ and its interior. Then

1. *Φ_x is well-defined: it does not depend on the particular curve Γ;*
2. *Φ_x is an algebra homomorphism;*
3. *$\Phi_x(\mathbb{1}_\mathbb{C}) = x$ and $\Phi_x(\underline{1}) = \mathbf{1}$;*
4. *$\sigma(\Phi_x(f)) = f^{\downarrow}\big(\sigma(x)\big)$.*

From points (2) and (3), it follows that $\Phi_x(p) = p(x)$ for any polynomial $p \in \mathbb{C}[X]$.
Note that equipping $\mathrm{Hol}(\sigma(x),\mathbb{C})$ with continuous convergence is not the same as uniform convergence, because functions in $\mathrm{Hol}(\sigma(x),\mathbb{C})$ may have unbounded domain, even though $\sigma(x)$ is compact.

Proof. (1) This follows from Proposition A.19.
(2) Take $f, g \in \mathrm{Hol}(\sigma(x),\mathbb{C})$ and $\lambda \in \mathbb{C}$. Then $\sigma(x) \subseteq \mathrm{dom}(f)\cap\mathrm{dom}(g)$ and we can find a curve Γ in $\mathrm{dom}(f)\cap\mathrm{dom}(g)$. By linearity of the integral, we have

$$\Phi_x\big(f+\lambda g\big) = \frac{1}{2\pi i}\oint_\Gamma \big(f(z)+\lambda g(z)\big)R_x(z)\,\mathrm{d}z \tag{A.77}$$

$$= \frac{1}{2\pi i}\oint_\Gamma f(z)R_x(z)\,\mathrm{d}z + \frac{\lambda}{2\pi i}\oint_\Gamma g(z)R_x(z)\,\mathrm{d}z \tag{A.78}$$

$$= \Phi_x(f) + \lambda\Phi_x(g). \tag{A.79}$$

To show multiplicativity, take two curves Γ_1, Γ_2 in $\mathrm{dom}(f) \cap \mathrm{dom}(g)$ such that Γ_2 is in the interior of Γ_1 and $\sigma(x)$ is in the interior of Γ_2. Then, using the first resolvent identity Proposition 0.3, we have

$$\Phi_x(f)\Phi_x(g) = \Big(\frac{1}{2\pi i}\Big)^2 \oint_{\Gamma_1} f(z)R_x(z)\,\mathrm{d}z \oint_{\Gamma_2} g(z')R_x(z')\,\mathrm{d}z' \tag{A.80}$$

$$= \Big(\frac{1}{2\pi i}\Big)^2 \oint_{\Gamma_1}\oint_{\Gamma_2} f(z)g(z')R_x(z)R_x(z')\,\mathrm{d}z'\,\mathrm{d}z \tag{A.81}$$

$$= \Big(\frac{1}{2\pi i}\Big)^2 \oint_{\Gamma_1}\oint_{\Gamma_2} f(z)g(z')\Big(\frac{R_x(z)-R_x(z')}{z'-z}\Big)\,\mathrm{d}z'\,\mathrm{d}z \tag{A.82}$$

$$= \Big(\frac{1}{2\pi i}\Big)^2 \oint_{\Gamma_1}\oint_{\Gamma_2} f(z)g(z')\frac{R_x(z)}{z'-z}\,\mathrm{d}z'\,\mathrm{d}z + \oint_{\Gamma_1}\oint_{\Gamma_2} f(z)g(z')\frac{R_x(z')}{z-z'}\,\mathrm{d}z'\,\mathrm{d}z \tag{A.83}$$

$$= \frac{1}{2\pi i}\oint_{\Gamma_2}\Big(\frac{1}{2\pi i}\oint_{\Gamma_1}\frac{f(z)}{z-z'}\,\mathrm{d}z\Big)g(z')R_x(z')\,\mathrm{d}z' + \frac{1}{2\pi i}\oint_{\Gamma_1} f(z)R_x(z)\Big(\frac{1}{2\pi i}\oint_{\Gamma_2}\frac{g(z')}{z'-z}\,\mathrm{d}z'\Big)\,\mathrm{d}z, \tag{A.84}$$

where the order of integration has been swapped in the second integral using Fubini's theorem. We have $\frac{1}{2\pi i}\oint_{\Gamma_1}\frac{f(z)}{z-z'}\,\mathrm{d}z = f(z')$ for all $z' \in \Gamma_2$ by Cauchy's integral formula , since all these z' lie inside Γ_1. We have $\oint_{\Gamma_2}\frac{g(z')}{z'-z}\,\mathrm{d}z' = 0$ for all $z \in \Gamma_1$ by Cauchy's theorem , since all these z lie outside Γ_2. Thus

$$\Phi_x(f)\Phi_x(g) = \frac{1}{2\pi i}\oint_{\Gamma_2} f(z')g(z')R_x(z')\,\mathrm{d}z' = \frac{1}{2\pi i}\oint_{\Gamma_2}(f\cdot g)(z')R_x(z')\,\mathrm{d}z' = \Phi_x(f\cdot g). \tag{A.85}$$

(3) Take $x \in A$ and let Γ be a circle centred at 0 with radius larger than $\|x\|$. Then, using Proposition A.2, we have

$$\Phi_x(\mathbb{1}_{\sigma(x)}) = \frac{1}{2\pi i}\oint_\Gamma zR_x(z)\,\mathrm{d}z \tag{A.86}$$

$$= \frac{1}{2\pi i}\oint_\Gamma \sum_{n=0}^\infty z\frac{x^n}{z^{n+1}}\,\mathrm{d}z \tag{A.87}$$

$$= \sum_{n=0}^\infty x^n \frac{1}{2\pi i}\oint_\Gamma z^{-n}\,\mathrm{d}z = a, \tag{A.88}$$

where we have used that $\oint_\Gamma z^{-n}\,\mathrm{d}z = 2\pi i$ if $n = 1$ and is zero otherwise, by the residue formula. Similarly, we calculate

$$\Phi_x(\underline{1}) = \frac{1}{2\pi i}\oint_\Gamma R_x(z)\,\mathrm{d}z = \sum_{n=0}^\infty x^n\frac{1}{2\pi i}\oint_\Gamma z^{-n-1}\,\mathrm{d}z = \mathbf{1}. \tag{A.89}$$

(4) First take $\lambda \in \sigma(x)$. We need to show that $f(\lambda) \in \sigma(\Phi_x(f))$, so $f(\lambda)\mathbf{1} - \Phi_x(f)$ is not invertible. Now $z \mapsto f(\lambda) - f(z)$ is holomorphic and equals 0 at $z = \lambda$. Then $f(z) - f(\lambda) = (\lambda - z)g(z)$ for some holomorphic g. Now, by (2) and (3), we have

$$f(\lambda)\mathbf{1} - \Phi_x(f) = \Phi_x\big(f(\lambda)\underline{1} - f\big) = \Phi_x\big((\lambda\underline{1} - \mathbb{1})\cdot g(z)\big) = (\lambda\mathbf{1} - x)\Phi_x(g). \tag{A.90}$$

If $f(\lambda)\mathbf{1} - \Phi_x(f)$ were invertible, then $\lambda\mathbf{1} - x$ would be invertible with inverse $\big(f(\lambda)\mathbf{1} - \Phi_x(f)\big)^{-1}\Phi_x(g)$. Since this is not true (by assumption $\lambda \in \sigma(x)$), we have that $f(\lambda)\mathbf{1} - \Phi_x(f)$ is not invertible.

Now suppose $\mu \notin f^{\downarrow}(\sigma(x))$. Then $\lambda - f(z)$ is non-zero on $\sigma(x)$, so $\sigma(x) \subseteq f^{-\downarrow}(\mathbb{C} \setminus \{0\})$. Also $f^{-\downarrow}(\mathbb{C}\setminus\{0\})$ is open. The function $(\underline{\lambda} - f)^{-1}$ is holomorphic on $f^{-\downarrow}(\mathbb{C}\setminus\{0\})$ and thus an element of $\mathrm{Hol}(\sigma(x), \mathbb{C})$. Then $\Phi_x\big((\underline{\lambda} - f)^{-1}\big)$ is the inverse of $\lambda\mathbf{1} - \Phi_x(f)$, so $\lambda \notin \sigma\big(\Phi_x(f)\big)$. □

A.1.3 Sylvester equation

Much of this section can be found in [64]. This textbook only considers the matrix case, but the arguments generalise readily. This section was included only because of the strong analogy with the operator equation (1.8). In particular, compare the solution $\widetilde{X}$ with Proposition A.25.

Let A be a Banach algebra. A Sylvester equation is an equation of the form

$$ax - xb = y \tag{A.91}$$

for some $a, b, x, y \in A$.

Proposition A.22. *Let A be a Banach algebra and $a, b, y \in A$. If $\sigma(a)$ and $\sigma(b)$ are disjoint, then the Sylvester equation $ax - xb = y$ has a unique solution x.*

Proof. Define the operator

$$T : A \to A : x \mapsto ax - bx. \tag{A.92}$$

This is a bounded linear operator on A (i.e. an element of $\mathcal{B}(A)$) and is equal to $\lambda_a - \rho_b$. Since λ_a and ρ_b commute, and $\mathcal{B}(A)$ is a unital Banach algebra, we can use Proposition A.7 and Proposition A.8 to get

$$\sigma(T) \subseteq \sigma(\lambda_a) - \sigma(\rho_b) \subseteq \sigma(a) - \sigma(b) \subseteq \mathbb{C} \setminus \{0\}. \tag{A.93}$$

Thus $0 \notin \sigma(T)$, which means that T is invertible. □

Proposition A.23. *Let A be a Banach algebra and $a, b, y \in A$. If there exists $0 < r_1 < r_2$ such that $\sigma(b) \subseteq \overline{\mathrm{B}}_{\mathbb{C}}(0, r_1)$ and $\sigma(a) \subseteq \overline{\mathrm{B}}_{\mathbb{C}}(0, r_2)^c$, then the solution of the Sylvester equation $ax - xb = y$ is given by*

$$x = \sum_{n=0}^{\infty} a^{-n-1} y b^n. \tag{A.94}$$

Note that a is invertible because $0 \notin \sigma(a)$.

Proof. Set $r = \frac{r_1 + r_2}{2}$. Then, by Proposition A.4, there exists $n_0 \in \mathbb{N}$ such that $\|b^n\| \leq r_1^n$ for all $n \geq n_0$. And, with Proposition A.5, there exists $n_1 \in \mathbb{N}$ such that $\|a^{-n}\| \leq r_2^{-n}$ for all $n \geq n_1$. Now

$$\sum_{n=0}^{\infty} \|a^{-n-1} y b^n\| = \sum_{n=0}^{\max\{n_0,n_1\}} \|a^{-n-1} y b^n\| + \sum_{n=\max\{n_0,n_1\}}^{\infty} \|a^{-n-1} y b^n\| \tag{A.95}$$

$$\leq \sum_{n=0}^{\max\{n_0,n_1\}} \|a^{-n-1} y b^n\| + \|y\| \sum_{n=\max\{n_0,n_1\}}^{\infty} \left(\frac{r_1}{r_2}\right)^n < \infty. \tag{A.96}$$

Since the series $\sum_{n=0}^{\infty} a^{-n-1} y b^n$ is absolutely convergent, it is also convergent.

We now verify that the series is indeed a solution of the Sylvester equation:

$$ax - xb = \sum_{n=0}^{\infty} a^{-n} y b^n - \sum_{n=0}^{\infty} a^{-n-1} y b^{n+1} \tag{A.97}$$

$$= \sum_{n=0}^{\infty} a^{-n} y b^n - \sum_{n=1}^{\infty} a^{-n} y b^n \tag{A.98}$$

$$= y. \tag{A.99}$$

□

Proposition A.24. *Let A be a unital Banach algebra and $a, b, y \in A$. Suppose there exists $\lambda \in \mathbb{R}$ such that*

$$\mathfrak{Re}^{\downarrow}\big(\sigma(a)\big) \subseteq]\lambda, \infty[\qquad \text{and} \qquad \mathfrak{Re}^{\downarrow}\big(\sigma(b)\big) \subseteq]-\infty, \lambda[. \tag{A.100}$$

Then the solution of the Sylvester equation $ax - xb = y$ is given by

$$x = \int_0^{\infty} e^{-ta} y e^{tb} \, \mathrm{d}t. \tag{A.101}$$

Proposition A.25. *Let A be a unital Banach algebra and $a, b, y \in A$. If Γ is a simple curve in $\mathbb{C}$ such that $\sigma(a)$ lies strictly inside Γ and $\sigma(b)$ lies strictly outside Γ, then the solution of the Sylvester equation $ax - xb = y$ is given by*

$$x = \frac{1}{2\pi i} \oint_{\Gamma} R_a(z) y R_b(z) \, \mathrm{d}z. \tag{A.102}$$

Proof. We calculate

$$ax - xb = \frac{1}{2\pi i} \oint_{\Gamma} \Big(a R_a(z) y R_b(z) - R_a(z) y R_b(z) b \Big) \, \mathrm{d}z \tag{A.103}$$

$$= \frac{1}{2\pi i} \oint_{\Gamma} \Big(z R_a(z) y R_b(z) - y R_b(z) - z R_a(z) y R_b(z) + R_a(z) y \Big) \, \mathrm{d}z \tag{A.104}$$

$$= \frac{1}{2\pi i} \oint_{\Gamma} \big(R_a(z) y - y R_b(z) \big) \, \mathrm{d}z \tag{A.105}$$

$$= \frac{1}{2\pi i} \oint_{\Gamma} R_a(z) \, \mathrm{d}z y - y \frac{1}{2\pi i} \oint_{\Gamma} R_b(z) \, \mathrm{d}z = y, \tag{A.106}$$

where we have used Lemma 0.5, Proposition A.19 and Theorem A.21. □

A.2 Operators on Banach spaces

In this section the notation $T : \mathrm{dom}(T) \subseteq V \to W$ and $T : V \not\to W$ will be used interchangeably to indicate that T is a partial function from V to W.

A.2.1 Closed operators and graph norm

Let $T : \mathrm{dom}(T) \subseteq X \to Y$ be an operator. Then T is a closed operator if $\mathrm{graph}(T)$ is closed in $X \oplus Y$.

This is not the same as a closed map in the topological sense!

A.2.1.1 The graph norm

Let $L : V \to W$ be a linear map between normed spaces. The graph of L

$$\{(v, w) \in V \oplus W \mid w = Lv\} \tag{A.107}$$

has a natural norm inherited from the direct sum:

$$\|(v, Lv)\| = \|v\|_V + \|Lv\|_W. \tag{A.108}$$

This norm can also be seen as a norm on V: the graph norm induced by L is defined as

$$\|v\|_L := \|v\|_V + \|Lv\|_W. \tag{A.109}$$

Proposition A.26. *Let $L : (V, \|\cdot\|_V) \nrightarrow (W, \|\cdot\|_W)$ be a linear map between normed spaces. Then $L : (\mathrm{dom}(L), \|\cdot\|_L) \to (W, \|\cdot\|_W)$ is bounded with norm K. Also*

1. *$K \leq 1$;*
2. *$K < 1$ if and only if $L : (\mathrm{dom}(V), \|\cdot\|_V) \to (W, \|\cdot\|_W)$ is bounded.*

Proof. Take any $v \in \mathrm{dom}(V)$. Then

$$\|L(v)\|_W \leq \|L(v)\|_W + \|v\|_V = \|v\|_L. \tag{A.110}$$

This shows the L is bounded and the norm is less than or equal to 1.
Now we can write $K = \sup_{v \in \mathrm{dom}(L) \setminus \{0\}} K_v$, where

$$K_v := \frac{\|L(v)\|_W}{\|v\|_L} = \sup_{v \in \mathrm{dom}(L) \setminus \{0\}} \frac{\|L(v)\|_W}{\|v\|_V + \|L(v)\|_W} \tag{A.111}$$

$$= \frac{\|L(v)\|_W + \|v\|_V - \|v\|_V}{\|v\|_V + \|L(v)\|_W} = 1 - \frac{\|v\|_V}{\|v\|_V + \|L(v)\|_W}. \tag{A.112}$$

If $L : (V, \|\cdot\|_V) \nrightarrow (W, \|\cdot\|_W)$ is bounded, then

$$K_v \leq 1 - \frac{\|v\|_V}{\|v\|_V + \|L\| \|v\|_V} = 1 - \frac{1}{1 + \|L\|} = \frac{\|L\|}{1 + \|L\|} < 1 \tag{A.113}$$

for all $v \in \mathrm{dom}(L) \setminus \{0\}$. This implies $K \leq \frac{\|L\|}{1+\|L\|} < 1$.
If $L : (V, \|\cdot\|_V) \to (W, \|\cdot\|_W)$ is unbounded, then there exists a sequence $\langle v_n \rangle$ of unit vectors such that $\|L(v_n)\|_W \to \infty$. Then $K_{v_n} = 1 - \frac{1}{1+\|L(v_n)\|_W} \to 1$ and $K = 1$. □

Lemma A.27. *Let $T : X \nrightarrow Y$ be an operator between normed spaces and $\langle x_n \rangle$ a sequence in $\mathrm{dom}(T)$. Then the following are equivalent:*

1. *$x_n \overset{\|\cdot\|_T}{\longrightarrow} x$;*
2. *$(x_n, Tx_n) \overset{\|\cdot\|_{X \oplus Y}}{\longrightarrow} (x, Tx)$;*
3. *$x_n \overset{\|\cdot\|_X}{\longrightarrow} x$ and $Tx_n \overset{\|\cdot\|_Y}{\longrightarrow} Tx$.*

Proof. We have the equivalences

$$\begin{aligned} x_n \overset{\|\cdot\|_T}{\longrightarrow} x &\iff \|x_n - x\|_T \longrightarrow 0 & \text{(A.114)}\\ &\iff \|x_n - x\|_X + \|Tx_n - Tx\|_Y \longrightarrow 0 & \text{(A.115)}\\ &\iff \|(x_n - x, Tx_n - Tx)\|_{X\oplus Y} \longrightarrow 0 & \text{(A.116)}\\ &\iff \|(x_n, Tx_n) - (x, Tx)\|_{X\oplus Y} \longrightarrow 0 & \text{(A.117)}\\ &\iff (x_n, Tx_n) \overset{\|\cdot\|_{X\oplus Y}}{\longrightarrow} (x, Tx). & \text{(A.118)} \end{aligned}$$

Now if $x_n \overset{\|\cdot\|_X}{\longrightarrow} x$ and $Tx_n \overset{\|\cdot\|_Y}{\longrightarrow} Tx$, then $\|x_n - x\|_X + \|Tx_n - Tx\|_Y \longrightarrow 0$. Conversely,

$$0 \le \|x_n - x\|_X \le \|x_n - x\|_X + \|Tx_n - Tx\|_Y, \tag{A.119}$$

implies $x_n \overset{\|\cdot\|_X}{\longrightarrow} x$ and $Tx_n \overset{\|\cdot\|_Y}{\longrightarrow} Tx$ is proved similarly. □

Corollary A.28. *The graph norm is strong than then original norm. Both norms are equivalent on* dom(T) if and only if *T is bounded.*

Corollary A.29. *Let $T : X \nrightarrow Y$ be an operator between normed spaces. Then the topology induced by the graph norm is equal to the initial topology w.r.t.* $\{\mathbb{1}_X : X \to (X, \|\cdot\|_X), T\}$.

A.2.1.2 Relatively bounded operators

Let $S, T : V \nrightarrow W$ be linear operators between normed spaces such that $\text{dom}(T) \subseteq \text{dom}(S)$. Then S is called relatively bounded w.r.t. T if S is a bounded operator, when it is restricted to $\text{dom}(T)$ and $\text{dom}(T)$ is equipped with the graph norm. We may write $S \in \mathcal{B}(\text{dom}(T), W)$ and consider the norm $\|S\|_{\text{dom}(T)\to W}$.

This definition of relative boundedness is the same as the usual one, which asserts the existence $c_0, c_1 \ge 0$ such that

$$\|S(v)\| \le c_0\|T(v)\| + c_1\|v\|. \tag{A.120}$$

A.2.1.3 Closed operators

Let X, Y be topological vector spaces and $T : \text{dom}(T) \subseteq X \to Y$ a linear operator. Then T is a closed operator if $\text{graph}(T)$ is closed in $X \oplus Y$.

There also exists a notion of "closed function" in topology: this is a function that maps closed sets to closed sets. It has nothing to do with the current setting.

Proposition A.30. *Let X, Y be topological vector spaces and $T : \text{dom}(T) \subseteq X \to Y$ a linear operator. Then*

1. *T is closed* if and only if *for all nets $\langle x_i \rangle_{i\in I}$ in* dom(T) *such that $x_i \to x \in X$ and $Tx_i \to y \in Y$, we have that $x \in \text{dom}(T)$ and $Tx = y$;*
2. *if T is continuous,* dom(T) *is closed and Y is Hausdorff, then T is closed;*
3. *if T is closed and injective, then $T^{-1} : \text{im}(T) \to \text{dom}(T)$ is closed.*

Lemma A.31. *Let X, Y be topological vector spaces and $T : \operatorname{dom}(T) \subseteq X \to Y$ a closed operator. Then*

1. *if $S : X \to Y$ is a continuous linear operator, then $S + T$ is a closed operator;*
2. *if $\lambda \in \mathbb{C}$, then λT is a closed operator.*

Proof. (1) We have $\operatorname{dom}(S + T) = \operatorname{dom}(T)$. Let $\langle x_i \rangle_{i \in I}$ be a net in $\operatorname{dom}(S + T)$ such that $x_i \to x \in X$ and $Sx_i + Tx_i \to y \in Y$. Then $Sx_i \to Sx$, so $Tx_i = Tx_i + Sx_i - Sx_i \to y - Sx$. Since T is closed, we have $y - Sx = Tx$ from Proposition A.30 and so $y = (S + T)x$. This implies, using Proposition A.30, that $S + T$ is closed.
(2) We have $\operatorname{graph}(\lambda T) = \lambda \operatorname{graph}(T)$. If $\lambda \neq 0$, then multiplication by λ is a homeomorphism, so $\lambda \operatorname{graph}(T)$ is closed. If $\lambda = 0$, then $\lambda \operatorname{graph}(T) = \operatorname{dom}(T) \times \{0\}$, which is closed since Y is Hausdorff. □

Proposition A.32. *Let $T \in \operatorname{Lin}(X, Y)$ be a closed operator between Banach spaces that is bounded below. Then $\operatorname{im}(T)$ is closed.*

Proof. Let T be bounded below by b and let $\langle Tx_n \rangle$ be a Cauchy sequence in $\operatorname{im}(T)$. Then $\|x_m - x_n\| \leq \frac{1}{b}\|T(x_m - x_n)\|$, so $\langle x_n \rangle$ is also Cauchy.
So we can find $x \in X, y \in Y$ such that $x_n \to x$ and $Tx_n \to y$. By closedness of T, we have $Tx = y$ and thus $y \in \operatorname{im}(T)$. □

Proposition A.33. *Let X, Y be Banach spaces and $T : X \not\to Y$ a linear operator. Then* $\operatorname{dom}(T)$*, equipped with the graph norm is a Banach space* if and only if *T is closed.*

In this case, being a Banach space is equivalent to being complete.

Proof. First assume $\operatorname{dom}(T)$, equipped with the graph norm, is a Banach space. We use Proposition A.30 to show that T is closed. Let $\langle x_n \rangle$ be a sequence in $\operatorname{dom}(T)$ such that $x_n \to x$ and $Tx_n \to y$. Then $\langle x_n \rangle$ is Cauchy in the graph norm. Since $\operatorname{dom}(T)$ is complete, we have $x_n \to x' \in \operatorname{dom}(T)$. Since X is Hausdorff (and the graph norm is stronger than the original convergence), we have $x' = x$. Finally, Lemma A.27 gives $Tx_n \to T(x)$. Since Y is also Hausdorff, this implies $T(x) = y$.
Now assume T is closed. Let $\langle x_n \rangle$ be a sequence that is Cauchy in the graph norm. Then both $\langle x_n \rangle$ and $\langle Tx_n \rangle$ are Cauchy sequences, the first in X and the second in Y. Since both X and Y are Banach spaces, there exists $x \in X$ and $y \in Y$ such that $x_n \to x$ and $Tx_n \to y$. Since T is closed, Proposition A.30 gives that $x \in \operatorname{dom}(T)$ and $y = T(x)$. Now $\langle x_n \rangle$ converges to x in graph norm. □

A.2.1.4 Closable operators

A linear operator is called closable if it has a closed linear extension.

Lemma A.34. *Let V, W be topological vector spaces and $T : \operatorname{dom}(T) \subseteq V \to W$ a linear operator defined on a subspace. Then the following are equivalent:*

1. *T is closable;*
2. *$\operatorname{cl}_{V \oplus W}\big(\operatorname{graph}(T)\big)$ is the graph of a linear operator $\overline{T}$;*
3. *$(0, w) \in \operatorname{cl}_{V \oplus W}\big(\operatorname{graph}(T)\big)$ implies $w = 0$ for all $w \in W$;*

4. if $\langle x_i \rangle_{i\in I}$ is a net in $\operatorname{dom}(T)$ *and $w \in W$ such that $x_i \to 0$ and $T(x_i) \to w$, then $w = 0$.*

In this case $\operatorname{dom}(\overline{T})$ *is a subspace.*

Corollary A.35. *Let V, W be topological vector spaces and $T : \operatorname{dom}(T) \subseteq V \to W$ a continuous operator. If W is Hausdorff, then T is closable.*

Proof. Let $\langle x_i \rangle_{i\in I}$ be a net in $\operatorname{dom}(T)$ that converges to 0. Then $T(x_i) \to 0$ by continuity. If $T(x_i) \to w$, then $w = 0$ by Hausdorffness. □

Let V, W be topological vector spaces and $T : \operatorname{dom}(T) \subseteq V \to W$ a closable linear operator. Then the operator $\overline{T}$ defined in Lemma A.34 is called the closure of T.

Proposition A.36. *Let V, W be topological vector spaces and $T : \operatorname{dom}(T) \subseteq V \to W$ a closable linear operator. Then*

1. $\operatorname{dom}(\overline{T}) \subseteq \operatorname{cl}_V(\operatorname{dom}(T))$*;*
2. *if W is Hausdorff and complete, then* $\operatorname{dom}(\overline{T}) = \operatorname{cl}_V(\operatorname{dom}(T))$.

Note that T is closable, by Corollary A.35.

Proposition A.37. *Let V, W be normed vector spaces and $T : \operatorname{dom}(T) \subseteq V \to W$ a bounded linear operator. Then $\overline{T}$ is bounded with $\|\overline{T}\| = \|T\|$.*

Note that T is closable, by Corollary A.35, because normed spaces are Hausdorff.

Proof. (1) Take $x \in \operatorname{dom}(\overline{T})$. Then there exists a sequence $\langle (x_n, Tx_n) \rangle_{n\in\mathbb{N}}$ in $\operatorname{graph}(T)$ that converges to $(x, \overline{T}(x)) \in \operatorname{graph}(\overline{T})$. This means that we can use the continuity of the norm to calculate

$$\|\overline{T}(x)\| = \lim_{n\to\infty} \|Tx_n\| \leq \lim_{n\to\infty} \|T\|\|x_n\| = \|T\|\|x\|, \tag{A.121}$$

so $\|\overline{T}\| \leq \|T\|$. Conversely,

$$\|T\| = \sup_{x\in\operatorname{dom}(T)} \frac{\|Tx\|}{\|x\|} = \sup_{x\in\operatorname{dom}(T)} \frac{\|\overline{T}x\|}{\|x\|} \leq \sup_{x\in\operatorname{dom}(\overline{T})} \frac{\|\overline{T}x\|}{\|x\|} = \|\overline{T}\|. \tag{A.122}$$

(2) One inclusion is given by Proposition A.36. Take $x \in \operatorname{cl}_V\big(\operatorname{dom}(T)\big)$. Then there exists a sequence $\langle x_n \rangle$ in $\operatorname{dom}(T)$ that converges to x. Since T is continuous and linear, it is uniformly continuous and $\langle Tx_n \rangle$ is a Cauchy sequence. Since W is complete, $\langle Tx_n \rangle$ converges to some $y \in W$. Then $(x_n, Tx_n) \to (x, y)$, so $\overline{T}(x) = y$ and $x \in \operatorname{dom}(\overline{T})$. □

Corollary A.38 (Bounded linear extension)**.** *Let X be a normed space, Y a Banach space and $T : \operatorname{dom}(T) \subseteq X \to Y$ be a bounded operator between normed spaces. Then T has a unique bounded extension to $\operatorname{cl}_X(\operatorname{dom}(T))$. This extension is given by the closure $\overline{T}$.*

In particular, if X is a dense subspace of a Banach space Y, then every operator in $\mathcal{B}(X)$ can be extended to an operator in $\mathcal{B}(Y)$, since we can first enlarge the codomain to Y and then apply the result.

Proof. The only part that has not been proved yet is uniqueness. Suppose S is another bounded extension of T to $\operatorname{cl}_X(\operatorname{dom}(T))$. Take $x \in \operatorname{cl}_X(\operatorname{dom}(T))$. Then there exists a sequence $\langle x_n \rangle$ in $\operatorname{dom}(T)$ such that $x_n \to x$ and we have

$$S(x) = \lim_{n\to\infty} S(x_n) = \lim_{n\to\infty} T(x_n) = \lim_{n\to\infty} \overline{T}(x_n) = \overline{T}(x). \tag{A.123}$$

□

A.2.1.5 Domain and core

Let $T : X \not\to Y$ be a closed operator between normed spaces and $D \subseteq \mathrm{dom}(T)$ a subspace. We call D a core or essential domain for T if $\{(x, Tx) \,|\, x \in D\}$ is dense in $\mathrm{graph}(T) \subseteq X \oplus Y$.

Proposition A.39. *Let $T : X \not\to Y$ be a closed operator between normed spaces and $D \subseteq \mathrm{dom}(T)$ a subspace. Then D is a core of T* if and only if *D is dense in* $\mathrm{dom}(T)$ *w.r.t. the graph norm $\|\cdot\|_T$ of T.*

Note that the norm is bounded by the graph norm, so the graph norm topology is stronger than the norm topology. Thus $\mathrm{cl}_{\|\cdot\|_T}(D) \subseteq \mathrm{cl}_{\|\cdot\|}(D)$ and it is not enough for D to be norm dense in $\mathrm{dom}(T)$.

Proof. Immediate by Lemma A.27. □

A.2.1.6 Resolvent bounds and continuity

Proposition A.40. *Let T be a closed operator on a Banach space X and $\lambda \in \rho(T)$. Let* $\mathrm{dom}(T)$ *be equipped with the graph norm. Then the resolvent $R_T(\lambda) : X \to \mathrm{dom}(T)$ is bounded and the norm satisfies*

$$\|R_T(\lambda)\|_{X\to\mathrm{dom}(T)} \leq 1 + (1 + |\lambda|)\|R_A(\lambda)\|. \tag{A.124}$$

Proof. Let $x \in X$ be a unit vector. Lemma 0.5 gives

$$\|TR_T(\lambda)x\| = \|x - \lambda R_T(\lambda)x\|_X \leq 1 + |\lambda|\|R_T(\lambda)\|. \tag{A.125}$$

The graph norm is then bounded by

$$\|R_T(\lambda)x\|_T = \|R_T(\lambda)x\| + \|TR_T(\lambda)x\| \leq 1 + (1 + |\lambda|)\|R_A(\lambda)\|. \tag{A.126}$$

□

Proposition A.41. *Let T be a closed operator on a Banach space X. Then R_T is holomorphic on $\sigma(T)$ in the topology generated by $\|\text{-}\|_{D\to X}$.*

In particular, R_T is continuous in this topology.

