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Quantum Symmetries and the Robustness of Dynamics

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A mia madre

A mio padre

A mia sorella

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Introduction

The construction of a quantum computer represents one of the major scientific and technological challenges of our time. However, building such a machine is extremely demanding, and current technology is still far from achieving this goal. One of the main applications of quantum computers is *quantum simulation* [1, 2], namely the ability to reproduce the dynamics of complex (not necessarily quantum) systems that cannot be efficiently studied using classical computation.

When a quantum simulation is used to reproduce the behavior of a complex system, approximations are unavoidable. The simulated dynamics cannot coincide exactly with those of the target system; they will inevitably represent a slightly modified version. For instance, it is common to implement *Trotter dynamics* to approximate the evolution of a quantum system within a simulation [3–5]. As a consequence, only those features of the target dynamics that remain stable under small modifications can be faithfully observed. Therefore, when studying a physical system, it is essential to identify the properties that exhibit robustness against perturbations.

This problem is broader than quantum simulation and is intrinsically connected to the modeling of physical systems. Whenever we attempt to provide a mathematical description of a system—whether quantum or classical—approximations are inevitable. To obtain explicit predictions, one must simplify the interactions. For instance, the behavior of a ferromagnet is often described by the Ising model, which neglects long-range couplings. This makes the model tractable, but in a real material such interactions are not exactly zero. This naturally raises the question: how reliable are the predictions of such models under perturbations? For short times these effects may be negligible, but over sufficiently long times perturbations can accumulate and produce significant deviations.

A famous example from classical mechanics is the dynamics of the Solar System. One can study the Earth–Sun system in isolation, neglecting the weaker interactions with other planets. This reduced model is exactly solvable, and the Earth follows a closed elliptical orbit. When the neglected interactions are reintroduced, the full system is no longer integrable, and a natural question arises: is the Solar System stable? This problem was famously addressed by Kolmogorov, Arnold, and Moser in the celebrated KAM theorem [6, 7]. They proved that many of the stable orbits of the simplified model survive in the full system, although slightly deformed. This illustrates a general lesson: to connect mathematical models with the real world, it is not enough to identify exact solutions of an idealized system; one must also determine whether these solutions persist when the model is perturbed.

A powerful way to address this question in quantum systems is through the study of *symmetries*, or equivalently, *conserved quantities* associated with the Hamiltonian [8, 9]. Quantum mechanics teaches us that symmetries correspond to the operators that commute with the Hamiltonian [10]. Once the Hamiltonian is known, its conserved quantities can, at least in principle, be identified. However, as mentioned above, in a quantum simulation only those symmetries that persist under perturbations can be observed. If a symmetry survives—perhaps slightly deformed but still effective—it is said to be *robust*; if it breaks down, it is *fragile* [11, 12]. Fragile symmetries are accidental: they are artifacts of the simplified model and disappear once more realistic effects are taken into account.

In this work, we analyze the problem of the long-time stability of conserved quantities under perturbations. The thesis is organized as follows:

- **Chapter 1** introduces the conserved quantities of a quantum system and discusses their algebraic characterization in terms of the Hamiltonian. It is well known that conserved quantities are the operators that commute with the Hamiltonian. However, when the Hamiltonian is unbounded, the meaning of "commutation" must be clarified. In this chapter, we define what it means for a bounded operator to commute with an unbounded one and present several equivalent formulations of this concept. This naturally leads to the notion of the commutant of a self-adjoint operator. In the final part of the chapter, we introduce the concept of symmetries in quantum systems and emphasize their connection with conserved quantities through a quantum version of Noether's theorem.

- **Chapter 2** investigates the long-time stability of quantum symmetries against perturbations of the system's Hamiltonian. We begin by introducing the notion of relatively bounded perturbations and show that a self-adjoint operator remains self-adjoint when modified by a sufficiently small relatively bounded perturbation (Kato–Rellich theorem). We then define *robust* and *fragile* symmetries against an arbitrary class of relatively bounded perturbations. Robust symmetries remain close to their initial value throughout their entire evolution, despite the perturbation of the Hamiltonian, while fragile symmetries exhibit large deviations from their initial value after sufficiently long times. Next, we provide an algebraic characterization of symmetries that are robust against a single perturbation, for Hamiltonians with discrete spectra. We show that every relatively bounded perturbation induces a family of subprojections of the spectral projections of the unperturbed Hamiltonian, and that the robust symmetries are precisely those commuting with this family of subprojections. Building on this single-perturbation analysis, we then determine which symmetries remain robust against an arbitrary set of perturbations $\mathcal{P}$. A particularly interesting physical situation arises when the perturbations themselves commute with a certain symmetry of the Hamiltonian. For instance, in a rotationally symmetric system, one may require that the perturbations respect the same symmetry. In Theorem 2.4.2, we show that in such cases the set of robust symmetries acquires a natural algebraic structure. We then investigate the symmetries that are robust against all possible (relatively bounded) perturbations. In Theorem 2.4.3, we show that they coincide with the bounded functions of the Hamiltonian, a result previously established for finite-dimensional quantum systems [11, 13]. Finally, we introduce the concept of a *quantum adiabatic invariant*, defined as the continuous deformation of a robust symmetry into a new symmetry of the perturbed Hamiltonian.

- **Chapter 3** focuses on the *wandering range* of a robust symmetry, which provides a quantitative measure of its deviation from the initial value under the perturbed dynamics. In particular, we study how the wandering range depends on the perturbation strength ε. In Example 2.1.1, we show that, in general, the wandering range is not necessarily of order ε. The chapter is devoted to identifying the conditions under which this scaling holds. We prove that the wandering range, when evaluated on an eigenvector of the unperturbed Hamiltonian or for a finite-rank symmetry, is indeed of order ε. In the last part of the chapter, we analyze in detail the wandering range of *completely robust symmetries* against bounded perturbations. In this case, we are able not only to establish that the wandering range is of order ε, but also to derive an explicit estimate for its value in terms of the perturbation norm and the minimal spectral gap of the Hamiltonian. The proof relies on Theorem 3.3.2, the detailed analysis of which constitutes the core of the following chapters.

- **Chapter 4** provides a first proof of Theorem 3.3.2, based on an iterative procedure known as *Quantum KAM iteration*. Throughout this analysis, we assume that the Hamiltonian H is self-adjoint with a purely point spectrum and non-vanishing spectral gap. In the first part, we introduce the main tool employed in the iteration—the *homological equation*. We discuss its solution and derive an upper bound in terms of the spectral gap of the Hamiltonian. We then explicitly construct the intertwining operator $W(\varepsilon)$ and the transformed perturbation $\widehat{V}(\varepsilon)$ of Theorem 3.3.2 as formal series expansions, and prove their convergence by exploiting the recursive combinatorial properties of a famous sequence: the Catalan numbers.

- **Chapter 5** presents an alternative approach to the construction of the intertwining operator $W(\varepsilon)$, known as the *Trotter approach*. In this framework, $W(\varepsilon)$ is expressed as an infinite product of unitary operators rather than as the exponential of a power series. As in the previous chapter, we assume that H is self-adjoint with a purely point spectrum and non-vanishing spectral gap. We first develop the formal construction of the relevant operators and then prove their boundedness, obtaining explicit estimates in terms of the spectral gap of the Hamiltonian. Finally, we discuss the numerical advantages of this formulation, which provides a computationally efficient scheme for the approximation of the effective dynamics.

- **Chapter 6** extends the analysis of the previous chapter to quantum systems whose

Hamiltonian exhibits a band spectrum, as typically occurs in periodic structures. We investigate the robustness of quantum symmetries in this setting and show that the symmetries belonging to the bicommutant of the band projections are completely robust against bounded perturbations of the Hamiltonian. The proof is once again based on the Quantum KAM Iteration, which can be naturally generalized to this broader class of Hamiltonians.

- **Chapter 7** proposes an alternative strategy for the construction of the operators $W(\varepsilon)$ and $\widehat{V}(\varepsilon)$ introduced in Theorem 3.3.2, for Hamiltonians with purely point spectra and non-vanishing spectral gap. We begin by briefly recalling the main elements of Kato's Perturbation Theory and then show that the operator $W(\varepsilon)$ can be obtained as the solution of a suitable differential equation. We construct its solution as a formal power series and prove its convergence by introducing a new sequence of numbers, which we call the *modified Catalan numbers*. Finally, we compare the resulting estimates with those obtained through the Quantum KAM Iteration.

Several results presented in this thesis are based on and extend the analysis developed in Refs. [12, 14, 15].

Chapter 1

Conserved quantities and symmetries

In this chapter, we introduce the algebraic framework underlying conserved quantities in quantum mechanics. We begin by defining the notion of commutation between a bounded operator and an unbounded self-adjoint Hamiltonian, clarifying how it can be formulated in terms of the resolvent, spectral projections, and bounded functions. This leads to the definition of the *commutant* of a Hamiltonian, which provides a rigorous algebraic characterization of conserved quantities.

In the second part, we connect this notion with the theory of symmetries, showing that continuous symmetries correspond to one-parameter unitary groups whose self-adjoint generators commute with the Hamiltonian. This establishes the quantum version of Noether's theorem.

1.1 Conserved quantities

Let $\mathcal{H}$ be a complex separable Hilbert space. We focus on isolated quantum systems, whose evolution is described by a one-parameter strongly continuous unitary group $\{U(t)\}_{t\in\mathbb{R}}$ satisfying

$$U(t) = \mathrm{e}^{-\mathrm{i}tH}, \qquad t \in \mathbb{R}, \tag{1.1}$$

where $H = H^\dagger$ is the (possibly unbounded) self-adjoint Hamiltonian of the system, defined on a dense domain $D(H) = D(H^\dagger) \subseteq \mathcal{H}$ [16].

We adopt the Heisenberg picture, in which states remain fixed while observables evolve in time. For every bounded operator $A \in B(\mathcal{H})$, its time evolution is given by

$$t \in \mathbb{R} \longmapsto A_t := U(t)^\dagger A U(t) = \mathrm{e}^{\mathrm{i}tH} A \mathrm{e}^{-\mathrm{i}tH} \in B(\mathcal{H}), \tag{1.2}$$

where A_t denotes the observable at time t [10].

Among all observables, some play a special role: the *conserved quantities*. They are those operators that remain constant under the Heisenberg evolution (1.2).

Definition 1.1.1. *A bounded operator $S \in B(\mathcal{H})$ is a* conserved quantity *of the Hamiltonian*

H if

$$e^{itH} S e^{-itH} = S, \qquad \forall\, t \in \mathbb{R}, \tag{1.3}$$

that is, if S is invariant under the Heisenberg evolution generated by H.[1]

Equivalently, S is a conserved quantity if and only if it commutes with the evolution group:

$$[S, e^{-itH}] := S e^{-itH} - e^{-itH} S = 0, \qquad \forall\, t \in \mathbb{R}. \tag{1.6}$$

If H is bounded, this condition can be expressed directly in terms of the Hamiltonian itself.

Theorem 1.1.1. *Let $H = H^\dagger \in B(\mathcal{H})$. Then a bounded operator $A \in B(\mathcal{H})$ is a conserved quantity if and only if*

$$[A, H] = 0.$$

Proof. For any $A \in B(\mathcal{H})$, its Heisenberg evolution is

$$A_t = e^{itH} A e^{-itH}, \qquad t \in \mathbb{R}. \tag{1.7}$$

Since H is bounded, the map $t \mapsto A_t$ is norm-differentiable, and

$$i \frac{d}{dt} A_t = [A_t, H], \qquad \forall t \in \mathbb{R}. \tag{1.8}$$

Hence,

$$A_t = A \iff \frac{d}{dt} A_t = 0 \tag{1.9}$$

$$\iff [A_t, H] = 0 \tag{1.10}$$

$$\iff e^{itH}[A, H] e^{-itH} = 0 \tag{1.11}$$

$$\iff [A, H] = 0, \tag{1.12}$$

where we used $A_t = e^{itH} A e^{-itH}$. □

This motivates the following algebraic definition.

[1]Even though we will deal only with bounded conserved quantities in this thesis, it is worth to define the unbounded conserved quantities.

Definition 1.1.2. *Let S be an unbounded operator with dense domain $D(S) \subset \mathcal{H}$. We say that S is a (unbounded) conserved quantity, if and only if*

$$e^{-itH} D(S) = D(S) \tag{1.4}$$

$$e^{itH} S e^{-itH} \psi = S\psi, \tag{1.5}$$

for all $\psi \in D(S)$.

Definition 1.1.3. *The* commutant *of a bounded operator H is the set of all bounded operators commuting with it:*

$$\{H\}' := \{A \in B(\mathcal{H}) : [A, H] = 0\}. \tag{1.13}$$

If H is bounded, the set of conserved quantities coincides exactly with its commutant. This provides an algebraic characterization of conserved quantities, independent of the explicit time evolution.

The situation becomes more delicate when H is unbounded. In this case, the commutator $[A, H]$ may fail to be well defined on the whole Hilbert space, since AH is defined on $D(H)$ while HA acts on the (generally different) domain $D(HA) = \{\psi \in \mathcal{H} : A\psi \in D(H)\}$. Thus, the expression $[A, H]\psi = AH\psi - HA\psi$ might not make sense even for all $\psi \in D(H)$.

To extend the algebraic notion of commutation to unbounded operators, we must require that both compositions are well defined on a common domain.

Definition 1.1.4. *Let H be a (possibly unbounded) operator with domain $D(H) \subseteq \mathcal{H}$. A bounded operator $A \in B(\mathcal{H})$ is said to* commute with H *if:*

- *$AD(H) \subseteq D(H)$;*
- *$AH\psi = HA\psi$ for all $\psi \in D(H)$.*

In the next section we show that Definition 1.1.4 can be expressed in terms of the resolvent operator of H when it is densely defined and closed.

1.2 Commutation with the Resolvent Operator

Let H be an unbounded closed operator with dense domain $D(H) \subset \mathcal{H}$. In this case, commutativity can be characterized in terms of the resolvent of H.

Theorem 1.2.1. *Let H be a (densely defined) closed operator, with domain $D(H)$. Then the following statements are equivalent:*

(i) A commutes with H;

(ii) $[A, R_\mu(H)] = 0$ for all $\mu \in \rho(H)$, the resolvent set of H, where $R_\mu(H) = (H - \mu\mathbb{I})^{-1}$.

(iii) $[A, R_\mu(H)] = 0$ for some $\mu \in \rho(H)$.

Proof. (i) ⇒ (ii). Assume that A commutes with H, that is,

$$AD(H) \subseteq D(H), \qquad AH\psi = HA\psi \quad \forall\, \psi \in D(H). \tag{1.14}$$

Let $\mu \in \rho(H)$ and $\psi \in \mathcal{H}$, and consider

$$R_\mu(H)A\psi. \tag{1.15}$$

Since $R_\mu(H)$ is a bounded operator, it is defined on the full Hilbert space $\mathcal{H}$. Hence,

$$\mathrm{Ran}(H-\mu\mathbb{I}) = D(R_\mu(H)) = \mathcal{H}. \tag{1.16}$$

Hence, there exists $\varphi \in D(H)$ such that

$$\psi = (H-\mu\mathbb{I})\varphi. \tag{1.17}$$

Substituting this into (1.15) gives

$$R_\mu(H)A\psi = R_\mu(H)A(H-\mu\mathbb{I})\varphi = R_\mu(H)(H-\mu\mathbb{I})A\varphi, \tag{1.18}$$

where the last equality follows from (1.14). Since $R_\mu(H) = (H-\mu\mathbb{I})^{-1}$ and $\varphi = R_\mu(H)\psi$, we obtain

$$R_\mu(H)A\psi = AR_\mu(H)\psi, \tag{1.19}$$

for all $\psi \in \mathcal{H}$, and therefore $[A, R_\mu(H)] = 0$.

(ii) ⇒ (iii). Trivial.

(iii) ⇒ (i). Assume now that

$$AR_\mu(H) = R_\mu(H)A, \tag{1.20}$$

for some $\mu \in \rho(H)$.

Step 1. $AD(H) \subseteq D(H)$.
Let $\varphi \in D(H)$. Since $\mathrm{Ran}(R_\mu(H)) = D(H)$, there exists $\psi \in \mathcal{H}$ such that

$$\varphi = R_\mu(H)\psi. \tag{1.21}$$

Using (1.20), we find

$$A\varphi = AR_\mu(H)\psi = R_\mu(H)A\psi. \tag{1.22}$$

Because the range of $R_\mu(H)$ equals $D(H)$, it follows that $A\varphi \in D(H)$, and hence $AD(H) \subseteq D(H)$.

Step 2. $AH\varphi = HA\varphi$ for all $\varphi \in D(H)$.
We can equivalently show that

$$A(H-\mu\mathbb{I})\varphi = (H-\mu\mathbb{I})A\varphi, \tag{1.23}$$

for some (and hence all) $\mu \in \rho(H)$. Using (1.21) and the identity $(H-\mu\mathbb{I})R_\mu(H) = \mathbb{I}$, we have

$$A(H-\mu\mathbb{I})\varphi = A(H-\mu\mathbb{I})R_\mu(H)\psi = A\psi, \tag{1.24}$$
$$(H-\mu\mathbb{I})A\varphi = (H-\mu\mathbb{I})R_\mu(H)A\psi = A\psi, \tag{1.25}$$

where the last equality follows from (1.20). Thus (1.23) holds for all $\varphi \in D(H)$, and the proof is complete. □

The equivalence proven above shows that the algebraic condition $HA \subseteq AH$ can be completely reformulated in terms of the resolvent of H. The resolvent family $\{R_\mu(H)\}_{\mu\in\rho(H)}$ thus serves as a bounded representative of the algebraic and spectral properties of H: although H itself may not be directly accessible due to domain issues, its resolvents fully determine its structure. For self-adjoint operators, these properties are encoded even more transparently by the spectral theorem, which associates to H a unique projection-valued measure $\{P_H(\Omega)\}_{\Omega\in\mathcal{B}(\mathbb{R})}$.[2] This will be the topic of the next section.

1.3 The commutant of a self-adjoint operator

Let $H = H^\dagger$ be a self-adjoint operator on the domain $D(H) = D(H^\dagger)$. According to the spectral theorem, there exists a unique projection-valued measure $\{P_H(\Omega)\}_{\Omega\in\mathcal{B}(\mathbb{R})}$ such that

$$H\psi = \int_{\mathbb{R}} \lambda\, dP_H(\lambda)\,\psi, \qquad \psi \in D(H). \tag{1.26}$$

This family of projections contains the complete spectral information of H and provides the foundation of the functional calculus, allowing one to define Borel functions of H.