Proof. Comparing with the proof of Corollary A.12, it is enough to prove that R_T is continuous in this topology.
The proof of Corollary A.12 can be adapted to this situation using Proposition A.40. □

A.2.2 Operators bounded below

Let T be a linear operator between normed spaces. We say T is bounded below if

$$\exists b > 0 : \forall v \in \mathrm{dom}(T) : \quad \|Tv\| \geq b\|v\| \tag{A.127}$$

Proposition A.42. *Let V, W be normed spaces and $T \in \mathrm{Lin}(V, W)$ an operator. Then T has a bounded inverse $T^{-1} : \mathrm{im}(T) \to V$* if and only if *$T$ is bounded below by some constant b.*
In this case

$$\|T^{-1}\| = \left(\inf_{x\neq 0} \frac{\|Tx\|}{\|x\|}\right)^{-1} \leq \frac{1}{b}. \tag{A.128}$$

Proof. First assume T bounded below. To show T is injective, take $x_1, x_2 \in \operatorname{dom} T$ such that $Tx_1 = Tx_2$. Then

$$0 = \|Tx_1 - Tx_2\| = \|T(x_1 - x_2)\| \geq b\|x_1 - x_2\| \geq 0. \tag{A.129}$$

So $\|x_1 - x_2\| = 0$ and thus $x_1 = x_2$. The existence of T^{-1} is then clear. For boundedness notice that $T^{-1}y \in \operatorname{dom}(T)$, so because T is bounded below,

$$b\|T^{-1}y\| \leq \|TT^{-1}y\| = \|y\| \quad \Longrightarrow \quad \|T^{-1}y\| \leq \frac{1}{b}\|y\|. \tag{A.130}$$

This also shows that $\|T^{-1}\| \leq 1/b$ for all lower bounds b. In other words $1/\|T^{-1}\| \geq \inf_{x\neq 0}\|Tx\|/\|x\|$.
Now assume T^{-1} bounded. Then for all $x \in \operatorname{dom}(T)$: $\|x\| = \|T^{-1}Tx\| \leq \|T^{-1}\|\|Tx\|$, so T is bounded below by $1/\|T^{-1}\|$.
This also shows that $1/\|T^{-1}\|$ is a lower bound, so $1/\|T^{-1}\| \leq \inf_{x\neq 0}\|Tx\|/\|x\|$. □

A.2.3 Major theorems about Banach spaces

Theorem A.43 (Uniform boundedness principle)**.** *Let $\mathcal{F} \subset \mathcal{B}(X, Y)$ be a family of bounded operators where X is a Banach space and Y a normed space, such that*

$$\sup\{\|Tx\| \mid T \in \mathcal{F}\} < \infty \qquad \text{for all } x \in X. \tag{A.131}$$

Then $\sup\{\|T\| \mid T \in \mathcal{F}\} < \infty$.

Corollary A.44 (Banach-Steinhaus)**.** *Let X be a Banach space and Y a normed space. Let $\langle T_n : X \to Y\rangle_{n\in\mathbb{N}}$ be a sequence of bounded operators that converges pointwise to some linear operator T. Then*

1. *$\{T_n\}_{n\in\mathbb{N}}$ is norm-bounded;*
2. *T is bounded.*

This does not imply that $\langle T_n\rangle$ converges to T in norm! The name "Banach-Steinhaus" is sometimes used to refer to the uniform boundedness principle.

Theorem A.45 (Open mapping theorem)**.** *Let X, Y be Banach spaces and $T : X \to Y$ a surjective bounded operator. Then T is an open map.*

Corollary A.46 (Bounded inverse theorem)**.** *Let X, Y be Banach spaces. If $T : X \to Y$ is is continuous, linear and bijective, then T is a homeomorphism.*

Proposition A.47. *Let $T : \operatorname{dom}(T) \subset X \to Y$ be a bounded linear operator. Then*

1. *if $\operatorname{dom}(T)$ is a closed subset of X, then T has closed graph;*
2. *if T has closed graph and Y is complete, then $\operatorname{dom}(T)$ is a closed subset of X.*

Theorem A.48 (Closed graph theorem)**.** *Let X, Y be Banach spaces and $T : X \to Y$ a linear operator with $\operatorname{dom}(T) = X$. Then T is continuous* if and only if *T is a closed operator.*

A.2.4 The Hahn-Banach theorems

Theorem A.49 (Hahn-Banach majorised by convex functionals)**.** *Let V be a real vector space, $U \subset V$ a subspace and p a convex functional on V. Let $f : U \to \mathbb{R}$ be a linear functional that is bounded by p:*

$$\forall u \in U : \quad f(u) \leq p(u). \tag{A.132}$$

Then f has an extension $\tilde{f} : V \to \mathbb{R}$ such that $\tilde{f}$ is a linear functional on V bounded by p:

$$\forall v \in V : \tilde{f}(v) \leq p(v) \qquad \textit{and} \qquad \forall u \in U : \tilde{f}(u) = f(u). \tag{A.133}$$

Corollary A.50 (Hahn-Banach majorised by sublinear functionals)**.** *Any majorant p that is sublinear is also convex and can be used in the Hahn-Banach theorem.*

Corollary A.51 (Hahn-Banach majorised by seminorms)**.** *Let $(\mathbb{C}, V, +)$ be a real or complex vector space, $U \subset V$ a subspace and p a seminorm on V. Let $f : U \to \mathbb{C}$ be a linear functional that is bounded by p:*

$$\forall u \in U : \quad |f(u)| \leq p(u). \tag{A.134}$$

Then f has an extension $\tilde{f} : V \to \mathbb{R}$ such that $\tilde{f}$ is a linear functional on V bounded by p:

$$\forall v \in V : |\tilde{f}(v)| \leq p(v) \qquad \textit{and} \qquad \forall u \in U : \tilde{f}(u) = f(u). \tag{A.135}$$

Theorem A.52 (Hahn-Banach separation theorem)**.** *Let V be a topological vector space. Suppose A, B are disjoint, non-empty, convex sets and that A is open. Then there exists a continuous linear functional $f : V \to \mathbb{C}$ such that $f^{\downarrow}[A]$ and $f^{\downarrow}[B]$ are disjoint.*

Proposition A.53. *Let (V, ξ) be a locally convex vector convergence space. Let B be a closed convex set and $v \notin B$, then there exists a continuous linear functional $f : V \to \mathbb{C}$ such that $f(v) \notin \overline{f^{\downarrow}[B]}$.*

Proposition A.54. *Let V be a Hausdorff locally convex topological vector space and $v \in V$. If $f(v) = 0$ for all $f \in V^*$, then $v = 0$.*

Proposition A.55. *Let X be a normed space and $Z \subset X$ a subspace. Any bounded linear functional in Z^* can be extended to a bounded linear functional in X^* with the same norm.*

Proof. Let $f : Z \to \mathbb{C}$ be such a functional. Extend f with the Hahn-Banach theorem Corollary A.51, using $p(x) = \|f\|_Z \|x\|$. □

Corollary A.56. *Let X be a normed space and $x_0 \neq 0$ an element of X. Then there exists a bounded linear functional ω_{x_0} such that*

$$\|\omega_{x_0}\| = 1 \qquad \textit{and} \qquad \omega_{x_0}(x_0) = \|x_0\|. \tag{A.136}$$

Proof. Extend the functional $f : \operatorname{span}\{x_0\} \to \mathbb{C}$ defined by

$$f(x) = f(a x_0) = a\|x_0\|. \tag{A.137}$$

□

A.3 Operators on Hilbert spaces

A.3.1 The adjoint

A.3.1.1 The adjoint as a relation

Let H, K be Hilbert spaces and $T : H \nrightarrow K$ an operator. An adjoint of T is an operator $S : K \nrightarrow H$ such that

$$\langle w, Tv\rangle_K = \langle Sw, v\rangle_H \quad \forall v \in \mathrm{dom}(T),\ \forall w \in \mathrm{dom}(S). \tag{A.138}$$

Lemma A.57. *Let $T : H \nrightarrow K$ be an operator between Hilbert spaces. Let S_1, S_2 be adjoints of T then for all $x \in \mathrm{dom}(S_1) \cap \mathrm{dom}(S_2)$ we have $S_1(x) - S_2(x) \in \mathrm{dom}(T)^\perp$.*
Conversely, let S be an adjoint of T and $x \in \mathrm{dom}(S)$. Then for all $v \in \mathrm{dom}(T)^\perp$ there exists an adjoint S' such that $S'(x) = S(x) + v$.

Proof. For all $u \in \mathrm{dom}(T)$ we have

$$\langle S_1(x) - S_2(x), u\rangle_H = \langle S_1(x), u\rangle_H - \langle S_2(x), u\rangle_H = \langle x, Tu\rangle_K - \langle x, Tu\rangle_K = 0. \tag{A.139}$$

So $(S_1(x) - S_2(x)) \in \mathrm{dom}(T)^\perp$.
For the converse, set $S' = S + \frac{\langle x, \cdot\rangle_K}{\langle x,x\rangle_K} v$. This is an adjoint: for all $a \in \mathrm{dom}(T), b \in \mathrm{dom}(S') = \mathrm{dom}(S)$ we have

$$\langle S'b, a\rangle_H = \langle Sb, a\rangle_H + \frac{\langle x, b\rangle_K}{\langle x, x\rangle_K}\langle v, a\rangle_H = \langle Sb, a\rangle_H = \langle b, Ta\rangle_K. \tag{A.140}$$

□

Corollary A.58. *Let $T : H \nrightarrow K$ be a densely defined operator between Hilbert spaces. Let S_1, S_2 be adjoints of T then for all $x \in \mathrm{dom}(S_1) \cap \mathrm{dom}(S_2)$ we have $S_1(x) = S_2(x)$.*

Proof. We have $\mathrm{dom}(T)^\perp = \overline{\mathrm{dom}(T)}^\perp = H^\perp = \{0\}$. So $S_1(x) - S_2(x) = 0$. □

Corollary A.59. *Let $T : H \nrightarrow K$ be an operator between Hilbert spaces. Then*

$$\bigcup\{\mathrm{graph}(S) \mid S \in (K \nrightarrow H) \text{ is an adjoint of } T\} \tag{A.141}$$

is the graph of an operator if and only if *T is densely defined.*

Let $T : H \nrightarrow K$ be an operator between Hilbert spaces. We define *the* adjoint T^* as the *relation* on (H, K) with graph

$$\mathrm{graph}(T^*) \coloneqq \bigcup\{\mathrm{graph}(S) \mid S \in (K \nrightarrow H) \text{ is an adjoint of } T\}. \tag{A.142}$$

Note that, by Corollary A.59, the adjoint is a function if and only if T is densely defined.

Lemma A.60. *Let $T : H \nrightarrow K$ be a densely defined operator between Hilbert spaces. If S is an adjoint of T that is defined everywhere, then $T^* = S$.*

Corollary A.61. *Let H be a Hilbert space. Then $\mathbb{1}_H^* = \mathbb{1}_H$.*

Example

Consider the left- and right-shift operators

$$S_L : \ell^2(\mathbb{N}) \to \ell^2(\mathbb{N}) : (x_n)_{n\in\mathbb{N}} \mapsto (x_{n+1})_{n\in\mathbb{N}} \tag{A.143}$$

$$S_R : \ell^2(\mathbb{N}) \to \ell^2(\mathbb{N}) : (x_n)_{n\in\mathbb{N}} \mapsto \left(\begin{cases} x_{n-1} & (n \geq 1) \\ 0 & (n = 0) \end{cases}\right)_{n\in\mathbb{N}}. \tag{A.144}$$

Then $S_L^* = S_R$ and $S_R^* = S_L$. To see this, take $\langle x_n\rangle, \langle y_n\rangle \in \ell^2(\mathbb{N})$. Then

$$\langle S_L\langle x_n\rangle, \langle y_n\rangle\rangle = \sum_{n\in\mathbb{N}} \overline{x_{n+1}} y_n = \overline{x_0}\cdot 0 + \sum_{n\in\mathbb{N}\setminus\{0\}} \overline{x_n} y_{n-1} = \langle\langle x_n\rangle, S_R\langle y_n\rangle\rangle. \tag{A.145}$$

Thus S_L is an adjoint of S_R and S_R is an adjoint of S_L. We have $S_L^* = S_R$ and $S_R^* = S_L$ from Lemma A.60.

Lemma A.62. *Let $T : H \not\rightarrow K$ be an operator between Hilbert spaces and $(x, y) \in K \times H$. Then $(x, y) \in T^*$* if and only if

$$\forall z \in \operatorname{dom}(T) : \ \langle x, T(z)\rangle = \langle y, z\rangle. \tag{A.146}$$

Proof. $\boxed{\Rightarrow}$ If $(x, y) \in T^*$, then there exists an adjoint $f : K \not\rightarrow H$ such that $f(x) = y$. Then for all $z \in \operatorname{dom}(T)$ we have $\langle x, T(z)\rangle = \langle f(x), z\rangle = \langle y, z\rangle$.
$\boxed{\Leftarrow}$ The function defined by $f(x) = y$ and extended to $\operatorname{span}\{x\}$ by linearity is an adjoint. □

Proposition A.63. *Let $T : H \not\rightarrow K$ be an operator between Hilbert spaces. Then*

$$\operatorname{dom}(T^*) = \{x \in K \mid \operatorname{dom}(T) \to \mathbb{C} : u \mapsto \langle x, Tu\rangle \textit{ is a bounded functional}\}. \tag{A.147}$$

This result is essentially due to the Riesz representation theorem.

Proof. $\boxed{\subseteq}$ If $\omega_x : u \mapsto \langle x, Tu\rangle$ is bounded, then its domain can be extended by continuity to $\overline{\operatorname{dom}(T)}$, which is a Hilbert space. This extended functional has a Riesz vector x^* such that $\omega_x = u \mapsto \langle x^*, u\rangle$. The linear operator with domain $\operatorname{span}\{x\}$ that maps x to x^* is then an adjoint.
$\boxed{\supseteq}$ If $x \in \operatorname{dom}(T^*)$, then, using the Cauchy-Schwarz inequality,

$$|\langle x, Tu\rangle| = |\langle T^*x, u\rangle| \leq \|T^*x\|\,\|u\|, \tag{A.148}$$

so the functional $u \mapsto \langle x, Tu\rangle$ is bounded. □

Corollary A.64. *The domain $\operatorname{dom}(T^*)$ is a vector space and in particular contains 0.*

Proposition A.65. *Let H, K be Hilbert spaces. Take $T \in (H \not\rightarrow K)$ and $S \in (K \not\rightarrow H)$. Then*

$$S \subseteq T^* \iff T \subseteq S^*. \tag{A.149}$$

In more abstract language, this can be rephrased as saying that $(*, *)$ is an antitone Galois connection between $((H \not\rightarrow K), \subseteq)$ and $((K \not\rightarrow H), \subseteq)$.

Proof. We have $S \subseteq T^*$ iff S is an adjoint of T iff T is an adjoint of S (since the definition of adjoint is symmetric in S and T) iff $T \subseteq S^*$. □

Corollary A.66. *Let $S, T : H \not\rightarrow K$ be operators between Hilbert spaces such that $S \subseteq T$. Then $T^* \subseteq S^*$.*

A.3.1.2 Properties of the adjoint relation

Proposition A.67. *Let T be an operator between Hilbert spaces and $\lambda \in \mathbb{C}$. If $\lambda \neq 0$, then*

$$\begin{pmatrix} \mathbb{1} & 0 \\ 0 & \overline{\lambda}\,\mathbb{1} \end{pmatrix} \operatorname{graph}(T^*) = (\lambda T)^*. \tag{A.150}$$

Note that if T^* is a function (i.e. if T is densely defined), then $\begin{pmatrix} \mathbb{1} & 0 \\ 0 & \overline{\lambda}\,\mathbb{1} \end{pmatrix} \operatorname{graph}(T^*) = \overline{\lambda} T^*$. We write the former in the proposition, because we have not made this assumption.
If $\lambda = 0$ and $T : H \not\rightarrow K$, then

$$\begin{pmatrix} \mathbb{1} & 0 \\ 0 & 0 \end{pmatrix} \operatorname{graph}(T^*) = \big(0 : \operatorname{dom}(T^*) \to H\big) \subseteq \big(0 : K \to H\big) = (0T)^*, \tag{A.151}$$

where the last equality is given by Proposition A.70.

Proof. For the inclusion $\subseteq$, take f to be an adjoint of T. It is enough to show that $\overline{\lambda} f$ is an adjoint of λT. This follows from

$$\langle \overline{\lambda} f(w), v\rangle = \lambda \langle f(w), v\rangle = \lambda \langle w, Tv\rangle = \langle w, \lambda T v\rangle \qquad \forall w \in \operatorname{dom}(f), v \in \operatorname{dom}(T). \tag{A.152}$$

For the other inclusion, let f be an adjoint of λT. It is enough to show that $\overline{\lambda^{-1}} f$ is an adjoint of T, because then $f = \overline{\lambda} \cdot \overline{\lambda^{-1}} f \subseteq \begin{pmatrix} \mathbb{1} & 0 \\ 0 & \overline{\lambda}\,\mathbb{1} \end{pmatrix} \operatorname{graph}(T^*)$. Indeed

$$\langle \overline{\lambda^{-1}} f(w), v\rangle = \lambda^{-1} \langle f(w), v\rangle = \langle w, \lambda^{-1} \lambda T v\rangle = \langle w, Tv\rangle \quad \forall w \in \operatorname{dom}(f), v \in \operatorname{dom}(T). \tag{A.153}$$

□

Proposition A.68. *Let $T : H \not\rightarrow K$ be an operator between Hilbert spaces. Then*

$$\operatorname{graph}(T^*) = \left(\begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \operatorname{graph}(T) \right)^{\perp} = \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \operatorname{graph}(T)^{\perp}. \tag{A.154}$$

If T is densely defined, then T^* is a closed operator.

Proof. We have

$$\operatorname{graph}(T^*) = \bigcup \{\operatorname{graph}(S) \,|\, S \in (K \not\rightarrow H) \text{ is an adjoint of } T\}. \tag{A.155}$$

Take an adjoint S and (w, Sw) in $\operatorname{graph}(S)$. Then for all $v \in \operatorname{dom}(T)$:

$$0 = \langle w, Tv\rangle_K - \langle Sw, v\rangle_H = \langle w, Tv\rangle_K + \langle Sw, -v\rangle_H = \langle (w, Sw), (Tv, -v)\rangle_{K \oplus H}. \tag{A.156}$$

So $(Tv, -v) = \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} (v, Tv) \in \operatorname{graph}(S)^{\perp}$.
The final equality is due to the fact that $\begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}$ is a surjective isometry.
If T is densely defined, then T^* is a function by Corollary A.59. It is closed since all orthogonal complements are closed. □

Corollary A.69. *Let $T : H \not\rightarrow K$ be a densely defined operator between Hilbert spaces. Then*

1. $\mathrm{graph}(T^{**}) = \overline{\mathrm{graph}(T)}$;
2. T^* *is densely defined* if and only if T *is closable;*
3. *If T is closable, then* $\overline{T} = T^{**}$.

Proof. From the proposition we have

$$\mathrm{graph}(T^{**}) = \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \mathrm{graph}(T^*)^\perp = \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \left(\begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \mathrm{graph}(T)^\perp \right)^\perp \tag{A.157}$$

$$= \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}^2 \mathrm{graph}(T)^{\perp\perp} = -\,\mathrm{graph}(T)^{\perp\perp} = \overline{\mathrm{graph}(T)}. \tag{A.158}$$

The right-hand side is the graph of an operator iff T is closable and the left-hand side is the graph of an operator iff T^* is densely defined, by Corollary A.59.
For a closable operator, the closure is defined by $\overline{\mathrm{graph}(T)} = \mathrm{graph}(\overline{T})$. ☐

Proposition A.70. *Let $T : H \to K$ be a densely defined operator between Hilbert spaces. Then* $\mathrm{dom}(T^*) = K$ if and only if T *is bounded.*

Proof. The direction $\Leftarrow$ is given by Proposition A.63.
For the other direction, note that T^* is closed by Proposition A.68. Then T^* is bounded by the closed graph theorem Theorem A.48. We use the direction $\Leftarrow$ to see that $\mathrm{dom}(T^{**}) = H$. Similarly, T^{**} is closed by Proposition A.68 and bounded by the closed graph theorem Theorem A.48. Thus $T \subseteq \overline{T} = T^{**}$ is bounded. ☐

An important application of this proposition is the Hellinger-Toeplitz theorem Theorem A.92.

Proposition A.71. *Let T, S be compatible operators between Hilbert spaces. Then*

1. $S^* + T^* \subseteq (S+T)^*$;
2. $S^*T^* \subseteq (TS)^*$.

Proof. (1) Let f be an adjoint of S and g an adjoint of T. It is enough to see that $f+g$ is an adjoint of $S+T$. Indeed $\forall w \in \mathrm{dom}(f+g), v \in \mathrm{dom}(S+T)$

$$\langle (f+g)(w), v\rangle = \langle f(w), v\rangle + \langle g(w), Tv\rangle = \langle w, Sv\rangle + \langle w, Tv\rangle = \langle w, (S+T)v\rangle. \tag{A.159}$$

(2) Let f be an adjoint of T and g an adjoint of S. It is enough to see that gf is an adjoint of TS. Indeed

$$\langle g\circ f(w), v\rangle = \langle f(w), Sv\rangle = \langle w, TSv\rangle \qquad \forall w \in \mathrm{dom}(g\circ f), v \in \mathrm{dom}(TS). \tag{A.160}$$

☐

Example

The inclusions in Proposition A.71 are, in general, not equalities.

- If S, T are densely defined, but $\mathrm{dom}(S+T) = \mathrm{dom}(S) \cap \mathrm{dom}(T)$ is not dense, then there can clearly not be an equality.
- Let $T : H \to K$ be a densely defined unbounded operator. Then $\mathrm{dom}(T^*) \neq K$ by

Proposition A.70. Now we have

$$T^* - T^* = \big(0 : \mathrm{dom}(T^*) \to H\big) \subsetneq \big(0 : K \to H\big) = \big(0 : \mathrm{dom}(T) \to K\big)^* = (T - T)^*. \tag{A.161}$$

The penultimate equality follows from Proposition A.70. In this case the domain of the sum is dense, but still there is no equality.

There exist various conditions that make the inclusions in Proposition A.71 equalities.

Proposition A.72. *Let T, S be compatible operators between Hilbert spaces.*

1. *if T is densely defined, $\mathrm{dom}(S) \subseteq \mathrm{dom}(T)$ and $\mathrm{dom}\big((S+T)^*\big) \subseteq \mathrm{dom}(T^*)$, then $S^*+T^* = (S+T)^*$;*
2. *if T is densely defined, $\mathrm{im}(S) \subseteq \mathrm{dom}(T)$ and $\mathrm{dom}\big((TS)^*\big) \subseteq \mathrm{dom}(T^*)$, then $S^*T^* = (TS)^*$;*
3. *if S is densely defined and $\mathrm{im}(S)$ has finite codimension, then $S^*T^* = (TS)^*$.*

Proof. (1) By Proposition A.71, we have

$$(S+T)^* - T^* \subseteq (S + T - T)^* = S^*, \tag{A.162}$$

where the last equality is due to $\mathrm{dom}(S) \subseteq \mathrm{dom}(T)$. Now take x, y such that $x \in \mathrm{dom}\big((S+T)^*\big)$. Then $T^*(x)$ exists and we have the implications

$$\begin{aligned} x(S+T)^*y &\iff x\big((S+T)^* - T^* + T^*\big)y && \text{(A.163)}\\ &\iff \exists z:\ x\big((S+T)^* - T^*\big)z \wedge (z + T^*(x) = y) && \text{(A.164)}\\ &\implies \exists z:\ x(S^*)z \wedge (z + T^*(x) = y) && \text{(A.165)}\\ &\iff x(S^* + T^*)y. && \text{(A.166)} \end{aligned}$$

Thus $(S+T)^* \subseteq S^* + T^*$.
(2) We need to prove $(TS)^* \subseteq S^*T^*$. Assume $(x, y) \in (TS)^*$. By Lemma A.62, we have

$$\forall z \in \mathrm{dom}(TS):\ \langle x, TS(z)\rangle = \langle y, z\rangle. \tag{A.167}$$

Because $\mathrm{im}(S) \subseteq \mathrm{dom}(T)$, we have $\mathrm{dom}(TS) = \mathrm{dom}(S)$. Also, by assumption, $x \in \mathrm{dom}(T^*)$. So we have

$$\forall z \in \mathrm{dom}(S):\ \langle x, TS(z)\rangle = \langle T^*(x), S(z)\rangle = \langle y, z\rangle, \tag{A.168}$$

which means that $\big(T^*(x), y\big) \in S^*$, so $(x, y) \in S^*T^*$.
(3) ∎

Corollary A.73. *If T is bounded and everywhere defined, then*

$$S^* + T^* = (S+T)^* \qquad \text{and} \qquad S^*T^* = (TS)^*. \tag{A.169}$$

A.3.1.3 Adjoints of densely defined operators

The adjoint of an operator is a function if and only the operator is densely defined.

Proposition A.74. *Let $S : K \not\rightarrow H$ and $T : H \not\rightarrow K$ be linear operators between Hilbert spaces. If*

$$\operatorname{im}(S \cap T^*) = H \qquad \textit{and} \qquad \operatorname{im}(T \cap S^*) = K, \tag{A.170}$$

then S and T are densely defined with $S^* = T$ and $T^* = S$.

Proposition A.75. *Let $T : H \not\rightarrow K$ be an operator between Hilbert spaces. Then*

$$\forall v \in K : \; (v, 0) \in T^* \iff v \in \operatorname{im}(T)^\perp. \tag{A.171}$$

If T^* is densely defined, this reduces to

1. $\ker(T^*) = \operatorname{im}(T)^\perp$*;*
2. $\ker(T) \subseteq \operatorname{im}(T^*)^\perp$*;*
3. *if T is closed, then* $\ker(T) = \operatorname{im}(T^*)^\perp$

Proof. (1) Because $\operatorname{dom}(T)$ is dense in H, we have $\operatorname{dom}(T)^\perp = \{0\}$. Take $v \in K$. We have the equivalences

$$\begin{aligned} v \in \operatorname{im}(T)^\perp &\iff \forall x \in \operatorname{dom}(T) : \langle v, T(x)\rangle = 0 && \text{(A.172)}\\ &\iff \forall x \in \operatorname{dom}(T) : \langle v, T(x)\rangle = \langle v, 0\rangle && \text{(A.173)}\\ &\iff (v, 0) \in T^*, && \text{(A.174)} \end{aligned}$$

using Lemma A.62.
Point (1) is a direct translation in the case that T^* is a function.
For point (2) note that $T \subseteq T^{**}$ (by Corollary A.69) implies that $(v, 0) \in T \implies (v, 0) \in T^{**}$.
For point (3): in this case $\ker(T) = \ker(T^{**}) = \operatorname{im}(T^*)^\perp$. □

Corollary A.76 (Closed range theorem for Hilbert spaces)**.** *Let T be a closed, densely defined operator between Hilbert spaces. Then the following are equivalent:*

1. $\operatorname{im}(T)$ *is closed;*
2. $\operatorname{im}(T^*)$ *is closed;*
3. $\operatorname{im}(T) = \ker(T^*)^\perp$*;*
4. $\operatorname{im}(T^*) = \ker(T)^\perp$*.*

Proposition A.77. *Let $T : H \not\rightarrow K$ be a densely defined operator between Hilbert spaces. Then*

1. $\operatorname{im}(T)$ *is dense in K* if and only if *T^* is injective;*
2. *if T and T^* are injective, then $(T^*)^{-1} = (T^{-1})^*$.*

Proof. (1) This is immediate from Proposition A.75 and the fact that a linear operator is injective if and only if it has a trivial kernel:

$$\operatorname{im}(T) \text{ is dense} \qquad \iff \qquad \{0\} = \operatorname{im}(T)^\perp = \ker(T^*). \tag{A.175}$$

(2) We have $\mathrm{graph}(T^{-1}) = \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \mathrm{graph}(T)$. Also note that $\begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}$ and $\begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}$ commute. Then we compute using Proposition A.68:

$$\mathrm{graph}((T^*)^{-1}) = \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \mathrm{graph}(T)^{\perp} \tag{A.176}$$

$$= \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \mathrm{graph}(T)^{\perp} \tag{A.177}$$

$$= \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \left(\begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \mathrm{graph}(T) \right)^{\perp} = \mathrm{graph}((T^{-1})^*), \tag{A.178}$$

using the fact that $\begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}$ is a surjective isometry to bring it inside the orthogonal complement. □

A.3.1.4 Adjoints of bounded operators

Proposition A.78. *Let $T : H \to K$ be a densely defined operator between Hilbert spaces. Then*

1. *if $T \in \mathcal{B}(H,K)$, then $T^* \in \mathcal{B}(K,H)$;*
2. *if $T^* \in \mathcal{B}(K,H)$, then T is bounded. If T is closed, then T is defined everywhere.*

Assume $T \in \mathcal{B}(H,K)$. Then

3. *$\|T\| = \|T^*\|$.*

Proof. (1) Assume $T \in \mathcal{B}(H,K)$. Then $u \mapsto \langle x, Tu\rangle$ is a bounded functional for all $x \in K$, so $\mathrm{dom}(T^*) = K$ by Proposition A.63. Also T^* is closed by Proposition A.68, so it is bounded by the closed graph theorem Theorem A.48.
(2) Assume $T^* \in \mathcal{B}(K,H)$. By the previous argument $T \subseteq \overline{T} = T^{**} \in \mathcal{B}(H,K)$.
(3) The function $(x,u) \mapsto \langle x, Tu\rangle$ is a bounded sesquilinear form. By Riesz representation, T^* must be the unique S from the proposition, which has norm $\|T\|$. □

Lemma A.79. *Let $S, T \in \mathcal{B}(H,K)$ and $\lambda \in \mathbb{C}$.*

1. *$(T^*)^* = T$;*
2. *$(S+T)^* = S^* + T^*$;*
3. *$(\lambda T)^* = \bar{\lambda} T^*$;*
4. *$\mathbb{1}_V^* = \mathbb{1}_V$.*

Let $T \in \mathcal{B}(H_1,H_2), S \in \mathcal{B}(H_2,H_3)$

5. *$(ST)^* = T^* S^*$.*

Proof. Since the adjoint of a bounded operator is bounded, Proposition A.78, these results are special cases of Proposition A.71, Proposition A.67 and Corollary A.69 (and 4 is a repeat of Corollary A.61).
They can also be proved using more elementary means. For example, to prove (1), we take arbitrary $v \in H$ and $w \in K$, Then

$$\langle w, Tv\rangle = \langle T^* w, v\rangle = \overline{\langle v, T^* w\rangle} = \overline{\langle (T^*)^* v, w\rangle} = \langle w, (T^*)^* v\rangle. \tag{A.179}$$

Since this holds for all w, we have $Tv = (T^*)^* v$ for all $v \in V$. □

Proposition A.80. *Let H, K be Hilbert spaces and $T : H \to K$ a bijective bounded linear operator with bounded inverse. Then $(T^*)^{-1}$ exists and*

$$(T^*)^{-1} = (T^{-1})^*. \tag{A.180}$$

Proof. We prove $(T^{-1})^*$ is both a left- and a right-inverse of T^*: $\forall x \in H, y \in K$

$$\langle T^*(T^{-1})^*x, y\rangle = \langle x, T^{-1}Ty\rangle = \langle x, y\rangle \tag{A.181}$$
$$\langle x, (T^{-1})^*T^*y\rangle = \langle TT^{-1}x, y\rangle = \langle x, y\rangle \tag{A.182}$$

So $T^*(T^{-1})^* = \mathbb{1}_H$ and $(T^{-1})^*T^* = \mathbb{1}_K$. □

Proposition A.81. *Let $T \in \mathcal{B}(H, K)$ with H, K Hilbert spaces. Then*

$$\|T^*T\| = \|T\|^2 = \|TT^*\|. \tag{A.183}$$

Proof. For $\|T^*T\| = \|T\|^2$ first observe that

$$\|T^*T\| \leq \|T^*\| \cdot \|T\| = \|T\|^2. \tag{A.184}$$

Conversely, $\forall x \in H$:

$$\|T(x)\|^2 = \langle Tx, Tx\rangle = \langle T^*Tx, x\rangle \leq \|T^*Tx\| \cdot \|x\| \leq \|T^*T\| \cdot \|x\|^2. \tag{A.185}$$

The other equality follows by applying the first to T^* and using $\|T^*\| = \|T\|$. □

A.3.2 Normal operators

A densely defined linear operator T on a Hilbert space H is normal if it is closed and $TT^* = T^*T$.