Indeed, given a measurable function $f : \mathbb{R} \to \mathbb{C}$, one defines

$$f(H)\psi = \int_{\mathbb{R}} f(\lambda)\, dP_H(\lambda)\,\psi, \tag{1.27}$$

for all $\psi \in D(f(H))$, where

$$D(f(H)) = \left\{ \psi \in \mathcal{H} : \int_{\mathbb{R}} |f(\lambda)|^2\, d\mu_\psi(\lambda) < +\infty \right\}, \tag{1.28}$$

and

$$\mu_\psi(\Omega) = \|P_H(\Omega)\psi\|^2, \qquad \Omega \in \mathcal{B}(\mathbb{R}), \tag{1.29}$$

is the spectral measure associated with the vector ψ.

The functional calculus makes it possible to restate commutation with H in terms of its spectral projections or any bounded function of H. The following theorem collects the

[2] Here $\mathcal{B}(\mathbb{R})$ denotes the Borel σ-algebra on $\mathbb{R}$.

equivalent formulations of this condition.

Theorem 1.3.1. *Let $H = H^\dagger$ be a self-adjoint operator on $\mathcal{H}$ and $A \in B(\mathcal{H})$. Then the following statements are equivalent:*

(i) $[A, R_\mu(H)] = 0$ *for all* $\mu \in \mathbb{C} \setminus \mathbb{R}$*;*

(ii) $[A, \mathrm{e}^{-\mathrm{i}tH}] = 0$ *for all* $t \in \mathbb{R}$*;*

(iii) $[A, P_H(\Omega)] = 0$ *for all Borel sets* $\Omega \subseteq \mathbb{R}$*;*

(iv) $[A, f(H)] = 0$ *for all bounded Borel functions* f*.*

Proof. (i) ⇒ (ii). Assume that $[A, R_\mu(H)] = 0$ for all $\mu \in \mathbb{C} \setminus \mathbb{R}$. We recall that the exponential of a self-adjoint operator can be expressed through the formula:

$$\mathrm{e}^{-\mathrm{i}tH}\psi = \lim_{n\to\infty} \left(\mathbb{I} + \mathrm{i}t\frac{H}{n}\right)^{-n} \psi, \qquad \forall\, \psi \in \mathcal{H}, \tag{1.30}$$

as shown in [17].

Moreover, for each n,

$$\left(\mathbb{I} + \mathrm{i}t\frac{H}{n}\right)^{-n} = \left(\frac{\mathrm{i}t}{n}\right)^{-n} R_{\frac{\mathrm{i}n}{t}}(H)^n. \tag{1.31}$$

Hence, for every $\psi \in \mathcal{H}$,

$$[A, \mathrm{e}^{-\mathrm{i}tH}]\psi = \lim_{n\to\infty} \left(\frac{\mathrm{i}t}{n}\right)^{-n} [A, R_{\frac{\mathrm{i}n}{t}}(H)^n]\psi = 0, \tag{1.32}$$

since by hypothesis $[A, R_{\frac{\mathrm{i}n}{t}}(H)] = 0$ for all n. Thus $[A, \mathrm{e}^{-\mathrm{i}tH}] = 0$.

(ii) ⇒ (iii). Assume that $[A, \mathrm{e}^{-\mathrm{i}tH}] = 0$ for all $t \in \mathbb{R}$. We first show that this implies

$$[A, f(H)] = 0, \tag{1.33}$$

for all bounded Schwartz functions $f \in \mathcal{S}(\mathbb{R})$.

Let $f \in \mathcal{S}(\mathbb{R})$ and denote by $\hat{f}$ its Fourier transform,

$$\hat{f}(s) = \int_{\mathbb{R}} f(\lambda)\, \mathrm{e}^{-\mathrm{i}s\lambda}\, \mathrm{d}\lambda. \tag{1.34}$$

Then the inverse transform reads

$$f(\lambda) = \frac{1}{2\pi} \int_{\mathbb{R}} \hat{f}(s)\, \mathrm{e}^{\mathrm{i}s\lambda}\, \mathrm{d}s. \tag{1.35}$$

By the spectral theorem and Fubini's theorem, this identity extends to the operator level:

$$f(H) = \frac{1}{2\pi} \int_{\mathbb{R}} \hat{f}(s)\, \mathrm{e}^{\mathrm{i}sH}\, \mathrm{d}s, \tag{1.36}$$

where the integral converges in the strong operator topology [16]. Then

$$[A, f(H)] = \frac{1}{2\pi}\int_{\mathbb{R}} \hat{f}(s)\,[A, \mathrm{e}^{\mathrm{i}sH}]\,\mathrm{d}s = 0, \tag{1.37}$$

since $[A, \mathrm{e}^{\mathrm{i}sH}] = 0$ for all s.

Now we show that this implies

$$[A, P_H(\Omega)] = 0, \tag{1.38}$$

for all Borel sets $\Omega \subseteq \mathbb{R}$. Recall that $P_H(\Omega) = \chi_\Omega(H)$, where χ_Ω denotes the characteristic function of Ω,

$$\chi_\Omega(\lambda) = \begin{cases} 1, & \lambda \in \Omega, \\ 0, & \lambda \notin \Omega. \end{cases} \tag{1.39}$$

The characteristic function can be approximated point-wise by a sequence of uniformly bounded Schwartz functions $f_n \in \mathcal{S}(\mathbb{R})$:

$$\chi_\Omega(\lambda) = \lim_{n\to\infty} f_n(\lambda). \tag{1.40}$$

By the functional calculus, this implies

$$f_n(H) \xrightarrow{n\to\infty} P_H(\Omega) \tag{1.41}$$

in the strong operator topology [16]. Since $[A, f_n(H)] = 0$ for all n, passing to the limit gives

$$[A, P_H(\Omega)] = 0. \tag{1.42}$$

(iii) ⇒ (iv). This follows directly from the spectral theorem and functional calculus. For any bounded Borel function f,

$$f(H) = \int_{\mathbb{R}} f(\lambda)\,\mathrm{d}P_H(\lambda). \tag{1.43}$$

If $[A, P_H(\Omega)] = 0$ for all Borel sets Ω, then by linearity of the integral with respect to the projection-valued measure,

$$[A, f(H)] = \int_{\mathbb{R}} f(\lambda)\,[A, \mathrm{d}P_H(\lambda)] = 0. \tag{1.44}$$

(iv) ⇒ (i). Trivial, since for every $\mu \in \mathbb{C} \setminus \mathbb{R}$,

$$R_\mu(H) = f_\mu(H), \tag{1.45}$$

where $f_\mu(\lambda) = \frac{1}{\lambda-\mu}$ is bounded because

$$|f_\mu(\lambda)| \leq \frac{1}{|\operatorname{Im}\mu|}, \tag{1.46}$$

where $\operatorname{Im}\mu$ denotes the imaginary part of the complex number μ.

Therefore, if $[A, f(H)] = 0$ for all bounded Borel f, it holds in particular for $f = f_\mu$, and hence $[A, R_\mu(H)] = 0$.

This completes the proof. □

This theorem provides a rigorous algebraic characterization of the conserved quantities of a closed quantum system.

A bounded operator $S \in B(\mathcal{H})$ is a conserved quantity if and only if

$$[S, \mathrm{e}^{-\mathrm{i}tH}] = 0, \qquad \forall\, t \in \mathbb{R}. \tag{1.47}$$

The equivalences established above show that this condition can be reformulated in several equivalent algebraic ways, involving any of the operator families associated with H: the resolvent $R_\mu(H)$, the spectral projections $P_H(\Omega)$, or the bounded Borel functions $f(H)$.

Accordingly, for a (possibly unbounded) self-adjoint Hamiltonian H, we define its *commutant* as the set of bounded operators that commute with all spectral projections (equivalently, with all bounded Borel functions of H or with the evolution group $\mathrm{e}^{-\mathrm{i}tH}$):

$$\{H\}' = \{P_H(\Omega) : \Omega \subseteq \mathbb{R} \text{ Borel}\}' \tag{1.48}$$

$$= \{f(H) : f : \mathbb{R} \to \mathbb{C},\ f \text{ bounded Borel}\}' \tag{1.49}$$

$$= \{\mathrm{e}^{-\mathrm{i}tH}, t \in \mathbb{R}\}'. \tag{1.50}$$

Here, for any subset $\mathcal{S} \subset B(\mathcal{H})$, we denote by $\mathcal{S}'$ its *commutant*,

$$\mathcal{S}' := \{A \in B(\mathcal{H}) : [A, S] = 0 \text{ for all } S \in \mathcal{S}\}. \tag{1.51}$$

The set $\{H\}'$ is a *von Neumann algebra*: it is a unital *-subalgebra of $B(\mathcal{H})$ that is closed under the strong (and equivalently, weak) operator topology. Among its elements, a particularly important subclass is given by those belonging to the *bicommutant* $\{H\}''$, which form the von Neumann algebra generated by H and will be discussed in the next subsection.

1.3.1 A privileged subalgebra: the bicommutant

Once the commutant of H has been introduced, it is natural to consider its commutant again, namely the *bicommutant* $\{H\}''$. Using the previous definition, we can write

$$\{H\}'' = \{f(H) : f : \mathbb{R} \to \mathbb{C},\ f \text{ bounded Borel}\}''. \tag{1.52}$$

This set consists of all bounded operators that commute with the entire commutant $\{H\}'$. Elements of $\{H\}''$ are therefore *special conserved quantities*: they commute not only with the Hamiltonian H itself, but also with all other conserved quantities of the system.

Consider now the set

$$\mathcal{A}_H = \{f(H) : f : \mathbb{R} \to \mathbb{C},\ f \text{ bounded Borel}\}. \tag{1.53}$$

One can show that $\mathcal{A}_H$ is an abelian von Neumann algebra [18]. Then, by the von Neumann bicommutant theorem,

$$\mathcal{A}_H'' = \mathcal{A}_H. \tag{1.54}$$

The algebra $\mathcal{A}_H$ is called the *abelian von Neumann algebra generated by H*. Hence, we conclude that the bicommutant of H coincides with the von Neumann algebra generated by H:

$$\{H\}'' = \mathcal{A}_H = \{f(H) : f : \mathbb{R} \to \mathbb{C},\ f \text{ bounded Borel}\}. \tag{1.55}$$

The operators in $\mathcal{A}_H$ thus form a distinguished class of conserved quantities. Each of them acts proportionally to the identity within every spectral subspace of H, and therefore cannot lift the degeneracies of the Hamiltonian. As will be shown in the next chapter, this property will be the key ingredient in establishing their robustness against perturbations.

In the next section, we turn to symmetry transformations in quantum mechanics and clarify their connection with conserved quantities.

1.4 Symmetry transformations in quantum mechanics

In quantum mechanics, the physical state of a system is not represented by an individual vector of the Hilbert space $\mathcal{H}$, but by a *ray*—that is, an equivalence class of normalized vectors differing only by a global phase. Explicitly, for every unit vector $\psi \in \mathcal{H}$, the corresponding ray is

$$\mathcal{R}_\psi = \{\, e^{i\theta}\psi : \theta \in \mathbb{R}\,\}. \tag{1.56}$$

All vectors in $\mathcal{R}_\psi$ describe the same physical state, since overall phases have no observable meaning. The set of all rays forms the *projective Hilbert space*

$$\mathbb{P}(\mathcal{H}) = \{\mathcal{R}_\psi : \psi \in \mathcal{H}, \|\psi\| = 1\}.$$

Physical predictions depend only on rays. In particular, the transition probability between two states is given by

$$P(\mathcal{R}_\psi \to \mathcal{R}_\phi) = |\langle\psi|\phi\rangle|^2 , \tag{1.57}$$

which is independent of the choice of representatives in each ray.

A *symmetry transformation* is a bijective map on the space of rays that preserves all transition probabilities [19]. If a transformation T sends $\mathcal{R}_\psi \mapsto \mathcal{R}'_\psi$ and $\mathcal{R}_\phi \mapsto \mathcal{R}'_\phi$, then

$$P(\mathcal{R}_\psi \to \mathcal{R}_\phi) = P(\mathcal{R}'_\psi \to \mathcal{R}'_\phi). \tag{1.58}$$

Such transformations represent the fundamental symmetries of the theory, since they preserve all physically measurable relations among states.

1.4.1 Projective representations

Wigner's theorem establishes that every symmetry transformation between rays is represented in Hilbert space by either a unitary or an antiunitary operator [9]. That is, for each transformation $\mathcal{R}_\psi \mapsto \mathcal{R}'_\psi$, there exists an operator U such that, if $\psi \in \mathcal{R}_\psi$, then $U\psi \in \mathcal{R}'_\psi$. Depending on the nature of U, one has:

$$\text{if } U \text{ is unitary:} \qquad \langle U\psi|U\phi\rangle = \langle\psi|\phi\rangle , \qquad U(\alpha\phi + \beta\psi) = \alpha U\phi + \beta U\psi, \tag{1.59}$$

$$\text{if } U \text{ is antiunitary:} \qquad \langle U\psi|U\phi\rangle = \langle\psi|\phi\rangle^* , \qquad U(\alpha\phi + \beta\psi) = \alpha^* U\phi + \beta^* U\psi. \tag{1.60}$$

The set of all symmetry transformations forms a group. If T_1 and T_2 are symmetries, their composition T_2T_1 is again a symmetry, and each transformation T has an inverse T^{-1}. According to Wigner's theorem, one can associate with each transformation T an operator $U(T)$ acting on $\mathcal{H}$. The composition of symmetry operations corresponds to operator multiplication, but only up to a phase factor:

$$U(T_2)U(T_1) = \mathrm{e}^{\mathrm{i}\phi(T_2,T_1)}\, U(T_2T_1), \tag{1.61}$$

where $\phi(T_2, T_1) \in \mathbb{R}$. Such a family $\{U(T)\}$ defines a *projective representation* of the symmetry group.

The associativity of operator multiplication implies a constraint on the phase factors:

$$\phi(T_2, T_1) + \phi(T_3, T_2T_1) = \phi(T_3, T_2) + \phi(T_3T_2, T_1), \tag{1.62}$$

known as the *two-cocycle condition.* If the phase function can be written as

$$\phi(T_1, T_2) = \alpha(T_1T_2) - \alpha(T_1) - \alpha(T_2), \tag{1.63}$$

then the condition (1.62) is automatically satisfied. In this case, redefining the operators as

$$\widetilde{U}(T) := \mathrm{e}^{\mathrm{i}\alpha(T)}\, U(T) \tag{1.64}$$

removes the phase in (1.61), yielding an ordinary representation:

$$\widetilde{U}(T_2)\widetilde{U}(T_1) = \widetilde{U}(T_2T_1). \tag{1.65}$$

Distinct projective representations differing by a redefinition of the form (1.63) belong to the same *two-cocycle class*. If the class contains the trivial cocycle $\phi = 0$, the representation can be made exact, and all symmetry operators may be taken as unitary or antiunitary. From now on we will assume this to be the case.

1.4.2 Connection with conserved quantities

Let us consider a one-parameter continuous group of symmetry transformations acting on the space of rays. Formally, this is a group homomorphism from the additive group $(\mathbb{R}, +)$ to the group G of symmetry transformations:

$$T : \theta \in \mathbb{R} \longmapsto T(\theta) \in G, \tag{1.66}$$
$$T(\theta_1 + \theta_2) = T(\theta_1)T(\theta_2) = T(\theta_2)T(\theta_1), \tag{1.67}$$

and we choose the parametrization such that $T(0)$ is the identity transformation.

According to Wigner's theorem, to each symmetry transformation $T(\theta)$ one can associate a unitary or antiunitary operator $U(T(\theta))$ acting on the Hilbert space $\mathcal{H}$, such that if $\psi \in \mathcal{H}$ represents the ray $\mathcal{R}_\psi$, then $U(T(\theta))\psi$ represents the transformed ray $T(\theta)\mathcal{R}_\psi$. Since the transformations $T(\theta)$ are continuously connected with the identity (and the identity is represented by a unitary operator), all elements of this one-parameter group are represented by unitary operators.

Thus, for every $\theta_1, \theta_2 \in \mathbb{R}$,

$$U(T(\theta_1 + \theta_2)) = U(T(\theta_1))\, U(T(\theta_2)). \tag{1.68}$$

Let us denote $S(\theta) := U(T(\theta))$. The family $\{S(\theta)\}_{\theta\in\mathbb{R}}$ is therefore a one-parameter unitary group on $\mathcal{H}$:

$$S(\theta_1 + \theta_2) = S(\theta_1)S(\theta_2), \tag{1.69}$$
$$S(0) = \mathbb{I}. \tag{1.70}$$

To ensure continuity of the symmetry action, one requires that $S(\theta)$ be *strongly continuous*, namely,

$$\lim_{\theta\to 0} \|S(\theta)\psi - \psi\| = 0, \qquad \forall\, \psi \in \mathcal{H}. \tag{1.71}$$

By Stone's theorem, there exists a unique self-adjoint operator Q (the *generator* of the symmetry) such that

$$S(\theta) = \mathrm{e}^{-\mathrm{i}\theta Q}, \qquad \theta \in \mathbb{R}. \tag{1.72}$$

We will show that Q is a conserved quantity whenever the Hamiltonian H admits $S(\theta)$ as a symmetry.

Let H be the self-adjoint Hamiltonian of the system, generating the time evolution $\mathrm{e}^{-\mathrm{i}tH}$. If the system admits $S(\theta) = \mathrm{e}^{-\mathrm{i}\theta Q}$ as a continuous symmetry, the expectation value of the evolution group must remain unchanged under the transformation

$$\psi \mapsto \mathrm{e}^{-\mathrm{i}\theta Q}\psi, \tag{1.73}$$

for all $\psi \in \mathcal{H}$. This requires that

$$\langle\psi|\mathrm{e}^{-\mathrm{i}tH}\psi\rangle = \langle \mathrm{e}^{-\mathrm{i}\theta Q}\psi|\mathrm{e}^{-\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}\theta Q}\psi\rangle\,, \qquad \forall\,\psi \in \mathcal{H}. \tag{1.74}$$

Equivalently,

$$\mathrm{e}^{\mathrm{i}\theta Q}\mathrm{e}^{-\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}\theta Q} = \mathrm{e}^{-\mathrm{i}tH}, \qquad \forall\,\theta \in \mathbb{R} \tag{1.75}$$

which means that $[\mathrm{e}^{-\mathrm{i}\theta Q}, \mathrm{e}^{-\mathrm{i}tH}] = 0$. It is easy to show that this implies that

$$\mathrm{e}^{-\mathrm{i}tH} D(Q) = D(Q) \tag{1.76}$$

and that for all $\psi \in D(Q)$

$$\mathrm{e}^{\mathrm{i}tH} Q \mathrm{e}^{-\mathrm{i}tH}\psi = Q\psi. \tag{1.77}$$

Then Q is a conserved quantity (in general unbounded). See [17].

Conversely, if we start from a conserved quantity $Q = Q^\dagger$, we can define a continuous unitary group

$$S(\theta) = \mathrm{e}^{-\mathrm{i}\theta Q}, \tag{1.78}$$

which represents a continuous symmetry of the system. This connection between continuous symmetries of the Hamiltonian H and conserved quantities, found in a quantum mechanical context, is actually a more general result, related to the Lie-algebra structure, that works also in classical mechanics, where it is known as Noether's theorem [7].