This is exactly the same definition as in the matrix case, except we need to additionally assert closedness. Self-adjoint and unitary operators are normal.

Lemma A.82. *Let $T : H \not\to H$ be a normal operator and $\lambda, \mu \in \mathbb{C}$. Then $\lambda T + \mu \mathbb{1}_H$ is normal.*

Proof. We have that $\lambda T + \mu \mathbb{1}_H$ is closed from Lemma A.31. We calculate

$$(\lambda T + \mu \mathbb{1}_H)^*(\lambda T + \mu \mathbb{1}_H) = |\lambda|^2 T^*T + \overline{\mu}\lambda T + \overline{\lambda}\mu T^* + |\mu|^2 = (\lambda T + \mu \mathbb{1}_H)(\lambda T + \mu \mathbb{1}_H)^* \tag{A.186}$$

using Corollary A.73 and Proposition A.67. □

Proposition A.83. *Let $T : H \not\to H$ be a densely defined operator on a Hilbert space. Then T is normal* if and only if $\operatorname{dom}(T) = \operatorname{dom}(T^*)$ *and* $\forall x \in \operatorname{dom}(T) : \|Tx\| = \|T^*x\|$.

Proof. First, assume T normal. Then, for all $x \in \operatorname{dom}(T^*T) = \operatorname{dom}(TT^*)$, we have $x \in \operatorname{dom}(T)$ and $x \in \operatorname{dom}(T^*)$ and

$$\|Tx\|^2 = |\langle Tx, Tx\rangle| = |\langle T^*Tx, x\rangle| = |\langle TT^*x, x\rangle| = |\langle T^*x, T^*x\rangle| = \|T^*x\|^2. \tag{A.187}$$

By Theorem A.104, $\operatorname{dom}(T^*T)$ is graph(T)-dense in $\operatorname{dom}(T)$. Thus, for all $x \in \operatorname{dom}(T)$, there exists a sequence $\langle x_n\rangle \in \operatorname{dom}(T^*T)^{\mathbb{N}}$ such that $x_n \overset{\operatorname{graph}(T)}{\longrightarrow} x$.

In particular, $Tx_n \to Tx$, which means $\langle Tx_n \rangle$ is a Cauchy sequence. Since $x_n, x_m \in \operatorname{dom}(T^*T)$, we have shown that $\|Tx_n - Tx_m\| = \|T^*x_n - T^*x_m\|$ and thus $\langle T^*x_n \rangle$ is Cauchy. It converges to some $y \in H$ by completeness and so $x \in \operatorname{dom}(T^*)$ and $T^*x = y$ by Proposition A.30, since T^* is closed Proposition A.68.
This shows that $\operatorname{dom}(T) \subseteq \operatorname{dom}(T^*)$. The same reasoning with T^* gives the opposite inclusion. Finally, we calculate

$$\|Tx\| = \lim_n \|Tx_n\| = \lim_n \|T^*x_n\| = \|T^*x\|. \tag{A.188}$$

For the converse, we first prove that T is closed, using Proposition A.30. Suppose $\langle x_n \rangle \in \operatorname{dom}(T)^{\mathbb{N}}$ converges to x and $\langle Tx_n \rangle$ also converges. Then $\langle Tx_n \rangle$ is Cauchy and, since $\|Tx_n - Tx_m\| = \|T^*x_n - T^*x_m\|$, the sequence $\langle T^*x_n \rangle$ is also Cauchy and thus convergent. Since T^* is closed Proposition A.68, we have $x \in \operatorname{dom}(T^*) = \operatorname{dom}(T)$ and $T^*x_n \to T^*x$ by Proposition A.30. Thus

$$\|Tx_n - Tx\| = \|T^*x_n - T^*x\| \to 0, \tag{A.189}$$

so $Tx_n \to Tx$.
Pick arbitrary $x, y \in \operatorname{dom}(T) = \operatorname{dom}(T^*)$. The polarisation identity gives

$$\langle Tx, Ty \rangle = \frac{1}{4}\sum_{k=0}^{3} i^k \|i^k Tx + Ty\|^2 = \frac{1}{4}\sum_{k=0}^{3} i^k \|i^k T^*x + T^*y\|^2 = \langle T^*x, T^*y \rangle. \tag{A.190}$$

Using Proposition A.63, we have

$$\begin{aligned} x \in \operatorname{dom}(T^*T) &\iff Tx \in \operatorname{dom}(T^*) && \text{(A.191)}\\ &\iff y \mapsto \langle Tx, Ty \rangle \text{ is a bounded functional} && \text{(A.192)}\\ &\iff y \mapsto \langle T^*x, T^*y \rangle \text{ is a bounded functional} && \text{(A.193)}\\ &\iff T^*x \in \operatorname{dom}(T^{**}) = \operatorname{dom}(T) && \text{(A.194)}\\ &\iff x \in \operatorname{dom}(TT^*), && \text{(A.195)} \end{aligned}$$

where we have used $T^{**} = T$ by Corollary A.69.
Finally, take $x \in \operatorname{dom}(T^*T) = \operatorname{dom}(TT^*)$ and $y \in \operatorname{dom}(T) = \operatorname{dom}(T^*)$. Then

$$\langle Tx, Ty \rangle = \langle T^*x, T^*y \rangle \implies \langle T^*Tx, y \rangle = \langle TT^*x, y \rangle \implies \langle (T^*Tx - TT^*)x, y \rangle = 0, \tag{A.196}$$

so $(T^*Tx - TT^*)x \in \operatorname{dom}(T)^{\perp} = \{0\}$ and $T^*Tx = TT^*x$. □

Corollary A.84. *If T is a normal operator, then $\ker T = \ker T^*$.*

Proof. We have $x \in \ker(T) \iff \|Tx\| = 0 \iff \|T^*x\| = 0 \iff x \in \ker(T^*)$. □

Corollary A.85. *If T is a normal operator and v is an eigenvector of T with eigenvalue λ, then v is an eigenvector of T^* with eigenvalue $\overline{\lambda}$.*

Proof. We have that $Tv = \lambda v$, so $(T - \lambda\mathbb{1})v = 0$. Since $T - \lambda\mathbb{1}$ is normal, Lemma A.82, we have $(T - \lambda\mathbb{1})^*v = 0$. Using Corollary A.73, Proposition A.67 and Corollary A.61, we calculate $T^*v = \overline{\lambda}v$. This means that v is an eigenvector of T^* with eigenvalue $\overline{\lambda}$. □

Corollary A.86. *If T is a normal operator and v, w are eigenvectors of T with distinct eigenvalues, then $v \perp w$.*

Proof. Suppose v has eigenvalue λ and w has eigenvalue μ. Then $v, w \in \operatorname{dom}(T^*)$ and we calculate

$$\mu\langle v, w\rangle = \langle v, \mu w\rangle = \langle v, Tw\rangle = \langle T^* v, w\rangle = \langle\overline{\lambda} v, w\rangle = \lambda\langle v, w\rangle. \tag{A.197}$$

Since $\mu \neq \lambda$, this implies $\langle v, w\rangle = 0$. ☐

Corollary A.87. *If T is a normal operator then $\sigma_r(T) = \emptyset$.*

Proof. If T is normal, then so is $\lambda\mathbb{1} - T$. Now $\lambda \in \sigma_{\mathrm{r}}(T)$ iff $\ker(\lambda\mathbb{1} - T) = \{0\}$ and $\operatorname{im}(\lambda\mathbb{1} - T)^\perp \neq \{0\}$, but $\operatorname{im}(\lambda\mathbb{1} - T)^\perp = \ker(\lambda\mathbb{1} - T)^* = \ker(\lambda\mathbb{1} - T)$. By Proposition A.75 and the previous corollary. This is a contradiction. ☐

A.3.3 Symmetric and self-adjoint operators

Let A be an operator on a Hilbert space.

- If $A^* = A$, we say A is self-adjoint.
- If $A^* = -A$, we say A is skew-adjoint.

We denote the set of self-adjoint operators on a Hilbert space H by $\mathfrak{SA}(H)$.

Lemma A.88. *Let A be a self-adjoint or skew-adjoint operator on a Hilbert space. Then*

1. *A is densely defined;*
2. *A is normal;*
3. *A is closed;*
4. *λA is self-adjoint (resp. skew-adjoint) for all $\lambda \in \mathbb{R}$.*

Proof. (1) From $A = A^*$ or $-A = A^*$, we have that A^* is a function. This implies that A is densely defined by Corollary A.59.
(2) Sicne A is densely defined, we can apply Proposition A.83.
(3) For any self-adjoint operator A, we have $A = A^* = A^{**} = \overline{A}$. Alternatively, note that all normal operators are closed (by definition).
(4) Since A is densely defined, we have $(\lambda A)^* = \overline{\lambda} A^* = \lambda A^* = \pm\lambda A^*$, by Proposition A.67. ☐

Lemma A.89. *Let A be an operator on a Hilbert space. Then A is self-adjoint* if and only if *iA is skew-adjoint.*

Proof. First suppose A is self-adjoint, then A is densely defined by Lemma A.88, so $(iA)^* = \overline{i}A^* = -iA^*$ by Proposition A.67.
Now suppose iA is skew-adjoint. Then iA is densely defined by Lemma A.88, so $A^* = \big(-i(iA)\big)^* = \overline{-i}(iA)^* = i(-iA) = A$, by Proposition A.67. ☐

A.3.3.1 Domain related matters

Lemma A.90. *Let A be a densely defined operator on a Hilbert space. Then*

1. *A is symmetric* if and only if *$A \subseteq A^*$;*
2. *if A is symmetric, then is A closable and $\overline{A} = A^{**}$ is symmetric.*

Proof. (1) A is symmetric iff it is an adjoint of itself, iff $A \subseteq A^*$.
(2) From (1) we see that A^* is densely defined, because the superset of a dense set is dense. Then A is closable by Corollary A.69.
To show symmetry of $\overline{A}$, we have (using the properties implied by Proposition A.65) $A^{**} \subseteq A^*$ from $A \subseteq A^*$ and thus

$$\overline{A} = A^{**} \subseteq A^* = A^{***} = \overline{A}^*. \tag{A.198}$$

□

A symmetric operator A is self-adjoint if and only if $\operatorname{dom}(A) = \operatorname{dom}(A^*)$.

Corollary A.91. *A closed and densely defined symmetric operator A is self-adjoint* if and only if A^* *is also symmetric.*

Proof. If A is self-adjoint, then A^* is self-adjoint and thus symmetric,
If A^* is symmetric, then $A \subseteq A^* \subseteq A^{**} = A$. □

Theorem A.92 (Hellinger-Toeplitz)**.** *Everywhere-defined symmetric operators are bounded.*

Proof. Assume $A : H \to H$ an everywhere-defined symmetric operator. Then $\operatorname{dom}(A) = H$. Also $A \subseteq A^*$ by Lemma A.90. Thus $H = \operatorname{dom}(A) \subseteq \operatorname{dom}(A^*) \subseteq H$. So $\operatorname{dom}(A^*) = H$. By Proposition A.70, A is bounded. □

Proposition A.93. *A self-adjoint operator cannot have a proper symmetric extension.*

Proof. Assume A self-adjoint and $A \subseteq B$ for some symmetric operator B. Then

$$A \subseteq B \subseteq B^* \subseteq A^* = A, \tag{A.199}$$

so $A = B$. We have used Lemma A.90 and Corollary A.66. □

Corollary A.94. *Let A be a densely defined symmetric operator. If $\overline{A}$ is self-adjoint, then it is the unique self-adjoint extension of A.*

Note that $\overline{A}$ is always an operator by Lemma A.90.

Proof. Let B be a self-adjoint extension of A. Then $\overline{A} = A^{**} \subseteq B^{**} = B$, by Corollary A.66. This means that B is symmetric extension of the self-adjoint operator $\overline{A}$, which, by the proposition, implies $B = \overline{A}$. □

In general it is possible for an unbounded, symmetric operator to not have a self-adjoint extension or have multiple self-adjoint extensions, even if it is densely defined.

A.3.3.2 Spectrum and related criteria

Lemma A.95. *The eigenvalues of a symmetric operator are real.*

Proof. Assume there exists an $x \in \ker(\lambda \mathbb{1}_H - A) \setminus \{0\}$. Then $Ax = \lambda x$ and thus

$$\lambda \|x\|^2 = \lambda \langle x, x\rangle = \langle x, \lambda x\rangle = \langle x, Ax\rangle = \langle Ax, x\rangle = \langle \lambda x, x\rangle = \overline{\lambda}\langle x, x\rangle = \overline{\lambda}\|x\|^2. \tag{A.200}$$

Because $\|x\|^2 \neq 0$, we have $\lambda = \overline{\lambda}$, meaning λ is real. □

Lemma A.96. *Let A be a symmetric operator on a complex Hilbert space H. If $\exists z \in \mathbb{C} \setminus \mathbb{R}$: $\operatorname{im}(A + z\,\mathbb{1}) = H$, then A is densely defined.*

Proof. Let $A + z\,\mathbb{1}$ be surjective and suppose, towards a contradiction that there exists an $y \perp \operatorname{dom}(A)$. Then $y = (A + z\,\mathbb{1})x$ for some $x \in \operatorname{dom}(A)$ by surjectivity. Then

$$0 = \mathfrak{Im}\langle x, y\rangle = \mathfrak{Im}\langle x, (A + z\,\mathbb{1})x\rangle = \cancel{\mathfrak{Im}\langle x, Ax\rangle} + \mathfrak{Im}\langle x, zx\rangle = \mathfrak{Im}(z)\|x\|^2. \tag{A.201}$$

By assumption, $\mathfrak{Im}(z) \neq 0$, so $x = 0$, meaning $y = (A + z\,\mathbb{1})x = 0$ and thus $\operatorname{dom}(A)^\perp = \{0\}$. □

Proposition A.97. *Let A be a symmetric operator on a complex Hilbert space H. Then $A + z\,\mathbb{1}_H$ is bounded below by $|\,\mathfrak{Im}\, z|$ for all $z \in \mathbb{C} \setminus \mathbb{R}$.*

Proof. We first calculate, $\forall x \in H$:

$$\mathfrak{Im}\langle x, (A + z\,\mathbb{1}_H)x\rangle = \cancel{\mathfrak{Im}\langle x, Ax\rangle} + \mathfrak{Im}\, z\|x\|^2. \tag{A.202}$$

Thus

$$|\,\mathfrak{Im}\, z|\;\|x\|^2 = |\,\mathfrak{Im}\langle x, (A + z\,\mathbb{1}_H)x\rangle| \leq |\langle x, (A + z\,\mathbb{1}_H)x\rangle| \leq \|x\|\;\|(A + z\,\mathbb{1}_H)x\|, \tag{A.203}$$

which means that $\|(A + z\,\mathbb{1}_H)x\| \geq |\,\mathfrak{Im}\, z|\;\|x\|$, so $A + z\,\mathbb{1}_H$ is bounded below by $|\,\mathfrak{Im}\, z|$. □

Corollary A.98. *Let A be a symmetric operator on a complex Hilbert space H. Then for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$, the resolvent $R_A(\lambda)$ well-defined and bounded by $\|R_A(\lambda)\| \leq 1/|\,\mathfrak{Im}\,\lambda|$.*

Note this does not mean $\mathbb{C} \setminus \mathbb{R} \subseteq \rho(A)$, as $\operatorname{dom}(R_A(\lambda))$ may not be all of H.

Proof. This is an application of Proposition A.42. □

Proposition A.99. *Let A be a symmetric operator on a Hilbert space H. The following are equivalent:*

1. $\forall z \in \mathbb{C} \setminus \mathbb{R} :\ \operatorname{im}(A + z\,\mathbb{1}) = H = \operatorname{im}(A + \overline{z}\,\mathbb{1})$*;*
2. $\exists z \in \mathbb{C} :\ \operatorname{im}(A + z\,\mathbb{1}) = H = \operatorname{im}(A + \overline{z}\,\mathbb{1})$*;*
3. *A is self-adjoint;*
4. $\sigma_r(A) = \emptyset$*;*
5. *A is closed and* $\forall z \in \mathbb{C} \setminus \mathbb{R} :\ \ker(A^* + z\,\mathbb{1}) = \{0\} = \ker(A^* + \overline{z}\,\mathbb{1})$*;*
6. *A is closed and* $\exists z \in \mathbb{C} \setminus \mathbb{R} :\ \ker(A^* + z\,\mathbb{1}) = \{0\} = \ker(A^* + \overline{z}\,\mathbb{1})$.

Notice that in (2) we include $\mathbb{R}$ and in (6) we exclude $\mathbb{R}$.

Corollary A.100. *Let A be a symmetric operator on a Hilbert space H. The following are equivalent:*

1. *A is essentially self-adjoint;*
2. $\exists z \in \mathbb{C} \setminus \mathbb{R} :\ \overline{\operatorname{im}(A + z\,\mathbb{1})} = H = \overline{\operatorname{im}(A + \overline{z}\,\mathbb{1})}$*;*
3. $\exists z \in \mathbb{C} \setminus \mathbb{R} :\ \ker(A^* + z\,\mathbb{1}) = \{0\} = \ker(A^* + \overline{z}\,\mathbb{1})$.

Corollary A.101. *Every surjective symmetric operator is self-adjoint.*

Proof. Take $z = 0$ in point (1). □

Proposition A.102. *Let A be a closed symmetric operator. Then one of the following cases holds:*

- *A is self-adjoint, in which case $\sigma(A) \subseteq \mathbb{R}$;*
- *$\sigma(A) = \overline{\mathbb{C}^{\uparrow}}$;*
- *$\sigma(A) = \overline{\mathbb{C}^{\downarrow}}$;*
- *$\sigma(A) = \mathbb{C}$.*

If A is not densely-defined, then the last case holds.

We have denoted the closed upper half plane $\overline{\mathbb{C}^{\uparrow}}$ and the closed lower half plane $\overline{\mathbb{C}^{\downarrow}}$.

Proposition A.103. *Let T be a densely defined operator on a Hilbert space H. Then*

1. *$T + T^*$ is symmetric;*
2. *T^*T and TT^* are symmetric.*

Proof. (1) We use Proposition A.71 to get

$$T + T^* \subseteq T^{**} + T^* \subseteq (T + T^*)^*. \tag{A.204}$$

We conclude by Lemma A.90.
(2) We use Proposition A.71 to get

$$T^*T \subseteq T^*T^{**} \subseteq (T^*T)^* \qquad \text{and} \qquad TT^* \subseteq T^{**}T^* \subseteq (TT^*)^*, \tag{A.205}$$

which means that T^*T and TT^* are symmetric by Lemma A.90. ☐

Theorem A.104 (von Neumann)**.** *Let T be a densely defined and closed operator on a Hilbert space H. Then*

1. *both T^*T and TT^* are self-adjoint;*
2. *both $\operatorname{dom}(T^*T)$ and $\operatorname{dom}(TT^*)$ are essential domains of T.*

Proof. (1) Because T^* is closed, $\operatorname{graph}(T^*)$ is closed in $H \oplus H$. Thus

$$H \oplus H = \operatorname{graph}(T^*) \oplus \operatorname{graph}(T^*)^{\perp} \tag{A.206}$$

$$= \operatorname{graph}(T^*) \oplus \left(\begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \operatorname{graph} T \right)^{\perp\perp} \tag{A.207}$$

$$= \operatorname{graph}(T^*) \oplus \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \operatorname{graph} T. \tag{A.208}$$

The last equality holds because $\operatorname{graph}(T)$ is closed (and $\begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}$ is a homeomorphism).
Then for all $v \in H$, we can write

$$\begin{pmatrix} 0 \\ v \end{pmatrix} = \begin{pmatrix} y \\ T^*y \end{pmatrix} + \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \begin{pmatrix} x \\ Tx \end{pmatrix} = \begin{pmatrix} y - Tx \\ T^*y + x \end{pmatrix}. \tag{A.209}$$

So $y = Tx$ and $v = T^*y + x = T^*Tx + x = (T^*T + \mathbb{1})x$, which means that $T^*T + \mathbb{1}$ is surjective. Since T^*T is symmetric, by Proposition A.103, it is self-adjoint by Proposition A.99.

We can show $TT^* + \mathbb{1}$ is surjective by writing

$$\begin{pmatrix} v \\ 0 \end{pmatrix} = \begin{pmatrix} y \\ T^*y \end{pmatrix} + \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \begin{pmatrix} x \\ Tx \end{pmatrix} = \begin{pmatrix} y - Tx \\ T^*y + x \end{pmatrix}, \tag{A.210}$$

so $x = -T^*y$ and $v = y - Tx = y + TT^*y = (TT^* + \mathbb{1})y$.
(2) We need to show that $\mathrm{dom}(T^*T)$ is dense in $\mathrm{dom}(T)$ w.r.t. the graph norm. Take $h \in \mathrm{dom}(T^*T)^{\perp_{\mathrm{graph}(T)}}$. Then, for all $x \in \mathrm{dom}(T^*T)$, we have

$$0 = \langle x, h\rangle_{\mathrm{graph}(T)} = \langle x, h\rangle + \langle Tx, Th\rangle = \langle x, h\rangle + \langle T^*Tx, h\rangle = \langle (\mathbb{1} + T^*T)x, h\rangle. \tag{A.211}$$

Thus $h \in \mathrm{im}(\mathbb{1} + T^*T)^\perp = H^\perp = \{0\}$ and thus $h = 0$ by the calculations in (1). So the orthogonal complement of $\mathrm{dom}(T^*T)$ w.r.t. the graph inner product is $\{0\}$, which shows density. The argument for $\mathrm{dom}(TT^*)$ is similar. □

Example

Let T be a densely defined operator. Then $T + T^*$ and T^*T are in general not self-adjoint. Closedness of T is enough to make T^*T self-adjoint. This is not the case for $T + T^*$.

- If T is not closed, then $T + T^* \subsetneq T^{**} + T^* \subseteq (T + T^*)^*$.
- It is even not necessarily self-adjoint if T is closed. Let T be a closed, symmetric, but not self-adjoint operator, for example.

A.4 The duality of bounded and trace class operators

This section is a review of the duality between $\mathcal{B}(\mathcal{H})$ and $\mathcal{B}_1(\mathcal{H})$, where $\mathcal{H}$ is some Hilbert space. The textbook [65] is a good source for the results in this section.

Let $\langle e_i\rangle_{i\in I}$ be some orthonormal basis of $\mathcal{H}$. Then the space of trace class operators is defined as

$$\mathcal{B}_1(\mathcal{H}) \coloneqq \{S \in \mathcal{B}(\mathcal{H}) \,|\, \sum_{i\in I} \langle e_i, |S| e_i\rangle < \infty\}. \tag{A.212}$$

If $S \in \mathcal{B}_1(\mathcal{H})$, then its trace can be defined as $\mathrm{Tr}(S) \coloneqq \sum_{i\in I} \langle e_i, Se_i\rangle$.
The trace norm $\|\_\|_1$ is defined as $\|S\|_1 \coloneqq \mathrm{Tr}(|S|)$.

It can be proved that this definition does not depend on the choice of orthonormal basis $\langle e_i\rangle_{i\in I}$. The trace of a trace class operator is always a finite number: any absolutely convergent series is convergent.

Proposition A.105. *The trace norm is a norm that makes the space of trace class operators $\mathcal{B}_1(\mathcal{H})$ a Banach space.*

Proposition A.106. *The space of trace class operators $\mathcal{B}_1(\mathcal{H})$ is an ideal in $\mathcal{B}(\mathcal{H})$ and*

$$\big|\mathrm{Tr}(TS)\big| \leq \|T\|\|S\|_1 \tag{A.213}$$

for all $T \in \mathcal{B}(\mathcal{H})$ and $S \in \mathcal{B}_1(\mathcal{H})$. In addition, $\mathrm{Tr}(TS) = \mathrm{Tr}(ST)$.

Proposition A.107. *For all $T \in \mathcal{B}(\mathcal{H})$, the function*

$$f_T : \mathcal{B}_1(\mathcal{H}) \to \mathbb{C} : S \mapsto \mathrm{Tr}(TS) \tag{A.214}$$

is a continuous functional with $\|f_T\| = \|T\|$. All continuous functionals on $\mathcal{B}_1(\mathcal{H})$ are of this form.

This proposition identifies $\mathcal{B}(\mathcal{H})$ with the dual of $\mathcal{B}_1(\mathcal{H})$. Conversely, $\mathcal{B}_1(\mathcal{H})$ is sometimes called the predual of $\mathcal{B}(\mathcal{H})$.
To emphasise duality, $\mathrm{Tr}(TS)$ is sometimes written as $\langle T, S\rangle$.

Lemma A.108. *For all $T \in \mathcal{B}(\mathcal{H})$, the functional f_T is positive* if and only if *T is positive.*

The positivity of the functional f_T means that $f_T(S) \geq 0$ for all positive $S \in \mathcal{B}_1(\mathcal{H})$.

Proof. First suppose f_T positive. Take arbitrary $|\psi\rangle \in \mathcal{H}$. Then $|\psi\rangle\langle\psi|$ is positive and trace class, so

$$\langle\psi|T\psi\rangle = \mathrm{Tr}\left(T|\psi\rangle\langle\psi|\right) = f_T\big(|\psi\rangle\langle\psi|\big) \geq 0. \tag{A.215}$$

Since $|\psi\rangle \in \mathcal{H}$ was taken arbitrarily, this shows the positivity of T.
Now suppose T positive. Let $S \in \mathcal{B}_1(\mathcal{H})$ be positive. Then

$$f_T(S) = \mathrm{Tr}(TS) = \mathrm{Tr}(\sqrt{T}S\sqrt{T}) \geq 0. \tag{A.216}$$

□

A.4.1 Schrödinger and Heisenberg pictures

A bounded linear operator on $\mathcal{B}_1(\mathcal{H})$ can be used to define a bounded operator on $\mathcal{B}(\mathcal{H})$. Suppose $\mathcal{F}$ is a bounded linear operator on $\mathcal{B}_1(\mathcal{H})$. Pick arbitrary $T \in \mathcal{B}(\mathcal{H})$. Then

$$\mathcal{B}_1(\mathcal{H}) \to \mathbb{C} : S \mapsto \mathrm{Tr}(T\mathcal{F}(S)) \tag{A.217}$$

is a bounded functional on $\mathcal{B}_1(\mathcal{H})$. According to Proposition A.107, there must exist $T' \in \mathcal{B}(\mathcal{H})$ such that this functional is equal to $f_{T'}$. This T' is unique.[4] The mapping

$$\mathcal{F}^* : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H}) : T \mapsto T' \tag{A.218}$$

is called the adjoint of $\mathcal{F}$.

Lemma A.109. *Let $\mathcal{F}$ be an operator on $\mathcal{B}_1(\mathcal{H})$. Then $\|\mathcal{F}^*\| = \|\mathcal{F}\|$.*

Proof. Take arbitrary $T \in \mathcal{B}(\mathcal{H})$. Then

$$\|\mathcal{F}^*(T)\| = \left\|f_{\mathcal{F}^*(T)}\right\| = \left\|f_T \circ \mathcal{F}\right\| \leq \|f_T\|\|\mathcal{F}\| = \|T\|\|\mathcal{F}\|. \tag{A.219}$$

For the converse inequality, let $S \in \mathcal{B}_1(\mathcal{H})$ have unit trace norm. Then Corollary A.56 gives the existence of $T \in \mathcal{B}(H)$ such that $\|T\| = 1$ and

$$\|\mathcal{F}(S)\|_1 = \left|f_T\big(\mathcal{F}(S)\big)\right| = \left|f_{\mathcal{F}^*(T)}(S)\right| \leq \|f_{\mathcal{F}^*(T)}\| = \|\mathcal{F}^*(T)\| \leq \|\mathcal{F}^*\|. \tag{A.220}$$

Since this holds for all such S, the other norm inequality holds. □

[4] Suppose there was another operator T'' such that $f_{T'} = f^{T''}$. Then $0 = \|f_{T'} - f_{T''}\| = \|T' - T''\|$, so $T' = T''$.

The operator $\mathcal{F}$ is said to be in the Schrödinger picture, since it operates on states in $\mathcal{B}_1(\mathcal{H})$. The adjoint $\mathcal{F}^*$ is said to be in the Heisenberg picture, since it operates on operators in $\mathcal{B}(\mathcal{H})$.