Chapter 2

Robustness of quantum symmetries against perturbations

In the previous chapter, we introduced the main tools for describing a quantum system: in particular, we discussed the Heisenberg evolution of observables and defined the conserved quantities. We showed that conserved quantities are intimately related to the continuous symmetries of the system. In what follows, we shall use the terms “conserved quantity” and “symmetry” interchangeably.[1]

In this chapter, we study the long-time stability of conserved quantities against perturbations of the system's Hamiltonian. We will see that some conserved quantities largely deviate from their initial value—the *fragile symmetries*—while others remain close to it—the *robust symmetries*. A precise algebraic characterization of these two behaviors will be provided.

We begin by introducing perturbations of self-adjoint operators, with particular attention to relatively bounded perturbations. Then, we establish a classification of robust symmetries by analyzing their stability with respect to an arbitrary family of perturbations. In particular, we address the following question: given a relatively bounded perturbation, which symmetries remain uniformly stable under the perturbed dynamics?

We will show that each perturbation induces a family of subprojections of the spectral projections of the unperturbed Hamiltonian. In Theorem 2.3.2, we prove that the robust symmetries are exactly those that commute with these subprojections. This result will then be used to study robustness with respect to an arbitrary set of perturbations $\mathcal{P}$. In particular, when $\mathcal{P}$ coincides with the set of relatively bounded operators commuting with a symmetry of the unperturbed Hamiltonian, the corresponding set of robust symmetries acquires a well-defined algebraic structure. We will also discuss the case of completely robust symmetries, i.e., conserved quantities that remain stable under *all* relatively bounded perturbations, and we will prove that they are precisely the bounded functions of the Hamiltonian. Finally, we introduce the concept of *Quantum Adiabatic Invariants*. The results presented in this

[1]Strictly speaking, this correspondence holds between continuous symmetries and *self-adjoint* conserved quantities. Nevertheless, throughout this thesis the term “symmetry” will also be used to refer to non-self-adjoint conserved quantities.

chapter form the core of the work reported in [12].

2.1 Perturbations

First of all, we need to define the notion of perturbation. We are interested in continuous modifications of the Hamiltonian that preserve its self-adjointness. This requirement is crucial, as we aim to study the stability of quantum symmetries under perturbations that do not compromise the unitarity of the evolution. One of the most natural types of perturbations is the linear one, namely

$$H(\varepsilon) = H + \varepsilon V. \tag{2.1}$$

However, the perturbation operator V cannot be arbitrary. In infinite-dimensional settings, even if V is self-adjoint, this does not guarantee that $H(\varepsilon)$ is self-adjoint. In fact, it may happen that $D(H) \cap D(V)$ is not dense in $\mathcal{H}$, or even trivial.

A well-known class of perturbations that ensures self-adjointness is that of H-bounded operators, which we define below.

Definition 2.1.1. *A linear operator V on $\mathcal{H}$ is said to be* H-bounded *if*

- *$D(H) \subseteq D(V)$;*
- *there exist nonnegative constants $a, b \geq 0$ such that for all $\psi \in D(H)$,*

$$\|V\psi\| \leq a\|H\psi\| + b\|\psi\|. \tag{2.2}$$

The greatest lower bound a_V of all admissible constants a in (2.2) *is called the* H-bound of *V.*

An equivalent condition to (2.2) is given by

$$\|V\psi\|^2 \leq a'^2 \|H\psi\|^2 + b'^2 \|\psi\|^2 \quad \forall \psi \in D(H), \tag{2.3}$$

where the constants a', b' are in general different from a, b in (2.2).

The Kato–Rellich theorem ensures the self-adjointness of the perturbed Hamiltonian $H + \varepsilon V$, provided that V is a symmetric H-bounded operator and $\varepsilon \in \mathbb{R}$ is small enough [20].

Theorem 2.1.1 (Kato–Rellich)**.** *Let V be a symmetric and H-bounded operator with H-bound a_V. Then for all $\varepsilon \in \mathbb{R}$ such that $|\varepsilon| a_V < 1$, the operator $H + \varepsilon V$ is self-adjoint on $D(H)$.*

Proof. To prove the self-adjointness of $H + \varepsilon V$, we use the standard criterion: it is enough to show that there exists $\lambda \in \mathbb{R}$ such that

$$\operatorname{Ran}(H + \varepsilon V \pm \mathrm{i}\lambda \mathbb{I}) = \mathcal{H}, \tag{2.4}$$

provided that $H + \varepsilon V$ is symmetric [10].

Clearly, $H + \varepsilon V$ is symmetric with domain $D(H)$. Since V is H-bounded, there exist constants $a, b \geq 0$ such that

$$\|V\psi\|^2 \leq a^2\|H\psi\|^2 + b^2\|\psi\|^2, \quad \forall\psi \in D(H). \tag{2.5}$$

Now observe that

$$a^2\|H\psi\|^2 + b^2\|\psi\|^2 = \|(aH \mp \mathrm{i}b)\psi\|^2, \tag{2.6}$$

so that (2.5) implies

$$\|V\psi\| \leq \|(aH \mp \mathrm{i}b)\psi\|, \quad \forall\psi \in D(H). \tag{2.7}$$

Let $c = b/a$, and fix $\varphi \in \mathcal{H}$. Since H is self-adjoint, the operator $H \mp \mathrm{i}c$ is surjective, so we can find $\psi \in D(H)$ such that

$$\varphi = (H \mp \mathrm{i}c)\psi. \tag{2.8}$$

Inverting this, we get

$$\psi = (H \mp \mathrm{i}c)^{-1}\varphi. \tag{2.9}$$

Plugging (2.9) into (2.7) yields

$$\|V(H \mp \mathrm{i}c)^{-1}\varphi\| \leq a\|\varphi\|, \tag{2.10}$$

which implies that the operator $B_{\pm} := V(H \mp \mathrm{i}c)^{-1}$ is bounded with

$$\|B_{\pm}\| \leq a. \tag{2.11}$$

Then the operator $\mathbb{I} - \varepsilon B_{\pm}$ is invertible for all $\varepsilon \in \mathbb{R}$ with $|\varepsilon|a < 1$, and hence maps $\mathcal{H}$ onto itself.

Now, observe that

$$H + \varepsilon V \mp \mathrm{i}c = (\mathbb{I} - \varepsilon B_{\pm})(H \mp \mathrm{i}c), \tag{2.12}$$

so that for all $\phi \in \mathcal{H}$,

$$\phi = (H + \varepsilon V \mp \mathrm{i}c)\alpha, \tag{2.13}$$

with

$$\alpha = (H \mp \mathrm{i}c)^{-1}(\mathbb{I} - \varepsilon B_{\pm})^{-1}\phi. \tag{2.14}$$

Therefore,

$$\mathrm{Ran}(H + \varepsilon V \mp \mathrm{i}c) = \mathcal{H}, \tag{2.15}$$

and $H + \varepsilon V$ is self-adjoint on $D(H)$. □

Example 2.1.1. Let H be the Hamiltonian of a one-dimensional harmonic oscillator with mass $m = 1$ and frequency $\omega = 1$ on the Hilbert space $L^2(\mathbb{R})$,

$$H = \frac{1}{2}\left(\hat{p}^2 + \hat{x}^2\right), \tag{2.16}$$

with domain $D(H) \subset H^2(\mathbb{R})$, [2] where $\hat{p} = -i\frac{d}{dx}$ is the momentum operator and $\hat{x}$ is the position operator. The Hamiltonian H has a discrete spectrum with simple eigenvalues

$$h_n = n + \frac{1}{2}, \quad n \in \mathbb{N}. \tag{2.17}$$

Let us consider the self-adjoint perturbation

$$V = \hat{p}, \tag{2.18}$$

with domain $D(V) = H^1(\mathbb{R})$.

We show that V is H-bounded and that its H-bound is 0. Indeed for all $\psi \in D(H)$ and $\delta > 0$, one has

$$\begin{aligned} \|\hat{p}\psi\|^2 &= \langle \hat{p}\psi|\hat{p}\psi\rangle = \langle \psi|\hat{p}^2\psi\rangle \leq \langle \psi|(\hat{p}^2 + \hat{x}^2)\psi\rangle \\ &= 2\langle \psi|H\psi\rangle \leq 2\|\psi\|\,\|H\psi\| \\ &\leq \delta^2\|H\psi\|^2 + \frac{1}{\delta^2}\|\psi\|^2 + 2\|\psi\|\,\|H\psi\| \\ &= \left(\delta\|H\psi\| + \frac{1}{\delta}\|\psi\|\right)^2. \end{aligned} \tag{2.19}$$

By taking the square root, one gets

$$\|\hat{p}\psi\| \leq \delta\|H\psi\| + \frac{1}{\delta}\|\psi\|, \tag{2.20}$$

for all positive δ arbitrarily small. Then

$$a_V = \inf_{\delta > 0} \delta = 0. \tag{2.21}$$

Obviously, if a symmetric operator V is bounded (which is always the case in finite-dimensional Hilbert spaces), then it is automatically self-adjoint, has H-bound zero, and the Kato–Rellich theorem applies for all $\varepsilon \in \mathbb{R}$.

2.2 $\mathcal{P}$-robustness

Consider a set $\mathcal{P}$ of symmetric operators with H-bound less than 1. Then, $H + \varepsilon V$ is self-adjoint for all $|\varepsilon| < 1$ and $V \in \mathcal{P}$. We want to classify the symmetries in terms of their

[2] Here $H^\ell(\mathbb{R})$ denotes the Sobolev space of order ℓ, that is, the space of functions $\psi \in L^2(\mathbb{R})$ whose weak derivatives up to order ℓ also belong to $L^2(\mathbb{R})$.

large-time evolution with respect to the family of perturbed Hamiltonians

$$H(\varepsilon) := H + \varepsilon V, \qquad \varepsilon \in (-1, 1), \tag{2.22}$$

with $V \in \mathcal{P}$, according to the following definition.

Definition 2.2.1. *Let $S \in \{H\}'$ be a symmetry of the Hamiltonian H, and let the* set $\mathcal{P}$ of perturbations of H *be a set of H-bounded symmetric operators.*

- *S is* $\mathcal{P}$-robust *if for all $V \in \mathcal{P}$ and for all $\psi \in \mathcal{H}$:*

$$\sup_{t\in\mathbb{R}} \left\| \left(\mathrm{e}^{\mathrm{i}t(H+\varepsilon V)} S \mathrm{e}^{-\mathrm{i}t(H+\varepsilon V)} - S\right)\psi \right\| \to 0, \quad \text{as } \varepsilon \to 0. \tag{2.23}$$

  The set of all $\mathcal{P}$-robust symmetries is denoted with $\mathcal{R}_{\mathcal{P}}(H)$. It contains the set $\hat{\mathcal{R}}_{\mathcal{P}}(H)$ of $\mathcal{P}$-unbroken *symmetries, for which $\mathrm{e}^{\mathrm{i}t(H+\varepsilon V)} S \mathrm{e}^{-\mathrm{i}t(H+\varepsilon V)} = S$.*

- *S is* $\mathcal{P}$-fragile *if it is not $\mathcal{P}$-robust, i.e. if there exists a perturbation $V \in \mathcal{P}$ and a vector $\psi \in \mathcal{H}$ such that*

$$\limsup_{\varepsilon\to 0} \left[\sup_{t\in\mathbb{R}} \left\| \left(\mathrm{e}^{\mathrm{i}t(H+\varepsilon V))} S \mathrm{e}^{-\mathrm{i}t(H+\varepsilon V)} - S\right)\psi \right\|\right] > 0. \tag{2.24}$$

- *If $\mathcal{P}$ contains only one element, namely $\mathcal{P} = \{V\}$, we say that S is V-*robust.

- *If $\mathcal{P}$ is the set of all symmetric and H-bounded operators, that is, if S is V-robust for all symmetric H-bounded perturbations V, we say that S is a* completely robust *symmetry. The set of all completely robust symmetries is denoted by $\mathcal{R}(H)$.*

In other words, a symmetry S is $\mathcal{P}$-robust if $\mathrm{e}^{\mathrm{i}t(H+\varepsilon V)} S \mathrm{e}^{-\mathrm{i}t(H+\varepsilon V)}\psi$ remains close, for small ε, to its unperturbed value $\mathrm{e}^{\mathrm{i}tH} S \mathrm{e}^{-\mathrm{i}tH}\psi = S\psi$ for every time $t \in \mathbb{R}$, for every possible perturbation $V \in \mathcal{P}$ and for every possible state $\psi \in \mathcal{H}$, that is

$$\mathrm{e}^{\mathrm{i}t(H+\varepsilon V)} S \mathrm{e}^{-\mathrm{i}t(H+\varepsilon V)} \approx S, \quad \text{for } |\varepsilon| \ll 1, \quad \text{uniformly in time } t. \tag{2.25}$$

In particular, S is $\mathcal{P}$-unbroken if it remains a symmetry of all the perturbed Hamiltonians, namely $\mathrm{e}^{\mathrm{i}t(H+\varepsilon V)} S \mathrm{e}^{-\mathrm{i}t(H+\varepsilon V)} = S$ for all times $t \in \mathbb{R}$ and perturbations $V \in \mathcal{P}$.

On the other hand, S is $\mathcal{P}$-fragile if, however small ε is, there is a perturbation $V \in \mathcal{P}$ and a vector $\psi \in \mathcal{H}$ such that $\mathrm{e}^{\mathrm{i}t(H+\varepsilon V)} S \mathrm{e}^{-\mathrm{i}t(H+\varepsilon V)}\psi$ drifts away from $S\psi$ and their distance accumulates over time.

In the next section we will study in detail the robustness of a symmetry against a single perturbation.

2.3 Robustness against a single perturbation

In order to perform our analysis on the symmetries, we introduce an assumption on the unperturbed self-adjoint Hamiltonian H: we assume that H has *compact resolvent*, i.e. $(H-z)^{-1}$ is a compact operator for some $z \in \mathbb{C}$. In such a case the spectrum of H consists entirely of isolated eigenvalues with finite multiplicity and its spectral decomposition reads

$$H\psi = \sum_{k\geq 1} h_k P_k \psi, \qquad \forall \psi \in D(H), \tag{2.26}$$

where $\{h_k\}_{k\geq 1} \subseteq \mathbb{R}$ are the distinct eigenvalues of H and $\{P_k\}_{k\geq 1}$ are its finite-rank eigenprojections:

$$P_k^\dagger = P_k, \quad P_k P_\ell = \delta_{kl} P_k, \quad \forall k, \ell \geq 1, \qquad \sum_{k\geq 1} P_k \psi = \psi, \quad \forall \psi \in \mathcal{H}. \tag{2.27}$$

A paradigmatic example that can be kept in mind is the Hamiltonian of the (n-dimensional isotropic) harmonic oscillator. Obviously, if the Hilbert space $\mathcal{H}$ is finite dimensional all Hamiltonians have compact resolvent.

Now we recall an important result on the spectral properties of the family $\{H(\varepsilon)\}_{\varepsilon\in(-1,1)}$ of perturbations of H [20].

Theorem 2.3.1 (Kato). *Let H be a self-adjoint operator with compact resolvent and spectral resolution* (2.26)*. Let V be a symmetric operator with H-bound less than 1. Then,*

1. *for all $\varepsilon \in (-1,1)$, the perturbed Hamiltonian $H(\varepsilon)$ in (2.22) has compact resolvent and its spectral decomposition reads*

$$H(\varepsilon)\psi = \sum_{n\geq 1} h_n(\varepsilon) P_n(\varepsilon)\psi, \qquad \forall \psi \in D(H), \tag{2.28}$$

   where $\{h_n(\varepsilon)\}_{n\geq 1}$ are the eigenvalues of $H(\varepsilon)$ and $\{P_n(\varepsilon)\}_{n\geq 1}$ are its finite-rank eigenprojections;

2. *for all $n \geq 1$, the maps $\varepsilon \in (-1,1) \mapsto h_n(\varepsilon) \in \mathbb{R}$, and $\varepsilon \in (-1,1) \mapsto P_n(\varepsilon) \in B(\mathcal{H})$, are analytic, with $h_n(\varepsilon) \neq h_m(\varepsilon)$ for $n \neq m$ and $\varepsilon \neq 0$;*

3. *the family $\{P_n(0)\}_{n\geq 1}$ is a family of subprojections of $\{P_k\}_{k\geq 1}$, namely for all $n \geq 1$ there is a unique $k \geq 1$ such that $P_n(0)P_k = P_k P_n(0) = P_n(0)$, so that $Ran(P_n(0)) \subseteq Ran(P_k)$.*

We are ready to give a complete algebraic characterization of all the V-robust symmetries.

Theorem 2.3.2. *Let H be a self-adjoint compact-resolvent operator and V be symmetric and H-bounded. Consider a symmetry $S \in \{H\}'$. Then*

1. *S is V-robust if and only if*

$$[S, P_n(0)] = 0, \quad \text{for all } n \geq 1, \tag{2.29}$$

where $\{P_n(\varepsilon)\}_{n\geq 1}$ are the eigenprojections of the perturbed Hamiltonian $H + \varepsilon V$;

2. *if V commutes with H and is self-adjoint, then S is V-robust if and only if $S \in \{V\}'$, i.e. S is V-unbroken.*

Furthermore, the set of V-robust symmetries

$$\mathcal{R}_{\{V\}}(H) = \{P_n(0) : n \geq 1\}' \tag{2.30}$$

is a von Neumann algebra with

$$\{H\}'' \subseteq \mathcal{R}_{\{V\}}(H) \subseteq \{H\}'. \tag{2.31}$$

and, if $V = V^\dagger$,

$$\{H, V\}' \subset \mathcal{R}_{\{V\}}(H). \tag{2.32}$$

Remark 2.3.1. In point (*ii*) of the previous theorem the expression V *commutes with* H means that the evolution groups they generate commute, i.e. $[\mathrm{e}^{\mathrm{i}tH}, \mathrm{e}^{\mathrm{i}sV}] = 0$ for all $t, s \in \mathbb{R}$. Clearly in such a case it is crucial that V be self-adjoint, and not simply symmetric, in order to define the evolution group generated by V, as well as its commutant $\{V\}'$ (see Chapter 1, Sec. 1.3).

Remark 2.3.2. In the case under consideration of a pure-point Hamiltonian H the bicommutant $\{H\}''$ in (1.52) reduces to the von Neumann algebra generated by the eigenprojections of H, namely,

$$\{H\}'' = \{P_k : k \geq 1\}'' = \Big\{\sum_{k\geq 1} a_k P_k \,:\, (a_k)_{k\geq 1} \in \ell^\infty\Big\}, \tag{2.33}$$

where the convergence of the series is in the strong topology.