Lemma A.110. *Let $\mathcal{F}, \mathcal{G}$ be operators on $\mathcal{B}_1(\mathcal{H})$ and $\lambda \in \mathbb{C}$. Then $(\mathcal{F} + \lambda\mathcal{G})^* = \mathcal{F}^* + \lambda\mathcal{G}^*$.*

Proposition A.111. *Let $\mathcal{F}$ be an operator on $\mathcal{B}_1(\mathcal{H})$. Then*

1. *$\mathcal{F}$ is positive* if and only if *$\mathcal{F}^*$ is positive;*
2. *$\mathcal{F}$ is trace-preserving* if and only if *$\mathcal{F}^*$ is unital.*

Proof. (1) First assume $\mathcal{F}$ positive and take arbitrary positive $T \in \mathcal{B}(\mathcal{H})$. Since

$$f_{\mathcal{F}^*(T)}(S) = f_T\big(\mathcal{F}(S)\big) \geq 0, \tag{A.221}$$

for all positive $S \in \mathcal{B}_1(\mathcal{H})$, from Lemma A.108, the same result implies that $\mathcal{F}^*(T)$ is positive. Now assume $\mathcal{F}^*$ is positive. Take arbitrary $S \in \mathcal{B}_1(\mathcal{H})$ and $|\psi\rangle \in \mathcal{H}$. Then

$$\langle\psi|\mathcal{F}(S)|\psi\rangle\rangle = \mathrm{Tr}\left(|\psi\rangle\langle\psi|\mathcal{F}(S)\right) = \mathrm{Tr}\left(\mathcal{F}^*(|\psi\rangle\langle\psi|)S\right) \geq 0. \tag{A.222}$$

(2) First assume $\mathcal{F}$ is trace-preserving and take arbitrary $S \in \mathcal{B}_1(\mathcal{H})$. Then

$$\mathrm{Tr}\left(\mathcal{F}^*(\mathbb{1})S\right) = \mathrm{Tr}\left(\mathbb{1}\,\mathcal{F}(S)\right) = \mathrm{Tr}\left(\mathcal{F}(S)\right) = \mathrm{Tr}(S) = \mathrm{Tr}(\mathbb{1}\,S). \tag{A.223}$$

Now assume $\mathcal{F}^*$ is unital and take arbitrary $S \in \mathcal{B}_1(\mathcal{H})$. Then

$$\mathrm{Tr}\left(\mathcal{F}(S)\right) = \mathrm{Tr}\left(\mathbb{1}\,\mathcal{F}(S)\right) = \mathrm{Tr}\left(\mathcal{F}^*(\mathbb{1})S\right) = \mathrm{Tr}(\mathbb{1}\,S) = \mathrm{Tr}(S). \tag{A.224}$$

$\square$

Appendix B

The existence of dynamics

B.1 Semigroups and evolution families

B.1.1 Semigroups and their generators

Good references for this section include [16] (as well as its abridged version [66]) and [67].

Let X be a normed space. We call a function $T : \mathbb{R}^+ \to \mathcal{B}(X)$ a semigroup of linear operators (or just semigroup) if

- $T(0) = \mathbb{1}_X$;
- $T(s+t) = T(s)T(t)$ for all $s, t \in \mathbb{R}^+$.

If T is strongly continuous, i.e. $t \mapsto T(t)x$ is continuous for all $x \in X$, then T is called a strongly continuous semigroup or C_0 semigroup.
If T is norm-continuous, then T is also called a uniformly continuous semigroup.
If $\|T(t)\| \leq 1$ for all $t \in \mathbb{R}^+$, then T is called a contraction semigroup.

Every uniformly continuous semigroup is strongly continuous, but the converse is not true. Every strongly continuous semigroup has a generator.

Proposition B.1. *Let X be a Banach space and $T : \mathbb{R}^+ \to \mathcal{B}(X)$ a function. Then the following are equivalent:*

1. *T is a uniformly continuous semigroup;*
2. *T is differentiable, $T(0) = \mathbb{1}$ and there exists $A \in \mathcal{B}(X)$ such that $\dfrac{\mathrm{d}T(t)}{\mathrm{d}t} = AT(t)$;*
3. *there exists an $A \in \mathcal{B}(X)$ such that $T(t) = e^{tA}$ for all $t \in \mathbb{R}^+$.*

In points (2) and (3) the operator A is the same.

It is remarkable that in this case some form of continuity is enough to imply differentiability. The bounded operator A completely determines the semigroup and is called the generator of the semigroup. If T is only strongly continuous, then there is still an operator A with similar properties, but it will no longer be a bounded operator.

Let $T : \mathbb{R}^+ \to \mathcal{B}(X)$ be a strongly continuous semigroup. The generator of T is the linear operator A on X defined by

$$Ax := \lim_{h \to 0^+} \frac{T(h)x - x}{h} \tag{B.1}$$

with domain

$$\mathrm{dom}(A) = \left\{ x \in X \,\middle|\, \lim_{h \to 0^+} \frac{T(h)x - x}{h} \text{ exists} \right\}. \tag{B.2}$$

Notice that the generator is indeed a linear operator. If T is a strongly continuous semigroup, then the following are equivalent: T is uniformly continuous, the generator of T is bounded, the generator of T is defined everywhere.

Lemma B.2. *Let $T : \mathbb{R}^+ \to \mathcal{B}(X)$ be an operator semigroup with generator A. If $x \in \mathrm{dom}(A)$, then $T(t)x \in \mathrm{dom}(A)$ and*

$$\frac{\mathrm{d}}{\mathrm{d}t} T(t)x = T(t)Ax = AT(t)x \tag{B.3}$$

for all $t \in [0, \infty]$.

In particular, A commutes with $T(t)$ and $T(t)$ maps the domain of A into the domain of A. There are two very nice theorems that characterise the operators that are generators of contraction semigroups

Theorem B.3 (Hille-Yosida)**.** *Let A be an operator on a Banach space X. The following are equivalent:*

1. *A generates a strongly continuous contraction semigroup;*
2. *A is closed, densely defined, $\sigma(A) \subseteq [0, +\infty]^c$ and, for all $r > 0$, $\|rR_A(r)\| \leq 1$.*

There is also a version of the Hille-Yosida theorem that characterises all strongly continuous semigroups, not just the contraction semigroups. This theorem is obtained by rescaling the semigroups with an exponential prefactor such that they become contractive. It is sometimes referred to by the names of Feller, Miyadera and Phillips.

Theorem B.4 (Lumer-Phillips)**.** *Let A be an operator on a Banach space X. The following are equivalent:*

1. *the closure of A generates a strongly continuous contraction semigroup;*
2. *A is densely defined, the range of $\lambda \mathbb{1} - A$ is dense in X for some $\lambda > 0$ and A is dissipative, which means that*

$$\|(r \mathbb{1} - A)x\| \geq r\|x\| \tag{B.4}$$

   for all $r > 0$ and x in the domain of A.

The following theorem is of utmost importance to quantum mechanics:

Theorem B.5 (Stone)**.** *Let $\mathcal{H}$ be a Hilbert space and $U : \mathbb{R}^+ \to \mathcal{B}(\mathcal{H})$ a strongly continuous semigroup. Then $U(t)$ is a unitary for all $t \in \mathbb{R}^+$* if and only if *U is generated by iH, where H is some self-adjoint operator.*

The operator H is, of course, commonly referred to as the Hamiltonian. A unitary semigroup is a contraction semigroup.

B.1.2 Evolution families

A function $U : \{(t,s) \in \mathbb{R}^2 \,|\, t \geq s\} \to \mathcal{B}(X)$ is called a (strongly continuous) evolution system if

- $U(t,s) = U(t,r)U(r,s)$ and $U(s,s) = \mathbb{1}_X$;
- it is a strongly continuous function.

Evolution systems are also called evolution families, evolution operators, evolution processes, propagators or fundamental solutions.

The operator should be U strongly continuous in both arguments simultaneously, which is stronger than just requiring strong continuity in each parameter separately.

Example

Let $f : \mathbb{R} \to \mathbb{C}$ be any continuous function. Then $U(t,s) = \exp\big(f(t) - f(s)\big)$ is a uniformly continuous evolution system.
Unlike in the semigroup case, see Proposition B.1, uniformly continuous evolution systems are not necessarily differentiable: take any f that is continuous, but not differentiable.

B.2 Continuous paths of bounded generators

Lemma B.6. *Let X be a Banach space, $s \in \mathbb{R}^+$ and $A : \mathbb{R}^+ \to \mathcal{B}(X)$ a strongly continuous function. Then the non-autonomous Cauchy problem*

$$\begin{cases} \dfrac{\mathrm{d}u(t)}{\mathrm{d}t} = A(t)u(t) \\ u(s) = x \end{cases} \tag{B.5}$$

has a unique classical solution for each inital value x.

Proof. For all $t \in \mathbb{R}^+$, we have $\sup_{s\in[0,t]} \|A(s)x\| < \infty$ from the extreme value theorem. The uniform boundedness principle Theorem A.43 implies $\sup_{s\in[0,t]} \|A(s)\| < \infty$. Now the existence and uniqueness of the classical solution follows from the Picard-Lindelöf theorem. ☐

Let $U(t,s) : X \to X$ be the function that maps x to $u(t)$, where u is the solution of the Cauchy problem in Lemma B.6.

In particular, this means that $\dfrac{\mathrm{d}U(t,s)x}{\mathrm{d}t} = A(t)U(t,s)x$.

Lemma B.7. *Let X be a Banach space, $s \leq r \leq t \in \mathbb{R}^+$ and $A : \mathbb{R}^+ \to \mathcal{B}(X)$ a continuous function. Then*

1. *$U(s,s) = \mathbb{1}_X$;*
2. *$U(t,s)$ is a linear operator;*
3. *$U(t,r)U(r,s) = U(t,s)$.*

Proof. (1) Take arbitrary $x \in X$. Then $t \mapsto U(t,s)x$ solves the initial value problem in Lemma B.6. In particular $U(s,s)x = x$. Since x was taken arbitrarily, this implies $U(s,s) = \mathbb{1}_X$.
(2) Take $x, y \in X$ and $\lambda \in \mathbb{C}$. We claim that $t \mapsto U(t,s)x + \lambda U(t,s)y$ solves the initial value problem

$$\begin{cases} \dfrac{\mathrm{d}u(t)}{\mathrm{d}t} = A(t)u(t) \\ u(s) = x + \lambda y. \end{cases} \tag{B.6}$$

Indeed, $U(s,s)x + \lambda U(s,s)y = x + \lambda y$ from (1) and

$$\frac{\mathrm{d}}{\mathrm{d}t}\big(U(t,s)x + \lambda U(t,s)y\big) = \frac{\mathrm{d}U(t,s)x}{\mathrm{d}t} + \lambda\,\frac{\mathrm{d}U(t,s)y}{\mathrm{d}t} \tag{B.7}$$

$$= A(t)U(t,s)x + \lambda A(t)U(t,s)y \tag{B.8}$$

$$= A(t)\big(U(t,s)x + \lambda U(t,s)y\big). \tag{B.9}$$

By uniqueness of the solution, Lemma B.6, we have $U(t,s)(x + \lambda y) = U(t,s)x + \lambda U(t,s)y$.
(3) Take arbitrary $x \in X$. It is clear that $t \mapsto U(t,s)x$ solves the initial value problem

$$\begin{cases} \dfrac{\mathrm{d}u(t)}{\mathrm{d}t} = A(t)u(t) \\ u(r) = U(r,s)x, \end{cases} \tag{B.10}$$

so we can conclude with the uniqueness of the solution, Lemma B.6. □

Lemma B.8. *Let X be a Banach space, $s \leq t \in \mathbb{R}^+$ and $A : \mathbb{R}^+ \to \mathcal{B}(X)$ a continuous function. Then*

1. *$U(t,s)$ is bounded with $\|U(t,s)\| \leq \exp\Big(\int_s^t \|A(r)\|\,\mathrm{d}r\Big)$;*
2. *$\|U(t,s) - \mathbb{1}_X\| \leq \exp\Big(\int_s^t \|A(r)\|\,\mathrm{d}r\Big) - 1 \leq \int_s^t \|A(r)\|\,\mathrm{d}r \exp\Big(\int_s^t \|A(r)\|\,\mathrm{d}r\Big)$;*
3. *for all $s' \leq t' \in \mathbb{R}^+$, we have*

$$\|U(t,s) - U(t',s')\| \leq \Big(\int_{\min\{s,s'\}}^{\max\{s,s'\}} \|A(r)\|\,\mathrm{d}r + \int_{\min\{t,t'\}}^{\max\{t,t'\}} \|A(r)\|\,\mathrm{d}r\Big) \exp\Big(\int_{\min\{s,s'\}}^{\max\{t,t'\}} \|A(r)\|\,\mathrm{d}r\Big). \tag{B.11}$$

Proof. (1) Let $x \in X$ be an arbitrary unit vector. Then

$$U(t,s)x = x + \int_s^t A(r)U(r,s)x\,\mathrm{d}r, \tag{B.12}$$

so

$$\|U(t,s)x\| \leq \|x\| + \int_s^t \|A(r)\|\,\|U(r,s)x\|\,\mathrm{d}r. \tag{B.13}$$

An application of the Bellman-Grönwall inequality gives

$$\|U(t,s)x\| \leq \|x\| \exp\Big(\int_s^t \|A(r)\|\,\mathrm{d}r\Big) = \exp\Big(\int_s^t \|A(r)\|\,\mathrm{d}r\Big). \tag{B.14}$$

Since x was taken arbitrarily, the result follows.

(2) Let $x \in X$ be an arbitrary unit vector. Then

$$\begin{aligned}
\big\|\big(U(t,s) - \mathbb{1}_X\big)x\big\| &= \Big\|\int_s^t A(r)U(r,s)x\,\mathrm{d}r\Big\| && \text{(B.15)}\\
&\le \int_s^t \|A(r)\|\,\|U(r,s)x\|\,\mathrm{d}r && \text{(B.16)}\\
&\le \int_s^t \|A(r)\|\,\exp\Big(\int_s^r \|A(r')\|\,\mathrm{d}r'\Big)\,\mathrm{d}r && \text{(B.17)}\\
&= \int_s^t \frac{\mathrm{d}}{\mathrm{d}r}\exp\Big(\int_s^r \|A(r')\|\,\mathrm{d}r'\Big)\,\mathrm{d}r && \text{(B.18)}\\
&= \exp\Big(\int_s^t \|A(r')\|\,\mathrm{d}r'\Big) - 1, && \text{(B.19)}
\end{aligned}$$

where we have used Lemma D.14 and Corollary D.32. The final inequality is due to the fact that $e^a - 1 \le ae^a$ for positive a.

(3) We either have

$$\|U(t,s) - U(t',s')\| = \|U(\max\{t,t'\},\min\{s,s'\}) - U(\min\{t,t'\},\max\{s,s'\})\| \qquad \text{(B.20)}$$

or

$$\|U(t,s) - U(t',s')\| = \|U(\max\{t,t'\},\max\{s,s'\}) - U(\min\{t,t'\},\min\{s,s'\})\|. \qquad \text{(B.21)}$$

Set $t_M := \max\{t,t'\}, t_m := \min\{t,t'\}, s_M := \max\{s,s'\}, s_m := \min\{s,s'\}$ and consider the first case. Then we necessarily have $t_m \ge s_M$ and we can calculate

$$\begin{aligned}
\|U(t_M,s_m) - U(t_m,s_M)\| &= \|U(t_M,t_m)U(t_m,s_M)U(s_M,s_m) - U(t_m,s_M)\| && \text{(B.22)}\\
&\le \|U(t_M,t_m)U(t_m,s_M)U(s_M,s_m) - U(t_M,t_m)U(t_m,s_M)\| && \text{(B.23)}\\
&\quad + \|U(t_M,t_m)U(t_m,s_M) - U(t_m,s_M)\| && \text{(B.24)}\\
&\le \|U(t_M,t_m)\|\|U(t_m,s_M)\|\|U(s_M,s_m) - \mathbb{1}_X\| && \text{(B.25)}\\
&\quad + \|U(t_M,t_m) - \mathbb{1}_X\|\|U(t_m,s_M)\| && \text{(B.26)}\\
&\le \exp\Big(\int_{t_m}^{t_M}\|A(r)\|\,\mathrm{d}r\Big)\exp\Big(\int_{s_M}^{t_m}\|A(r)\|\,\mathrm{d}r\Big)\exp\Big(\int_{s_m}^{s_M}\|A(r)\|\,\mathrm{d}r\Big)\int_{s_m}^{s_M}\|A(r)\|\,\mathrm{d}r && \text{(B.27)}\\
&\quad + \exp\Big(\int_{t_m}^{t_M}\|A(r)\|\,\mathrm{d}r\Big)\exp\Big(\int_{s_M}^{t_m}\|A(r)\|\,\mathrm{d}r\Big)\int_{t_m}^{t_M}\|A(r)\|\,\mathrm{d}r && \text{(B.28)}\\
&= \exp\Big(\int_{s_m}^{t_M}\|A(r)\|\,\mathrm{d}r\Big)\int_{s_m}^{s_M}\|A(r)\|\,\mathrm{d}r && \text{(B.29)}\\
&\quad + \exp\Big(\int_{s_M}^{t_M}\|A(r)\|\,\mathrm{d}r\Big)\int_{t_m}^{t_M}\|A(r)\|\,\mathrm{d}r && \text{(B.30)}\\
&\le \exp\Big(\int_{s_m}^{t_M}\|A(r)\|\,\mathrm{d}r\Big)\Big(\int_{s_m}^{s_M}\|A(r)\|\,\mathrm{d}r + \int_{t_m}^{t_M}\|A(r)\|\,\mathrm{d}r\Big). && \text{(B.31)}
\end{aligned}$$

Now consider the second case. We either have $t_m \ge s_M$ or $s_M \ge t_m$. In the first subcase, we have

$$\|U(t_M,s_M)-U(t_m,s_m)\| = \|U(t_M,t_m)U(t_m,s_M)-U(t_m,s_M)U(s_M,s_m)\| \tag{B.32}$$
$$\leq \|U(t_M,t_m)U(t_m,s_M)-U(t_m,s_M)\| \tag{B.33}$$
$$+\|U(t_m,s_M)-U(t_m,s_M)U(s_M,s_m)\| \tag{B.34}$$
$$\leq \exp\Big(\int_{s_M}^{t_M}\|A(r)\|\,\mathrm{d}r\Big)\int_{t_m}^{t_M}\|A(r)\|\,\mathrm{d}r \tag{B.35}$$
$$+\exp\Big(\int_{s_m}^{t_m}\|A(r)\|\,\mathrm{d}r\Big)\int_{s_m}^{s_M}\|A(r)\|\,\mathrm{d}r \tag{B.36}$$
$$\leq \exp\Big(\int_{s_m}^{t_M}\|A(r)\|\,\mathrm{d}r\Big)\Big(\int_{s_m}^{s_M}\|A(r)\|\,\mathrm{d}r+\int_{t_m}^{t_M}\|A(r)\|\,\mathrm{d}r\Big). \tag{B.37}$$

Finally, in the second subcase, we have

$$\|U(t_M,s_M)-U(t_m,s_m)\| \leq \|U(t_M,s_M)-U(t_M,s_M)U(s_M,t_m)U(t_m,s_m)\| \tag{B.38}$$
$$+\|U(t_M,s_M)U(s_M,t_m)U(t_m,s_m)-U(t_m,s_m)\| \tag{B.39}$$
$$\leq \|U(t_M,s_M)\|\|\mathbb{1}_X-U(s_M,s_m)\| \tag{B.40}$$
$$+\|U(t_M,t_m)-\mathbb{1}_X\|\|U(t_m,s_m)\| \tag{B.41}$$
$$\leq \exp\Big(\int_{s_m}^{t_M}\|A(r)\|\,\mathrm{d}r\Big)\int_{s_m}^{s_M}\|A(r)\|\,\mathrm{d}r \tag{B.42}$$
$$+\exp\Big(\int_{s_m}^{t_M}\|A(r)\|\,\mathrm{d}r\Big)\int_{t_M}^{t_m}\|A(r)\|\,\mathrm{d}r \tag{B.43}$$
$$= \exp\Big(\int_{s_m}^{t_M}\|A(r)\|\,\mathrm{d}r\Big)\Big(\int_{s_m}^{s_M}\|A(r)\|\,\mathrm{d}r+\int_{t_m}^{t_M}\|A(r)\|\,\mathrm{d}r\Big). \tag{B.44}$$

□

Corollary B.9. *Let X be a Banach space and $A:\mathbb{R}^+\to\mathcal{B}(X)$ a continuous function. Then $U:\{(t,s)\in\mathbb{R}^2\,|\,t\geq s\}\to\mathcal{B}(X)$ is a uniformly continuous evolution system.*

Proof. The lemma combined with Lemma B.7 gives that U is a evolution system.
For uniform continuity at (t_0,s_0), set $M=\max_{r\in[0,t_0+1]}\|A(r)\|$, which exists due to the extreme value theorem. Then we have, assuming $|s-s_0|\leq 1$ and $|t-t_0|\leq 1$, that

$$\|U(t,s)-U(t_0,s_0)\|\leq 2Me^{M\big(\max\{t,t_0\}-\min\{s,s_0\}\big)}. \tag{B.45}$$

This clearly goes to zero as $(t,s)\to(t_0,s_0)$. □

Lemma B.10. *Let X be a Banach space, $s\leq t\in\mathbb{R}^+$ and $A:\mathbb{R}^+\to\mathcal{B}(X)$ a continuous function. Then*

1. $U(t,s)=\mathbb{1}_X+\displaystyle\int_s^t A(r)U(r,s)\,\mathrm{d}r$;
2. $\dfrac{\mathrm{d}U(t,s)}{\mathrm{d}t}=A(t)U(t,s)$;

3. $\dfrac{\mathrm{d}U(t,s)}{\mathrm{d}s} = -U(t,s)A(s)$.

Proof. (1) Since $U(t,s)$ is norm-continuous, Corollary B.9, so is $A(r)U(r,s)$ and the integral exists due to Corollary D.21.
Since

$$U(t,s)x = x + \int_s^t A(r)U(r,s)x \,\mathrm{d}r \tag{B.46}$$

for all $x \in X$ (this is exactly the fixed-point condition of the Picard-Lindelöf theorem), the result follows from Corollary D.24.
(2) Immediate from (1) and the fundamental theorem of calculus Theorem D.31.
(3) We have

$$\begin{aligned}
\lim_{h\to 0^+} \frac{U(t,s+h) - U(t,s)}{h} &= \lim_{h\to 0^+} \frac{U(t,s+h) - U(t,s+h)U(s+h,s)}{h} &\text{(B.47)}\\
&= \lim_{h\to 0^+} U(t,s+h)\frac{\mathbb{1}_X - U(s+h,s)}{h} &\text{(B.48)}\\
&= -\lim_{h\to 0^+} U(t,s+h)\frac{U(s+h,s) - U(s,s)}{h} &\text{(B.49)}\\
&= -U(t,s)\,\frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=s} U(t,s) = -U(t,s)A(s), &\text{(B.50)}
\end{aligned}$$

where we have used (2) and the continuity of the multiplication. The calculation in the limit $h \to 0^-$ is similar and so the result follows. □

B.3 The hyperbolic case

Let X be a Banach space, $D \subseteq X$ a dense subspace and $A : \mathbb{R}^+ \to \mathrm{Lin}(X)$ a function such that

- $\mathrm{dom}\big(A(t)\big) = D$, for all $t \in \mathbb{R}^+$;
- $A(t)$ generates a contraction semigroup, for all $t \in \mathbb{R}^+$;
- the function $\mathbb{R}^+ \to X : t \mapsto A(t)y$ is in $\mathcal{C}^1(\mathbb{R}^+, X)$ for all $y \in Y$.

In this case we say $A(t)$ generates a hyperbolic non-autonomous Cauchy problem.

Lemma B.11. *Let X be a Banach space, $D \subseteq X$ a dense subspace, $t \geq 0$ and $A : \mathbb{R}^+ \to \mathrm{Lin}(D, X)$ a hyperbolic generator. Then*

1. $(\mathbb{1}_X - A(t))(\mathbb{1}_X - A(s))^{-1} : X \to X$ *is bounded, for all* $s, t \in \mathbb{R}^+$
2. $(\mathbb{1}_X - A(t))^{-1}(\mathbb{1}_X - A(s)) : (D, \|\text{-}\|_{A(s)}) \to (D, \|\text{-}\|_{A(t)})$ *is bounded, for all* $s, t \in \mathbb{R}^+$;
3. *the graph norm of $A(t)$ determines the same topology on D, for all $t \in \mathbb{R}^+$.*

Here $\|\text{-}\|_{A(s)}$ is the graph norm of $A(s)$.

Note that $(\mathbb{1}_X - A(t))(\mathbb{1}_X - A(s))^{-1}$ and $(\mathbb{1}_X - A(t))^{-1}(\mathbb{1}_X - A(s))$ are well-defined, since $1 \in \rho(A(t))$, Theorem B.3. We also have that any of the graph norms makes D a Banach space, Proposition A.33.

Proof. (1,2) We have that $(\mathbb{1}_X - A(s)) : (D, \|\text{-}\|_{A(s)}) \to X$ is bounded due to Proposition A.26. We have that $(\mathbb{1}_X - A(t))^{-1} : X \to D \subseteq X$ is bounded as an operator from X to D equipped with the graph norm, see Proposition A.40.
(3) We have that $(\mathbb{1}_X - A(t))^{-1}(\mathbb{1}_X - A(0)) : (D, \|\text{-}\|_{A(0)}) \to (D, \|\text{-}\|_{A(t)})$ is bounded, linear and bijective. This implies that it is a homeomorphism, Corollary A.46 (where we have used that both spaces are Banach, Proposition A.33). □

There is now only one reasonable topology to put on D, but there are many norms that generate it. For definiteness, let D be equipped with the graph norm of $A(0)$.

Lemma B.12. *Let X be a Banach space, $D \subseteq X$ a dense subspace, $t \in \mathbb{R}^+$ and $A : \mathbb{R}^+ \to \mathrm{Lin}(D, X)$ a hyperbolic generator. Then*

1. *the operator $B(s) : D \to X : y \mapsto \dfrac{\mathrm{d}A(s)y}{\mathrm{d}s}$ is bounded;*
2. *the operator $B(s) : D \to X : y \mapsto \dfrac{\mathrm{d}A(s)y}{\mathrm{d}s}$ is bounded uniformly for $s \in [0, t]$;*
3. *there exists $M_t \geq 0$ such that $\|A(s') - A(s)\|_{D\to X} \leq |s' - s|M$ for all $s, s' \in [0, t]$.*

Proof. (1) For all $y \in D$, we have

$$B(s) = \lim_{n\to\infty} \frac{A(s + n^{-1}) - A(s)}{h} y, \tag{B.51}$$

so $B(s)$ is the pointwise limit of bounded operators, Lemma B.11. It is bounded due to Corollary A.44.
(2) For all y, the function $s \mapsto \|B(s)y\|$ is continuous. The extreme value theorem implies $\sup_{s\in[0,t]} \|B(s)y\| < \infty$ and the uniform boundedness principle Theorem A.43 implies $\sup_{s\in[0,t]} \|B(s)\| < \infty$.
(3) Let $y \in D$ be a unit vector. Then

$$A(s')y - A(s)y = \int_s^{s'} \frac{\mathrm{d}}{\mathrm{d}r} A(r)y \,\mathrm{d}r = \int_s^{s'} B(r)y \,\mathrm{d}r. \tag{B.52}$$

Now $B(r)$ is uniformly bounded on $[0, t]$. Let $M_t \geq 0$ denote this bound. Then

$$\|A(s')y - A(s)y\|_X \leq \int_s^{s'} \|B(r)y\|_X \,\mathrm{d}r \leq |s' - s|M_t. \tag{B.53}$$

The bound is independent of y, so $\|A(s') - A(s)\|_{D\to X} \leq |s' - s|M_t$. □

Corollary B.13. *Let X be a Banach space, $D \subseteq X$ a dense subspace, $t \in \mathbb{R}^+$ and $A : \mathbb{R}^+ \to \mathrm{Lin}(D, X)$ a hyperbolic generator. Then $A : \mathbb{R}^+ \to \mathcal{B}(D, X)$ is norm-continuous.*

Lemma B.14. *Let X be a Banach space, $D \subseteq X$ a dense subspace, $0 \leq t$ and $A : \mathbb{R}^+ \to \mathrm{Lin}(D, X)$ a hyperbolic generator. Then*

$$C : [0, t] \times [0, t] \to \mathcal{B}(X) : (s_0, s_1) \mapsto (\mathbb{1}_X - A(s_0))(\mathbb{1}_X - A(s_1))^{-1} \tag{B.54}$$

is uniformy bounded.

Proof. We have that $\frac{\mathrm{d}}{\mathrm{d}s} C(s,0)$ is strongly continuous. The extreme value theorem gives pointwise boundedness: $\sup_{s\in[0,t]} \left\| \frac{\mathrm{d}}{\mathrm{d}s} C(s,0)x \right\| < \infty$ for all $x \in X$. The uniform boundedness principle gives norm boundedness $\left\| \frac{\mathrm{d}}{\mathrm{d}s} C(s,0) \right\| < \infty$. Now let $x \in X$ be a unit vector and $s \in [0,t]$. Then

$$\|C(s,0)x - C(s_0,0)x\| \leq \int_{s_0}^{s} \left\| \frac{\mathrm{d}}{\mathrm{d}r} C(r,0)x \right\| \mathrm{d}r \leq |s_0 - s| \left\| \frac{\mathrm{d}}{\mathrm{d}s} C(s,0) \right\|. \tag{B.55}$$

Since the resolvent $(\mathbb{1}_X - A(s))^{-1}$ is also strongly continuously differentiable, a similar argument gives that $C(0,s)$ is bounded uniformly in s. Now $C(s_0,s_1) = C(s_0,0)C(0,s_1)$ gives the result. □

Lemma B.15. *Let X be a Banach space, $D \subseteq X$ a dense subspace, $t \in \mathbb{R}^+$ and $A : \mathbb{R}^+ \to \operatorname{Lin}(D,X)$ a hyperbolic generator. Then*

1. *there exists $K_t \geq 0$ such that $\|y\|_D \leq K_t \|y\|_{A(s)}$, for all $y \in D$ and $s \in [0,t]$;*
2. *there exists $L_t \geq 0$ such that $\|y\|_{A(s_0)} \leq \big(1 + L_t|s_1 - s_0|\big)\|y\|_{A(s_1)}$.*

Proof. (1) The function $\mathbb{R}^+ \to \mathcal{B}(X,D) : s \mapsto (\mathbb{1}_X - A(s))^{-1}$ is continuous, from Proposition A.3. This implies that $\|(\mathbb{1}_X - A(s))^{-1}\|_{X\to D}$ is also continuous in s. The extreme value theorem implies $K_t \coloneqq \sup_{s\in[0,t]} \|(\mathbb{1}_X - A(s))^{-1}\|_{X\to D} < \infty$.
Now, for all $y \in D$, we have

$$\|y\|_D = \|(\mathbb{1}_X - A(s))^{-1}(\mathbb{1}_X - A(s))y\|_D \tag{B.56}$$
$$\leq \|(\mathbb{1}_X - A(s))^{-1}\|_{X\to D} \|(\mathbb{1}_X - A(s))y\|_X \tag{B.57}$$
$$\leq K_t\big(\|y\|_X + \|A(s)y\|_X\big) = K_t\|y\|_{A(s)}. \tag{B.58}$$

(2) Set $L_t \coloneqq K_t M_t$, where M_t is defined in Lemma B.12. Calculate

$$\|y\|_{A(s_0)} \leq \|y\|_X + \|A(s_0)\|_X \tag{B.59}$$
$$\leq \|y\|_X + \|A(s_1)y\|_X + \|A(s_0)y - A(s_1)y\|_X \tag{B.60}$$
$$\leq \|y\|_{A(s_1)} + |s_0 - s_1| M_t \|y\|_D \tag{B.61}$$
$$\leq \|y\|_{A(s_1)} + |s_0 - s_1| M_t K_t \|y\|_{A(s_1)} = \big(1 + L_t|s_1 - s_0|\big)\|y\|_{A(s_1)}. \tag{B.62}$$

□

Theorem B.16. *Let X be a Banach space, $D \subseteq X$ a dense subspace and $A : \mathbb{R}^+ \to \operatorname{Lin}(D,X)$ a hyperbolic generator. Then there exists a strongly continuous evolution system $U : \{(t,s) \in \mathbb{R}^2 \mid t \geq s\} \to \mathcal{B}(X)$ such that*

1. *$\|U(t,s)\| \leq 1$ for all $s \leq t \in \mathbb{R}^+$;*
2. *$U(t,s)^{\downarrow}(D) \subseteq D$ for all $s \leq t \in \mathbb{R}^+$;*
3. *$\frac{\mathrm{d}}{\mathrm{d}t} U(t,s)y = A(t)U(t,s)y$;*
4. *$\frac{\mathrm{d}}{\mathrm{d}s} U(t,s)y = -U(t,s)A(s)y$.*

This evolution system is unique.

Proof. We will first construct $U(t,s)$ for all $s \le t \in [0,N]$, where N is some fixed integer. We can then show that these solutions are compatible, so we can let $U(t,s)$ be defined for all $s \le t \in \mathbb{R}^+$.
Fix $N \in \mathbb{N}$. Since each $A(t)$ generates a strongly continuous contraction semigroup, let S_t be the semigroup generated by $A(t)$. Also fix $M_N \ge 0$ as in Lemma B.12. For all $n \in \mathbb{N}$, define

$$U_n(t,s) = S_{\frac{N}{n}\lfloor \frac{n}{N}t\rfloor}\Big(t - \Big\lfloor \frac{nt}{N}\Big\rfloor \frac{N}{n}\Big)\Big(\prod_{k=\lceil \frac{n}{N}s\rceil}^{\lfloor \frac{n}{N}t\rfloor} S_{k\frac{N}{n}}\Big(\frac{N}{n}\Big)\Big) S_{\frac{N}{n}\lfloor \frac{n}{N}s\rfloor}\Big(\Big\lceil \frac{n}{N}s\Big\rceil \frac{N}{n} - s\Big). \tag{B.63}$$

Since each S_t maps D to D, it is clear, from Lemma B.2, that

$$\frac{\mathrm{d}}{\mathrm{d}t} U_n(t,s)y = A\Big(\frac{N}{n}\Big\lfloor \frac{n}{N}t\Big\rfloor\Big)U_n(t)y \tag{B.64}$$

$$\frac{\mathrm{d}}{\mathrm{d}s} U_n(t,s)y = -U_n(t)A\Big(\frac{N}{n}\Big\lfloor \frac{n}{N}s\Big\rfloor\Big)y \tag{B.65}$$

for all $y \in D$ and all $s \le t$, except at the discretisation points $k\frac{N}{n}$. It is also clear that $U_n(t,s)$ is strongly continuous evolution family.
For $m, n \in \mathbb{N}$, we have

$$U_n(t,s)y - U_m(t,s)y = -\int_s^t \frac{\mathrm{d}}{\mathrm{d}r} U_n(t,r)U_m(r,s)y\,\mathrm{d}r \tag{B.66}$$

$$= \int_s^t U_n(t,r)\Big(A\Big(\frac{N}{n}\Big\lfloor \frac{n}{N}r\Big\rfloor\Big) - A\Big(\frac{N}{m}\Big\lfloor \frac{m}{N}r\Big\rfloor\Big)\Big)U_m(r,s)y\,\mathrm{d}r. \tag{B.67}$$

We would like to take the norm, but for the central part to have a well-defined norm, the right-hand part needs to have its norm taken in D, i.e. we need to bound $\|U_m(r,s)y\|_D$. The basic fact we use is the observation that $\|S_{t_0}(s_0)\|_{A(t_0)\to A(t_0)} \le 1$. With the estimates in Lemma B.15, we first write

$$\|U_m(r,s)y\|_D \le K_N \|U_m(r,s)y\|_{A\left(\frac{N}{n}\lfloor \frac{n}{N}t\rfloor\right)}. \tag{B.68}$$

Since $U_m(r,s)y$ is a big product, the idea is to recursively remove the leftmost factor (with has norm ≤ 1 in the right graph norm) and then change graph norm to the right one for the next factor, which can be done up to a multiplicative error factor (Lemma B.15). There are at most m factors in $U_m(r,s)y$, so

$$\|U_m(r,s)y\|_D \le K_N\Big(1 + L_N\frac{N}{m}\Big)^m \|y\|_{A(s)} \le K_N e^{L_N N}\|y\|_{A(s)}. \tag{B.69}$$

We are now ready to take the norm:

$$\|U_n(t,s)y - U_m(t,s)y\|_X = K_N e^{L_N N}\|y\|_{A(s)} \int_s^t \Big\| A\Big(\frac{N}{n}\Big\lfloor \frac{n}{N}r\Big\rfloor\Big) - A\Big(\frac{N}{m}\Big\lfloor \frac{m}{N}r\Big\rfloor\Big)\Big\|_{D\to X}\mathrm{d}r \tag{B.70}$$

$$\le K_N e^{L_N N}\|y\|_{A(s)} M_N (t-s)\frac{N}{\min\{m,n\}}. \tag{B.71}$$

Due to the continuity of A, Corollary B.13, this implies that $\langle U_n(t,s)y\rangle_{n\in\mathbb{N}}$ is a Cauchy sequence in X. It has a limit, which we call $U(t,s)y$.

It is clear that $U(t,s)$ is a bounded operator that defined on a dense subset of X. We can extend by continuity to the whole of X. Now $U(t,s)$ being an evolution system and (1), (2) are immediate (of course still restricted to $[0,N]$).
Next, we tackle (3) and (4). We have, for $n \in \mathbb{N}$, $t \in [0,N]$ and $h > 0$, variation of parameters Proposition D.36 gives

$$U_n(t+h,t) - S_t(h) = \int_0^h S_t(h-r)\Big(A\Big(\frac{N}{n}\Big\lfloor\frac{n}{N}(t+r)\Big\rfloor\Big) - A(t)\Big)U_n(t+r,t)\,\mathrm{d}r. \tag{B.72}$$

Taking the norm gives

$$\Big\|\frac{U_n(t+h,t)y - y}{h} - \frac{S_t(h)y-y}{h}\Big\| \leq \frac{1}{h}\Big\|\int_0^h S_t(h-r)\Big(A\Big(\frac{N}{n}\Big\lfloor\frac{n}{N}(t+r)\Big\rfloor\Big) - A(t)\Big)U_n(t+r,t)\,\mathrm{d}r\Big\| \tag{B.73}$$

$$\leq M_N K_N e^{L_N N}\Big|\frac{N}{n}\Big\lfloor\frac{n}{N}(t+h)\Big\rfloor - t\Big| \leq M_N K_N e^{L_N N}\|y\|_{A(t)}h. \tag{B.74}$$

Taking the limit $n \to \infty$ gives

$$\Big\|\frac{U(t+h,t)y - y}{h} - \frac{S_t(h)y-y}{h}\Big\| \leq M_N K_N e^{L_N N}h. \tag{B.75}$$

Replacing y by $U(t,s)y$ and taking the limit $h \to 0$ gives (3). The argument for (4) is similar.
Finally we check uniqueness: suppose there was some other evolution system V that satisfied the requirements. Then, for all $y \in D$,

$$U(t,s)y - V(t,s)y = \int_s^t \frac{\mathrm{d}}{\mathrm{d}r}\big(U(t,t+s-r)V(t,t+s-r)y\big)\,\mathrm{d}r \tag{B.76}$$

$$= \int_s^t U(t,t+s-r)\big(A(t+s-r) - A(t+s-r)\big)V(t,t+s-r)y\,\mathrm{d}r = 0. \tag{B.77}$$

Since this holds on a dense subset of X, it holds on all X. We also conclude that the construction of U is independent of N: taking a different N must give the same result, by uniqueness. □

Appendix C

Trotter product formulas

C.1 Time-independent Lie-Trotter product formulas

The basic structure of the proofs in this section is as follows: first a “single step” approximation is proved – these are collected in subsection C.1.2 – then these approximations are iterated to Lie-Trotter-Suzuki formulas. First some useful lemmas about exponentials are proved.
Much of this material is essentially due to M. Suzuki. See in particular [68].

C.1.1 Some useful lemmas bounding exponentials

Lemma C.1 (Kubo's identity [69])**.** *Let A be a unital Banach algebra and $a, b \in A$. Then*

$$[a, e^b] = \int_0^1 e^{(1-t)b}[a, b]e^{tb}\,\mathrm{d}t. \tag{C.1}$$

Proof. We have

$$[a, e^b] = \left[e^{(1-t)b}ae^{tb}\right]_{t=0}^{t=1} \tag{C.2}$$

$$= \int_0^1 \frac{\mathrm{d}}{\mathrm{d}t}\left(e^{(1-t)b}ae^{tb}\right)\mathrm{d}t \tag{C.3}$$

$$= \int_0^1 e^{(1-t)b}[a, b]e^{tb}\,\mathrm{d}t \tag{C.4}$$

from the second fundamental theorem of calculus Corollary D.32. □

Corollary C.2. *Let A be a unital Banach algebra and $a, b \in A$. Then*

$$\|e^a b - be^a\| \leq \|ab - ba\|e^{\|a\|}. \tag{C.5}$$

We can also give a more elementary proof using the series expansion.

Alternate proof. Take arbitrary $n \in \mathbb{N}$. Then we have

$$\|a^n b - ba^n\| = \left\| \sum_{k=0}^{n-1} a^{k+1} b a^{n-k-1} - a^k b a^{n-k} \right\| \tag{C.6}$$

$$= \left\| \sum_{k=0}^{n-1} a^k (ab - ba) a^{n-k-1} \right\| \tag{C.7}$$

$$\leq \sum_{k=0}^{n-1} \|a\|^k \, \|ab - ba\| \|a\|^{n-k-1} \tag{C.8}$$

$$= \|ab - ba\| \sum_{k=0}^{n-1} \|a\|^{n-1} = n \|ab - ba\| \|a\|^{n-1}. \tag{C.9}$$

Now calculate

$$\|e^a b - be^a\| = \left\| \Big(\sum_{n=0}^{\infty} \frac{a^n}{n!} b \Big) - \Big(\sum_{n=0}^{\infty} b \frac{a^n}{n!} \Big) \right\| \tag{C.10}$$

$$= \left\| \Big(\sum_{n=1}^{\infty} \frac{a^n}{n!} b \Big) - \Big(\sum_{n=1}^{\infty} b \frac{a^n}{n!} \Big) \right\| \tag{C.11}$$

$$\leq \sum_{n=1}^{\infty} \frac{\|a^n b - ba^n\|}{n!} \tag{C.12}$$

$$\leq \sum_{n=1}^{\infty} \frac{n \|ab - ba\| \|a\|^{n-1}}{n!} \tag{C.13}$$

$$= \|ab - ba\| \sum_{n=1}^{\infty} \frac{\|a\|^{n-1}}{(n-1)!} = \|ab - ba\| e^{\|a\|}. \tag{C.14}$$

□

Lemma C.3. *Let A be a unital Banach algebra, $n \in \mathbb{N}$ and $a, b \in A$. Then*

1. $\|\mathbf{1} + a\| \leq e^{\|a\|}$;
2. $\|\mathbf{1} + a + a^2/2\| \leq e^{\|a\|}$;
3. $\|e^a - \mathbf{1}\| \leq \|a\| e^{\|a\|}$;
4. $\|e^a - (\mathbf{1} + a)\| \leq \|a^2\| e^{\|a\|}$;
5. $\|e^a - (\mathbf{1} + a + a^2/2)\| \leq \|a^3\| e^{\|a\|}$;
6. $\|a^n - b^n\| \leq n \|a - b\| \max\{\|a\|, \|b\|\}^{n-1}$.

Proof. (1) We have

$$\|\mathbf{1} + a\| \leq 1 + \|a\| \leq \sum_{k=0}^{\infty} \frac{\|a\|^k}{k!} = e^{\|a\|}. \tag{C.15}$$

(2) We have

$$\|\mathbf{1} + a + a^2/2\| \leq 1 + \|a\| + \|a\|^2/2 \leq \sum_{k=0}^{\infty} \frac{\|a\|^k}{k!} = e^{\|a\|}. \tag{C.16}$$

(3) By straightforward calculation,

$$\|e^a - \mathbf{1}\| = \left\| \sum_{k=1}^{\infty} \frac{a^k}{k!} \right\| \tag{C.17}$$

$$= \left\| \sum_{k=0}^{\infty} \frac{a^{k+1}}{(k+1)!} \right\| \tag{C.18}$$

$$\leq \|a\| \sum_{k=0}^{\infty} \frac{\|a\|^k}{(k+1)!} \tag{C.19}$$

$$\leq \|a\| \sum_{k=0}^{\infty} \frac{\|a\|^k}{k!} = \|a\| e^{\|a\|}. \tag{C.20}$$

(4) By straightforward calculation,

$$\|e^a - (\mathbf{1} + a)\| = \left\| \sum_{k=2}^{\infty} \frac{a^k}{k!} \right\| \tag{C.21}$$

$$= \left\| \sum_{k=0}^{\infty} \frac{a^{k+2}}{(k+2)!} \right\| \tag{C.22}$$

$$\leq \|a^2\| \sum_{k=0}^{\infty} \frac{\|a\|^k}{(k+2)!} \tag{C.23}$$

$$\leq \|a^2\| \sum_{k=0}^{\infty} \frac{\|a\|^k}{k!} = \|a^2\| e^{\|a\|}. \tag{C.24}$$

(5) By straightforward calculation,

$$\|e^a - (\mathbf{1} + a + a^2/2)\| = \left\| \sum_{k=3}^{\infty} \frac{a^k}{k!} \right\| \tag{C.25}$$

$$= \left\| \sum_{k=0}^{\infty} \frac{a^{k+3}}{(k+3)!} \right\| \tag{C.26}$$

$$\leq \|a^3\| \sum_{k=0}^{\infty} \frac{\|a\|^k}{(k+3)!} \tag{C.27}$$

$$\leq \|a^3\| \sum_{k=0}^{\infty} \frac{\|a\|^k}{k!} = \|a^3\| e^{\|a\|}. \tag{C.28}$$

(6) Consider the following telescoping sum:

$$a^n - b^n = \sum_{k=0}^{n-1} a^{k+1} b^{n-k-1} - a^k b^{n-1} = \sum_{k=0}^{n-1} a^k (a-b) b^{n-k-1}. \tag{C.29}$$

The norm can then be bounded by

$$\|a^n - b^n\| \leq \sum_{k=0}^{n-1} \|a\|^k \|a-b\| \|b\|^{n-k-1} \leq n\|a-b\| \max\{\|a\|, \|b\|\}^{n-1}. \tag{C.30}$$

□

Lemma C.4. *Let A be a unital Banach algebra and $a, b \in A$. Then*

$$e^a x e^{-a} - e^b x e^{-b} = \int_0^1 \left(e^{ta}[a,x]e^{-ta} - e^{tb}[b,x]e^{-tb}\right) \mathrm{d}t. \tag{C.31}$$

Proof. Since $e^{at}xe^{-at} - e^{bt}xe^{-bt}$ is zero when evaluated at $t = 0$, we have

$$e^a x e^{-a} - e^b x e^{-b} = \int_0^1 \frac{\mathrm{d}}{\mathrm{d}t} \left(e^{at}xe^{-at} - e^{bt}xe^{-bt}\right) \mathrm{d}t \tag{C.32}$$

$$= \int_0^1 \left(e^{ta}[a,x]e^{-ta} - e^{tb}[b,x]e^{-tb}\right) \mathrm{d}t, \tag{C.33}$$

from the second fundamental theorem of calculus Corollary D.32. $\square$

Lemma C.5. *Let A be a unital Banach algebra and $a, b \in A$. Then*

$$\exp(a+b) = \exp(a)\exp(b) + O_0\Big(\frac{1}{2}\big\|[a,b]\big\| e^{\|a\|+\|b\|}\Big). \tag{C.34}$$

Proof. Applying variation of parameters, Proposition D.36, with $S(t) = e^{ta}e^{tb}$ and $T(t) = e^{t(a+b)}$ at $t = 1$ gives

$$e^a e^b - e^{a+b} = \int_0^1 \left(e^{(1-s)(a+b)} a e^{sa} e^{sb} + e^{(1-s)(a+b)} e^{sa} b e^{sb} - e^{(1-s)(a+b)}(a+b) e^{sa} e^{sb}\right) \mathrm{d}s \tag{C.35}$$

$$= \int_0^1 e^{(1-s)(a+b)}\big(e^{sa}b - be^{sa}\big)e^{sb} \,\mathrm{d}s. \tag{C.36}$$

Then the triangle inequality and Corollary C.2 give

$$\|e^{a+b} - e^a e^b\| \leq \int_0^1 e^{(1-s)(\|a\|+\|b\|)} \big\|e^{sa}b - be^{sa}\big\| e^{s\|b\|} \,\mathrm{d}s \tag{C.37}$$

$$\leq \int_0^1 e^{(1-s)(\|a\|+\|b\|)} \big(s\|ab - ba\| e^{s\|a\|}\big) e^{s\|b\|} \,\mathrm{d}s \tag{C.38}$$

$$= \|ab - ba\| e^{\|a\|+\|b\|} \int_0^1 s \,\mathrm{d}s = \frac{1}{2}\|ab - ba\| e^{\|a\|+\|b\|}. \tag{C.39}$$

$\square$

C.1.2 Splitting lemmas

Lemma C.6 (Marchuk-Strang splitting)**.** *Let A be a unital Banach algebra and $a, b \in A$. Then*

$$\exp(a+b) = \exp(a/2)\exp(b)\exp(a/2) + O_0\bigg(\Big(\frac{1}{12}\Big\|\big[b,[b,a]\big]\Big\| + \frac{1}{24}\Big\|\big[a,[a,b]\big]\Big\|\Big) e^{\|a\|+\|b\|}\bigg). \tag{C.40}$$

This leads to a second-order Trotter-Suzuki decomposition. In numerical integration the analogous method is called Størmer-Verlet.

Proof. Applying variation of parameters, Proposition D.36, with $S(t) = e^{ta/2}e^{tb}e^{ta/2}$ and $T(t) = e^{t(a+b)}$ at $t = 1$ gives

$$e^{\frac{a}{2}}e^{b}e^{\frac{a}{2}} - e^{a+b} = \int_0^1 \Big(e^{(1-s)(a+b)}\big(\frac{a}{2}e^{\frac{sa}{2}}e^{sb}e^{\frac{sa}{2}} + e^{\frac{sa}{2}}be^{sb}e^{\frac{sa}{2}} + e^{\frac{sa}{2}}e^{sb}\frac{a}{2}e^{\frac{sa}{2}}\big) - e^{(1-s)(a+b)}(a+b)e^{\frac{sa}{2}}e^{sb}e^{\frac{sa}{2}} \Big)\,\mathrm{d}s \tag{C.41}$$

$$= \int_0^1 e^{(1-s)(a+b)}\Big(\frac{a}{2}e^{\frac{sa}{2}}e^{sb} + e^{\frac{sa}{2}}be^{sb} + e^{\frac{sa}{2}}e^{sb}\frac{a}{2} - (a+b)e^{\frac{sa}{2}}e^{sb}\Big)e^{\frac{sa}{2}}\,\mathrm{d}s \tag{C.42}$$

$$= \int_0^1 e^{(1-s)(a+b)}\Big(e^{\frac{sa}{2}}[e^{sb}, \frac{a}{2}] + [e^{\frac{sa}{2}}, b]e^{sb}\Big)e^{\frac{sa}{2}}\,\mathrm{d}s \tag{C.43}$$

$$\tag{C.44}$$

Next we use Lemma C.1 and Lemma C.4 to calculate

$$e^{\frac{sa}{2}}[e^{sb}, \frac{a}{2}] + [e^{\frac{sa}{2}}, b]e^{sb} = \int_0^1\int_0^1 \Big(e^{\frac{sa}{2}}e^{(1-t)sb}[sb, \frac{a}{2}]e^{tsb} + e^{(1-t')\frac{sa}{2}}[\frac{sa}{2}, b]e^{t'\frac{sa}{2}}e^{sb}\Big)\,\mathrm{d}t\,\mathrm{d}t' \tag{C.45}$$

$$= \frac{s}{2}\int_0^1\int_0^1 e^{\frac{sa}{2}}\Big(e^{(1-t)sb}[b,a]e^{-(1-t)sb} + e^{-t'\frac{sa}{2}}[a,b]e^{t'\frac{sa}{2}}\Big)e^{sb}\,\mathrm{d}t\,\mathrm{d}t' \tag{C.46}$$

$$= \frac{s}{2}\int_0^1\int_0^1\int_0^1 e^{\frac{sa}{2}}\Big(e^{u(1-t)sb}\big[(1-t)sb, [b,a]\big]e^{-u(1-t)sb} \tag{C.47}$$

$$- e^{-ut'\frac{sa}{2}}\big[-t'\frac{sa}{2}, [b,a]\big]e^{ut'\frac{sa}{2}}\Big)e^{sb}\,\mathrm{d}u\,\mathrm{d}t\,\mathrm{d}t'. \tag{C.48}$$

Taking the norm gives

$$\Big\|e^{\frac{sa}{2}}[e^{sb}, \frac{a}{2}] + [e^{\frac{sa}{2}}, b]e^{sb}\Big\| \le \frac{s}{2}\int_0^1\int_0^1\int_0^1 e^{\frac{s}{2}\|a\|}\Big((1-t)s\Big\|\big[b,[b,a]\big]\Big\| + \frac{st'}{2}\Big\|\big[a,[a,b]\big]\Big\|\Big)e^{s\|b\|}\,\mathrm{d}u\,\mathrm{d}t\,\mathrm{d}t' \tag{C.49}$$

$$= \frac{s}{2}e^{\frac{s}{2}\|a\|}\Big(\Big(\int_0^1 (1-t)\,\mathrm{d}t\Big)s\Big\|\big[b,[b,a]\big]\Big\| + \frac{s}{2}\Big(\int_0^1 t'\,\mathrm{d}t'\Big)\Big\|\big[a,[a,b]\big]\Big\|\Big)e^{s\|b\|} \tag{C.50}$$

$$= \frac{s}{4}e^{\frac{s}{2}\|a\|}\Big(s\Big\|\big[b,[b,a]\big]\Big\| + \frac{s}{2}\Big\|\big[a,[a,b]\big]\Big\|\Big)e^{s\|b\|}. \tag{C.51}$$

Plugging this back in the first calculation gives

$$\big\|e^{\frac{a}{2}}e^{b}e^{\frac{a}{2}} - e^{a+b}\big\| \le \int_0^1 e^{(1-s)(\|a\|+\|b\|)}\Big(\frac{s}{4}e^{\frac{s}{2}\|a\|}\Big(s\Big\|\big[b,[b,a]\big]\Big\| + \frac{s}{2}\Big\|\big[a,[a,b]\big]\Big\|\Big)e^{s\|b\|}\Big)e^{\frac{s}{2}\|a\|}\,\mathrm{d}s \tag{C.52}$$

$$= \int_0^1 e^{\|a\|+\|b\|}\Big(\frac{s}{4}\Big(s\Big\|\big[b,[b,a]\big]\Big\| + \frac{s}{2}\Big\|\big[a,[a,b]\big]\Big\|\Big)\Big)\,\mathrm{d}s \tag{C.53}$$

$$= e^{\|a\|+\|b\|}\Big(\frac{1}{12}\Big\|\big[b,[b,a]\big]\Big\| + \frac{1}{24}\Big\|\big[a,[a,b]\big]\Big\|\Big). \tag{C.54}$$

□

Lemma C.7 (Symmetric spitting)**.** *Let A be a unital Banach algebra and $a, b \in A$. Then*

$$\exp(a+b) = \frac{1}{2}\big(e^a e^b + e^b e^a\big) + O_0\bigg(\frac{1}{12}\Big(\big\|\,[a,[a,b]]\,\big\| + \big\|\,[b,[a,b]]\,\big\| + 4\|a\|\,\big\|[a,b]\big\|\Big)e^{\|a\|+\|b\|}\bigg). \tag{C.55}$$

Proof. Applying variation of parameters, Proposition D.36, with $S(t) = \frac{1}{2}\big(e^{ta}e^{tb} + e^{tb}e^{ta}\big)$ and $T(t) = e^{t(a+b)}$ at $t = 1$ gives

$$\frac{1}{2}\big(e^a e^b + e^b e^a\big) - e^{a+b} = \frac{1}{2}\int_0^1 e^{(1-s)(a+b)}\Big(ae^{sa}e^{sb} + e^{sa}be^{sb} + be^{sb}e^{sa} + e^{sa}ae^{sb} - (a+b)\big(e^{sa}e^{sb} + e^{sb}e^{sa}\big)\Big)\,\mathrm{d}s \tag{C.56}$$

$$= \frac{1}{2}\int_0^1 e^{(1-s)(a+b)}\Big([e^{sa}, b]e^{sb} + [e^{sb}, a]e^{sa}\Big)\,\mathrm{d}s. \tag{C.57}$$

Next we use Lemma C.1 to calculate

$$[e^{sa}, b]e^{sb} + [e^{sb}, a]e^{sa} = \int_0^1\int_0^1 \Big(e^{(1-t)sa}[sa, b]e^{tsa}e^{sb} + e^{(1-t')sb}[sb, a]e^{t'sb}e^{sa}\Big)\,\mathrm{d}t\,\mathrm{d}t' \tag{C.58}$$

$$= s\int_0^1\int_0^1 \Big(e^{(1-t)sa}[a, b]e^{-(1-t)sa}e^{sa}e^{sb} - e^{(1-t')sb}[a, b]e^{-(1-t')sb}e^{sb}e^{sa}\Big)\,\mathrm{d}t\,\mathrm{d}t'. \tag{C.59}$$

Now, for $u \in [0, 1]$, define

$$F(u) \coloneqq e^{(1-t)sua}[a, b]e^{-(1-t)sua}e^{sua}e^{sb} - e^{(1-t')sub}[a, b]e^{-(1-t')sub}e^{sb}e^{sua}. \tag{C.60}$$

Since $F(0) = 0$, the second fundamental theorem of calculus Corollary D.32 gives

$$F(1) = \int_0^1 \frac{\mathrm{d}}{\mathrm{d}u}F(u)\,\mathrm{d}u \tag{C.61}$$

$$= \int_0^1 \Big(e^{(1-t)sua}\big[(1-t)sa, [a, b]\big]e^{-(1-t)sua}e^{sua}e^{sb} + e^{(1-t)sua}[a, b]e^{-(1-t)sua}sae^{sua}e^{sb} \tag{C.62}$$

$$- e^{(1-t')sub}\big[(1-t')sb, [a, b]\big]e^{-(1-t')sub}e^{sb}e^{sua} - e^{(1-t')sub}[a, b]e^{-(1-t')sub}e^{sb}sae^{sua}\Big)\,\mathrm{d}u. \tag{C.63}$$

Taking the norm gives

$$\|F(1)\| \leq \int_0^1 \Big((1-t)s\big\|\,[a,[a,b]]\,\big\| + (1-t')s\big\|\,[b,[a,b]]\,\big\| + 2s\|a\|\,\big\|[a,b]\big\|\Big)e^{su\|a\|}e^{s\|b\|}\,\mathrm{d}u \tag{C.64}$$

$$= s\Big((1-t)\big\|\,[a,[a,b]]\,\big\| + (1-t')\big\|\,[b,[a,b]]\,\big\| + 2\|a\|\,\big\|[a,b]\big\|\Big)e^{s\|b\|}\int_0^1 e^{su\|a\|}\,\mathrm{d}u \tag{C.65}$$

$$= s\Big((1-t)\big\|\,[a,[a,b]]\,\big\| + (1-t')\big\|\,[b,[a,b]]\,\big\| + 2\|a\|\,\big\|[a,b]\big\|\Big)e^{s\|b\|}\frac{e^{s\|a\|} - 1}{s\|a\|} \tag{C.66}$$

$$\leq s\Big((1-t)\big\|\,[a,[a,b]]\,\big\| + (1-t')\big\|\,[b,[a,b]]\,\big\| + 2\|a\|\,\big\|[a,b]\big\|\Big)e^{s\|b\|}e^{s\|a\|}. \tag{C.67}$$

This means that

$$\big\|[e^{sa},b]e^{sb}+[e^{sb},a]e^{sa}\big\| \le s^2\int_0^1\int_0^1 \Big((1-t)\big\|\,[a,[a,b]]\,\big\|+(1-t')\big\|\,[b,[a,b]]\,\big\|+2\|a\|\,\big\|[a,b]\big\|\Big)e^{s(\|b\|+\|a\|)}\,\mathrm{d}t\,\mathrm{d}t' \tag{C.68}$$

$$= s^2\Big(\frac{1}{2}\big\|\,[a,[a,b]]\,\big\|+\frac{1}{2}\big\|\,[b,[a,b]]\,\big\|+2\|a\|\,\big\|[a,b]\big\|\Big)e^{s(\|b\|+\|a\|)} \tag{C.69}$$

$$= \frac{s^2}{2}\Big(\big\|\,[a,[a,b]]\,\big\|+\big\|\,[b,[a,b]]\,\big\|+4\|a\|\,\big\|[a,b]\big\|\Big)e^{s(\|b\|+\|a\|)}. \tag{C.70}$$

Finally,

$$\Big\|\frac{1}{2}(e^ae^b+e^be^a)-e^{a+b}\Big\| \le \frac{1}{2}\int_0^1 e^{(1-s)(\|a\|+\|b\|)}\frac{s^2}{2}\Big(\big\|\,[a,[a,b]]\,\big\|+\big\|\,[b,[a,b]]\,\big\|+4\|a\|\,\big\|[a,b]\big\|\Big)e^{s(\|b\|+\|a\|)}\,\mathrm{d}s \tag{C.71}$$

$$\le \frac{1}{4}\Big(\big\|\,[a,[a,b]]\,\big\|+\big\|\,[b,[a,b]]\,\big\|+4\|a\|\,\big\|[a,b]\big\|\Big)e^{\|a\|+\|b\|}\int_0^1 s^2\,\mathrm{d}s \tag{C.72}$$

$$= \frac{1}{12}\Big(\big\|\,[a,[a,b]]\,\big\|+\big\|\,[b,[a,b]]\,\big\|+4\|a\|\,\big\|[a,b]\big\|\Big)e^{\|a\|+\|b\|}. \tag{C.73}$$

□

C.1.3 Lie-Trotter-Suzuki product formulas

Proposition C.8 (Lie-Trotter-Suzuki product formulae)**.** *Let A be a unital Banach algebra, $a, b \in A$ and $n \in \mathbb{N}$. Then*

1. $\exp(a+b) = \Big(\exp\Big(\frac{a}{n}\Big)\exp\Big(\frac{b}{n}\Big)\Big)^n + O_0\Big(\frac{1}{2n}\big\|[a,b]\big\|e^{\|a\|+\|b\|}\Big)$;
2. $\exp(a+b) = \Big(\exp\Big(\frac{a}{2n}\Big)\exp\Big(\frac{b}{n}\Big)\exp\Big(\frac{a}{2n}\Big)\Big)^n + O_0\Big(\frac{1}{12n^2}\Big(\Big\|\,[b,[b,a]]\,\Big\|+\frac{1}{2}\Big\|\,[a,[a,b]]\,\Big\|\Big)e^{\|a\|+\|b\|}\Big)$;
3. $\exp(a+b) = \Big(\frac{1}{2}(e^{\frac{a}{n}}e^{\frac{b}{n}}+e^{\frac{b}{n}}e^{\frac{a}{n}})\Big)^n + O_0\Big(\frac{1}{12n^2}\Big(\big\|\,[a,[a,b]]\,\big\|+\big\|\,[b,[a,b]]\,\big\|+4\|a\|\,\big\|[a,b]\big\|\Big)e^{\|a\|+\|b\|}\Big)$.