The symmetries of the Hamiltonian H are the bounded operators which commute with the Hamiltonian H, or equivalently with (the Abelian von Neumann algebra $\{H\}''$ generated by) the family of its eigenprojections $\{P_k\}_{k\geq 1}$. On the other hand, the V-robust symmetries are the ones which commute with (the larger Abelian von Neumann algebra generated by) the subprojections $\{P_n(0)\}_{n\geq 1}$ of $\{P_k\}_{k\geq 1}$ induced by V.

The robust symmetries form a von Neumann algebra: thus the product and the linear combination of robust symmetries is still robust and so is the (strong) limit of a sequence of robust symmetries.

Theorem 2.3.2 is a corollary, via Kato's Theorem 2.3.1, of the following more general result concerning the stability of symmetries against a broader class of continuous self-adjoint deformations of H. We refer to such deformations as *admissible*, and we define them below.

Definition 2.3.1. (Admissible deformation) *Let H be a self-adjoint operator with purely point spectrum. Let I be a real neighborhood of 0. Let $\varepsilon \in I \mapsto H(\varepsilon)$ be a deformation of H. We say that $H(\varepsilon)$ is an admissible deformation if*

1. *$H(\varepsilon)\psi = \sum_{n\geq 1} h_n(\varepsilon)\, P_n(\varepsilon)\psi$, for all $\psi \in D(H)$ and all $\varepsilon \in I$;*

2. *$\varepsilon \mapsto h_n(\varepsilon)$ are continuous real-valued functions, with $h_n(\varepsilon) \neq h_m(\varepsilon)$ for $n \neq m$ and all $\varepsilon \in I \setminus \{0\}$;*

3. *$\{P_n(\varepsilon)\}_{n\geq 1}$ is a complete orthogonal family of projections, and there exists a strongly continuous family of unitary operators $U(\varepsilon)$ such that*

$$P_n(\varepsilon) = U(\varepsilon)\, P_n(0)\, U(\varepsilon)^\dagger \qquad \text{for all } \varepsilon \in I. \tag{2.34}$$

The following theorem generalizes Theorem 2.3.2 to admissible deformations.

Theorem 2.3.3. *Let H be a pure-point self-adjoint operator. Let I be a real neighborhood of 0. Let $\varepsilon \in I \mapsto H(\varepsilon)$ be an admissible deformation of H,*

Let S be a symmetry of H, i.e. $S \in \{H\}'$. Then,

$$\sup_{t\in\mathbb{R}} \left\| \left(\mathrm{e}^{\mathrm{i}tH(\varepsilon)} S \mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - S\right) \psi \right\| \to 0, \quad \text{as } \varepsilon \to 0, \tag{2.35}$$

for all $\psi \in \mathcal{H}$, if and only if

$$S \in \{P_n(0) : n \geq 1\}'. \tag{2.36}$$

When (2.35) *holds, we say that the symmetry S is* robust against the deformation $H(\varepsilon)$.

Remark 2.3.3. Here we consider deformations $H(\varepsilon)$ of a pure-point Hamiltonian H (not assumed to have a compact resolvent), which are not necessarily of the form (2.22), whence $H(\varepsilon)$ are no longer guaranteed to have a compact resolvent. However, their spectrum is still required to be pure point, but the eigenvalues can have finite accumulation points and infinite degeneracy. Finally, the eigenvalues and the eigenprojections are only required to be continuous.

The proofs of Theorems 2.3.2 and 2.3.3 are postponed to Subsection 2.3.3, after proving two preliminary lemmas. The first one deals with the construction of an eternal block-diagonal approximation of the deformed Hamiltonian $H(\varepsilon)$ in Theorem 2.3.3, which generates a unitary group commuting with the one generated by H (and then block-diagonal), and approximating the group generated by $H(\varepsilon)$ uniformly in time (eternally). The second lemma regards the splitting of the perturbed evolution of a symmetry in two parts: a fragile component and a robust one.

2.3.1 Eternal Block-Diagonal Approximation

Consider a continuous deformation $\varepsilon \in I \mapsto H(\varepsilon)$ of a pure-point self-adjoint operator H, as in Theorem 2.3.3. For all $\varepsilon \in I$ define the self-adjoint operator

$$\tilde{H}(\varepsilon) := U(\varepsilon)^\dagger H(\varepsilon) U(\varepsilon) = \sum_{n\geq 1} h_n(\varepsilon) P_n(0), \tag{2.37}$$

on the domain $U(\varepsilon)^\dagger D(H)$, and consider the unitary group $t \mapsto \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)}$ it generates. We now show that this group is an approximation of $t \mapsto \mathrm{e}^{-\mathrm{i}tH(\varepsilon)}$ uniform in time.

Lemma 2.3.1. *Let $\varepsilon \mapsto H(\varepsilon)$ be an admissible continuous deformation of a pure-point self-adjoint operator H, as in Theorem 2.3.3. Then, for all $\psi \in \mathcal{H}$,*

$$\sup_{t\in\mathbb{R}} \left\| \left(\mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)} \right) \psi \right\| \to 0, \quad \text{as } \varepsilon \to 0. \tag{2.38}$$

Proof. Let $\psi \in \mathcal{H}$ and $t \in \mathbb{R}$, we have that

$$\begin{aligned}
\left\| (\mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)})\psi \right\| &= \left\| (U(\varepsilon)\mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)} U(\varepsilon)^\dagger - \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)})\psi \right\| \\
&= \left\| \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)} U(\varepsilon)^\dagger - U(\varepsilon)^\dagger \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)} \right\| \qquad (2.39) \\
&= \left\| \left[\mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)}, U(\varepsilon)^\dagger \right] \psi \right\| \qquad (2.40) \\
&= \left\| \left[\mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)}, U(\varepsilon)^\dagger - \mathbb{I} \right] \psi \right\| \\
&\leq \|(U(\varepsilon) - \mathbb{I})\psi\| + \left\| (U(\varepsilon) - \mathbb{I})\mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)}\psi \right\|, \qquad (2.41)
\end{aligned}$$

where in the step (2.39) we use the invariance of the norm under unitary operator, in step (2.40) the fact that the identity operator commutes with everything and in the step (2.41) the triangular inequality.

Since $H(\varepsilon)$ is an admissible deformation, by property (*iii*) of Definition 2.3.1 we have that $\|(U(\varepsilon) - \mathbb{I})\psi\| \to 0$, as $\varepsilon \to 0$. Let us consider the second term of (2.41) and the resolution of the identity applied to ψ:

$$\psi = \sum_{n\geq 1} P_n(0)\psi.$$

For all $N \in \mathbb{N}^*$, we can write

$$\psi = \psi_{\leq N} + \psi_{>N}, \tag{2.42}$$

where

$$\psi_{\leq N} = \sum_{n=1}^{N} P_n(0)\psi, \qquad \psi_{>N} = \sum_{n=N+1}^{+\infty} P_n(0)\psi, \tag{2.43}$$

and

$$\|\psi_{>N}\| \to 0, \quad \text{as } N \to \infty, \tag{2.44}$$

since the series has to converge. By plugging (2.42) into the second term of (2.41), we get:

$$\begin{aligned}
\left\|(U(\varepsilon)-\mathbb{I})\mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)}\psi\right\| &= \left\|(U(\varepsilon)-\mathbb{I})\mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)}(\psi_{\le N}+\psi_{>N})\right\| \\
&\le \left\|(U(\varepsilon)-\mathbb{I})\mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)}\psi_{\le N}\right\| + \|U(\varepsilon)-\mathbb{I}\|\,\|\psi_{>N}\| \qquad (2.45)\\
&\le \left\|(U(\varepsilon)-\mathbb{I})\mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)}\psi_{\le N}\right\| + 2\,\|\psi_{>N}\| \\
&\le \left\|(U(\varepsilon)-\mathbb{I})\mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)}\sum_{n=1}^{N}P_n(0)\psi\right\| + 2\,\|\psi_{>N}\| \\
&= \left\|\sum_{n=1}^{N}\mathrm{e}^{-\mathrm{i}th_n(\varepsilon)}(U(\varepsilon)-\mathbb{I})P_n(0)\psi\right\| + 2\,\|\psi_{>N}\| \\
&\le \sum_{n=1}^{N}\|(U(\varepsilon)-\mathbb{I})P_n(0)\psi\| + 2\,\|\psi_{>N}\|,
\end{aligned}$$

where in step (2.45) we have used that

$$\|U(\varepsilon)-\mathbb{I}\| \le \|U(\varepsilon)\| + 1 = 2, \tag{2.46}$$

since $U(\varepsilon)$ is unitary.

Let $\eta > 0$, then by (2.44) there is $N_0 > 0$ such that

$$\|\psi_{>N_0}\| < \frac{\eta}{6},$$

Moreover, by the strong continuity of $\varepsilon \mapsto U(\varepsilon)$, there is $\varepsilon_0 > 0$ such that for all $\varepsilon \in I$, with $|\varepsilon| < \varepsilon_0$, and for all $n = 1, \dots, N_0$:

$$\|(U(\varepsilon)-\mathbb{I})P_n(0)\psi\| < \frac{\eta}{3N_0},$$

and

$$\|(U(\varepsilon)-\mathbb{I})\psi\| < \frac{\eta}{3}.$$

Then for all $|\varepsilon| < \varepsilon_0$:

$$\begin{aligned}
\left\|(\mathrm{e}^{-\mathrm{i}tH(\varepsilon)}-\mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)})\psi\right\| &\le \|(U(\varepsilon)-\mathbb{I})\psi\| + \left\|(U(\varepsilon)-\mathbb{I})\mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)}\psi\right\| \\
&\le \|(U(\varepsilon)-\mathbb{I})\,\psi\| + \sum_{n=1}^{N_0}\|(U(\varepsilon)-\mathbb{I})P_n(0)\psi\| + 2\,\|\psi_{>N_0}\| \\
&< \frac{\eta}{3} + N_0\frac{\eta}{3N_0} + 2\frac{\eta}{3} \\
&= \frac{\eta}{3} + \frac{\eta}{3} + \frac{\eta}{3} = \eta.
\end{aligned}$$

This proves the limit (2.38). □

Remark 2.3.4. The proof of Lemma 2.3.1 is based on the property

$$\sup_{t\in\mathbb{R}} \left\| (U(\varepsilon) - \mathbb{I}) \, \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)} \psi \right\| \to 0, \quad \text{as } \varepsilon \to 0, \qquad \forall \psi \in \mathcal{H}. \tag{2.47}$$

For this property to hold the assumption of pure-point spectrum of $H(\varepsilon)$, and thus of $\tilde{H}(\varepsilon)$, is crucial. Indeed, if the Hamiltonian has a pure-point spectrum, the orbit of a generic $\psi \in \mathcal{H}$ has a compact closure (see e.g. [17]). In such a case a vector, during its evolution, spends most of the time, apart a small error uniform in time, in a finite-dimensional manifold. Then the operation of taking the supremum over time does not span the full Hilbert space, but just a finite-dimensional submanifold, where (2.47) is trivially satisfied because of the strong continuity of $\{U(\varepsilon)\}_{\varepsilon\in I}$. On the other hand, when the spectrum is not pure point such property is not in general satisfied.

2.3.2 Fragile and robust components of a symmetry

In the following lemma we split the evolution of a symmetry with respect to the perturbed dynamics in two parts: a fragile component and a robust one.

Lemma 2.3.2. *Let H and $H(\varepsilon)$ be as in Theorem 2.3.3 and $\tilde{H}(\varepsilon)$ be as in* (2.37). *Let $S \in \{H\}'$ be a symmetry of the Hamiltonian H. Define for all $\varepsilon \in I$ and $t \in \mathbb{R}$*

$$A(t,\varepsilon) := \mathrm{e}^{\mathrm{i}tH(\varepsilon)} \left[S, \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)} \right], \tag{2.48}$$

$$B(t,\varepsilon) := \mathrm{e}^{\mathrm{i}tH(\varepsilon)} \left[S, \mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)} \right], \tag{2.49}$$

so that

$$\mathrm{e}^{\mathrm{i}tH(\varepsilon)} S \mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - S = A(t,\varepsilon) + B(t,\varepsilon). \tag{2.50}$$

Then for all $\psi \in \mathcal{H}$,

$$\sup_{t\in\mathbb{R}} \| B(t,\varepsilon)\psi \| \to 0, \quad \text{as } \varepsilon \to 0. \tag{2.51}$$

Remark 2.3.5. As Eq. (2.51) makes clear, the operator $B(t,\varepsilon)$ describes a robust component of the perturbed evolution of S. Indeed, its contribution is negligible, uniformly in time, for ε sufficiently small. On the other hand, as we will see, $A(t,\varepsilon)$ is responsible for a possible non-negligible divergence of the symmetry from its initial value. For this reason it represents a fragile component of the evolution of S.

Let us prove Lemma 2.3.2.

Proof. Let $\varepsilon \in I$, $t \in \mathbb{R}$, and $\psi \in \mathcal{H}$, then

$$\begin{aligned} \mathrm{e}^{\mathrm{i}tH(\varepsilon)} S \mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - S &= \mathrm{e}^{\mathrm{i}tH(\varepsilon)} \left[S, \mathrm{e}^{-\mathrm{i}tH(\varepsilon)} \right] \\ &= \mathrm{e}^{\mathrm{i}tH(\varepsilon)} \left[S, \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)} \right] + \mathrm{e}^{\mathrm{i}tH(\varepsilon)} \left[S, \mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)} \right] \\ &= A(t,\varepsilon) + B(t,\varepsilon). \end{aligned}$$

Moreover,

$$\begin{aligned}
\|B(t,\varepsilon)\psi\| &= \left\| \mathrm{e}^{\mathrm{i}tH(\varepsilon)} \left[S, \mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)} \right] \psi \right\| \\
&= \left\| \left[S, \mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)} \right] \psi \right\| \\
&\leq \left\| S \left(\mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)} \right) \psi \right\| + \left\| \left(\mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)} \right) S\psi \right\| \\
&\leq \|S\| \left\| \left(\mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)} \right) \psi \right\| + \left\| \left(\mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)} \right) S\psi \right\| .
\end{aligned}$$

Thus, by using Lemma 2.3.1, we get the thesis (2.51). □

2.3.3 Proof of Theorems

We are now ready to prove the two main theorems of this section. We start with Theorem 2.3.3, and then we will prove Theorem 2.3.2.

Proof of Theorem 2.3.3. We want to prove that if S is robust against the admissible deformation $H(\varepsilon)$, namely if (2.35) holds, then S commutes with $P_n(0)$ for all $n \geq 1$. We prove the negation of such implication, namely we assume that there exists $n \geq 1$ such that $[S, P_n(0)] \neq 0$ and show that this implies that S is fragile, i.e. (2.35) does not hold.

Since $[S, P_n(0)] \neq 0$, there exists an integer $m \neq n$ such that $P_m(0) S P_n(0) \neq 0$ or $P_n(0) S P_m(0) \neq 0$. Let us assume, for definiteness, that the first inequality holds, and thus that there exist two unit vectors $\psi_n \in P_n(0)\mathcal{H}$ and $\psi_m \in P_m(0)\mathcal{H}$, such that

$$\langle \psi_m \,|\, S\psi_n \rangle \neq 0.$$

Let $\varepsilon \in I$ and $t \in \mathbb{R}$. By Lemma 2.3.2 we have that

$$\begin{aligned}
\left\| \left(\mathrm{e}^{\mathrm{i}tH(\varepsilon)} S \mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - S \right) \psi_n \right\| &= \| (A(t,\varepsilon) + B(t,\varepsilon))\, \psi_n \| \\
&\geq \left| \|A(t,\varepsilon)\psi_n\| - \|B(t,\varepsilon)\psi_n\| \right| ,
\end{aligned}$$

with

$$\sup_{t\in\mathbb{R}} \|B(t,\varepsilon)\psi_n\| \to 0, \quad \text{as } \varepsilon \to 0.$$

On the other hand, by (2.48),

$$\begin{aligned}
\|A(t,\varepsilon)\psi_n\| &= \left\| \mathrm{e}^{\mathrm{i}tH(\varepsilon)} \left[S, \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)} \right] \psi_n \right\| = \left\| \left[S, \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)} \right] \psi_n \right\| \\
&= \left\| \left(\mathrm{e}^{\mathrm{i}t\tilde{H}(\varepsilon)} S \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)} - S \right) \psi_n \right\| \\
&= \left\| \left(\mathrm{e}^{\mathrm{i}t\tilde{H}(\varepsilon)} S \mathrm{e}^{-\mathrm{i}th_n(\varepsilon)} - S \right) \psi_n \right\| \\
&= \sup_{\|\phi\|=1} \left| \left\langle \phi \,\middle|\, \left(\mathrm{e}^{\mathrm{i}t\tilde{H}(\varepsilon)} S \mathrm{e}^{-\mathrm{i}th_n(\varepsilon)} - S \right) \psi_n \right\rangle \right| ,
\end{aligned}$$

where we made use of $\tilde{H}(\varepsilon)\psi_n = h_n(\varepsilon)\psi_n$. By using the properties of the supremum and the equality $\tilde{H}(\varepsilon)\psi_m = h_m(\varepsilon)\psi_m$, we get

$$\begin{aligned} \|A(t,\varepsilon)\psi_n\| &\geq \left|\left\langle \psi_m \,\middle|\, \left(\mathrm{e}^{\mathrm{i}th_m(\varepsilon)} S \mathrm{e}^{-\mathrm{i}th_n(\varepsilon)} - S\right)\psi_n\right\rangle\right| \\ &= \left|\mathrm{e}^{\mathrm{i}t(h_m(\varepsilon)-h_n(\varepsilon))} - 1\right| \left|\langle \psi_m \,|\, S\psi_n\rangle\right| \\ &= 2\left|\sin\left(\frac{t(h_m(\varepsilon)-h_n(\varepsilon))}{2}\right)\right| \left|\langle \psi_m \,|\, S\psi_n\rangle\right| . \end{aligned}$$

Now,

$$\sup_{t\in\mathbb{R}} \left|\sin\left(\frac{t(h_m(\varepsilon)-h_n(\varepsilon))}{2}\right)\right| = 1,$$

for all $\varepsilon \in I \setminus \{0\}$, by property (ii) in Theorem 2.3.3. Therefore,

$$\liminf_{\varepsilon\to 0} \sup_{t\in\mathbb{R}} \left\|\left(\mathrm{e}^{\mathrm{i}tH(\varepsilon)} S \mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - S\right)\psi_n\right\| \geq 2\left|\langle \phi_m \,|\, S\psi_n\rangle\right| \neq 0,$$

and S is fragile against the deformation $H(\varepsilon)$.