In particular $\exp(a+b) = \lim_{n\to\infty}\big(\exp\big(\frac{a}{n}\big)\exp\big(\frac{b}{n}\big)\big)^n$.

The big oh hides no constants.

Proof. (1) We calculate

$$\Big\|\exp(a+b)-\Big(\exp\Big(\frac{a}{n}\Big)\exp\Big(\frac{b}{n}\Big)\Big)^n\Big\| = \Big\|\exp\Big(\frac{a+b}{n}\Big)^n-\Big(\exp\Big(\frac{a}{n}\Big)\exp\Big(\frac{b}{n}\Big)\Big)^n\Big\| \tag{C.74}$$

$$\le n\Big\|\exp\Big(\frac{a+b}{n}\Big)-\exp\Big(\frac{a}{n}\Big)\exp\Big(\frac{b}{n}\Big)\Big\|e^{(\|a\|+\|b\|)\frac{n-1}{n}} \tag{C.75}$$

$$\le n\Big(\frac{1}{2n^2}\big\|[a,b]\big\|e^{(\|a\|+\|b\|)\frac{1}{n}}\Big)e^{(\|a\|+\|b\|)\frac{n-1}{n}} \tag{C.76}$$

$$= \frac{1}{2n}\big\|[a,b]\big\|e^{\|a\|+\|b\|}. \tag{C.77}$$

using Lemma C.3 and Lemma C.5.
(2) We calculate

$$\left\| e^{a+b} - \left(e^{\frac{a}{2n}} e^{\frac{b}{n}} e^{\frac{a}{2n}}\right)^n \right\| = \left\| \left(e^{\frac{a+b}{n}}\right)^n - \left(e^{\frac{a}{2n}} e^{\frac{b}{n}} e^{\frac{a}{2n}}\right)^n \right\| \tag{C.78}$$

$$\leq n \left\| e^{\frac{a+b}{n}} - e^{\frac{a}{2n}} e^{\frac{b}{n}} e^{\frac{a}{2n}} \right\| e^{(\|a\|+\|b\|)\frac{n-1}{n}} \tag{C.79}$$

$$\leq n\left(\frac{1}{12n^3}\left(\left\|[b,[b,a]]\right\| + \frac{1}{2}\left\|[a,[a,b]]\right\|\right) e^{(\|a\|+\|b\|)\frac{1}{n}}\right) e^{(\|a\|+\|b\|)\frac{n-1}{n}} \tag{C.80}$$

$$= \frac{1}{12n^2}\left(\left\|[b,[b,a]]\right\| + \frac{1}{2}\left\|[a,[a,b]]\right\|\right) e^{\|a\|+\|b\|}. \tag{C.81}$$

using Lemma C.3 and Lemma C.6.
(3) We calculate

$$\left\| e^{a+b} - \left(\frac{1}{2}\left(e^{\frac{a}{n}} e^{\frac{b}{n}} + e^{\frac{b}{n}} e^{\frac{a}{n}}\right)\right)^n \right\| = \left\| \left(e^{\frac{a+b}{n}}\right)^n - \left(\frac{1}{2}\left(e^{\frac{a}{n}} e^{\frac{b}{n}} + e^{\frac{b}{n}} e^{\frac{a}{n}}\right)\right)^n \right\| \tag{C.82}$$

$$\leq n \left\| e^{\frac{a+b}{n}} - \frac{1}{2}\left(e^{\frac{a}{n}} e^{\frac{b}{n}} + e^{\frac{b}{n}} e^{\frac{a}{n}}\right) \right\| e^{(\|a\|+\|b\|)\frac{n-1}{n}} \tag{C.83}$$

$$\leq \frac{1}{12n^2}\left(\left\|[a,[a,b]]\right\| + \left\|[b,[a,b]]\right\| + 4\|a\| \left\|[a,b]\right\|\right) e^{\|a\|+\|b\|}. \tag{C.84}$$

using Lemma C.3 and Lemma C.7. □

C.2 Time-dependent Trotter product formulas

C.2.1 Moduli of continuity

Let (X, d_x) and (Y, d_Y) be metric spaces. Let $f : X \to Y$ and $\omega : \overline{\mathbb{R}^+} \to \overline{\mathbb{R}^+}$ be functions. We call ω a modulus of continuity for f if

- ω is increasing;
- $\lim_{t\to 0^+} \omega(t) = 0$;
- $d_Y\big(f(x), f(y)\big) \leq \omega\big(d_X(x, y)\big)$ for all $x, y \in X$.

The notation $\overline{\mathbb{R}^+}$ means the extended half line, i.e. $[0, +\infty]$.

Lemma C.9. *Let $(X, d_x), (Y, d_Y)$ be metric spaces and $f : X \to Y$ a function. Consider the following function*

$$\omega_0 : \overline{\mathbb{R}^+} \to \overline{\mathbb{R}^+} : a \mapsto \sup\{d_Y\big(f(x), f(y)\big) \mid d_X(x, y) \leq a\}. \tag{C.85}$$

Then

1. *ω_0 is increasing;*
2. *if ω is a modulus of continuity for f, then $\omega_0 \leq \omega$.*

Proof. (1) Immediate.
(2) Take $a \in \overline{\mathbb{R}^+}$. Take arbitrary $x, y \in X$ such that $d_X(x,y) \leq a$. Then

$$d_Y\big(f(x), f(y)\big) \leq \omega\big(d_X(x,y)\big) \leq \omega(a). \tag{C.86}$$

Taking the supremum over all such x, y gives $\omega_0(a) \leq \omega(a)$. □

Proposition C.10. *Let $(X, d_x), (Y, d_Y)$ be metric spaces and $f : X \to Y$ a function. Consider the following function*

$$\omega_0 : \overline{\mathbb{R}^+} \to \overline{\mathbb{R}^+} : a \mapsto \sup\{d_Y\big(f(x), f(y)\big) \mid d_X(x,y) \leq a\}. \tag{C.87}$$

Then the following are equivalent:

1. *f is uniformly continuous;*
2. *ω_0 is a modulus of continuity for f, i.e. $\lim_{t \to 0^+} \omega_0(t) = 0$;*
3. *f has a modulus of continuity.*

Proof. (1) ⇒ (2) With Lemma C.9, it is straightforward to see that ω_0 is a modulus of continuity for f if and only if $\lim_{t \to 0^+} \omega_0(t) = 0$.
Take arbitrary $\epsilon > 0$. Take a $\delta > 0$ that satisfies the $\epsilon - \delta$ definition of uniform continuity and arbitrary $a \in \overline{\mathbb{R}^+}$ such that $a \leq \delta$. Take arbitrary $x, y \in X$ such that $d_X(x,y) \leq a \leq \delta$. Then $d_Y\big(f(x), f(y)\big) \leq \epsilon$, by definition of δ. Taking the supremum over such x, y gives $\omega_0(a) \leq \epsilon$. (Here we have also implicitly used that the set of such x, y is not empty, indeed taking $x = y$ yields an element).
(2) ⇒ (3) Immediate.
(3) ⇒ (1) Let $\omega : \overline{\mathbb{R}^+} \to \overline{\mathbb{R}^+}$ be a modulus of continuity. Take arbitrary $\epsilon > 0$. Since ω is continuous at 0, we can take $\delta > 0$ that satisfies the $\epsilon - \delta$ definition of continuity. Take arbitrary $x, y \in X$ such that $d_X(x,y) \leq \delta$. Then

$$d_Y\big(f(x), f(y)\big) \leq \omega\big(d_X(x,y)\big) \leq \epsilon \tag{C.88}$$

and we conclude that f is uniformly continuous. □

Lemma C.11. *Let A be a Banach algebra, $a \leq b \in \mathbb{R}$ and $f : [a,b] \to A$ a continuously differentiable function. Then*

$$\omega : \overline{\mathbb{R}^+} \to \overline{\mathbb{R}^+} : x \mapsto x \sup_{s \in [a,b]} \|f'\| \tag{C.89}$$

is a modulus of continuity for f.

Proof. Take $s, t \in [a,b]$. Then

$$\|f(s) - f(t)\| \leq \int_s^t \|f'(r)\| \,\mathrm{d}r \tag{C.90}$$

$$\leq |t - s| \sup_{s \in [a,b]} \|f'\| = \omega(|t - s|). \tag{C.91}$$

□

C.2.2 The product formula

Lemma C.12. *Let X be a Banach space, $s \le t \in \mathbb{R}^+$ and $A : \mathbb{R}^+ \to \mathcal{B}(X)$ a continuous function. Set $K_{s,t} := \sup_{r\in[s,t]}\|A(r)\|$ and $\omega_A : \overline{\mathbb{R}^+} \to \overline{\mathbb{R}^+}$ a modulus of uniformity for A on $[s,t]$. Then*

$$U(t,s) = e^{(t-s)A(s)} + O_0\Big(e^{(t-s)K_{s,t}}(t-s)\omega_A(t-s)\Big). \tag{C.92}$$

Note that $K_{s,t}$ is finite due to the extreme value theorem and A has a modulus of continuity on $[s,t]$ due to the Heine-Cantor theorem and Proposition C.10.

Proof. Variation of parameters, Proposition D.36, with Lemma B.10 gives

$$U(t,s) - e^{(t-s)A(s)} = \int_s^t \left(e^{(t-r)A(s)}A(r)U(r,s) - e^{(t-r)A(s)}A(s)U(r,s)\right)\mathrm{d}r \tag{C.93}$$

$$= \int_s^t e^{(t-r)A(s)}\big(A(r)-A(s)\big)U(r,s)\,\mathrm{d}r. \tag{C.94}$$

Taking the norm and bounding using Lemma B.8 and Lemma D.14 gives

$$\|U(t,s) - e^{(t-s)A(s)}\| \le \int_s^t e^{(t-r)\|A(s)\|}\|A(r)-A(s)\|e^{\int_s^r\|A(r')\|\,\mathrm{d}r'}\,\mathrm{d}r \tag{C.95}$$

$$\le \int_s^t e^{(t-r)K_{s,t}}\|A(r)-A(s)\|e^{(r-s)K_{s,t}}\,\mathrm{d}r \tag{C.96}$$

$$= e^{(t-s)K_{s,t}}\int_s^t \|A(r)-A(s)\|\,\mathrm{d}r \tag{C.97}$$

$$\le e^{(t-s)K_{s,t}}(t-s)\omega_A(t-s). \tag{C.98}$$

□

Proposition C.13. *Let X be a Banach space, $s \le t \in \mathbb{R}^+$ and $A : \mathbb{R}^+ \to \mathcal{B}(X)$ a continuous function. Set $K_{s,t} := \sup_{r\in[s,t]}\|A(r)\|$ and $\omega_A : \overline{\mathbb{R}^+} \to \overline{\mathbb{R}^+}$ a modulus of uniformity for A on $[s,t]$. Then*

$$U(t,s) = \prod_{k=0}^{n-1} e^{\frac{t-s}{n}A\left(s+k\frac{t-s}{n}\right)} + O_0\left((t-s)e^{(t-s)K_{s,t}}\omega_A\left(\frac{t-s}{n}\right)\right). \tag{C.99}$$

Proof. We expand the telescoping sum

$$\prod_{k=0}^{n-1} e^{\frac{t-s}{n}A\left(s+k\frac{t-s}{n}\right)} - U(t,s) = \sum_{m=0}^{n-1} U\left(t, s+(t-s)\frac{m+1}{n}\right)\left(\prod_{k=0}^{m} e^{\frac{t-s}{n}A\left(s+k\frac{t-s}{n}\right)}\right) \tag{C.100}$$

$$- U\left(t, s+(t-s)\frac{m}{n}\right)\left(\prod_{k=0}^{m-1} e^{\frac{t-s}{n}A\left(s+k\frac{t-s}{n}\right)}\right) \tag{C.101}$$

$$= \sum_{m=0}^{n-1} U\left(t, s+(t-s)\frac{m+1}{n}\right) \tag{C.102}$$

$$\cdot\left(e^{\frac{t-s}{n}A\left(s+m\frac{t-s}{n}\right)} - U\left(s+(t-s)\frac{m+1}{n}, s+(t-s)\frac{m}{n}\right)\right)\prod_{k=0}^{m-1} e^{\frac{t-s}{n}A\left(s+k\frac{t-s}{n}\right)}. \tag{C.103}$$

Now we can use Lemma B.8 to bound

$$\left\|U\Big(t, s+(t-s)\frac{m+1}{n}\Big)\right\| \leq \exp\Big(\int_{s+(t-s)\frac{m+1}{n}}^{t} \|A(r)\|\,\mathrm{d}r\Big) \tag{C.104}$$

$$\leq e^{\left(t-s-(t-s)\frac{m+1}{n}\right)K_{s,t}} \tag{C.105}$$

$$\leq e^{\left((t-s)\frac{n-m-1}{n}\right)K_{s,t}}. \tag{C.106}$$

We can also bound

$$\left\|\prod_{k=0}^{m-1} e^{\frac{t-s}{n}A\left(s+k\frac{t-s}{n}\right)}\right\| \leq \prod_{k=0}^{m-1} e^{\frac{t-s}{n}K_{s,t}} \tag{C.107}$$

$$= e^{(t-s)\frac{m}{n}K_{s,t}}. \tag{C.108}$$

The last factor is bounded using Lemma C.12:

$$\left\|e^{\frac{t-s}{n}A\left(s+m\frac{t-s}{n}\right)} - U\Big(s+(t-s)\frac{m+1}{n}, s+(t-s)\frac{m}{n}\Big)\right\| \leq e^{\frac{t-s}{n}K_{s,t}}\frac{t-s}{n}\omega_A\Big(\frac{t-s}{n}\Big). \tag{C.109}$$

Putting these three bounds together gives

$$\left\|\prod_{k=0}^{n-1} e^{\frac{t-s}{n}A\left(s+k\frac{t-s}{n}\right)} - U(t,s)\right\| \leq \sum_{k=0}^{n-1} e^{\left((t-s)\frac{n-m-1}{n}\right)K_{s,t}} e^{(t-s)\frac{m}{n}K_{s,t}} e^{\frac{t-s}{n}K_{s,t}}\frac{t-s}{n}\omega_A\Big(\frac{t-s}{n}\Big) \tag{C.110}$$

$$= \sum_{k=0}^{n-1} e^{(t-s)K_{s,t}}\frac{t-s}{n}\omega_A\Big(\frac{t-s}{n}\Big) \tag{C.111}$$

$$= (t-s)e^{(t-s)K_{s,t}}\omega_A\Big(\frac{t-s}{n}\Big). \tag{C.112}$$

□

Appendix D

Bochner integration in locally convex topological vector spaces

D.1 Some background on locally convex topological vector spaces

A topological vector space is a vector space that is equipped with a topology. It is locally convex if the neighbourhood filter of the origin has a base of convex sets. This is not a particularly insightful property, but it turns out to equivalent to something much more meaningful:

Proposition D.1. *Let V be a topological vector space. Then the following are equivalent:*

1. *V is locally convex;*
2. *for any $v \in V$ and any net $\langle v_i \rangle_{i \in I}$ the following are equivalent:*
   (a) *$v_i \to v$ in V;*
   (b) *$p(v_i - v) \to 0$ for all continuous seminorms $p : V \to \mathbb{R}^+$.*

We say that the topology of V is generated by its continuous seminorms. It is clear that the implication $(a) \implies (b)$ holds in any topological vector space (this is prcisely what it means for p to be continuous). It is the other implication that is significant: it says that convergence (and, by extension, other topological notions like continuity and closure) can be tested by using seminorms to map the problem to the real numbers.
As an immediate example, any normed space V is locally convex. Since $(a) \implies (b)$ is trivial, we only need to consider the other implication. Since the norm is a continuous seminorm, (b) implies $\|v_i - v\| \to 0$, which, by definition, means that $v_i \to v$ in V.
In general, any space whose topology is generated by some set of seminorms is locally convex. Here are some notable examples

- Let U, W be Banach spaces. Then the strong operator topology on the bounded operators $\mathcal{B}(U, W)$ is generated by the seminorms of pointwise evaluation:

$$\mathcal{B}(U, W) \to \mathbb{R}^+ : L \mapsto \|L(x)\|. \tag{D.1}$$

  This is the topology that was meant whenever "strong continuity" was mentioned.

- If the topology of a topological vector space is generated by its linear functionals, then it is called a weak topology. Any weak topology is locally convex.
- The Schwarz space of rapidly decreasing functions.
- The spaces of (Schwarz) distributions and tempered distributions. The Dirac delta lives in these spaces.

Since "locally convex topological vector space" is quite a mouthful, it is often abbreviated to LCTVS.

D.2 A very rough and opinionated overview of Lebesgue integration

The aim of this section is to give a basic outline of the Lebesgue integral. This should function more to jog the memory and fix notation, than than as an introduction to the subject.
The Lebesgue integral can be constructed by following the following steps:

1. First, start with a way of measuring some sets $A \subseteq \Omega$. This is a function μ that maps some sets to a positive number. For example, the finite intervals $[a,b] \subseteq \mathbb{R}$ can be measured by $\mu([a,b]) = |b-a|$. This way of measuring should be σ-additive: suppose A_n is a measurable set, for all n, such that all distinct A_n, A_m are disjoint and $\bigcup_{n\in\mathbb{N}} A_n$ is measurable, then
$$\mu\Big(\bigcup_{n\in\mathbb{N}} A_n\Big) = \sum_{n\in\mathbb{N}} \mu(A_n). \tag{D.2}$$
Note that the set of measurable sets is not yet supposed closed under countable unions, intersections or complements.
2. Define the elementary integral I. This is a linear function that operates on the space of functions $s : \Omega \to \mathbb{R}^+$ such that
   - the image $\mathrm{im}(s)$ is a finite set;
   - all preimages of s are measurable.

   Such functions s are called (measurable) simple functions and the set of such functions is denoted $\mathrm{SF}(\Omega, \mathbb{R}^+)$. Now I is defined as
$$I(s) = \sum_{s(x)\in\mathrm{im}(s)} s(x) \cdot \mu\big(\{x' \in \Omega \,|\, s(x') = s(x)\}\big). \tag{D.3}$$
3. Consider a seminorm $\int^*$ (the "outer integral") on the space of functions $(\Omega \to \mathbb{R}^+)$ that makes I continuous (the full definition is given at the end of this section).
4. Define the Lebesgue integral to be the closure of $I : (\Omega \to \mathbb{R}^+) \to \mathbb{R}^+$, when $(\Omega \to \mathbb{R}^+)$ is equipped with the topology generated by $\int^*$.

This procedure for constructing the integral is not exactly the usual one. Usually μ (which is called a pre-measure) is extended to all subsets of Ω. This defines an "outer measure" μ^* (its use is analogous to the outer integral). This μ^* is then restricted to the set of "Carathéodory measurable" sets. At this point it is a measure. Now define the integral as

$$\int f \, \mathrm{d}\mu \coloneqq \sup\bigl\{I(s) \bigm| s \in \mathrm{SF}(\Omega, \mathbb{R}^+)\bigr\}. \tag{D.4}$$

Here the simple functions are taken to be measurable w.r.t. the measure, not the original pre-measure.

Now there arises a problem: the integral $\int f \, \mathrm{d}\mu$ defined via this procedure is not necessarily linear! (This is unlike the previous construction, where linearity is manifest). In order to recover linearity, this definition of the integral is restricted to the Borel-measurable functions f.

With this restriction, this classical procedure gives the same integral as the alternative outlined above. It has the disadvantage that the notion of measurability is somewhat unmotivated. (At least it felt that way to me).

Classical real analysis textbooks introduce measurability (of functions between arbitrary measurable spaces) as an important concept per se. I believe this is somewhat misleading. Measurability is necessary to enforce linearity. But, more exactly, *Borel*-meaurability is necessary. This is essentially due to the following result:

Proposition D.2. *Let $(\Omega, \mathcal{A})$ be a measurable space and $f : \Omega \to \mathbb{R}^+$ a function. Then the following are equivalent*

1. *f is Borel-measurable;*
2. *there exists an increasing sequence $\langle s_n \rangle_{n \in \mathbb{N}}$ of measurable simple functions such that $s_n \to f$ pointwise.*

This explains why the Borel-σ-algebra is so important. Much more important that, say, the Lebesgue-σ-algebra, that in some sense is the more natural one to equip the real line with.

The conclusion of the classical construction of the Lebesgue integral has the following conclusion:

Proposition D.3. *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space and $f : \Omega \to \mathbb{R}^+$ a function. Then f is integrable* if and only if *f is measurable and*

$$\sup\bigl\{I(s) \bigm| s \in \mathrm{SF}(\Omega, \mathbb{R}^+)\bigr\} < \infty. \tag{D.5}$$

This equivalence actually breaks in the context of our more general integral on LCTVSs. In this context restricting to Borel-measurable functions is unnecessarily restrictive. This is in some sense the reason why this approach is more general than previous approaches [70, 71] and it bolsters my belief that the way integration (in particular as regards measurability) is often taught is not the best way.

Finally, the definition of the outer integral is given.

Let I be an elementary integral. Then the outer integral is defined as

$$\int^* f \, \mathrm{d}\mu \coloneqq \inf \bigl\{K \in \mathbb{R}^+ \bigm| \exists \text{ increasing } \langle s_n \rangle \text{ in } \mathrm{SF}(\Omega, \mathbb{R}^+) \text{ such that } f = \sup\{f \wedge s_n\} \text{ and } I(s_n) \le K \text{ for all } n \in \mathbb{N}\bigr\}. \tag{D.6}$$

This outer integral for scalar functions will be used extensively in the sequel.

D.3 Bochner integration

In this section Bochner integration for LCTVSs is developed, in the manner outlined above. Many of the results and, indeed, the proofs are classical. Their scope has been considerably expanded.
The integral developed here is more general than previous approaches [70, 71]. An example will be given that shows separation.

D.3.1 The Bochner topology

Let $(\Omega, \mathcal{A}, \mu)$ be a measure space and (V, ξ) be a LCTVS. Let $p : V \to \mathbb{R}^+$ be a continuous finite seminorm and define

$$I_p : (\Omega \to V) \to \overline{\mathbb{R}^+} : f \mapsto \int_\Omega^* p \circ f \,\mathrm{d}\mu. \tag{D.7}$$

We call the seminorm topology on $(\Omega \to V)$ generated by $\{I_p \mid p \in S\}$ the Bochner topology.

Notice that $I_p(f)$ is not necessarily finite, it may also be $+\infty$. We still call $I_p : (\Omega \to V) \to \overline{\mathbb{R}^+}$ a seminorm (i.e. it as absolutely homogenous and subadditive). If we want to impose that a seminorm be finite, we either say it is a finite seminorm, or write $\mathbb{R}^+$ as the codomain.

Lemma D.4. *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space and (V, ξ) be a LCTVS. If S is a set of finite seminorms that generates ξ, then $\{I_p \mid p \in S\}$ generates the Bochner topology.*

Proof. It is enough to prove that the seminorm topology generated by $\{I_p \mid p \in S\}$ makes I_q is continuous for any continuous finite seminorm q on V.
Pick such a seminorm q. Then there exists a finite subset $A \subseteq S$ and $C > 0$ such that $q(v) \leq C \max_{p\in A} p(v)$ for all $v \in V$. This implies, for all $f \in (\Omega \to V)$,

$$I_q(f) = \int_\Omega^* q \circ f \,\mathrm{d}\mu \leq C \int_\Omega^* \sum_{p\in A} p \circ f \,\mathrm{d}\mu \leq C \sum_{p\in A} \int_\Omega^* p \circ f \,\mathrm{d}\mu = \Big(C \sum_{p\in A} I_p\Big)(f). \tag{D.8}$$

Since $C \sum_{p\in A} I_p$ is a continuous seminorm, this implies that I_q is also a continuous seminorm. □

Lemma D.5. *Let (V, ξ) be a locally convex TVS, $A \subseteq V$ a subset and $x \in V$. Then $x \in \mathrm{cl}_\xi(A)$* if and only if *for each continuous seminorm $p : V \to \mathbb{R}^+$ there exists $a \in A$ such that $p(a - x) \leq 1$.*

This result uses choice.

Proof. First suppose $x \in \mathrm{cl}_\xi(A)$. Then there exists a net $\langle x_i \rangle_{i\in I}$ in A such that $x_i \xrightarrow{\xi} x$. For each continuous seminorm, we have $p(x_i - x) \to 0$, so there exists an $i \in I$ such that $p(x_i - x) \leq 1$.
For the converse, fix, for each continuous finite seminorm p some $y_p \in A$ such that $p(y_p - x) \leq 1$. Since the set of continuous finite seminorms is directed, this is a net in A. We claim it converges to x. With Proposition D.1, it is enough to prove that $q(y_p - x) \xrightarrow{p\to\infty} 0$ for all continuous finite seminorms q on V. Fix $\epsilon > 0$. Then, for all $p \geq \epsilon^{-1} q$, we have

$$q(y_p - x) \leq (\epsilon p)(y_p - x) \leq \epsilon. \tag{D.9}$$

We conclude that $y_p \to x$ and so $x \in \mathrm{cl}_\xi(A)$. □

Lemma D.6. *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space and (V, ξ) be a LCTVS. Let $(\Omega \to V)_F$ be the subspace of functions f such that $I_p(f) < \infty$, for all continuous finite seminorms $p : V \to \mathbb{R}^+$. Let $A \subseteq (\Omega \to V)_F$ a subset and $f \in (X \to V)$. Then $f \in \mathrm{cl}_\xi(A)$* if and only if *for each continuous seminorm $p : V \to \mathbb{R}^+$ there exists $a \in A$ such that $\int^*_\Omega p \circ (a - f)\, \mathrm{d}\mu \leq 1$.*

This result uses choice.

Proof. The direction $\Rightarrow$ follows from Lemma D.5.
For the converse, we also aim to use Lemma D.5. Let $t : (\Omega \to V)_F \to \mathbb{R}^+$ be a finite seminorm. Then there exists a finite set $B \subseteq S$ such that

$$t \leq C \max_{q \in S} \int^*_\Omega q \circ (\_)\, \mathrm{d}\mu \leq \int^*_\Omega C \max_{q \in S} q \circ (\_)\, \mathrm{d}\mu. \tag{D.10}$$

Since $C \max_{q\in S} q$ is a continuous finite seminorm on V, there exists $a \in A$ such that $t(a - f) \leq \int^*_\Omega C \max_{q\in S} q \circ (a - f)\, \mathrm{d}\mu \leq 1$. □

D.3.2 Essentially separably-valued functions

Lemma D.7. *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space, (V, ξ) a topological vector space, $f : \Omega \to V$ a Borel-measurable function and $s : \Omega \to V$ a measurable simple function (i.e. a measurable function whose image is a finite set). Then $f + s$ is Borel-measurable.*

Proof. We can write $s = \sum_{k=0}^n a_k \cdot \chi_{A_k}$, where $a_k \in V$ and $\{A_k\}_{k=0}^n$ is a measurable partition of Ω.
Now take arbitrary Borel set $B \subseteq V$ and calculate

$$\begin{aligned}(f + s)^{\text{-}\downarrow}(B) &= \{\omega \in \Omega \mid f(\omega) + s(\omega) \in B\} && \text{(D.11)}\\ &= \bigcup_{k=0}^n \{\omega \in A_k \mid f(\omega) + s(\omega) \in B\} && \text{(D.12)}\\ &= \bigcup_{k=0}^n \{\omega \in A_k \mid f(\omega) + a_k \in B\} && \text{(D.13)}\\ &= \bigcup_{k=0}^n \{\omega \in A_k \mid f(\omega) \in B - a_k\} && \text{(D.14)}\\ &= \bigcup_{k=0}^n A_k \cap f^{\text{-}\downarrow}(B - a_k), && \text{(D.15)}\end{aligned}$$

which is measurable since f, s are Borel-measurable. □

Let $(\Omega, \mathcal{A}, \mu)$ be a measure space, (V, ξ) a LCTVS and $f : \Omega \to V$ a function. Then we call f an essentially separably-valued function if, for all continuous seminorms $p : V \to \mathbb{R}^+$ there exists

- a null set $N_p \subseteq \Omega$; and
- a countable set $C_p \subseteq V$

such that $f^{\downarrow}(N_p^c) \subseteq \mathrm{cl}_p(C_p)$.

Lemma D.8. *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space, $\{X_n\}_{n\in\mathbb{N}}$ a measurable partition on Ω, (V, ξ) a LCTVS and $f : \Omega \to V$ a function. If $f|_{X_n}$ is essentially separably-valued for all $n \in \mathbb{N}$, then f is essentially separably valued.*

Proof. We find $N_{n,p}, C_{n,p}$ for each X_n separately. Then $N_p \coloneqq \bigcup_{n\in\mathbb{N}} N_{n,p}$ is a null set and $C_p \coloneqq \bigcup_{n\in\mathbb{N}} C_{n,p}$ is countable. We also have

$$f^{\downarrow}(N_p^c) = f^{\downarrow}\Big(\bigcup_{n\in\mathbb{N}} X_n \setminus N_{n,p}\Big) \tag{D.16}$$

$$= \bigcup_{n\in\mathbb{N}} f^{\downarrow}(X_n \setminus N_{n,p}) \tag{D.17}$$

$$\subseteq \bigcup_{n\in\mathbb{N}} \mathrm{cl}_p(C_{n,p}) \tag{D.18}$$

$$\subseteq \mathrm{cl}_p\Big(\bigcup_{n\in\mathbb{N}} C_{n,p}\Big) = \mathrm{cl}_p(C_p). \tag{D.19}$$

□

Lemma D.9. *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space, (V, ξ) a LCTVS and $f : \Omega \to V$ a function. If $f^{\downarrow}(\Omega)$ is relatively compact, then f is essentially separably-valued.*

This proof uses countable choice.

Proof. Let $p : V \to \mathbb{R}^+$ be a continuous seminorm and set $U_p \coloneqq p^{\text{-}\downarrow}([0, 1[)$. For all $n \in \mathbb{N}$, the set $\{x + n^{-1}U_p \mid x \in V\}$ is an open cover of V. Due to the relative compactness of $f^{\downarrow}(\Omega)$, there exists a finite subset $F_n \subseteq V$ such that

$$f^{\downarrow}(\Omega) \subseteq \bigcup_{x\in F_n} x + n^{-1}U_p. \tag{D.20}$$

We have that $C_p \coloneqq \bigcup_{n\in\mathbb{N}} F_n$ is countable and we claim that C_p satisfies $f^{\downarrow}(\Omega) \subseteq \mathrm{cl}_p(C_p)$. Take arbitrary $\omega \in \Omega$ and $\epsilon > 0$. Then there exists $n \in \mathbb{N}$ such that $n^{-1} \leq \epsilon$. There exists $x \in F_n$ such that $f(\omega) \in x + n^{-1}U_p$, so $p\big(f(\omega) - x\big) \leq n^{-1} \leq \epsilon$. Thus $f(\omega) \in \mathrm{cl}_p(C_p)$. □

Corollary D.10. *Let (V, ξ) be a LCTVS and $f : \mathbb{R} \to V$ a continuous function. Then f is essentially separably-valued.*

Proof. We partition $\mathbb{R} = \bigcup_{n=0}^{\infty} [-n-1, -n[\cup [n, n+1[$. Then the image of f is relatively compact on each part of the partition, so we can conclude with Lemma D.8. □

D.3.3 The Bochner integral

Let $(\Omega, \mathcal{A}, \mu)$ be a measure space and (V, ξ) a LCTVS. A function $s : \Omega \to V$ is called a simple function if its image is a finite set. It is called an integrable simple function if, in addition, the measure of $s^{\text{-}\downarrow}(V \setminus \{0\})$ is finite.
The set of simple functions is denoted $\mathrm{SF}(\Omega, V)$. The set of integrable simple functions is denoted $\mathrm{SF}_i(\Omega, V)$.