Now we prove the converse implication. Suppose that $[S, P_n(0)] = 0$ for all $n \geq 1$. Then we get that $A(t,\varepsilon) = 0$ for all $\varepsilon \in I$ and $t \in \mathbb{R}$. Therefore, by using Lemma 2.3.2, we have:

$$\sup_{t\in\mathbb{R}} \left\|\left(\mathrm{e}^{\mathrm{i}tH(\varepsilon)} S \mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - S\right)\psi\right\| = \sup_{t\in\mathbb{R}} \|B(t,\varepsilon)\psi\| \to 0, \quad \text{as } \varepsilon \to 0,$$

for all $\psi \in \mathcal{H}$, i.e. S is robust against the deformation $H(\varepsilon)$. □

We end this subsection by finally proving Theorem 2.3.2.

Proof of Theorem 2.3.2. The theorem is a corollary of Theorem 2.3.3.

In order to prove (i), we will prove that $H(\varepsilon) = H + \varepsilon V$ is an admissible deformation of H, that is, we will show it satisfies the properties of the Definition 2.3.1. This is a consequence of Kato's perturbation Theorem 2.3.1.

Indeed, the property (i) of Definition 2.3.1 is the spectral resolution given in Theorem 2.3.1(i).

Moreover, by Theorem 2.3.1(ii), $\varepsilon \mapsto h_n(\varepsilon)$ are analytic for $\varepsilon \in (-1,1)$ and $h_n(\varepsilon) \neq h_m(\varepsilon)$ for $n \neq m$ and $\varepsilon \neq 0$. Therefore, they are continuous and there exists an interval $I \subseteq (-1,1)$ with $0 \in I$ such that $h_n(\varepsilon) \neq h_m(\varepsilon)$ for $\varepsilon \in I \setminus \{0\}$, and (ii) of Definition 2.3.1 is satisfied.

It remains to prove that Definition 2.3.1(iii) holds too. For all $\varepsilon \in (-1,1)$ consider the operator

$$W(\varepsilon) = \sum_{n\geq 1} P_n(\varepsilon) P_n(0),$$

implementing the following transformations between the spectral projections $P_m(\varepsilon)$ and $P_m(0)$: for all $m \geq 1$

$$W(\varepsilon)P_m(0) = P_m(\varepsilon)P_m(0) = P_m(\varepsilon)W(\varepsilon).$$

In general $W(\varepsilon)$ is not a unitary operator. However, following Kato [20, Secs. 4.6 and 6.8], we can define the operator

$$U(\varepsilon) = \sum_{n\geq 1} P_n(\varepsilon)P_n(0)(\mathbb{I} - R_n(\varepsilon))^{-1/2},$$

where

$$R_n(\varepsilon) = (P_n(\varepsilon) - P_n(0))^2$$

and

$$(\mathbb{I} - R_n(\varepsilon))^{-1/2} = \sum_{j\geq 0} \binom{-1/2}{j} R_n(\varepsilon), \tag{2.52}$$

which is well defined for $\|R_n(\varepsilon)\|<1$. The operator $R_n(\varepsilon)$ commutes with both $P_n(\varepsilon)$ and $P_n(0)$. Indeed

$$\begin{aligned} R_n(\varepsilon)P_n(0) &= (P_n(\varepsilon) - P_n(0))^2 P_n(0) \\ &= (P_n(\varepsilon) + P_n(0) - P_n(\varepsilon)P_n(0) - P_n(0)P_n(\varepsilon))P_n(0) \\ &= (P_n(\varepsilon)P_n(0) + P_n(0) - P_n(\varepsilon)P_n(0) - P_n(0)P_n(\varepsilon)P_n(0)) \\ &= P_n(0) - P_n(0)P_n(\varepsilon)P_n(0) \\ &= P_n(0) - P_n(0)P_n(\varepsilon)P_n(0) - P_n(0)P_n(\varepsilon) + P_n(0)P_n(\varepsilon) \\ &= P_n(0)R_n(\varepsilon). \end{aligned}$$

By proceeding in the same exactly way, one can show that $R_n(\varepsilon)P_n(\varepsilon) = P_n(\varepsilon)R_n(\varepsilon)$. It is possible to prove now that $U(\varepsilon)$ is a unitary operator. Indeed

$$\begin{aligned} U(\varepsilon)^\dagger U(\varepsilon) &= \sum_{n,m} P_n(0)P_n(\varepsilon)(\mathbb{I} - R_n(\varepsilon))^{-1/2}(\mathbb{I} - R_m(\varepsilon))^{-1/2}P_m(\varepsilon)P_m(0) \\ &= \sum_{n,m} (\mathbb{I} - R_n(\varepsilon))^{-1/2}(\mathbb{I} - R_m(\varepsilon))^{-1/2}P_n(0)P_n(\varepsilon)P_m(\varepsilon)P_m(0) \\ &= \sum_{n\geq 1} (\mathbb{I} - R_n(\varepsilon))^{-1}P_n(0)P_n(\varepsilon)P_n(0), \end{aligned}$$

where we have used the fact that $R_n(\varepsilon)$ commutes with both $P_n(0)$ and $P_m(\varepsilon)$ and the orthogonality of $\{P_n(\varepsilon)\}$. We can show now that

$$(\mathbb{I} - R_n(\varepsilon))^{-1}P_n(0)P_n(\varepsilon)P_n(0) = P_n(0), \tag{2.53}$$

which is equivalent to

$$P_n(0)P_n(\varepsilon)P_n(0) = (\mathbb{I} - R_n(\varepsilon))P_n(0). \tag{2.54}$$

Let us evaluate the right hand side of the previous equality.

$$\begin{aligned}(\mathbb{I} - R_n(\varepsilon))P_n(0) &= (\mathbb{I} - (P_n(\varepsilon) - P_n(0))^2)P_n(0) && (2.55)\\ &= (\mathbb{I} - P_n(\varepsilon) - P_n(0) + P_n(\varepsilon)P_n(0) + P_n(0)P_n(\varepsilon))P_n(0) && (2.56)\\ &= P_n(0) - P_n(\varepsilon)P_n(0) + P_n(\varepsilon)P_n(0) + P_n(0)P_n(\varepsilon)P_n(0) && (2.57)\\ &= P_n(0)P_n(\varepsilon)P_n(0). && (2.58)\end{aligned}$$

Then

$$U(\varepsilon)^\dagger U(\varepsilon) = \sum_{n\geq 1} P_n(0) = \mathbb{I}, \tag{2.59}$$

since the $P_n(0)$'s form a resolution of the identity. Similarly, one can obtain $U(\varepsilon)U(\varepsilon)^\dagger = \mathbb{I}$. Then $U(\varepsilon)$ is a unitary operator. Furthermore,

$$U(\varepsilon)P_n(0) = (\mathbb{I} - R_n(\varepsilon))^{-1/2}P_n(\varepsilon)P_n(0) = P_n(\varepsilon)U(\varepsilon) \tag{2.60}$$

Then, since $U(\varepsilon)$ is a unitary operator, we have

$$P_n(\varepsilon) = U(\varepsilon)P_n(0)U(\varepsilon)^\dagger. \tag{2.61}$$

It remains to prove that $U(\varepsilon)$ is strongly continuous at $\varepsilon = 0$, that is,

$$\lim_{\varepsilon\to 0} \|(U(\varepsilon) - \mathbb{I})\psi\| = 0, \qquad \text{for all } \psi \in \mathcal{H}. \tag{2.62}$$

Let $\psi \in \mathcal{H}$. Using the resolution of the identity associated with the family $\{P_n(0)\}_{n\geq 1}$, we write

$$\psi = \sum_{n\geq 1} P_n(0)\psi, \tag{2.63}$$

with convergence in norm. For every $N \in \mathbb{N}^*$, define

$$\psi_{\leq N} := \sum_{n=1}^{N} P_n(0)\psi, \qquad \psi_{>N} := \sum_{n=N+1}^{\infty} P_n(0)\psi, \tag{2.64}$$

so that

$$\psi = \psi_{\leq N} + \psi_{>N}. \tag{2.65}$$

Since the series converges, we have

$$\|\psi_{>N}\| \xrightarrow[N\to\infty]{} 0. \tag{2.66}$$

We now estimate

$$\|(U(\varepsilon)-\mathbb{I})\psi\| \leq \|(U(\varepsilon)-\mathbb{I})\psi_{\leq N}\| + \|(U(\varepsilon)-\mathbb{I})\psi_{>N}\| \tag{2.67}$$

$$\leq \sum_{n=1}^{N} \|(U(\varepsilon)-\mathbb{I})P_n(0)\psi\| + 2\,\|\psi_{>N}\|\,. \tag{2.68}$$

Using the definition

$$U(\varepsilon) := \sum_{n\geq 1}(\mathbb{I}-R_n(\varepsilon))^{-1/2}P_n(\varepsilon)P_n(0),$$

we obtain

$$(U(\varepsilon)-\mathbb{I})P_n(0)\psi = \left[(\mathbb{I}-R_n(\varepsilon))^{-1/2}P_n(\varepsilon)P_n(0)-P_n(0)\right]\psi. \tag{2.69}$$

By Kato's theorem 2.3.1, both $P_n(\varepsilon)$ and $R_n(\varepsilon) := (P_n(\varepsilon)-P_n(0))^2$ depend analytically on ε, and hence

$$\left\|\left[(\mathbb{I}-R_n(\varepsilon))^{-1/2}P_n(\varepsilon)P_n(0)-P_n(0)\right]\psi\right\| \xrightarrow[\varepsilon\to 0]{} 0. \tag{2.70}$$

Therefore, for every $\eta>0$, there exist $\varepsilon_0>0$ and $N_0\in\mathbb{N}$ such that for all $|\varepsilon|<\varepsilon_0$ and $1\leq n\leq N_0$,

$$\left\|\left[(\mathbb{I}-R_n(\varepsilon))^{-1/2}P_n(\varepsilon)P_n(0)-P_n(0)\right]\psi\right\| < \frac{\eta}{2N_0}, \tag{2.71}$$

and

$$\|\psi_{>N_0}\| < \frac{\eta}{4}. \tag{2.72}$$

Then, for all such ε, we conclude

$$\|(U(\varepsilon)-\mathbb{I})\psi\| \leq \sum_{n=1}^{N_0}\frac{\eta}{2N_0} + 2\cdot\frac{\eta}{4} = \frac{\eta}{2}+\frac{\eta}{2} = \eta, \tag{2.73}$$

which proves the desired strong continuity.

Therefore, $H(\varepsilon)=H+\varepsilon V$ is an admissible deformation of H and by Theorem 2.3.3 one gets (i).

Now we prove (ii). Since V and H commute and are both self-adjoint, we have that for all $\varepsilon\in I$ and $t\in\mathbb{R}$:

$$\mathrm{e}^{itH(\varepsilon)} = \mathrm{e}^{it(H+\varepsilon V)} = \mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{\mathrm{i}t\varepsilon V} = \mathrm{e}^{\mathrm{i}t\varepsilon V}\mathrm{e}^{\mathrm{i}tH}.$$

Hence for all $\psi\in\mathcal{H}$

$$\begin{aligned}
\sup_{t\in\mathbb{R}}\left\|\left(\mathrm{e}^{\mathrm{i}tH(\varepsilon)}S\mathrm{e}^{-\mathrm{i}tH(\varepsilon)}-S\right)\psi\right\| &= \sup_{t\in\mathbb{R}}\left\|\left(\mathrm{e}^{\mathrm{i}t\varepsilon V}\mathrm{e}^{\mathrm{i}tH}S\mathrm{e}^{-\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}t\varepsilon V}-S\right)\psi\right\| \\
&= \sup_{t\in\mathbb{R}}\left\|\left(\mathrm{e}^{\mathrm{i}t\varepsilon V}S\mathrm{e}^{-\mathrm{i}t\varepsilon V}-S\right)\psi\right\| \\
&= \sup_{\tau\in\mathbb{R}}\left\|\left(\mathrm{e}^{\mathrm{i}\tau V}S\mathrm{e}^{-\mathrm{i}\tau V}-S\right)\psi\right\| \\
&= \sup_{\tau\in\mathbb{R}}\left\|\left[\mathrm{e}^{\mathrm{i}\tau V},S\right]\psi\right\|
\end{aligned}$$

which is ε-independent and vanishes for all ψ if and only if $S \in \{V\}'$.

The last assertion is a direct consequence of (i) and definition (1.50), by noting that in this case the bicommutant of H is the von Neumann algebra generated by the eigenprojections P_n, and that $\{H, V\}' = \hat{\mathcal{R}}_{\{V\}}$ is the set of V-unbroken symmetries. □

Remark 2.3.6. According to Definition 2.2.1 a symmetry $S \in \{H\}'$ is V-fragile if

$$\limsup_{\varepsilon \to 0} \sup_{t \in \mathbb{R}} \left\| \left(\mathrm{e}^{\mathrm{i}t(H+\varepsilon V)} S \mathrm{e}^{-\mathrm{i}t(H+\varepsilon V)} - S \right) \psi \right\| > 0, \tag{2.74}$$

for some $\psi \in \mathcal{H}$. However, looking at the proof of Theorem 2.3.3, one gets that S is V-fragile if and only if

$$\liminf_{\varepsilon \to 0} \sup_{t \in \mathbb{R}} \left\| \left(\mathrm{e}^{\mathrm{i}t(H+\varepsilon V)} S \mathrm{e}^{-\mathrm{i}t(H+\varepsilon V)} - S \right) \psi \right\| > 0, \tag{2.75}$$

for some $\psi \in \mathcal{H}$.

2.4 $\mathcal{P}$-robustness and complete robustness

In Section 2.3, we have studied in detail the set of the symmetries robust against a single perturbation. In this section we want to characterize the set of the symmetries robust against an arbitrary set $\mathcal{P}$ of symmetric H-bounded perturbations.

As a consequence of Theorem 2.3.2 we have the following result:

Theorem 2.4.1. *Let $\mathcal{P}$ be a set of symmetric H-bounded perturbations and $S \in \{H\}'$ be a symmetry of the Hamiltonian H. Then, S is $\mathcal{P}$-robust if and only if*

$$[S, P_n^{(V)}(0)] = 0, \quad \textit{for all } n \geq 1 \textit{ and } V \in \mathcal{P}, \tag{2.76}$$

where $\{P_n^{(V)}(\varepsilon)\}_{n \geq 1}$ are the eigenprojections of the perturbed Hamiltonian $H + \varepsilon V$. Therefore,

$$\mathcal{R}_{\mathcal{P}}(H) = \bigcap_{V \in \mathcal{P}} \mathcal{R}_{\{V\}}(H), \tag{2.77}$$

with $\mathcal{R}_{\{V\}}(H) = \{P_n^{(V)}(0) \; : \; n \geq 1\}'$, is a von Neumann algebra of bounded operators containing the bicommutant $\{H\}''$.

As in the case of a single perturbation, the set of robust symmetries $\mathcal{R}_{\mathcal{P}}(H)$ forms a von Neumann algebra, thus it is closed with respect to the algebraic operations, as well as to taking the adjoint and taking strong limits. However, for a generic set $\mathcal{P}$ of perturbations $\mathcal{R}_{\mathcal{P}}(H)$ is no longer the commutant of an Abelian algebra and has a more complex structure, which depends on $\mathcal{P}$.

In the following two subsections we will look at the fine structure of the set of robust symmetries in the mathematical (and physical) interesting situation where the set of perturbations has itself a natural algebraic structure.

2.4.1 Symmetry-restricted perturbations

We want to analyze some interesting classes $\mathcal{P}$ of perturbations of the Hamiltonian H. There are plenty of physical situations where, by fundamental reasons, the dynamical laws of the system must be invariant under some symmetry group. Paradigmatic examples are given by the isotropy of space which implies rotational symmetry, or by the principle of relativity which implies relativistic invariance, etc. Those protected symmetries restricts the class of possible dynamics and thus of possible Hamiltonians H *and* their perturbations $\mathcal{P}$.

Let us consider n protected Hermitian symmetries $J_1, J_2, \dots, J_n \in \{H\}'$, that in general are not assumed to commute among themselves. In the above physical examples, these can be, e.g., the generators of the rotation group, or, in relativistic systems, of the Lorentz group.

What happens when the set of perturbations is made by the Hermitian operators of $\{J_1, J_2, \dots, J_n\}'$? This is exactly the largest set of perturbations that leave the above n symmetries unbroken. We are going to prove that the set $\mathcal{R}_\mathcal{P}(H)$ of robust symmetries against this kind of perturbations has a very nice algebraic structure.

We first consider the situation of a single protected symmetry. Let $J \in \{H\}'$ be a Hermitian symmetry of H and consider as set of perturbations $\mathcal{P} = \{J\}'_h$, the Hermitian elements of the commutant of J, which is the largest set of perturbations which keep J unbroken. This would be, for example, the case of a system with cylindrical symmetry where, say, $J = J_z$ is conserved. In such a case the set of robust symmetries (against this kind of perturbations) acquires the algebraic structure of a bicommutant.

Lemma 2.4.1. *Let H be self-adjoint with compact resolvent and $J \in \{H\}'$ be a Hermitian symmetry of H. Let $\mathcal{P} = \{J\}'_h$, where $\{J\}'_h$ are the Hermitian elements of $\{J\}'$. Then, a symmetry $S \in \{H\}'$ is $\mathcal{P}$-robust if and only if $S \in \{H, J\}''$, where*

$$\{H, J\}'' = \{Q_k \,:\, k \geq 1\}'' \tag{2.78}$$

is the bicommutant of H and J, with Q_k being the common eigenprojections of H and J. Therefore,

$$\mathcal{R}_\mathcal{P}(H) = \{H, J\}''. \tag{2.79}$$

Proof. We start by proving that if S is a $\mathcal{P}$-robust symmetry then $S \in \{H, J\}''$.

Notice first that, by von Neumann's bicommutant theorem

$$\{H, J\}'' = \{Q_k \,:\, k \geq 1\}'' = \Big\{ \sum_{k\geq 1} a_k Q_k \,:\, (a_k)_{k\geq 1} \in \ell^\infty \Big\}, \tag{2.80}$$

where the convergence of the series is in the strong topology. Consider perturbations in $V = V^\dagger \in \{H, J\}'$. Then $V\psi = \sum_{k\geq 1} Q_k V Q_k \psi$, for all $\psi \in \mathcal{H}$. Since V commutes with H, by Theorem 2.3.2(ii), we get that

$$[S, V] = 0, \quad \text{for all } V = V^\dagger \in \{H, J\}'. \tag{2.81}$$

By choosing $V = \sum_{k\geq 1}(1/k)Q_k$ we get

$$S = \sum_{k\geq 1} Q_k S Q_k,$$

in the strong topology. By choosing for any $k \geq 1$ the perturbation in the form $V = Q_k W Q_k$ with arbitrary $W = W^\dagger$ we get

$$[Q_k S Q_k, Q_k W Q_k] = 0, \quad \text{for all } W = W^\dagger \in B(\mathcal{H}),$$

which gives, according to Schur's lemma, $Q_k S Q_k = s_k Q_k$, for some $s_k \in \mathbb{R}$ with $|s_k| \leq \|S\|$. We conclude that

$$S = \sum_{k\geq 1} s_k Q_k \in \{H, J\}''.$$

Now we prove that if $S \in \{H, J\}''$ then S is a $\mathcal{P}$-robust symmetry, with $\mathcal{P} = \{J\}'_h$. According to (2.80), there is a sequence $(s_k)_{k\geq 1} \in \ell^\infty$ such that

$$S = \sum_{k\geq 1} s_k Q_k,$$

in the strong topology.

Let us fix a perturbation $V \in \{J\}'_h$. Since both H and V commute with J, then the same has to be true for $H(\varepsilon) = H + \varepsilon V$, with $\varepsilon \in I$. This clearly means that

$$[Q_k, P_n(\varepsilon)] = 0,$$

for $\varepsilon \in I$, $\varepsilon \neq 0$ and $n, k \geq 1$. By taking the limit $\varepsilon \to 0$ and by using the continuity of $P_n(\varepsilon)$, we get

$$[Q_k, P_n(0)] = 0.$$

Thus, for all $n \geq 1$ and $\psi \in \mathcal{H}$,

$$[S, P_n(0)]\, \psi = \sum_{k\geq 1} s_k \,[Q_k, P_n(0)]\, \psi = 0,$$

so that S is V-robust by Theorem 2.3.2(ii). By the arbitrariness of V we get the thesis. □

We are now ready to tackle the generic situation of an arbitrary family of protected symmetries.

Theorem 2.4.2. *Let H be self-adjoint with compact resolvent. Let $\mathcal{P} = \mathcal{J}'_h$, with $\mathcal{J} \subseteq \{H\}'_h$ being a family of Hermitian protected symmetries of H. Then*

$$\mathcal{R}_{\mathcal{P}}(H) = (\{H\} \cup \mathcal{J})''. \tag{2.82}$$

Proof. We are going to prove the double inclusion. First of all let us prove that $\mathcal{R}_{\mathcal{P}}(H) \supseteq$

$(\{H\} \cup \mathcal{J})''$.

Let $\mathcal{P}_J = \{J\}'_h$ for $J \in \mathcal{J}$. Since $\mathcal{P} = \mathcal{J}'_h = \bigcap_{J\in\mathcal{J}} \mathcal{P}_J$, every $\mathcal{P}_J$-robust symmetry is also $\mathcal{P}$-robust, that is

$$\bigcup_{J\in\mathcal{J}} \mathcal{R}_{\mathcal{P}_J}(H) \subseteq \mathcal{R}_{\mathcal{P}}(H).$$

Now, by the previous theorem we get that $\mathcal{R}_{\mathcal{P}_J}(H) = \{H, J\}''$, whence

$$\bigcup_{J\in\mathcal{J}} \{H, J\}'' \subseteq \mathcal{R}_{\mathcal{P}}.$$

Taking the bicommutant of both members, considering that $\mathcal{R}_{\mathcal{P}}$ is a von Neumann algebra, i.e. $\mathcal{R}''_{\mathcal{P}} = \mathcal{R}_{\mathcal{P}}$, we get

$$\Big(\bigcup_{J\in\mathcal{J}} \{H, J\}''\Big)'' \subseteq \mathcal{R}_{\mathcal{P}}.$$

By using the properties of the bicommutant we can compute the left hand side

$$\Big(\bigcup_{J\in\mathcal{J}} \{H, J\}''\Big)'' = \Big(\bigcup_{J\in\mathcal{J}} \{H, J\}\Big)'' = (\{H\} \cup \mathcal{J})''.$$

Then we have proved that

$$(\{H\} \cup \mathcal{J})'' \subseteq \mathcal{R}_{\mathcal{P}}.$$

Now we are going to prove that $\mathcal{R}_{\mathcal{P}} \subseteq (\{H\} \cup \mathcal{J})''$. Consider $S \in \mathcal{R}_{\mathcal{P}}$. We have to show that $[S, B] = 0$, for all $B \in (\{H\} \cup \mathcal{J})'$. Let us decompose B as

$$B = V_1 + \mathrm{i}V_2,$$

where

$$V_1 = \frac{B + B^\dagger}{2} \quad V_2 = \frac{B - B^\dagger}{2\mathrm{i}}.$$

Since H and $J \in \mathcal{J}$ are self-adjoint operators, $(\{H\} \cup \mathcal{J})'$ is a von Neumann algebra. Then since $B \in (\{H\} \cup \mathcal{J})'$, also $B^\dagger \in (\{H\} \cup \mathcal{J})'$ and then $V_i \in (\{H\} \cup \mathcal{J})'$, for $i = 1, 2$. Then, since S is $\mathcal{P}$-robust and $V_1, V_2 \in \mathcal{P}$ commute with H, by Theorem 2.3.2(ii) we have that

$$[S, V_1] = [S, V_2] = 0,$$

that is $[S, B] = 0$. Therefore,

$$\mathcal{R}_{\mathcal{P}} \subseteq (\{H\} \cup \mathcal{J})'',$$

and the theorem is proved. □

2.4.2 Completely robust symmetries

Finally, we provide a characterization of the completely robust symmetries of H, that are robust against unrestricted perturbations.

Theorem 2.4.3. *Let H be self-adjoint with compact resolvent. Let $S \in \{H\}'$ be a symmetry of H. Then S is a completely robust symmetry if and only if $S \in \{H\}''$, where $\{H\}''$ is the bicommutant* (2.33) *of the Hamiltonian H. Therefore,*

$$\mathcal{R}(H) = \{H\}''. \tag{2.83}$$

Proof. It follows from Lemma 2.4.1 with $J = \mathbb{I}$. □

The characterization of completely robust symmetries as the elements of the bicommutant of H, that are the bounded functions of the Hamiltonian, was proved in [11] for finite-dimensional quantum systems. Theorem 2.4.3 generalizes this result also to unbounded Hamiltonians with compact resolvent in an infinite-dimensional Hilbert space.

The extension of the validity of this characterization to unbounded Hamiltonians could have been anticipated. Indeed, heuristically, the long-time dynamics is expected to be unaffected by the ultraviolet (i.e. high energy) behavior of the Hamiltonian. And the assumption of compact resolvent, which allows the application of Kato's perturbation theorem and ensures the stability of the pure-point spectrum, is an infrared (i.e. low energy) condition on the spectrum of H.

2.5 Quantum adiabatic invariants

When the Hamiltonian of a quantum system is continuously deformed, a symmetry is in general no longer a conserved quantity with respect to the perturbed dynamics. However, if a symmetry is robust against the perturbation, it is possible to continuously deform it and obtain a new symmetry of the perturbed dynamics, called an *adiabatic invariant.*

Theorem 2.5.1. *Let $H(\varepsilon)$ be an admissible deformation of H as in Theorem 2.3.3 and let $\{U(\varepsilon)\}_{\varepsilon\in I}$ be the corresponding strongly continuous family of unitary operators. Let $S \in \{H\}'$ be a robust symmetry against the deformation $H(\varepsilon)$. We define for all $\varepsilon \in I$*

$$S_\varepsilon := U(\varepsilon) S U(\varepsilon)^\dagger. \tag{2.84}$$

Then S_ε is a symmetry for the system with Hamiltonian $H(\varepsilon)$, i.e. $S_\varepsilon \in \{H(\varepsilon)\}'$, for all $\varepsilon \in I$.

Proof. Let $\varepsilon \in I$. Since S is a robust symmetry, according to Theorem 2.3.3, S commutes with all the projections $\{P_n(0)\}_{n\geq 1}$, hence S commutes with $\tilde{H}(\varepsilon)$ in (2.37). Moreover, since

$H(\varepsilon) = U(\varepsilon)\tilde{H}(\varepsilon)U(\varepsilon)^\dagger$, then

$$\begin{aligned} e^{itH(\varepsilon)} S_\varepsilon e^{-itH(\varepsilon)} &= e^{itH(\varepsilon)} U(\varepsilon) S U(\varepsilon)^\dagger e^{-itH(\varepsilon)} \\ &= U(\varepsilon) e^{it\tilde{H}(\varepsilon)} S e^{-it\tilde{H}(\varepsilon)} U(\varepsilon)^\dagger \\ &= U(\varepsilon) S U(\varepsilon)^\dagger \\ &= S_\varepsilon. \end{aligned}$$

□

Remark 2.5.1. Equation (2.84) is just one possible definition of an adiabatic invariant. Indeed, it is enough to define for all $\varepsilon \in I$

$$S_\varepsilon := U(\varepsilon)\bar{S}_\varepsilon U(\varepsilon)^\dagger, \tag{2.85}$$

where $\bar{S}_\varepsilon$ is any operator in $\{\tilde{H}(\varepsilon)\}'$ such that

$$\bar{S}_\varepsilon \psi \to S\psi, \quad \text{as } \varepsilon \to 0, \qquad \forall \psi \in \mathcal{H}. \tag{2.86}$$

Such construction works if and only if S is a robust symmetry. This suggests an alternative definition of a robust symmetry: S is robust against the continuous deformation $H(\varepsilon)$ if it can be continuously deformed in such a way it is conserved with respect to the perturbed dynamics generated by $H(\varepsilon)$.

From this point of view a robust symmetry can be viewed as a symmetry which is not broken by the perturbations, but instead is only bent by them. In classical mechanics this is indeed the way in which one defines the invariant KAM tori [21].

Chapter 3

Wandering range of Quantum Adiabatic Invariants

In the previous chapter, we defined robust symmetries against perturbations and provided a precise algebraic characterization for admissible deformations of the unperturbed Hamiltonian.

In this chapter, we introduce the concept of the *wandering range* of a robust symmetry. Roughly speaking, this quantity measures the maximal deviation of a given robust symmetry throughout the entire perturbed evolution. It depends on the strength ε of the perturbation and vanishes as $\varepsilon \to 0$. However, in general, this dependence is not linear in ε, as will be illustrated by an explicit example.

We then address the following question: under which conditions is the wandering range of a robust symmetry linear in the strength of the perturbation? This behavior may clearly depend on the specific symmetry under consideration, on the nature of the perturbation, and/or on the particular state on which the wandering range is evaluated.

In the first part of the chapter, we study the wandering range on eigenvectors of the unperturbed Hamiltonian and for finite-rank symmetries. In both cases, we show that—under the assumption of admissible perturbations and an additional technical hypothesis—the wandering range is of order ε.

In the final part, we examine the wandering range of completely robust symmetries under bounded perturbations. Also in this setting, we find that the wandering range is of order ε. Remarkably, in this case, it is not necessary to assume admissible perturbations: it is sufficient for the unperturbed Hamiltonian to have a purely point spectrum with a spectral gap, without imposing any specific condition on the spectrum of the perturbed Hamiltonian [14].

3.1 Wandering range and adiabatic invariants

According to Definition 2.2.1, a symmetry S is V-robust if, for all $\varphi \in \mathcal{H}$:

$$\delta_{H+\varepsilon V}(S;\varphi) = \sup_{t\in\mathbb{R}} \left\| (\mathrm{e}^{it(H+\varepsilon V)} S \mathrm{e}^{-it(H+\varepsilon V)} - S)\varphi \right\| \to 0, \quad \text{as } \varepsilon \to 0. \tag{3.1}$$

Here we want to discuss the speed of convergence of the above limit.

For this purpose it would be useful to have an explicit upper bound of the divergence $\delta_{H+\varepsilon V}(S;\varphi)$, which physically represents the *wandering range* of the perturbed evolution of the symmetry $\mathrm{e}^{it(H+\varepsilon V)} S \mathrm{e}^{-it(H+\varepsilon V)}$ around its unperturbed evolution S.

For finite-dimensional systems the following uniform bound for robust symmetries holds:

$$\sup_{t\in\mathbb{R}} \left\| \mathrm{e}^{it(H+\varepsilon V)} S \mathrm{e}^{-it(H+\varepsilon V)} - S \right\| \leq \frac{14\sqrt{d}\|V\|\|S\|}{\eta}|\varepsilon|, \tag{3.2}$$

where d is the number of distinct eigenvalues of H and η is its minimal spectral gap [11].

A natural question arises from the bound obtained for finite-dimensional systems: given a V-robust symmetry $S \in \{H\}'$ and a unit vector $\varphi \in \mathcal{H}$, one can ask whether it is possible to find a constant $C_\varphi > 0$ and $\varepsilon^*_\varphi \in (0,1)$ such that for all $\varepsilon \in (-\varepsilon^*_\varphi, \varepsilon^*_\varphi)$:

$$\sup_{t\in\mathbb{R}} \left\| (\mathrm{e}^{\mathrm{i}t(H+\varepsilon V)} S \mathrm{e}^{-\mathrm{i}t(H+\varepsilon V)} - S)\varphi \right\| \leq C_\varphi \left|\varepsilon\right|. \tag{3.3}$$

Or, even more, whether the above bound holds in operator norm, i.e. for positive C and ε^* independent of φ. If this were the case, one would have that the wandering range $\delta_{H+\varepsilon V}(S;\varphi)$ of the robust symmetry S is of $O(\varepsilon)$ (and uniformly in φ for a bound in operator norm).

The answer to the above question is negative (when $\mathcal{H}$ is infinite-dimensional): in general, the convergence (3.1) is not uniform in φ (with $\|\varphi\| = 1$), and hence it does not hold in the operator norm. Moreover, there exist vectors φ such that the wandering range is of order $O(|\varepsilon|^\gamma)$, with $\gamma > 0$ arbitrarily small. This behavior is reminiscent of the phenomenon of Arnold diffusion in classical mechanics [22]. This is illustrated in the following example.

Example 3.1.1. Let H be the Hamiltonian of a one-dimensional harmonic oscillator with mass $m = 1$ and frequency $\omega = 1$ on the Hilbert space $L^2(\mathbb{R})$,

$$H = \frac{1}{2}\left(\hat{p}^2 + \hat{x}^2\right), \tag{3.4}$$

with domain $D(H) \subset H^2(\mathbb{R})$, where $\hat{p} = -i\frac{d}{dx}$ is the momentum operator and $\hat{x}$ is the position operator. The Hamiltonian H has compact resolvent and its spectrum is discrete with simple eigenvalues

$$h_n = n + \frac{1}{2}, \quad n \in \mathbb{N} \tag{3.5}$$

and normalized eigenfunctions

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{1}{\sqrt{\pi}}\right)^{1/2} e^{-x^2/2} H_n(x), \tag{3.6}$$

where $H_n(x)$ are the Hermite polynomials.

Let us consider the self-adjoint H-bounded perturbation (see Example 2.1.1)

$$V = \hat{p}, \tag{3.7}$$

with domain $D(V) = H^1(\mathbb{R})$.

For all $\varepsilon \in \mathbb{R}$ the perturbed Hamiltonian reads

$$H(\varepsilon) = H + \varepsilon V = \frac{1}{2}\left(\hat{p}^2 + \hat{x}^2 + 2\varepsilon\hat{p}\right) = \frac{1}{2}\left((\hat{p}+\varepsilon)^2 + \hat{x}^2\right) - \frac{\varepsilon^2}{2}\mathbb{I}, \tag{3.8}$$

with domain $D(H(\varepsilon)) = D(H)$, that is the Hamiltonian of a harmonic oscillator with shifted momentum, with spectrum

$$h_n(\varepsilon) = h_n - \frac{\varepsilon^2}{2}, \quad n \in \mathbb{N} \tag{3.9}$$

and eigenfunctions

$$\psi_n(x,\varepsilon) = \mathrm{e}^{-\mathrm{i}\varepsilon x}\psi_n(x). \tag{3.10}$$

An easy computation shows that the family of unitary operators $\{U(\varepsilon)\}_{\varepsilon\in\mathbb{R}}$ in Lemma 2.3.1 is given by

$$U(\varepsilon) = \mathrm{e}^{\mathrm{i}\varepsilon\hat{x}}, \quad \varepsilon \in \mathbb{R}. \tag{3.11}$$

Indeed, by using the Dirac notation, since the eigenvalues are non-degenerate,

$$P_n(\varepsilon) = |\psi_n(x,\varepsilon)\rangle\langle\psi_n(x,\varepsilon)| = \mathrm{e}^{-\mathrm{i}\varepsilon x}|\psi_n(x)\rangle\langle\psi_n(x)|\,\mathrm{e}^{\mathrm{i}\varepsilon x} = \mathrm{e}^{-\mathrm{i}\varepsilon\hat{x}}P_n(0)\mathrm{e}^{\mathrm{i}\varepsilon\hat{x}}, \tag{3.12}$$

where we have denoted with $P_n(\varepsilon)$ and $P_n(0)$ the spectral projections of $H(\varepsilon)$ and H respectively.[1]

Then, the eternal block-diagonal approximation (2.37) reads

$$\tilde{H}(\varepsilon) = e^{-\mathrm{i}\varepsilon\hat{x}}H(\varepsilon)e^{\mathrm{i}\varepsilon\hat{x}} = H - \frac{\varepsilon^2}{2}\mathbb{I}. \tag{3.13}$$

This means that H and $\tilde{H}(\varepsilon)$ share the eigenprojections for all $\varepsilon \in \mathbb{R}$, hence all the symmetries of H are V-robust, namely for all $S \in \{H\}'$ and for all $\psi \in L^2(\mathbb{R})$,

$$\delta_{H(\varepsilon)}(S;\psi) = \sup_{t\in\mathbb{R}} \left\|(\mathrm{e}^{\mathrm{i}tH(\varepsilon)}S\mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - S)\psi\right\| \to 0, \quad \text{as } \varepsilon \to 0. \tag{3.14}$$

[1]In general $P_n(0)$ do not coincide with the projections of the unperturbed Hamiltonian. However, this is true when there is no degeneracy.