Lemma D.11. *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space, (V, ξ) a LCTVS, $s \in \mathrm{SF}_i(\Omega, V)$ and $p : V \to \mathbb{R}^+$ a seminorm. Then*

$$p\Big(\int_\Omega s \,\mathrm{d}\mu\Big) \leq \int_\Omega p \circ s \,\mathrm{d}\mu. \tag{D.21}$$

Proof. We calculate

$$p\Big(\int_\Omega s \,\mathrm{d}\mu\Big) = p\Big(\sum_{v\in \mathrm{im}(s)\setminus\{0\}} v\cdot \mu\big(s^{\text{-}\downarrow}(v)\big)\Big) \tag{D.22}$$

$$\leq \sum_{v\in \mathrm{im}(s)\setminus\{0\}} p(v)\cdot \mu\big(s^{\text{-}\downarrow}(v)\big) \tag{D.23}$$

$$= \sum_{\lambda\in \mathrm{im}(p\circ s)\setminus\{0\}} \sum_{v\in \mathrm{im}(s)\setminus\{0\}\cap p^{\text{-}\downarrow}(\lambda)} p(v)\cdot \mu(s^{\text{-}\downarrow}(v)) \tag{D.24}$$

$$= \sum_{\lambda\in \mathrm{im}(p\circ s)\setminus\{0\}} \lambda\cdot \mu\Big(\sum_{v\in \mathrm{im}(s)\setminus\{0\}\cap p^{\text{-}\downarrow}(\lambda)} s^{\text{-}\downarrow}(v)\Big) \tag{D.25}$$

$$= \sum_{\lambda\in \mathrm{im}\,\big(p\circ s\big)\setminus\{0\}} \lambda\cdot \mu\big((p\circ s)^{\text{-}\downarrow}(\lambda)\big) \tag{D.26}$$

$$= \int_\Omega p\circ s \,\mathrm{d}\mu. \tag{D.27}$$

□

Lemma D.12. *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space and (V, ξ) a LCTVS. Let $(\Omega \to V)$ be equipped with the Bochner topology. Then*

1. *the elementary integral on $\mathrm{SF}_i(\Omega, V)$ is continuous;*
2. *if V is Hausdorff, then it is closable and the domain of the closure is a subset of $\mathrm{cl}\big(\mathrm{SF}_i(\Omega, V)\big)$;*
3. *if V is complete and Hausdorff, then its domain is $\mathrm{cl}\big(\mathrm{SF}_i(\Omega, V)\big)$.*

The closure $\mathrm{cl}\big(\mathrm{SF}_i(\Omega, V)\big)$ is taken in the Bochner topology.

Proof. (1) Let $\langle s_i\rangle_{i\in I}$ be a net in $\mathrm{SF}_i(\Omega, V)$ that converges to $s \in \mathrm{SF}_i(\Omega, V)$ in the Bochner topology. Take an arbitrary continuous seminorm $p : V \to \mathbb{R}^+$. Then we use Lemma D.11 to calculate

$$p\Big(\int_\Omega s_i \,\mathrm{d}\mu - \int_\Omega s \,\mathrm{d}\mu\Big) = p\Big(\int_\Omega s_i - s \,\mathrm{d}\mu\Big) \leq \int_\Omega p\circ (s_i - s)\,\mathrm{d}\mu. \tag{D.28}$$

The last integral converges to 0 as $i \to \infty$ by definition of the Bochner topology. This implies that $p\Big(\int_\Omega s_i \,\mathrm{d}\mu - \int_\Omega s \,\mathrm{d}\mu\Big) \to 0$ and thus, since p was taken arbitrarily, $\int_\Omega s_i \,\mathrm{d}\mu \to \int_\Omega s \,\mathrm{d}\mu$. We conclude that the elementary integral is continuous.
(2) This is given by Corollary A.35 and Proposition A.36.
(3) This is given by Proposition A.36. □

Let $(\Omega, \mathcal{A}, \mu)$ be a measure space and (V, ξ) a Hausdorff LCTVS. Let $(\Omega \to V)$ be equipped with the Bochner topology. We call the closure of the elementary integral on $\mathrm{SF}_i(\Omega, V)$ the Bochner integral.
Functions in the domain of the Bochner integral are called Bochner integrable functions.
The set of Bochner integrable functions is denoted $\mathcal{L}^1(\Omega, V)$.

This closure is a well-defined linear operator, by Lemma D.12.

Example

Consider the vector space $([0,1] \to \mathbb{R})$ with pointwise convergence. Let μ be the counting measure on $[0,1]$ which is defined on the σ-algebra of all subsets of $[0,1]$. For all $x \in [0,1]$, consider the function

$$\delta_x : [0,1] \to \mathbb{R} : a \mapsto \begin{cases} 1 & (a = x) \\ 0 & (a \neq x). \end{cases} \tag{D.29}$$

Now consider the function

$$f : [0,1] \to ([0,1] \to \mathbb{R}) : x \mapsto \delta_x. \tag{D.30}$$

Let F be the net of finite subsets of $[0,1]$ and set

$$s_A : [0,1] \to ([0,1] \to \mathbb{R}) : x \mapsto \begin{cases} \delta_x & (x \in A) \\ 0 & (x \notin A) \end{cases} \tag{D.31}$$

for all $A \in F$. Then

$$\int_{[0,1]}^{*} |\operatorname{ev}_a| \circ (s_A - f) \,\mathrm{d}\mu = \begin{cases} 0 & (a \in A) \\ 1 & (a \notin A) \end{cases} \tag{D.32}$$

so $s_A \to f$ in the Bochner topology. We also have

$$\int_{[0,1]} s_A \,\mathrm{d}\mu = \chi_A \to \underline{1}, \tag{D.33}$$

so f is Bochner integrable with $\int_0^1 f \,\mathrm{d}\mu = \underline{1}$.
Then f is Bochner integrable according to the definition in [70], but not according to [71]. Now suppose μ is not defined on the σ-algebra of all subsets of $[0,1]$, but rather the countable-cocountable σ-algebra. According to our definition f is still Bochner-integrable, but it is not Bochner-integrable according to the definition of [70], since it is not Borel-measurable: the set $C \coloneqq \{\delta_x \mid x \in [0,1/2]\}$ is closed, but the preimage $f^{\text{-}\downarrow}(C) = [0,1/2]$ is neither countable, nor cocountable.

Lemma D.13. *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space, (V,ξ) a complete Hausdorff LCTVS, $E \in \mathcal{A}$ and $f \in \mathcal{L}^1(\Omega, V)$. Then $f \cdot \chi_E$ is Bochner integrable.*

Proof. From Lemma D.12, there exists a net $\langle s_i \rangle_{i\in I}$ in $\mathrm{SF}_i(\Omega, V)$ that converges to f in the Bochner topology. Now we claim $\langle s_i \cdot \chi_E \rangle$ converges to $f \cdot \chi_E$. Indeed, let $p : V \to \mathbb{R}^+$ be a continuous seminorm. Then

$$\int_{\Omega}^{*} p \circ (s_i \cdot \chi_E - f \cdot \chi_E) \,\mathrm{d}\mu = \int_{\Omega}^{*} \chi_E \cdot \big(p \circ (s_i - f)\big) \,\mathrm{d}\mu \leq \int_{\Omega}^{*} p \circ (s_i - f) \,\mathrm{d}\mu \to 0. \tag{D.34}$$

Since p was taken arbitrarily, we have $f \cdot \chi_E \in \operatorname{cl}\big(\mathrm{SF}_i(\Omega, V)\big)$. Since V is complete, we have that $f \cdot \chi_E$ is Bochner integrable, Lemma D.12. ☐

Let $(\Omega, \mathcal{A}, \mu)$ be a measure space, (V, ξ) a complete Hausdorff LCTVS, $E \in \mathcal{A}$ and

$f \in \mathcal{L}^1(\Omega, V)$. Then we define

$$\int_E f \,\mathrm{d}\mu := \int_\Omega f \cdot \chi_E \,\mathrm{d}\mu. \tag{D.35}$$

Lemma D.14. *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space, (V, ξ) a Hausdorff LCTVS, $p : V \to \mathbb{R}^+$ a continuous seminorm and $f \in \mathcal{L}^1(\Omega, V)$. Then*

$$p\Big(\int_\Omega f \,\mathrm{d}\mu\Big) \leq \int_\Omega^* p \circ f \,\mathrm{d}\mu < \infty. \tag{D.36}$$

Proof. There exists a net $\langle s_i \rangle_{i \in I}$ in $\mathrm{SF}_i(\Omega, V)$ such that $s_i \to f$ in the Bochner topology and $\int_\Omega s_i \,\mathrm{d}\mu \xrightarrow{\xi} \int_\Omega f \,\mathrm{d}\mu$.
Now we calculate

$$p\Big(\int_\Omega f \,\mathrm{d}\mu\Big) = p\Big(\lim_{i\to\infty} \int_\Omega s_i \,\mathrm{d}\mu\Big) \tag{D.37}$$
$$= \lim_{i\to\infty} p\Big(\int_\Omega s_i \,\mathrm{d}\mu\Big) \tag{D.38}$$
$$\leq \lim_{i\to\infty} \int_\Omega p \circ s_i \,\mathrm{d}\mu \tag{D.39}$$
$$= \int_\Omega^* p \circ \big(\lim_{i\to\infty} s_i\big) \,\mathrm{d}\mu = \int_\Omega^* p \circ f \,\mathrm{d}\mu, \tag{D.40}$$

where we have used that p is continuous, Lemma D.11 and the fact that the Bochner topology makes the seminorm $\int_\Omega^* p \circ (\_) \,\mathrm{d}\mu$ continuous.
Finally, the convergence of $s_i \to f$ in the Bochner topology means, in particular, that there exists $i_0 \in I$ such that $\int_\Omega p \circ (f - s_i) \,\mathrm{d}\mu \leq 1$. Now

$$\int_\Omega^* p \circ f \,\mathrm{d}\mu \leq \int_\Omega^* p \circ s_i \,\mathrm{d}\mu + \int_\Omega^* p \circ (f - s_i) \,\mathrm{d}\mu \leq \int_\Omega^* p \circ s_i \,\mathrm{d}\mu + 1 < \infty. \tag{D.41}$$

□

Lemma D.15. *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space, $f : \Omega \to \mathbb{R}$ a function and $\langle f_n : \Omega \to \mathbb{R} \rangle$ a sequence of measurable functions such that $\int_\Omega^* (f - f_n) \,\mathrm{d}\mu \to 0$. Then*

1. *there is a subsequence $\langle f_{n_k} \rangle_{k \in \mathbb{N}}$ that converges a.e. to f;*
2. *f is a.e. equal to a measurable function;*
3. *if $\int_\Omega^* |f| \,\mathrm{d}\mu < \infty$, then it is a.e. equal to an integrable function.*

Lemma D.16. *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space, (V, ξ) a Hausdorff LCTVS, $p : V \to \mathbb{R}^+$ a continuous seminorm and $f : \Omega \to V$ a function. If f is Bochner integrable, then $p \circ f : \Omega \to \mathbb{R}^+$ is a.e. equal to an integrable function.*

Proof. Since f is Bochner integrable, Lemma D.12 implies that, for all $n \in \mathbb{N}$, there exists $s_n \in \mathrm{SF}_i(\Omega, V)$ such that

$$\int_\Omega^* \big|p \circ f - p \circ s_n\big| \,\mathrm{d}\mu \leq \int_\Omega^* p \circ (f - s_n) \,\mathrm{d}\mu \leq n^{-1}. \tag{D.42}$$

The result then follows from Lemma D.15. □

Proposition D.17 (Bochner integrability criterion)**.** *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space, (V, ξ) a Hausdorff LCTVS and $f : \Omega \to V$ a function. Then $f \in \mathrm{cl}\big(\mathrm{SF}_i(\Omega, V)\big)$* if and only if

1. *$p \circ (f - t) : \Omega \to \mathbb{R}^+$ is a.e. equal to an integrable function, for all continuous seminorms $p : V \to \mathbb{R}^+$ and all $t \in \mathrm{SF}_i(\Omega, V)$; and*
2. *f is essentially separably-valued.*

This proof uses choice.
If f is Bochner integrable, then $f \in \mathrm{cl}\big(\mathrm{SF}_i(\Omega, V)\big)$. If V is complete, then the converse also holds, see Lemma D.12.

Proof. First suppose $f \in \mathrm{cl}\big(\mathrm{SF}_i(\Omega, V)\big)$. Pick an arbitrary continuous seminorm $p : V \to \mathbb{R}^+$. Using countable choice, we can pick, for all $n \in \mathbb{N}$, some $s_n \in \mathrm{SF}_i(\Omega, V)$ such that $\int_\Omega^* p \circ (f - s_n) \leq n^{-1}$. Now the reverse triangle inequality gives

$$0 \leq \int_\Omega^* \big|p \circ (f - t) - p \circ (s_n - t)\big| \,\mathrm{d}\mu \leq \int_\Omega^* p \circ (f - s_n) \to 0, \tag{D.43}$$

so Lemma D.15 gives that $p \circ (f - t)$ is a.e. equal to an integrable function.
We now consider essential separability. From point (1), we have that $p \circ (f - s_n)$ is a.e. equal to an integrable function $g_n : \Omega \to \mathbb{R}^+$. Set $A_n \coloneqq \{p \circ (f - s_n) \neq g_n\}$. With Lemma D.15 we have the existence of a subsequence $\langle g_{n_k}\rangle_{k\in\mathbb{N}}$ that converges a.e. to 0. Let A be the null set of points where $\langle g_{n_k}\rangle_{k\in\mathbb{N}}$ does not converge to 0 and set $N_p \coloneqq A \cup \bigcup_{n\in\mathbb{N}} A_n$, which is a null set. For all $\omega \in N_p^c$, we have

$$p\big(f(\omega) - s_{n_k}(\omega)\big) = g_{n_k}(\omega) \overset{k\to\infty}{\longrightarrow} 0, \tag{D.44}$$

so $f(\omega) \in \mathrm{cl}_p\Big(\bigcup_{n\in\mathbb{N}} \mathrm{im}(s_n)\Big)$. Setting $C_p \coloneqq \bigcup_{n\in\mathbb{N}} \mathrm{im}(s_n)$, which is a countable set, shows essential separability.
We now show the converse direction. Let $p : V \to \mathbb{R}^+$ be a continuous seminorm and take $n \in \mathbb{N}$. Let N_p, C_p be the sets witnessing essential separability. Fix some enumeration $\langle c_k\rangle_{k\in\mathbb{N}}$ of C_p. There exists a null set E such that $p \circ f$ is equal to a measurable function on E^c. Set, for all $\delta > 0$,

$$D_\delta \coloneqq E^c \cap (p \circ f)^{-\downarrow}([\delta, +\infty[), \tag{D.45}$$

which is a measurable set with

$$\delta\mu(D_\delta) = \int_\Omega \delta\chi_{D_\delta} \leq \int_\Omega^* p \circ f \,\mathrm{d}\mu < \infty. \tag{D.46}$$

Now, for all $n \in \mathbb{N}$, there exists a null set $E_{\delta,n}$ such that $p\circ(f - c_n \cdot \chi_{D_\delta})$ is equal to a measurable function on $E_{\delta,n}^c$. Recursively define (with $B_{\delta,0} = \emptyset$)

$$\begin{aligned} B_{\delta,n+1} \coloneqq& \big\{\omega \in D_\delta \,\big|\, p\big(f(\omega) - c_{n+1}\big) \leq \delta\big\} \setminus (E_{\delta,n+1} \cup B_n) && \text{(D.47)}\\ =& D_\delta \cap \big(p \circ (f - c_{n+1} \cdot \chi_{D_\delta})\big)^{-\downarrow}([0, \delta]) \setminus (E_{\delta,n+1} \cup B_n), && \text{(D.48)} \end{aligned}$$

which is a disjoint sequence of measurable sets. Now define $u_n \coloneqq \sum_{k=1}^n c_k \cdot \chi_{B_{n^{-1},k}}$. Set $X \coloneqq N_p \cup E \cup \bigcup_{n,k\in\mathbb{N}} E_{n^{-1},k}$, which is a null set. We claim that $p \circ (f - u_n)$ converges pointwise to 0 on X^c. Take arbitrary $\omega \in X^c$ and $n \in \mathbb{N}$. If $(p \circ f)(\omega) < n^{-1}$, then $\omega \in D_{n^{-1}}^c$, so

$$p\big(f(\omega) - u_n(\omega)\big) = (p \circ f)(\omega) \leq n^{-1}. \tag{D.49}$$

Otherwise, we have $(p \circ f)(\omega) \geq n^{-1}$ and so $\omega \in D_{n^{-1}}$. Since $f(\omega) \in \mathrm{cl}_p(C_p)$, there exists $m := \min\{l \in \mathbb{N} \,|\, p(f(\omega) - c_l) \leq n^{-1}\}$. We have $\omega \in B_m$ and so

$$p\big(f(\omega) - u_n(\omega)\big) = p\big(f(\omega) - c_m\big) \leq n^{-1} \leq (p \circ f)(\omega). \tag{D.50}$$

Since $n \in \mathbb{N}$ was taken arbitrarily, we conclude that $p\circ(f-u_n) \to 0$ pointwise (in fact uniformly) on X^c.

We have also shown that $p \circ (f - u_n) \leq p \circ f$ on X^c. We have that $p \circ (f - u_n)$ is equal to an integrable function, except on a null set F_n. Set $Y := X \cup \bigcup_{n\in\mathbb{N}} F_n$, which is a null set. Since $p \circ (f - u_n) \leq p \circ f$ a.e., we can use the scalar dominated convergence theorem to observe that

$$\lim_{n\to\infty} \int_\Omega^* p \circ (f - u_n) \,\mathrm{d}\mu \to 0. \tag{D.51}$$

In particular, for all finite continuous seminorms p, there exists u_{n_0} such that $\int_\Omega^* p\circ(f-u_n) \leq 1$. We conclude with Lemma D.6. ☐

Corollary D.18. *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space, (V, ξ) a complete Hausdorff LCTVS and $f : \Omega \to V$ a function. If f is Borel-measurable, then*

1. *$\int_\Omega^* p \circ f \,\mathrm{d}\mu < \infty$ for all continuous seminorms $p : V \to \mathbb{R}^+$; and*
2. *f is essentially separably-valued;*

imply that f is Bochner integrable.

Proof. Let $p : V \to \mathbb{R}^+$ be a continuous seminorm and $t \in \mathrm{SF}_i(\Omega, V)$. Since p is continuous, it is Borel-measurable. We also have that $(f - t)$ is Borel-measurable, from Lemma D.7. Then $p \circ (f - t)$ is measurable and, with

$$\int_\Omega^* p \circ (f - t) \,\mathrm{d}\mu \leq \int_\Omega^* p \circ f \,\mathrm{d}\mu + \int_\Omega^* p \circ t \,\mathrm{d}\mu < \infty, \tag{D.52}$$

we have that $p \circ (f - t)$ is integrable, Proposition D.3.

Now we have that $f \in \mathrm{cl}\,\big(\mathrm{SF}_i(\Omega, V)\big)$, so we can conclude with Lemma D.12. ☐

Corollary D.19. *Let (V, ξ) be a LCTVS and $f : \mathbb{R} \to V$ a continuous function such that*

$$\int_{-\infty}^{*\,\infty} p \circ f \,\mathrm{d}\mu < \infty. \tag{D.53}$$

Then f is Bochner integrable.

Proof. We have that f is essentially separably-valued from Corollary D.10. ☐

Corollary D.20. *Let $(\Omega, \mathcal{A}, \mu)$ be a finite measure space, (V, ξ) a complete Hausdorff LCTVS and $f : \Omega \to V$ a Borel-measurable function. If $f^{\downarrow}(\Omega)$ is relatively compact, then f is Bochner integrable.*

Proof. We have that f is essentially separable from Lemma D.9.

Let p be a continuous finite seminorm. We then have that $(p \circ f)^{\downarrow}(\Omega)$ is relatively compact and thus also bounded by some $K \in \mathbb{R}^+$. Then

$$\int_\Omega^* p \circ f \,\mathrm{d}\mu \leq K\mu(\Omega) < \infty. \tag{D.54}$$

☐

Corollary D.21. *Let (X, ξ) be a compact convergence space equipped with a finite Borel measure μ, (V, ξ) a complete Hausdorff LCTVS and $f : \Omega \to V$ a continuous function. Then f is Bochner integrable.*

In particular, this applies when $X = [a, b] \subseteq \mathbb{R}$, since the Lebesgue measure is a Borel measure.

Proof. Since f continuous, it is clearly Borel-measurable and $f^{\downarrow}(X)$ is compact because X is compact. □

Theorem D.22 (Dominated convergence for Bochner integrals)**.** *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space, (V, ξ) a complete Hausdorff LCTVS generated by a set S of seminorms and $\langle f_n \rangle$ a sequence of Bochner integrable functions that converges pointwise to a function f.*
If, for all $p \in S$, there exists a positive integrable function $g_p : \Omega \to \mathbb{R}^+$ such that $p \circ f_n \leq g$ a.e. for all $n \in \mathbb{N}$, then f is Bochner integrable and

$$\lim_{n\to\infty} \int_\Omega f_n \,\mathrm{d}\mu = \int_\Omega f \,\mathrm{d}\mu. \tag{D.55}$$

Proof. For all $n \in \mathbb{N}$, Lemma D.16 implies that $p \circ f_n$ is a.e. equal to a Borel-measurable function. Let A_n be a null set such that $p \circ f_n$ is equal to the Borel-measurable function for all $x \in A_n^c$. Set $A \coloneqq \bigcup_{n\in\mathbb{N}} A_n$, which is also a null set. Let f_n' be equal to f_n on A^c and equal to 0 on A. Similarly set f' equal to f on A^c and equal to 0 on A.
Take arbitrary $p \in S$. Since p is continuous, we have that $p \circ f_n' \to p \circ f'$ pointwise, so $p \circ f'$ is also measurable.
Now $p \circ (f' - f_n') \leq p \circ f' + p \circ f_n' \leq 2g_p$ a.e., so the scalar dominated convergence theorem gives that $p \circ f'$ is integrable and that

$$\lim_{n\to\infty} \int_\Omega^* p \circ (f - f_n') = \lim_{n\to\infty} \int_\Omega p \circ (f' - f_n') \,\mathrm{d}\mu = 0. \tag{D.56}$$

Together with Lemma D.4 this implies that $f_n' \to f$ in the Bochner topology. Now Lemma D.12 gives that f is Bochner integrable.
Finally we have

$$p\Big(\int_\Omega f \,\mathrm{d}\mu - \int_\Omega f_n \,\mathrm{d}\mu\Big) = p\Big(\int_\Omega (f - f_n) \,\mathrm{d}\mu\Big) \leq \int_\Omega^* p \circ (f - f_n) \,\mathrm{d}\mu \to 0, \tag{D.57}$$

from Lemma D.14, so $\int_\Omega f_n \,\mathrm{d}\mu \xrightarrow{\xi} \int_\Omega f \,\mathrm{d}\mu$. □

Proposition D.23. *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space, V, W Hausdorff LCTVSs, $T \in \mathcal{B}(V, W)$ and $f \in \mathcal{L}^1(\Omega, V)$. Then $T \circ f$ is Bochner integrable and*

$$\int_\Omega (T \circ f) \,\mathrm{d}\mu = T\Big(\int_\Omega f \,\mathrm{d}\mu\Big). \tag{D.58}$$

Proof. There exists a net $\langle s_i \rangle_{i\in I}$ in $\mathrm{SF}_i(\Omega, V)$ such that $s_i \to f$ in the Bochner topology and $\int_\Omega s_i \,\mathrm{d}\mu \xrightarrow{\xi} \int_\Omega f \,\mathrm{d}\mu$.
The net $\langle T \circ s_i \rangle_{i\in I}$ is a net in $\mathrm{SF}_i(\Omega, W)$. Let $p : W \to \mathbb{R}^+$ be a continuous seminorm. Then

$$\int_\Omega^* p \circ \big(T \circ s_i - T \circ f\big) \,\mathrm{d}\mu = \int_\Omega^* p \circ T \circ (s_i - f) \,\mathrm{d}\mu \to 0, \tag{D.59}$$

since $p \circ T$ is a continuous seminorm on V and $s_i \to f$ in the Bochner topology. This means that $T \circ s_i \to T \circ f$ in the Bochner topology. We also have

$$\int_\Omega T \circ s_i \,\mathrm{d}\mu = \sum_{T(v)\in \mathrm{im}(T\circ s_i)\setminus\{0\}} T(v)\cdot \mu\big((T\circ s_i)^{\text{-}\downarrow}(Tv)\big) \tag{D.60}$$

$$= \sum_{v\in \mathrm{im}(s_i)\setminus\{0\}} T(v)\cdot \mu\big(s_i^{\text{-}\downarrow}(v)\big) \tag{D.61}$$

$$= T\Big(\sum_{v\in \mathrm{im}(s_i)\setminus\{0\}} v\cdot \mu\big(s_i^{\text{-}\downarrow}(v)\big)\Big) \tag{D.62}$$

$$= T\Big(\int_\Omega s_i \,\mathrm{d}\mu\Big) \to T\Big(\int_\Omega f \,\mathrm{d}\mu\Big) \tag{D.63}$$

from the continuity of T. We conclude that $T \circ f$ is Bochner integrable. □

Corollary D.24. *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space, X a Banach space and $T : \Omega \to \mathcal{B}(X)$ be a function. If T is integrable, then for all $x \in X$, Tx is integrable and*

$$\Big(\int_\Omega T \,\mathrm{d}\mu\Big) x = \int_\Omega Tx \,\mathrm{d}\mu. \tag{D.64}$$

Proof. The evaluation map ev_x is linear and bounded by $\|x\|$ for all $x \in X$. □

Lemma D.25. *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space, (V, ξ) a Hausdorff LCTVS, $f \in \mathcal{L}^1(\Omega, V)$, $p : V \to \mathbb{R}^+$ a continuous seminorm and $\epsilon > 0$. Then there exists $s \in \mathrm{SF}_i(\Omega, V)$ and $A \in \mathcal{A}$ such that*

- *$\mu(A) \le \epsilon$;*
- *$p\big(f(\omega) - s(\omega)\big) \le \epsilon$ for all $\omega \in A^c$; and*
- *$\int^*_\Omega p \circ |s| \,\mathrm{d}\mu \le \int^*_\Omega p \circ |f| \,\mathrm{d}\mu + \epsilon^2$.*

Proof. From Lemma D.12, we have the existence of $s \in \mathrm{SF}_i(\Omega, V)$ such that

$$\int^*_\Omega p \circ |f - s| \,\mathrm{d}\mu \le \epsilon^2. \tag{D.65}$$

From Lemma D.16, we have that $p \circ |f - s|$ is equal to a measurable function $g : \mathbb{R} \to \mathbb{R}^+$, except on a null set A_0.
Now set $A \coloneqq \{g > \epsilon\} \cup A_0$ and calculate

$$\epsilon\mu(A) = \epsilon \int_\Omega [g > \epsilon] \vee \chi_{A_0} \,\mathrm{d}\mu \tag{D.66}$$

$$\le \int_\Omega g \cdot \big([g > \epsilon] \vee \chi_{A_0}\big) \,\mathrm{d}\mu \tag{D.67}$$

$$\le \int_\Omega g \cdot \big([g > \epsilon] \vee \chi_{A_0}\big) \,\mathrm{d}\mu + \int_\Omega g \cdot \big([g \le \epsilon] \wedge \chi_{A_0}\big) \,\mathrm{d}\mu \tag{D.68}$$

$$= \int_\Omega g \,\mathrm{d}\mu \tag{D.69}$$

$$= \int^*_\Omega p \circ |f - s| \,\mathrm{d}\mu \le \epsilon^2. \tag{D.70}$$

This implies $\mu(A) \leq \epsilon$.
Next, take $\omega \in A^c = \{g \leq \epsilon\} \cap A_0$, so $p\big(f(\omega) - s(\omega)\big) = g(\omega) \leq \epsilon$.
Finally, we have

$$\int_\Omega^* p \circ |s| \,\mathrm{d}\mu \leq \int_\Omega^* p \circ |f| \,\mathrm{d}\mu + \int_\Omega^* p \circ |f - s| \,\mathrm{d}\mu \leq \int_\Omega^* p \circ |f| \,\mathrm{d}\mu + \epsilon^2. \tag{D.71}$$

□

Lemma D.26. *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space and $f : \Omega \to \mathbb{R}$ an integrable function. Then*

$$\forall \epsilon > 0 : \exists \delta > 0 : \forall E \in \mathcal{A} : \quad \mu(E) \leq \delta \implies \int_E f \,\mathrm{d}\mu \leq \epsilon. \tag{D.72}$$

Theorem D.27 (Hille's theorem)**.** *Let $(\Omega, \mathcal{A}, \mu)$ be a finite measure space, V, W Hausdorff LCTVSs, $T : V \not\to W$ a closed operator and $f : \Omega \to V$ a function such that $\operatorname{im}(f) \subseteq \operatorname{dom}(T)$. If both f and $T \circ f$ are Bochner integrable, then $\int_\Omega f \,\mathrm{d}\mu \in \operatorname{dom}(T)$ and*

$$\int_\Omega (T \circ f) \,\mathrm{d}\mu = T\Big(\int_\Omega f \,\mathrm{d}\mu\Big). \tag{D.73}$$

As stated the theorem is only applicable to finite measure spaces. It should be straightforward to extend, at least to σ-finite measure spaces.

Proof. Let $p : V \to \mathbb{R}^+$ be an arbitrary continuous seminorm. Take $n \in \mathbb{N}$ and use Lemma D.25 to find $s_n, t_n \in \mathrm{SF}_i(\Omega, V)$ and $S_n, T_n \in \mathcal{A}$ such that

$$p\big(f(\omega) - s_n(\omega)\big) \leq (2n)^{-1} \qquad \text{for all } \omega \in S_n^c, \tag{D.74}$$

with $\mu(S_n) \leq (2n)^{-1}$, and

$$p\big((T \circ f)(\omega) - t_n(\omega)\big) \leq (2n)^{-1} \qquad \text{for all } \omega \in T_n^c, \tag{D.75}$$

with $\mu(T_n) \leq (2n)^{-1}$. Set

$$D_n \coloneqq \Big\{(v, w) \in V \times W \,\Big|\, \Big(s_n^{-\downarrow}(\{v\}) \cap S_n^c \cap t_n^{-\downarrow}(\{w\}) \cap T_n^c \neq \emptyset\Big) \wedge \big((v, w) \neq (0, 0)\big)\Big\} \tag{D.76}$$

and pick some

$$\omega_{v,w} \in s_n^{-\downarrow}(\{v\}) \cap t_n^{-\downarrow}(\{w\}) \cap S_n^c \cap T_n^c \tag{D.77}$$

for all $(v, w) \in D_n$. Now define

$$u_n \coloneqq \sum_{(v,w) \in D_n} f(\omega_{v,w}) \cdot \chi_{s_n^{-\downarrow}(\{v\}) \cap t_n^{-\downarrow}(\{w\}) \cap S_n^c \cap T_n^c}. \tag{D.78}$$

Now take arbitrary $\omega \in S_n^c \cap T_n^c$. If $s_n(\omega) = 0 = t_n(\omega)$, then

$$p\big(f(\omega) - u_n(\omega)\big) = p\big(f(\omega)\big) = p\big(f(\omega) - s_n(\omega)\big) \leq (2n)^{-1} \leq n^{-1} \tag{D.79}$$

and

$$p\big((T \circ f)(\omega) - u_n(\omega)\big) = p\big((T \circ f)(\omega)\big) = p\big((T \circ f)(\omega) - t_n(\omega)\big) \leq (2n)^{-1} \leq n^{-1} \tag{D.80}$$

Otherwise, $\big(s_n(\omega), t_n(\omega)\big) \in D_n$ and $s_n(\omega_{(s_n(\omega),t_n(\omega))}) = s_n(\omega)$, so

$$\begin{aligned} p\big(f(\omega) - u_n(\omega)\big) &= p\big(f(\omega) - f(\omega_{(s_n(\omega),t_n(\omega))})\big) && \text{(D.81)} \\ &\leq p\big(f(\omega) - s_n(\omega)\big) + p\big(s_n(\omega) - f(\omega_{(s_n(\omega),t_n(\omega))})\big) && \text{(D.82)} \\ &\leq p\big(f(\omega) - s_n(\omega)\big) + p\big(s_n(\omega_{(s_n(\omega),t_n(\omega))}) - f(\omega_{(s_n(\omega),t_n(\omega))})\big) && \text{(D.83)} \\ &\leq 2(2n)^{-1} = n^{-1}. && \text{(D.84)} \end{aligned}$$

Similarly, $t_n(\omega_{(s_n(\omega),t_n(\omega))}) = t_n(\omega)$, so

$$\begin{aligned} p\big((T\circ f)(\omega) - (T\circ u_n)(\omega)\big) &= p\big((T\circ f)(\omega) - (T\circ f)(\omega_{(s_n(\omega),t_n(\omega))})\big) && \text{(D.85)} \\ &\leq p\big((T\circ f)(\omega) - t_n(\omega)\big) + p\big(t_n(\omega) - (T\circ f)(\omega_{(s_n(\omega),t_n(\omega))})\big) && \text{(D.86)} \\ &\leq p\big((T\circ f)(\omega) - t_n(\omega)\big) + p\big(t_n(\omega_{(s_n(\omega),t_n(\omega))}) - (T\circ f)(\omega_{(s_n(\omega),t_n(\omega))})\big) && \text{(D.87)} \\ &\leq 2(2n)^{-1} = n^{-1}. && \text{(D.88)} \end{aligned}$$

Next we calculate, with Lemma D.14, that

$$\begin{aligned} p\Big(\int_\Omega f\,\mathrm{d}\mu - \int_\Omega u_n\,\mathrm{d}\mu\Big) &\leq \int_\Omega^* p\circ(f-u_n)\,\mathrm{d}\mu && \text{(D.89)} \\ &\leq \int_\Omega^* p\circ\big((f-u_n)\cdot\chi_{S_n\cup T_n} + (f-u_n)\cdot\chi_{S_n^c\cap T_n^c}\big)\,\mathrm{d}\mu && \text{(D.90)} \\ &\leq \int_\Omega^* p\circ\big((f-u_n)\cdot\chi_{S_n\cup T_n}\big)\,\mathrm{d}\mu + \int_\Omega^* p\circ\big((f-u_n)\cdot\chi_{S_n^c\cap T_n^c}\big)\,\mathrm{d}\mu && \text{(D.91)} \\ &= \int_\Omega^* (p\circ f)\cdot\chi_{S_n\cup T_n}\,\mathrm{d}\mu + \int_\Omega^* \big(p\circ(f-u_n)\big)\cdot\chi_{S_n^c\cap T_n^c}\,\mathrm{d}\mu && \text{(D.92)} \\ &\leq \int_\Omega^* (p\circ f)\cdot\chi_{S_n\cup T_n}\,\mathrm{d}\mu + n^{-1}\mu(\Omega). && \text{(D.93)} \end{aligned}$$

Since $p\circ f$ is equal a.e. to an integrable function $g : \Omega \to \mathbb{R}^+$, Lemma D.16, we have

$$p\Big(\int_\Omega f\,\mathrm{d}\mu - \int_\Omega u_n\,\mathrm{d}\mu\Big) \leq \int_\Omega^* (p\circ f)\cdot\chi_{S_n\cup T_n}\,\mathrm{d}\mu + n^{-1}\mu(\Omega) = \int_\Omega^* g\cdot\chi_{S_n\cup T_n}\,\mathrm{d}\mu + n^{-1}\mu(\Omega) \xrightarrow{n\to\infty} 0, \tag{D.94}$$

from Lemma D.26. This implies that $\int_\Omega u_n\,\mathrm{d}\mu \to \int_\Omega f\,\mathrm{d}\mu$.

Similarly, $p\circ T\circ f$ is equal a.e. to an integrable function $g':\Omega\to\mathbb{R}^+$. We calculate

$$\begin{aligned}
p\Big(\int_\Omega T\circ f\,\mathrm{d}\mu-\int_\Omega T\circ u_n\,\mathrm{d}\mu\Big) &\leq \int_\Omega^* p\circ(T\circ f-T\circ u_n)\,\mathrm{d}\mu && \text{(D.95)}\\
&\leq \int_\Omega^* p\circ\big((T\circ f-T\circ u_n)\cdot\chi_{S_n\cup T_n}\big)\,\mathrm{d}\mu+\int_\Omega^* p\circ\big((T\circ f-T\circ u_n)\cdot\chi_{S_n^c\cap T_n^c}\big)\,\mathrm{d}\mu && \text{(D.96)}\\
&= \int_\Omega^* (p\circ T\circ f)\cdot\chi_{S_n\cup T_n}\,\mathrm{d}\mu+\int_\Omega^* \big(p\circ(T\circ f-T\circ u_n)\big)\cdot\chi_{S_n^c\cap T_n^c}\,\mathrm{d}\mu && \text{(D.97)}\\
&\leq \int_\Omega^* (p\circ T\circ f)\cdot\chi_{S_n\cup T_n}\,\mathrm{d}\mu+n^{-1}\mu(\Omega) && \text{(D.98)}\\
&= \int_\Omega^* g'\cdot\chi_{S_n\cup T_n}\,\mathrm{d}\mu+n^{-1}\mu(\Omega)\overset{n\to\infty}{\longrightarrow}0, && \text{(D.99)}
\end{aligned}$$

so $T\Big(\int_\Omega u_n\,\mathrm{d}\mu\Big)=\int_\Omega T\circ u_n\,\mathrm{d}\mu\to\int_\Omega T\circ f\,\mathrm{d}\mu$.

Since T is closed, we conclude that $\int_\Omega f\,\mathrm{d}\mu\in\mathrm{dom}(T)$ and $\int_\Omega(T\circ f)\,\mathrm{d}\mu=T\Big(\int_\Omega f\,\mathrm{d}\mu\Big)$. □

D.3.4 The fundamental theorems of calculus

Proposition D.28. *Let (V,ξ) be a Hausdorff LCTVS, $a<b\in\mathbb{R}$ and $f:\,]a,b[\,\to V$ a differentiable function. If $f'=\underline{0}$, then there exists $v\in V$ such that $f=\underline{v}$.*

Proof. Let $\omega:V\to\mathbb{C}$ be some continuous linear functional and $x\in\,]a,b[$.
Then, using the mean value theorem there exists $c\in\,]a,x[$ such that

$$\omega\big(f(x)-f(a)\big)=(x-a)\big(\omega\circ f\big)'(c)=(x-a)\omega\big(f'(c)\big)=0. \tag{D.100}$$

Since this holds for all continuous linear functionals ω, we have $f(x)-f(a)=0$ from Proposition A.54. Since this holds for all $x\in\,]a,b[$, the result follows. □

Corollary D.29. *Let (V,ξ) be a Hausdorff LCTVS, $a<b\in\mathbb{R}$ and $f,g:\,]a,b[\,\to V$ differentiable functions. If $f'=g'$, then there exists $v\in V$ such that $f=g+\underline{v}$.*

Proof. Apply the proposition to $f-g$. □

Proposition D.30. *Let (V,ξ) be a complete Hausdorff LCTVS, $a,b\in[-\infty,+\infty]$ and $f:[a,b]\to V$ be a Bochner integrable function. Then the function*

$$F:[a,b]\to\mathbb{R}^+:x\mapsto\int_a^x f(t)\,\mathrm{d}t \tag{D.101}$$

is continuous.

Here f is not assumed continuous.

Proof. Let $\langle x_n\rangle_{n\in\mathbb{N}}$ be a sequence in $[a,b]$ that converges to $x\in[a,b]$. Then $f\cdot\chi_{[a,x_n]}$ is a sequence of integrable functions, Lemma D.13, that converges pointwise to $f\cdot\chi_{[a,x]}$. For all continuous seminorms $p : V \to \mathbb{R}^+$, we have $p \circ (f \cdot \chi_{[a,x]}) \leq p \circ f$, which is equal a.e. to an integrable function, Proposition D.17. Now dominated convergence, Theorem D.22, gives

$$\lim_{n\to\infty} F(x_n) = \lim_{n\to\infty} \int_a^{x_n} f \,\mathrm{d}t = \lim_{n\to\infty} \int_a^b f \cdot \chi_{[a,x_n]} \,\mathrm{d}t = \int_a^b f \cdot \chi_{[a,x]} \,\mathrm{d}t = \int_a^x f \,\mathrm{d}t = F(x), \tag{D.102}$$

which implies the continuity of F. □

Theorem D.31 (First fundamental theorem of calculus)**.** *Let (V, ξ) be a complete Hausdorff LCTVS, $a \in \mathbb{R}, b \in \mathbb{R} \cup \{\infty\}$ and $f : [a, b] \to V$ be a continuous function. Set*

$$F : [a, b] \to V : x \mapsto \int_a^x f(t) \,\mathrm{d}t. \tag{D.103}$$

Then F is differentiable on $[a, b]$ with $F'(x) = f(x)$ for all $x \in [a, b]$.

Note that F is well-defined due to Corollary D.21. The derivative at the endpoints is defined as a one-sided limit.

Proof. For any $x, h \in \mathbb{R}$ such that $x, x + h \in [a, b]$, we have

$$F(x + h) - F(x) = \int_a^{x+h} f(t) \,\mathrm{d}t - \int_a^x f(t) \,\mathrm{d}t = \int_x^{x+h} f(t) \,\mathrm{d}t. \tag{D.104}$$

Then

$$\frac{F(x + h) - F(x)}{h} - f(x) = \frac{1}{h} \int_x^{x+h} f(t) \,\mathrm{d}t - \frac{1}{h} \int_x^{x+h} \underline{f(x)} \,\mathrm{d}t = \frac{1}{h} \int_x^{x+h} \big(f - \underline{f(x)}\big) \,\mathrm{d}t. \tag{D.105}$$

Let $p : V \to \mathbb{R}^+$ be a continuous seminorm. Then Lemma D.14 gives

$$p\Big(\frac{F(x + h) - F(x)}{h} - f(x)\Big) \leq \frac{1}{|h|} \int_x^{x+h} p\big(f(t) - f(x)\big) \,\mathrm{d}x \leq \max_{t\in[x,x+h]} p\big(f(t) - f(x)\big). \tag{D.106}$$

We claim that this converges to 0 as $h \to 0$. Indeed, fix $\epsilon > 0$. Then continuity of p, f implies the existence of some $\delta > 0$ such that $p\big(f(t) - f(x)\big) \leq \epsilon$ for all t such that $|x - t| \leq \delta$. In particular, $\max_{t\in[x,x+h]} p\big(f(t) - f(x)\big) \leq \epsilon$ if $|h| \leq \delta$, which proves the claim.
Since the continuous seminorm p was taken arbitrarily, we conclude $F'(x) = f(x)$. □

Corollary D.32 (Weak second fundamental theorem of calculus)**.** *Let (V, ξ) be a complete Hausdorff LCTVS, $a, b \in \mathbb{R}$ and $f : [a, b] \to V$ be a differentiable function such that $f' : [a, b] \to V$ is continuous. Then, for all $x \in [a, b]$,*

$$f(x) = f(a) + \int_a^x f'(t) \,\mathrm{d}t. \tag{D.107}$$

In particular $\int_a^b f'(t) \,\mathrm{d}t = f(b) - f(a)$.

This result is said to be weak because it makes the a priori (strong) assumption that f' is continuous.

Proof. The function f' is integrable by Corollary D.21. Set $g : [a, b] \to \mathbb{R} : x \mapsto \int_a^x f'(t) \,\mathrm{d}t$, which is differentiable by the first fundamental theorem and $g' = f'$ for all $x \in \,]a, b[$.
We can now apply Corollary D.29 to obtain $f(x) = v + \int_a^x f'(t) \,\mathrm{d}t$. Extend by continuity to the closed interval and evaluate at a to get the result. □

D.3.4.1 Integration by parts

Proposition D.33 (Integration by parts)**.** *Let U, V, W be topological vector spaces, with W complete Hausdorff and locally convex, $B : U \oplus V \to W$ a continuous bilinear function, $a < b \in \mathbb{R}$, and $f : [a, b] \to U$, $g : [a, b] \to V$ continuously differentiable functions. Then*

$$\int_a^b B\big(f'(t), g(t)\big)\,\mathrm{d}t = B\big(f(b), g(b)\big) - B\big(f(a), g(a)\big) - \int_a^b B\big(f(t), g'(t)\big)\,\mathrm{d}t. \tag{D.108}$$

In particular, these integrals are well-defined, Corollary D.21.

Proof. The Leibniz rule gives

$$B(f, g)' = B(f', g) + B(f, g'), \tag{D.109}$$

which is a continuous function. We can then use the second fundamental theorem of calculus, Corollary D.32, to get

$$B\big(f(x), g(x)\big) = B\big(f(a), g(a)\big) + \int_a^x B\big(f(t), g(t)\big)'\,\mathrm{d}t \tag{D.110}$$

$$= B\big(f(a), g(a)\big) + \int_a^x B\big(f'(t), g(t)\big)\,\mathrm{d}t + \int_a^x B\big(f(t), g'(t)\big)\,\mathrm{d}t \tag{D.111}$$

for all $x \in [a, b]$. Setting $x = b$ and rearranging gives the result. □

The crux of the proof of integration by parts is the applicability of the second fundamental theorem of calculus:

$$B\big(f(x), g(x)\big) = B\big(f(a), g(a)\big) + \int_a^x B\big(f(t), g(t)\big)'\,\mathrm{d}t. \tag{D.112}$$

The continuity of the derivative of f and g is sufficient give this conclusion, but far from necessary. For example, piecewise continuity is clearly also sufficient. If f, g are complex-valued and B is the usual product, then the obvious hypothesis is that f, g be absolutely continuous. In the vector-valued case, the question is more subtle and typically involves a discussion of the Radon-Nikodym property.
The following is probably far from an optimal result, but is useful in the context of this thesis.

Proposition D.34. *Let V be a Banach space, $a < b \in \mathbb{R}$, and $g : [a, b] \to V$ a continuously differentiable function. Suppose $f : [a, b] \to \mathbb{C}$ is absolutely continuous. Then*

$$f(x)g(x) = f(a)g(a) + \int_a^x \big(f'(t)g(t) + f(t)g'(t)\big)\,\mathrm{d}t \tag{D.113}$$

for all $x \in [a, b]$.

Of course the derivative f' is only defined a.e. This proof is essentially the usual proof that for any absolutely continuous f, $f' = 0$ a.e. implies that f is constant, but adapted to this special case with a vector-valued function. Compare, e.g., with theorem 4.5.4 in [72].

Proof. With Lemma D.35 and Theorem D.31, we see that

$$0 = \frac{\mathrm{d}}{\mathrm{d}x}\left(f(x)g(x) - \int_a^x \big(f'(t)g(t) + f(t)g'(t)\big)\,\mathrm{d}t\right) \tag{D.114}$$

holds almost everywhere. Let the set on which it holds be called A. Pick arbitrary $c \in [a, b]$ and $\epsilon > 0$. Since f is absolutely continuous, there exists $\delta_0 > 0$ such that for any finite set $\{]a_k, b_k[\}_{k=0}^N$ of disjoint subintervals of $[a, c]$, such that $\sum_{k=0}^N (b_k - a_k) \leq \delta_0$, the following holds:

$$\sum_{k=0}^{N} |f(b_k) - f(a_k)| \leq \frac{\epsilon}{4 \max_{t\in[a,c]} \|g(t)\|}. \tag{D.115}$$

The function

$$h : [a, c] \to \mathbb{R} : x \mapsto \int_a^x \|f'(t)g(t) + f(t)g'(t)\| \,\mathrm{d}t, \tag{D.116}$$

so there exists $\delta_1 > 0$ such that for any finite set $\{]a_k, b_k[\}_{k=0}^N$ of disjoint subintervals of $[a, c]$, such that $\sum_{k=0}^N (b_k - a_k) \leq \delta_1$, the following holds:

$$\sum_{k=0}^{N} |h(b_k) - h(a_k)| \leq \frac{\epsilon}{4}. \tag{D.117}$$

For all $x \in A$, there exists y_x such that

$$\left\| f(y)g(y) - f(x)g(x) - \int_x^y \big(f'(t)g(t) + f(t)g'(t)\big) \,\mathrm{d}t \right\| \leq \frac{\epsilon(y - x)}{2(c - a)} \tag{D.118}$$

for all $y \in [x, y_x]$. The set of all intervals $[x, y]$ with $y \in [x, y_x]$, forms a Vitali covering of $[a, c]$. Due to the Vitali covering lemma, a finite subset of disjoint intervals can be found that covers B up to a set of measure less than

$$\leq \min \left\{ \delta_0, \delta_1, \epsilon 4^{-1} \big(\max_{t\in[a,c]} \|g'(t)\| \big)^{-1} \big(\max_{t\in[a,c]} |f(t)| \big)^{-1} \right\}. \tag{D.119}$$

Denote this set $\{[x_k, y_k]\}_{k=1}^N$, ordered such that $y_k \leq x_{k+1}$. Set $y_0 = a$ and $x_{N+1} = c$. Then the following difference can be expressed as a telescoping sum:

$$f(c)g(c) - f(a)g(a) - \int_a^c \big(f'(t)g(t) + f(t)g'(t)\big) \,\mathrm{d}t \tag{D.120}$$

$$= \sum_{k=0}^{N} f(x_{k+1})g(x_{k+1}) - f(y_k)g(y_k) - \int_{y_k}^{x_{k+1}} \big(f'(t)g(t) + f(t)g'(t)\big) \,\mathrm{d}t \tag{D.121}$$

$$+ \sum_{k=1}^{N} f(y_k)g(y_k) - f(x_k)g(x_k) - \int_{x_k}^{y_k} \big(f'(t)g(t) + f(t)g'(t)\big) \,\mathrm{d}t. \tag{D.122}$$

The aim is now to bound the norm. The first term in the top sum (D.121) can be further expanded as follows:

$$\sum_{k=0}^{N} \|f(x_{k+1})g(x_{k+1}) - f(y_k)g(y_k)\| \tag{D.123}$$

$$\leq \sum_{k=0}^{N} \|f(x_{k+1})g(x_{k+1}) - f(y_k)g(x_{k+1})\| + \|f(y_k)g(x_{k+1}) - f(y_k)g(y_k)\| \tag{D.124}$$

$$\leq \sum_{k=0}^{N} |f(x_{k+1}) - f(y_k)| \max_{t\in[a,c]} \|g(t)\| + \sum_{k=0}^{N} \left\| \int_{y_k}^{x_{k+1}} g'(t) \,\mathrm{d}t \right\| \max_{t\in[a,c]} |f(t)|. \tag{D.125}$$

The first term of (D.125) is bounded by $\frac{\epsilon}{4}$ due to the absolute continuity of f. The second is bounded by

$$\sum_{k=0}^{N}\int_{y_k}^{x_{k+1}}\|g'(t)\|\,\mathrm{d}t\max_{t\in[a,c]}|f(t)| \leq \sum_{k=0}^{N}(x_{k+1}-y_k)\max_{t\in[a,c]}\|g'(t)\|\max_{t\in[a,c]}|f(t)| \leq \frac{\epsilon}{4}. \tag{D.126}$$

We consider the sum (D.121). With (D.118) this is bounded by $\frac{\epsilon}{2}$. Putting all these bounds together, the norm of (D.120) is bounded by ϵ. Since this holds for all $\epsilon > 0$. This norm must be zero, which gives the result. □

Lemma D.35. *Let V be a Banach space, $a < b \in \mathbb{R}$, and $g : [a,b] \to V$ a continuously differentiable function. Suppose $f : [a,b] \to \mathbb{C}$ is absolutely continuous. Then*

$$f'g = \frac{\mathrm{d}}{\mathrm{d}x}\int_a^x f'g\,\mathrm{d}t \tag{D.127}$$

almost everywhere.

Proof. Since f' is Lebesgue integrable, it is to too hard to see that $f'g$ is integrable. Take $x \in [a,b]$. Then

$$\lim_{h\to 0}\Big\|f'(x)g(x) - \frac{1}{h}\int_x^{x+h} f'(t)g(t)\,\mathrm{d}t\Big\| \tag{D.128}$$

$$= \lim_{h\to 0}\Big\|\frac{1}{h}\int_x^{x+h}\big(f'(x)g(x) - f'(t)g(t)\big)\,\mathrm{d}t\Big\|$$

$$\leq \lim_{h\to 0}\frac{1}{h}\int_x^{x+h}\Big(\big\|f'(x)g(x) - f'(x)g(t)\big\| + \big\|f'(x)g(t) - f'(t)g(t)\big\|\Big)\,\mathrm{d}t \tag{D.129}$$

$$\leq \lim_{h\to 0}\Big(|f'(x)|\max_{t\in[x,x+h]}\big\|g(x)-g(t)\big\| + \max_{t\in[a,b]}\|g(t)\|\frac{1}{h}\int_x^{x+h}|f'(x)-f'(t)|\,\mathrm{d}t\Big), \tag{D.130}$$

which converges to 0 almost everywhere due to the continuity of g and the Lebesgue differentiation theorem. □

D.3.4.2 Variation of parameters

Proposition D.36. *Let A be a complete, Hausdorff, LCTVS that is also a unital algebra such that the multiplication is continuous in each component separately. Let $s \leq t \in \mathbb{R}^+$ and $S, T : [s,t] \to A$ be continuously differentiable functions with $S(s) = \mathbf{1} = T(s)$. Then*

$$S(t) - T(t) = \int_s^t \big(T(t+s-r)S'(r) - T'(t+s-r)S(r)\big)\,\mathrm{d}r. \tag{D.131}$$

This can be seen as a continuous version of a telescoping sum. Compare, e.g., with Lemma C.3. The two examples of A that are of great importance to us are the algebra of bounded operators on a Hilbert space with (1) the norm topology and (2) the strong operator topology.

Proof. We calculate

$$\int_s^t \big(T(t+s-r)S'(r) - T'(t+s-r)S(r)\big)\,\mathrm{d}r$$
$$= \int_r^t \frac{\mathrm{d}}{\mathrm{d}r}\big(T(t+s-r)S(r)\big)\,\mathrm{d}s \tag{D.132}$$
$$= T(t+s-t)S(t) - T(t+s-s)S(s) = S(t) - T(t), \tag{D.133}$$

where we have used the Leibniz rule and the second fundamental theorem of calculus Corollary D.32. ☐

D.4 Campbell's theorem

We prove a stochastic version of Campbell's theorem.
Given a sequence $X, X_0, X_1, \ldots : \Omega \to \mathbb{R}$ of i.i.d. random variables and a Poisson process $N : \mathbb{R}^+ \times \Omega \to \mathbb{N}$ with jump times T_n and a function $f : [0,1] \times \mathbb{R} \to X$, we define

$$\int_0^1 f\big(s, X_{N_s}\big)\,\mathrm{d}N_s \coloneqq \sum_{m=0}^{\infty} [T_m \leq 1] f(T_m, X_{m-1}). \tag{D.134}$$

Proposition D.37. *Let $\lambda : \mathbb{R}^+ \to \mathbb{R}^+$ be a function, $(\Omega, \mathcal{A}, \mu)$ a probability space, $N : \mathbb{R}^+ \times \Omega \to \mathbb{R}$ be a Poisson process with rate λ and jump times T_m. Let $X, X_0, X_1, \ldots : \Omega \to \mathbb{R}$ be a sequence of i.i.d. random variables. Let $\mathfrak{X}$ be a Banach space and $f : [0,1] \times \mathbb{R} \to \mathfrak{X}$ a bounded function such that $s \mapsto f(s,x)$ is continuous for all $x \in \mathbb{R}$ and $x \mapsto f(s,x)$ is measurable for all $s \in [0,1]$. Then*

$$\mathbb{E}\Big[\int_0^1 f\big(s, X_{N_s}\big)\,\mathrm{d}N_s\Big] = \int_0^1 \mathbb{E}[f(s,X)]\lambda(s)\,\mathrm{d}s. \tag{D.135}$$

Proof. We claim that

$$\lim_{n\to\infty} \sum_{k=0}^{n-1} f\Big(\frac{k}{n}, X_{N_{\frac{k}{n}}}\Big)\big(N_{\frac{k+1}{n}} - N_{\frac{k}{n}}\big) = \sum_{m=0}^{\infty} [T_m \leq 1] f(T_m, X_{m-1}), \tag{D.136}$$

with convergence in mean. Terms in the first sum are non-zero if and only if there exists $m \in \mathbb{N}$ such that $\frac{k}{n} \leq T_m \leq \frac{k+1}{n}$. This implies $k \leq nT_m \leq k+1$, so $k = \lfloor nT_m \rfloor$. There is almost surely an n_0 such that each interval $\Big[\frac{k}{n_0}, \frac{k+1}{n_0}\Big]$ contains at most one jump point. For all $n \geq n_0$ we have

$$\sum_{k=0}^{n-1} f\Big(\frac{k}{n}, X_{N_{\frac{k}{n}}}\Big)\big(N_{\frac{k+1}{n}} - N_{\frac{k}{n}}\big) - \sum_{m=0}^{\infty} [T_m \leq 1] f(T_m, X_{m-1}) \tag{D.137}$$
$$= \sum_{m=0}^{\infty} [T_m \leq 1]\bigg(f\Big(\frac{\lfloor nT_m \rfloor}{n}, X_{N_{\frac{\lfloor nT_m \rfloor}{n}}}\Big) - f(T_m, X_{m-1})\bigg) \tag{D.138}$$
$$= \sum_{m=0}^{\infty} [T_m \leq 1]\bigg(f\Big(\frac{\lfloor nT_m \rfloor}{n}, X_{m-1}\Big) - f(T_m, X_{m-1})\bigg). \tag{D.139}$$

We now want to take the limit $n \to \infty$ and conclude that this is 0. This is true if we can pull the limit inside the sum: $s \mapsto f(s,x)$ was assumed continuous for all x, so the sequence of random variables converges a.s. and, since the function f was assumed bounded, the dominated convergence theorem implies convergence in mean. We also justify pulling the limit inside the sum using dominated convergence. Since f is bounded, it is enough to verify that $\sum_{m=0}^{\infty} \mathbb{E}[T_m \leq 1] < \infty$. We calculate

$$\sum_{m=0}^{\infty} \mathbb{E}[T_m \leq 1] = \sum_{m=0}^{\infty} \mathbb{E}[N(1) \geq m] \tag{D.140}$$

$$= \sum_{m=0}^{\infty} \sum_{n=m}^{\infty} \mathbb{E}[N(1) = m] \tag{D.141}$$

$$= \sum_{m=0}^{\infty} \sum_{n=m}^{\infty} \frac{\left(\int_0^1 \lambda \, \mathrm{d}s\right)^n}{n!} e^{-\int_0^1 \lambda \, \mathrm{d}s} \tag{D.142}$$

$$= \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{\left(\int_0^1 \lambda \, \mathrm{d}s\right)^{n+m}}{(n+m)!} e^{-\int_0^1 \lambda \, \mathrm{d}s} \tag{D.143}$$

$$\leq \sum_{m=0}^{\infty} \frac{\left(\int_0^1 \lambda \, \mathrm{d}s\right)^m}{m!} e^{-\int_0^1 \lambda \, \mathrm{d}s} \sum_{n=0}^{\infty} \frac{\left(\int_0^1 \lambda \, \mathrm{d}s\right)^n}{n!} \tag{D.144}$$

$$= \sum_{m=0}^{\infty} \frac{\left(\int_0^1 \lambda \, \mathrm{d}s\right)^m}{m!} = e^{\int_0^1 \lambda \, \mathrm{d}s} < \infty. \tag{D.145}$$

Next we have that $N_{\frac{k}{n}} = N_{\frac{k}{n}} - N_0$ and $N_{\frac{k+1}{n}} - N_{\frac{k}{n}}$ are independent. We then calculate

$$\mathbb{E}\Big[\lim_{n\to\infty} \sum_{k=0}^{n-1} f\Big(\frac{k}{n}, X_{N_{\frac{k}{n}}}\Big)\big(N_{\frac{k+1}{n}} - N_{\frac{k}{n}}\big)\Big] = \lim_{n\to\infty} \sum_{k=0}^{n-1} \mathbb{E}\Big[f\Big(\frac{k}{n}, X_{N_{\frac{k}{n}}}\Big)\Big] \mathbb{E}\big[N_{\frac{k+1}{n}} - N_{\frac{k}{n}}\big] \tag{D.146}$$

$$= \lim_{n\to\infty} \sum_{k=0}^{n-1} \mathbb{E}\Big[f\Big(\frac{k}{n}, X\Big)\Big] \int_{\frac{k}{n}}^{\frac{k+1}{n}} \lambda \, \mathrm{d}s \tag{D.147}$$

$$= \lim_{n\to\infty} \sum_{k=0}^{n-1} \int_{\frac{k}{n}}^{\frac{k+1}{n}} \mathbb{E}\Big[f\Big(\frac{k}{n}, X\Big)\Big] \lambda \, \mathrm{d}s \tag{D.148}$$

$$= \lim_{n\to\infty} \sum_{k=0}^{n-1} \int_{\frac{k}{n}}^{\frac{k+1}{n}} \mathbb{E}\Big[f\Big(\frac{\lfloor ns \rfloor}{n}, X\Big)\Big] \lambda \, \mathrm{d}s \tag{D.149}$$

$$= \lim_{n\to\infty} \int_0^1 \mathbb{E}\Big[f\Big(\frac{\lfloor ns \rfloor}{n}, X\Big)\Big] \lambda \, \mathrm{d}s \tag{D.150}$$

$$= \int_0^1 \mathbb{E}\big[f(s, X)\big] \lambda \, \mathrm{d}s. \tag{D.151}$$

The final equality relies on two more applications of the dominated convergence theorem: once to move the limit inside the integral and once to move it inside the expectation value. $\square$

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