We want to construct a (robust) symmetry S of H and a vector ψ of the Hilbert space $L^2(\mathbb{R})$ such that (3.3) is not true. Consider the following symmetry of H

$$S = \frac{\mathbb{I} - \Pi}{2}, \tag{3.15}$$

where Π is the parity operator, $\Pi\psi(x) = \psi(-x)$, for $\psi \in L^2(\mathbb{R})$. Notice that the parity operator can be written in the following way:

$$\Pi = \mathrm{i}\mathrm{e}^{-\mathrm{i}\pi H}. \tag{3.16}$$

Indeed since $\{\psi_n(x)\}_{n\geq 0}$ form an orthonormal basis for $L^2(\mathbb{R})$, we can write

$$\psi(x) = \sum_{n\geq 0} c_n \psi_n(x) \tag{3.17}$$

for every $\psi \in L^2(\mathbb{R})$. Then, by recalling that

$$(\Pi\psi_n)(x) = (-1)^n \psi_n(x), \tag{3.18}$$

we have

$$\begin{aligned}
(\Pi\psi)(x) &= \sum_{n\geq 0} c_n (\Pi\psi_n)(x) = \sum_{n\geq 0} (-1)^n c_n \psi_n(x) && (3.19)\\
&= \sum_{n\geq 0} \mathrm{e}^{-\mathrm{i}n\pi} c_n \psi_n(x) = \mathrm{i} \sum_{n\geq 0} \mathrm{e}^{-\mathrm{i}\left(n+\frac{1}{2}\right)\pi} c_n \psi_n(x) && (3.20)\\
&= \mathrm{i} \sum_{n\geq 0} \mathrm{e}^{-\mathrm{i}h_n\pi} c_n \psi_n(x) = \left(\mathrm{i}\mathrm{e}^{-\mathrm{i}\pi H}\psi\right)(x). && (3.21)
\end{aligned}$$

Consider now the family wave functions

$$\psi_\alpha(x) = \frac{1}{(1+x^2)^{\alpha/4}}, \quad x \in \mathbb{R}, \tag{3.22}$$

with $\alpha > 1$. Since $S\psi_\alpha = 0$, we have that for all $\varepsilon \in \mathbb{R}$:

$$\begin{aligned}
\sup_{t\in\mathbb{R}} \left\| \left(\mathrm{e}^{\mathrm{i}tH(\varepsilon)} S \mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - S\right) \psi_\alpha \right\| &= \sup_{t\in\mathbb{R}} \left\| S\mathrm{e}^{-\mathrm{i}tH(\varepsilon)}\psi_\alpha \right\| \\
&= \sup_{t\in\mathbb{R}} \left\| S\mathrm{e}^{\mathrm{i}\varepsilon\hat{x}} \mathrm{e}^{-\mathrm{i}t(H-\varepsilon^2/2)} \mathrm{e}^{-\mathrm{i}\varepsilon\hat{x}} \psi_\alpha \right\| \\
&= \sup_{t\in\mathbb{R}} \left\| S\mathrm{e}^{\mathrm{i}\varepsilon\hat{x}} \mathrm{e}^{-\mathrm{i}tH} \mathrm{e}^{-\mathrm{i}\varepsilon\hat{x}} \psi_\alpha \right\| \\
&\geq \left\| S\mathrm{e}^{\mathrm{i}\varepsilon\hat{x}} \mathrm{e}^{-\mathrm{i}\pi H} \mathrm{e}^{-\mathrm{i}\varepsilon\hat{x}} \psi_\alpha \right\| \\
&= \left\| -\mathrm{i}S\mathrm{e}^{\mathrm{i}\varepsilon\hat{x}} \Pi\, \mathrm{e}^{-\mathrm{i}\varepsilon\hat{x}} \psi_\alpha \right\|, \qquad (3.23)
\end{aligned}$$

where in the last equality we used (3.16). For all $\varepsilon \in \mathbb{R}$,

$$
\begin{aligned}
\left(-\mathrm{i}S\mathrm{e}^{\mathrm{i}\varepsilon\hat{x}}\Pi\mathrm{e}^{-\mathrm{i}\varepsilon\hat{x}}\psi_\alpha\right)(x) &= \left(-\mathrm{i}S\mathrm{e}^{\mathrm{i}\varepsilon\hat{x}}\Pi\right)\left(\mathrm{e}^{-\mathrm{i}\varepsilon x}\psi_\alpha(x)\right) \\
&= \left(-\mathrm{i}S\mathrm{e}^{\mathrm{i}\varepsilon\hat{x}}\right)\left(\mathrm{e}^{\mathrm{i}\varepsilon x}\psi_\alpha(x)\right) \qquad (3.24)\\
&= (-\mathrm{i}S)\left(\mathrm{e}^{2\mathrm{i}\varepsilon x}\psi_\alpha(x)\right) \qquad (3.25)\\
&= \frac{\mathrm{e}^{2\mathrm{i}\varepsilon x}-\mathrm{e}^{-2\mathrm{i}\varepsilon x}}{2\mathrm{i}}\psi_\alpha(x) \qquad (3.26)\\
&= \sin(2\varepsilon x)\psi_\alpha(x), \quad x \in \mathbb{R},
\end{aligned}
$$

where in (3.24) and (3.26) we have used that $\psi_\alpha(-x) = \psi_\alpha(x)$.

Then, we have that

$$
\begin{aligned}
\left\|-\mathrm{i}S\mathrm{e}^{\mathrm{i}\varepsilon\hat{x}}\Pi\mathrm{e}^{-\mathrm{i}\varepsilon\hat{x}}\psi_\alpha\right\|^2 &= \int_{\mathbb{R}} \sin^2(2\varepsilon x)\,|\psi_\alpha(x)|^2\,\mathrm{d}x = \int_{\mathbb{R}} \frac{\sin^2(2\varepsilon x)}{(1+x^2)^{\frac{\alpha}{2}}}\mathrm{d}x \\
&= |\varepsilon|^{\alpha-1}\int_{\mathbb{R}} \frac{\sin^2(2x)}{(\varepsilon^2+x^2)^{\frac{\alpha}{2}}}\mathrm{d}x \\
&\geq |\varepsilon|^{\alpha-1}\int_{\mathbb{R}} \frac{\sin^2(2x)}{(1+x^2)^{\frac{\alpha}{2}}}\mathrm{d}x, \qquad (3.27)
\end{aligned}
$$

where the last inequality is true for $|\varepsilon| < 1$. Therefore, for all $\varepsilon \in (-1, 1)$:

$$
\delta_{H(\varepsilon)}(S;\psi_\alpha) = \sup_{t\in\mathbb{R}} \left\|\left(\mathrm{e}^{\mathrm{i}tH(\varepsilon)}S\mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - S\right)\psi_\alpha\right\| \geq c_\alpha|\varepsilon|^{\frac{\alpha-1}{2}}, \qquad (3.28)
$$

where

$$
c_\alpha = \left(\int_{\mathbb{R}} \frac{\sin^2(2x)}{(1+x^2)^{\frac{\alpha}{2}}}dx\right)^{\frac{1}{2}} < +\infty, \qquad (3.29)
$$

because $\alpha > 1$. Therefore, (3.3) cannot hold if $\alpha \in (1, 3)$. In fact, the speed of convergence can be arbitrarily slow for $\alpha \approx 1$.

This example also shows that the convergence cannot be in operator norm. Indeed, since $c_\alpha/\|\psi_\alpha\| \to 1/\sqrt{2}$, as $\alpha \downarrow 1$, then

$$
\begin{aligned}
\sup_{t\in\mathbb{R}} \left\|\mathrm{e}^{\mathrm{i}tH(\varepsilon)}S\mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - S\right\| &\geq \left\|\mathrm{e}^{\mathrm{i}\pi H(\varepsilon)}S\mathrm{e}^{-\mathrm{i}\pi H(\varepsilon)} - S\right\| \\
&\geq \sup_{\alpha>1} \frac{\left\|\left(\mathrm{e}^{\mathrm{i}\pi H(\varepsilon)}S\mathrm{e}^{-\mathrm{i}\pi H(\varepsilon)} - S\right)\psi_\alpha\right\|}{\|\psi_\alpha\|} \geq \frac{1}{\sqrt{2}}. \qquad (3.30)
\end{aligned}
$$

We would like to see now, in which cases instead, the wandering range has a linear dependence on ε and when the uniform topology can be used.

This can depend on several factors: on the particular state on which the wandering range is evaluated, on the symmetry under consideration, or on the chosen perturbation. In the following sections we analyze three specific cases: when ψ is an eigenvector of the unperturbed Hamiltonian H, when the symmetry in question is of finite rank, and when the perturbation is bounded.

3.2 Eigenvectors of the Hamiltonian and finite-rank symmetries

Let $H = H^\dagger$ be our unperturbed Hamiltonian. As usual, we assume that it has a purely point spectrum. Its spectral decomposition reads

$$H\psi = \sum_{k\geq 1} h_k P_k \psi, \qquad \forall \psi \in D(H), \tag{3.31}$$

where $\{h_k\}_{k\geq 1} \subset \mathbb{R}$ are the distinct eigenvalues of H and $\{P_k\}_{k\geq 1}$ are its spectral projections:

$$P_k^\dagger = P_k, \quad P_k P_\ell = \delta_{k\ell} P_k, \quad \forall k, \ell \geq 1, \qquad \sum_{k\geq 1} P_k \psi = \psi, \quad \forall \psi \in \mathcal{H}. \tag{3.32}$$

In the following theorem we will show that for particular states and/or particular symmetries, the wandering range is of order ε. We will consider an admissible deformation of H, defined in 2.3.1, by adding a particular regularity condition on the operators $U(\varepsilon)$.

Theorem 3.2.1. *Let H be a self-adjoint operator with purely point spectrum, and let $H(\varepsilon)$ admissible. Assume that for all $n \geq 1$, there exists $C_n > 0$ such that*

$$\|(U(\varepsilon) - \mathbb{I})P_n(0)\| \leq C_n |\varepsilon|^\alpha, \tag{3.33}$$

for ε sufficiently small and some $\alpha > 0$.

Let S be a robust symmetry for $H(\varepsilon)$. Then the following statements hold:

(i) If $\psi \in \mathcal{H}$ is an eigenvector of H, belonging to an eigenspace of finite dimension, then there exist $\varepsilon_\psi \in (0, 1)$ and $C_\psi > 0$ such that for all $\varepsilon \in (-\varepsilon_\psi, \varepsilon_\psi)$:

$$\sup_{t\in\mathbb{R}} \left\|(\mathrm{e}^{\mathrm{i}tH(\varepsilon)} S \mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - S)\psi\right\| \leq C_\psi |\varepsilon|^\alpha; \tag{3.34}$$

(ii) If S is a finite-rank operator, then there exist $\varepsilon^* \in (0, 1)$ and $C > 0$ such that for all $\varepsilon \in (-\varepsilon^*, \varepsilon^*)$:

$$\sup_{t\in\mathbb{R}} \left\|\mathrm{e}^{\mathrm{i}tH(\varepsilon)} S \mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - S\right\| \leq C|\varepsilon|^\alpha. \tag{3.35}$$

Then, we have a linear wandering range when the property (3.33) is satisfied with $\alpha \geq 1$.

Proof. The proof of (i) is based on the following claim:

$$\sup_{t\in\mathbb{R}} \left\|(\mathrm{e}^{\mathrm{i}tH(\varepsilon)} S \mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - S)P_n(0)\right\| \leq 4\,\|S\|\, C_n\, |\varepsilon|\,, \tag{3.36}$$

where C_n is the positive constant of (3.33).

Let us introduce the following family of self-adjoint operator

$$\tilde{H}(\varepsilon) = U(\varepsilon)^\dagger H(\varepsilon) U(\varepsilon) = \sum_{n\geq 1} h_n(\varepsilon) P_n(0), \tag{3.37}$$

which we referred to in the previous chapter as the *eternal block-diagonal approximation* of $H(\varepsilon)$.

Since S is robust against $H(\varepsilon)$, according to the Theorem 2.3.3, $[S, P_m(0)] = 0$ for all $m \geq 1$. Hence $[S, \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)}] = 0$ for all $t \in \mathbb{R}$ and $\varepsilon \in I$. Therefore, for all $t \in \mathbb{R}$ and $\varepsilon \in I$:

$$\begin{aligned} \left\|(\mathrm{e}^{\mathrm{i}tH(\varepsilon)} S \mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - S) P_n(0)\right\| &= \left\|\mathrm{e}^{\mathrm{i}tH(\varepsilon)} \left[S, \mathrm{e}^{-\mathrm{i}tH(\varepsilon)}\right] P_n(0)\right\| \\ &= \left\|\left[S, \mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)}\right] P_n(0)\right\| \\ &\leq 2\|S\| \left\|\left(\mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)}\right) P_n(0)\right\| && (3.38) \\ &\leq 4\|S\| \left\|\left(U(\varepsilon) - \mathbb{I}\right) P_n(0)\right\| && (3.39) \\ &\leq 4 \|S\| \, C_n \, |\varepsilon| \, . && (3.40) \end{aligned}$$

where in (3.38) we used that

$$H(\varepsilon) = U(\varepsilon) \tilde{H}(\varepsilon) U(\varepsilon)^\dagger \tag{3.41}$$

and in (3.39) we have applied (3.33).

Now we prove (i). Since ψ is an eigenvector of H there is $k \geq 1$ such that $\psi = P_k \psi$. Since, by hypothesis, P_k has finite rank, there exist $1 \leq d_k < \infty$ such that

$$\psi = P_k \psi = \sum_{n=1}^{d_k} P_n(0) \psi, \tag{3.42}$$

where we have used that the $P_n(0)$'s form a family of subprojections of the P_k's.

Then

$$\sup_{t\in\mathbb{R}} \left\|(\mathrm{e}^{\mathrm{i}tH(\varepsilon)} S \mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - S)\psi\right\| \leq \sum_{n=1}^{d_k} \left\|(\mathrm{e}^{\mathrm{i}tH(\varepsilon)} S \mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - S) P_n(0)\psi\right\|. \tag{3.43}$$

Hence, the bound (3.34) follows immediately by (3.36), with

$$C_\psi = 4 \|S\| \, \|\psi\| \sum_{n=1}^{d_k} C_n. \tag{3.44}$$

Now we prove (ii). Since S is a finite-rank robust symmetry, then there is $d \geq 1$ such that

$$S = \sum_{m=1}^{d} P_m(0) S P_m(0).$$

We have that for all $t \in \mathbb{R}$:

$$\begin{aligned}\left\|(\mathrm{e}^{\mathrm{i}tH(\varepsilon)}S\mathrm{e}^{-\mathrm{i}tH(\varepsilon))} - S)\right\| &= \left\|\left[S, \mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)}\right]\right\| \\ &\leq \left\|S\left(\mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)}\right)\right\| + \left\|\left(\mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)}\right)S\right\|.\end{aligned}$$

Therefore,

$$\begin{aligned}\sup_{t\in\mathbb{R}}\left\|(\mathrm{e}^{\mathrm{i}tH(\varepsilon)}S\mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - S)\right\| &\leq 2\|S\|\sum_{m=1}^{d}\sup_{t\in\mathbb{R}}\left\|\left(\mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - \mathrm{e}^{-\mathrm{i}t\tilde{H}(\varepsilon)}\right)P_m(0)\right\| \\ &\leq 4\|S\|\sum_{m=1}^{d}\|(U(\varepsilon) - \mathbb{I})\,P_m(0)\|\,,\end{aligned}$$

hence (3.35) follows immediately by (3.33), with

$$C = 4\,\|S\|\sum_{m=1}^{d}C_m \tag{3.45}$$

□

The previous theorem implies the following corollary for linear perturbations.

Theorem 3.2.2. *Let H be a self adjoint operator with compact resolvent. Let V a H-bounded perturbation and S be a V-robust symmetry. Then the following propositions are true:*

(i) if $\psi \in \mathcal{H}$ is an eigenvector of H, which belong to an eigenspace of finite dimension, then there is $\varepsilon_\psi \in (0,1)$ and $C_\psi > 0$ such that for all $\varepsilon \in (-\varepsilon_\psi, \varepsilon_\psi)$:

$$\sup_{t\in\mathbb{R}}\left\|(\mathrm{e}^{\mathrm{i}t(H+\varepsilon V)}S\mathrm{e}^{-\mathrm{i}t(H+\varepsilon V)} - S)\psi\right\| \leq C_\psi\,|\varepsilon|\,; \tag{3.46}$$

(ii) if S is a finite rank operator, then there is $\varepsilon^* \in (0,1)$ and $C > 0$ such that for all $\varepsilon \in (-\varepsilon^*, \varepsilon^*)$:

$$\sup_{t\in\mathbb{R}}\left\|\mathrm{e}^{\mathrm{i}t(H+\varepsilon V)}S\mathrm{e}^{-\mathrm{i}t(H+\varepsilon V)} - S\right\| \leq C\,|\varepsilon|\,. \tag{3.47}$$

Proof. In order to prove the theorem, we need to show that $H(\varepsilon) = H + \varepsilon V$ satisfies the hypotheses of Theorem 3.2.1, namely that it constitutes an admissible deformation fulfilling condition (3.33), with $\alpha = 1$. We have already shown in the previous chapter that $H(\varepsilon)$ is indeed an admissible deformation of H; therefore, it remains to verify that condition (3.33) holds. Let us recall that, in this case, the operator $U(\varepsilon)$ is given by

$$U(\varepsilon) = \sum_{n\geq 1}(\mathbb{I} - R_n(\varepsilon))^{-1/2}P_n(\varepsilon)P_n(0), \tag{3.48}$$

where $R_n(\varepsilon) = \big(P_n(\varepsilon) - P_n(0)\big)^2$ and $P_n(\varepsilon)$ denote the spectral projections of $H(\varepsilon)$. We have already proved that $U(\varepsilon)$ defines a family of unitary operators satisfying $P_n(\varepsilon) =$

$U(\varepsilon)P_n(0)U(\varepsilon)^\dagger$. It remains to prove (3.33), with $\alpha = 1$. We have

$$\begin{aligned}
\|(U(\varepsilon) - \mathbb{I})\, P_n(0)\| &= \left\|(\mathbb{I} - R_n(\varepsilon))^{-1/2} P_n(\varepsilon) P_n(0) - P_n(0)\right\| && (3.49)\\
&\leq \left\|(\mathbb{I} - R_n(\varepsilon))^{-1/2} P_n(\varepsilon) P_n(0) - P_n(\varepsilon) P_n(0)\right\| && (3.50)\\
&+ \|P_n(\varepsilon) P_n(0) - P_n(0)\| && (3.51)\\
&\leq \|P_n(\varepsilon) - P_n(0)\| + \left\|(1 - R_n(\varepsilon))^{-1/2} - \mathbb{I}\right\|. && (3.52)
\end{aligned}$$

According to Kato's Theorem 2.3.1, the projections $P_n(\varepsilon)$ depend analytically on ε and, in particular, are differentiable. Hence, there exist constants $k_n > 0$ such that

$$\|P_n(\varepsilon) - P_n(0)\| \leq k_n |\varepsilon|, \tag{3.53}$$

for all sufficiently small ε.

Let us consider now the norm

$$\left\|(\mathbb{I} - R_n(\varepsilon))^{-1/2} - \mathbb{I}\right\|. \tag{3.54}$$

By considering the Neumann series for $(\mathbb{I} - R_n(\varepsilon))^{-1/2}$ and by applying the triangular inequality, we get

$$\left\|(\mathbb{I} - R_n(\varepsilon))^{-1/2} - \mathbb{I}\right\| \leq d_n \, |\varepsilon|^2, \tag{3.55}$$

for ε sufficiently small.

$$\begin{aligned}
\left\|(\mathbb{I} - R_n(\varepsilon))^{-1/2} - \mathbb{I}\right\| &= \left\|\sum_{j\geq 1} \binom{-1/2}{j} (-R_n(\varepsilon))^j\right\|\\
&\leq \sum_{j\geq 1} \left|\binom{-1/2}{j}\right| \|R_n(\varepsilon)\|^j.
\end{aligned}$$

Notice that

$$\begin{aligned}
\left|\binom{-1/2}{j}\right| &= \frac{|-1/2|\,|-1/2-1|\cdots|-1/2-j+1|}{j!}\\
&= \frac{1/2\cdot 3/2\cdots(2j-1)/2}{j!}\\
&= \frac{1\cdot 3\cdots(2j-1)}{2^j j!} = \frac{(2j-1)!!}{j!2^j}.
\end{aligned}$$

By using the known identity

$$(2j-1)!! = \frac{(2j)!}{j!2^j}, \tag{3.56}$$

we get

$$\left|\binom{-1/2}{j}\right| = \frac{(2j)!}{4^j (j!)^2} = \frac{1}{4^j}\binom{2j}{j}.$$

Then

$$\left\|(\mathbb{I}-R_n(\varepsilon))^{-1/2}-1\right\| \le \sum_{j\ge 1}\binom{2j}{j}\left\|\frac{R_n(\varepsilon)}{4}\right\|^j = \sum_{j\ge 1}\binom{2j}{j}x^j,$$

where $x=\|R_n(\varepsilon)/4\|$. The sum of the right hand can be evaluated analytically for $x<1/4$:

$$\sum_{j\ge 1}\binom{2j}{j}x^j = \frac{1-\sqrt{1-4x}}{\sqrt{1-4x}}. \tag{3.57}$$

The sum of a convergent power series in x (vanishing at $x=0$) is clearly of order x. Then

$$\left\|(\mathbb{I}-R_n(\varepsilon))^{-1/2}-\mathbb{I}\right\| = O(\|R_n(\varepsilon)\|) = O(\|P_n(\varepsilon)-P_n(0)\|^2) = O(\varepsilon^2). \tag{3.58}$$

We conclude that there exists $C_n>0$ such that

$$\|(U(\varepsilon)-\mathbb{I})\,P_n(0)\| \le C_n\,|\varepsilon|\,, \tag{3.59}$$

for ε sufficiently small. □

In this section, we have seen particular classes of vector and/or symmetries for which the wandering range is of order ε. In the next section we want to analyze instead, a particular class of perturbations for which the wandering range is linear. These are the bounded perturbations.

3.3 Bounded perturbations

Let H be a self-adjoint operator with purely point spectrum. Its spectral decomposition reads

$$H\psi = \sum_{k\ge 1} h_k P_k \psi, \tag{3.60}$$

where $\{h_k\}_{k\ge 1}$ are the distinct (increasingly ordered) eigenvalues of H, and $\{P_k\}_{k\ge 1}$ are the corresponding orthogonal spectral projections.

We focus on a particular class of symmetries, namely the elements of the bicommutant

$$\{H\}'' = \{f(H) : f:\mathbb{R}\to\mathbb{C} \text{ Borel bounded}\}, \tag{3.61}$$

which consists of all bounded Borel functions of H. Any operator $S\in\{H\}''$ can be written as

$$S = \sum_{k\ge 1} s_k P_k, \tag{3.62}$$

where $(s_k)_{k\geq 1}$ is a uniformly bounded sequence of complex number.

We have shown in the previous chapter that $\{H\}''$ is the set of completely robust symmetries for Hamiltonians with compact resolvent.

In this section, we show that this class of symmetries remains robust against all bounded perturbations also for some Hamiltonians without compact resolvent.

Consider a family of perturbed Hamiltonians

$$H(\varepsilon) := H + \varepsilon V(\varepsilon), \tag{3.63}$$

parametrized by $\varepsilon \in I \subset \mathbb{R}$. We say that the perturbation is *(uniformly) bounded* if there exists a constant $C > 0$ such that

$$\|V(\varepsilon)\| \leq C \qquad \text{for all } \varepsilon \in I. \tag{3.64}$$

The goal of this section is to show that, under this class of perturbations, the wandering range of a symmetry $S \in \{H\}''$ remains uniformly of order ε. This is made precise by the following result.

Theorem 3.3.1 (Robust symmetries against bounded perturbations)**.** *Let H be a self-adjoint operator with purely point spectrum $\{h_k\}_{k\geq 1}$. Let $(V(\varepsilon))_{\varepsilon\in I}$ be a family of perturbations of H, and let $S \in \{H\}'$ be a symmetry of H. Assume that:*

1. *H has a positive minimal spectral gap, i.e.*

$$\eta := \inf_{k\neq \ell} |h_k - h_\ell| > 0; \tag{3.65}$$

2. *$(V(\varepsilon))_{\varepsilon\in I}$ is uniformly bounded, i.e. there exists $C > 0$ such that for all $\varepsilon \in I$:*

$$\|V(\varepsilon)\| \leq C; \tag{3.66}$$

3. *S is in the bicommutant of H, i.e.*

$$S \in \{H\}'' = \{A \in B(\mathcal{H}) : [A, B] = 0 \ \ \forall B \in \{H\}'\}. \tag{3.67}$$

Then,

$$\sup_{t\in\mathbb{R}} \left\|\mathrm{e}^{\mathrm{i}tH(\varepsilon)} S \mathrm{e}^{-\mathrm{i}tH(\varepsilon)} - S\right\| \leq \frac{4C\beta\|S\|}{\eta} |\varepsilon|, \tag{3.68}$$

for some $\beta > 0$ and ε sufficiently small.

Remark 3.3.1. Assumption (ii) guarantees that the right-hand side of inequality (3.68) is of order ε, confirming the linearity of the wandering range of S in the perturbation.

Remark 3.3.2. The deformations considered in this theorem are not necessarily admissible. Indeed, we are not making any assumption on the spectrum of the perturbed Hamiltonian $H(\varepsilon)$.

Remark 3.3.3. The Hamiltonian H is not necessarily assumed to have a compact resolvent. It is required to have a purely point spectrum and a non-vanishing spectral gap, although its eigenvalues may, in general, exhibit infinite degeneracy.

3.3.1 Strategy of the proof

The proof of Theorem 3.3.1 is based on the following auxiliary result.

Theorem 3.3.2. *There exist two families of operators $W(\varepsilon)$ and $\hat{V}(\varepsilon)$ with the following properties:*

1. $\hat{V}(\varepsilon) = \hat{V}(\varepsilon)^\dagger$ *commutes with* H.
2. $W(\varepsilon)$ *is unitary.*
3. $W(\varepsilon)D(H) \subseteq D(H)$.
4. $W(0) = \mathbb{I}$.
5. *The operators* $H + \varepsilon V(\varepsilon)$ *and* $H + \varepsilon\hat{V}(\varepsilon)$ *are unitarily equivalent through* $W(\varepsilon)$*:*
$$W(\varepsilon)^\dagger (H + \varepsilon V(\varepsilon)) W(\varepsilon)\psi = (H + \varepsilon\hat{V}(\varepsilon))\psi, \tag{3.69}$$
for all $\psi \in D(H)$.
6. $W(\varepsilon)$ *satisfies the following inequality:*
$$\|W(\varepsilon) - \mathbb{I}\| \leq \beta\frac{C}{\eta}\,|\varepsilon|\,, \tag{3.70}$$
for all ε *such that*
$$|\varepsilon| \leq \frac{\eta}{C\rho}, \tag{3.71}$$
for suitable constants $\beta, \rho > 0$.

Remark 3.3.4. The operators $W(\varepsilon)$ and $\hat{V}(\varepsilon)$ are not uniquely defined, and different strategies can be employed for their construction. In the following chapters, we present two such approaches: the Quantum KAM Iteration, discussed in two variants (Chapters 4 and 5), and Kato's perturbative method (Chapter 6). The specific values of the parameters β and ρ depend on the chosen strategy.

We postpone the proof of the previous theorem, which involves the explicit construction and estimation of the operators $\hat{V}(\varepsilon)$ and $W(\varepsilon)$, to the following chapters. Assuming this result, we now proceed to prove Theorem 3.3.1.

Proof of Theorem 3.3.1. Let $S \in \{H\}''$. We have

$$\left\| \mathrm{e}^{\mathrm{i}t(H+\varepsilon V(\varepsilon))} S \mathrm{e}^{-\mathrm{i}t(H+\varepsilon V(\varepsilon))} - S \right\| = \left\| \left[\mathrm{e}^{\mathrm{i}t(H+\varepsilon V(\varepsilon))}, S \right] \right\| \tag{3.72}$$

$$= \left\| \left[\mathrm{e}^{\mathrm{i}t(H+\varepsilon V(\varepsilon))} - \mathrm{e}^{\mathrm{i}t(H+\varepsilon \hat{V}(\varepsilon))}, S \right] \right\| \tag{3.73}$$

$$\leq 2 \left\| S \right\| \left\| \mathrm{e}^{\mathrm{i}t(H+\varepsilon V(\varepsilon))} - \mathrm{e}^{\mathrm{i}t(H+\varepsilon \hat{V}(\varepsilon))} \right\| ,$$

where in step (3.73) we used that $S \in \{H\}''$, i.e. S commutes with all the operators in $\{H\}'$, in particular with $\hat{V}(\varepsilon)$.

By using the unitary equivalence above, we obtain

$$\left\| \mathrm{e}^{\mathrm{i}t(H+\varepsilon V(\varepsilon))} S \mathrm{e}^{-\mathrm{i}t(H+\varepsilon V(\varepsilon))} - S \right\| \leq 2 \left\| S \right\| \left\| \mathrm{e}^{\mathrm{i}t(H+\varepsilon V(\varepsilon))} - W(\varepsilon) \mathrm{e}^{\mathrm{i}t(H+\varepsilon \hat{V}(\varepsilon))} W(\varepsilon)^{\dagger} \right\| \tag{3.74}$$

$$= 2 \left\| S \right\| \left\| \left[\mathrm{e}^{\mathrm{i}t(H+\varepsilon V(\varepsilon))}, W(\varepsilon) - \mathbb{I} \right] \right\| \tag{3.75}$$

$$\leq 4 \left\| S \right\| \left\| W(\varepsilon) - \mathbb{I} \right\| \tag{3.76}$$

$$\leq 4 \left\| S \right\| \beta \frac{C}{\eta} \left| \varepsilon \right| ,$$

where in step (3.76) we used (3.70). □

Remark 3.3.5. In the proof of Theorem 3.3.1, and in particular in step (3.76), we established the estimate

$$\left\| \mathrm{e}^{\mathrm{i}t(H+\varepsilon V(\varepsilon))} S \mathrm{e}^{-\mathrm{i}t(H+\varepsilon V(\varepsilon))} - S \right\| \leq 4 \left\| S \right\| \left\| W(\varepsilon) - \mathbb{I} \right\| . \tag{3.77}$$

On the other hand, the trivial bound

$$\left\| \mathrm{e}^{\mathrm{i}t(H+\varepsilon V(\varepsilon))} S \mathrm{e}^{-\mathrm{i}t(H+\varepsilon V(\varepsilon))} - S \right\| \leq 2 \left\| S \right\| \tag{3.78}$$

is always valid. Therefore, when proving the auxiliary theorem, we can restrict to those values of ε such that

$$\left\| W(\varepsilon) - \mathbb{I} \right\| \leq \frac{1}{2}, \tag{3.79}$$

since otherwise the trivial bound already implies the claim.

Chapter 4

Quantum KAM Iteration

In the previous chapter we have analyzed some particular cases in which the wandering range of a robust symmetry is linear in the strength of the perturbation. In particular, at the end of that chapter we have seen that this is the case for functions of the unperturbed Hamiltonian, when subject to bounded perturbations.

The proof of this last property is based on the validity of Theorem 3.3.2, namely on the existence (with suitable properties) of a family of unitary operators $W(\varepsilon)$ and self-adjoint operators $\hat{V}(\varepsilon)$ such that

$$H + \varepsilon\hat{V}(\varepsilon) = W(\varepsilon)^\dagger (H + \varepsilon V(\varepsilon))W(\varepsilon), \tag{4.1}$$

with $\hat{V}(\varepsilon) \in \{H\}'$.

In this chapter we present a first strategy for proving this claim. We shall search for the operators $\hat{V}(\varepsilon)$ and $W(\varepsilon)$ in terms of formal power series in ε, and determine them order by order through an iterative construction. At each order the procedure reduces to solving a commutator equation, known in the literature as the *homological equation*, which will be analyzed in detail in the first section.

This recursive procedure is called *Quantum KAM Iteration*, since it closely mirrors the iteration scheme of the Kolmogorov–Arnold–Moser theorem in classical mechanics [6, 7]. We will prove the convergence of this quantum iteration by making use of a celebrated combinatorial sequence, the Catalan numbers (see Appendix A). Finally, we will show that the operators constructed in this way satisfy all the requirements of Theorem 3.3.2 [14].

4.1 The Homological Equation

In this section we introduce a key lemma concerning the so-called *homological equation*, also known as the commutator equation. This equation will play a central role in the proof of Theorem 3.3.2. We shall first fix some notation, then present the formal solution and establish quantitative estimates. Let $H = H^\dagger$ be a Hamiltonian with purely point spectrum.

Then, its spectral decomposition reads

$$H\psi = \sum_{k\geq 1} h_k P_k \psi \quad \forall \psi \in D(H), \tag{4.2}$$

where $\{h_k\}_{k\geq 1}$ is the set of distinguished eigenvalues of H and $\{P_k\}_{k\geq 1}$ is the complete set of spectral projections. We assume that the spectrum of H has a non vanishing minimal spectral gap, i.e.

$$\eta = \inf_{k\neq \ell} |h_k - h_\ell| > 0. \tag{4.3}$$

Given an operator $A \in B(\mathcal{H})$, we define its *block-diagonal part* with respect to the Hamiltonian H as

$$[A] = \sum_{k\geq 1} P_k A P_k, \tag{4.4}$$

where $\{P_k\}$ are the spectral projections of H. Conversely, the *off-diagonal part* of A is defined as

$$\{A\} = A - [A] = \sum_{k\neq \ell} P_k A P_\ell. \tag{4.5}$$

Lemma 4.1.1 (Homological Equation)**.** *Let H be a self-adjoint unbounded operator, with purely point spectrum and a non-vanishing minimal spectral gap $\eta > 0$. Let $B \in B(\mathcal{H})$ be a bounded operator. Then, there is a unique operator $X \in B(\mathcal{H})$ satisfying the following conditions:*

(i) $XD(H) \subseteq D(H)$;

(ii) For all $\psi \in D(H)$,

$$\mathrm{i}[X, H]\psi = \{B\}\psi; \tag{4.6}$$

(iii) The block-diagonal part of X vanishes, i.e.,

$$[X] = 0; \tag{4.7}$$

and it is given by

$$X = \mathrm{i} \sum_{k\neq \ell} \frac{P_k B P_\ell}{h_k - h_\ell}. \tag{4.8}$$

Moreover, if B is self-adjoint then X is self-adjoint. Finally, the following estimates hold:

$$\|X\| \leq \frac{\pi}{\sqrt{3}\eta} \|B\|, \tag{4.9}$$

$$\|HX\psi\| \leq \left(2\|\psi\| + \frac{\pi}{\sqrt{3}\eta}\|H\psi\|\right) \|B\|, \qquad \forall\, \psi \in D(H). \tag{4.10}$$

Equation (4.6) *is known in literature as homological equation.*

Proof. Let $\psi \in \mathcal{H}$. Since equation (4.6) must hold for all $\phi \in D(H)$, it must in particular hold for $\phi = \psi_\ell := P_\ell \psi$, for any $\ell \geq 1$. In this case, we obtain

$$\mathrm{i}\,(h_\ell X P_\ell - H X P_\ell)\,\psi = \{B\} P_\ell \psi. \tag{4.11}$$

By left-multiplying both sides by P_k, with $k \geq 1$, we find

$$(h_k - h_\ell) P_k X P_\ell \psi = \mathrm{i} P_k \{B\} P_\ell \psi. \tag{4.12}$$

For $k = \ell$, the equation is automatically satisfied for any choice of X, while for $k \neq \ell$ it gives

$$P_k X P_\ell \psi = \mathrm{i} \frac{P_k B P_\ell}{h_k - h_\ell} \psi. \tag{4.13}$$

Summing over all $k \neq \ell$ and removing the dependence on ψ, we obtain the operator identity

$$\{X\} = \mathrm{i} \sum_{k \neq \ell} \frac{P_k B P_\ell}{h_k - h_\ell}, \tag{4.14}$$

Thus, the homological equation determines only the off-diagonal part of X, leaving its block-diagonal part arbitrary. Therefore, the solution is unique up to the addition of a block-diagonal operator. By fixing the block-diagonal part to zero, i.e., by imposing $[X] = 0$, we select the unique solution:

$$X = \mathrm{i} \sum_{k \neq \ell} \frac{P_k B P_\ell}{h_k - h_\ell}. \tag{4.15}$$

Furthermore, if $B = B^\dagger$ it is straightforward to verify that (formally) $X = X^\dagger$.

Clearly, it is necessary to verify the convergence of the series defining X. Let $\psi \in \mathcal{H}$. Using the orthogonality of the projections P_k, we obtain:

$$\|X\psi\|^2 \;\leq\; \|B\|^2 \sum_{\ell \geq 1} \sum_{k \neq \ell} \frac{\|P_k \psi\|^2}{|h_k - h_\ell|^2}. \tag{4.16}$$

Exchanging the order of summation gives:

$$\|X\psi\|^2 \;\leq\; \|B\|^2 \sum_{k \geq 1} \|P_k \psi\|^2 \sum_{\ell \neq k} \frac{1}{|h_k - h_\ell|^2}.$$

We now use the fact that H has a non-vanishing spectral gap $\eta > 0$. Since the eigenvalues $\{h_k\}_{k \geq 1}$ are ordered increasingly, we have:

$$|h_k - h_\ell| \geq \eta |k - \ell|. \tag{4.17}$$

[1]

Applying this bound yields:

$$\|X\psi\|^2 \leq \frac{\|B\|^2}{\eta^2} \sum_{k \geq 1} \|P_k\psi\|^2 \sum_{\ell \neq k} \frac{1}{(k-\ell)^2}. \tag{4.18}$$

Changing variables in the second sum by setting $j = \ell - k$, we find:

$$\begin{aligned}
\|X\psi\|^2 &\leq \frac{\|B\|^2}{\eta^2} \sum_{k \geq 1} \|P_k\psi\|^2 \sum_{j=-k+1}^{-1} \frac{1}{j^2} + \sum_{j=1}^{\infty} \frac{1}{j^2} \\
&= \frac{\|B\|^2}{\eta^2} \sum_{k \geq 1} \|P_k\psi\|^2 \left(\sum_{j=1}^{k-1} \frac{1}{j^2} + \frac{\pi^2}{6} \right) \\
&< \frac{\|B\|^2}{\eta^2} \sum_{k \geq 1} \|P_k\psi\|^2 \left(\sum_{j=1}^{+\infty} \frac{1}{j^2} + \frac{\pi^2}{6} \right) \\
&= \frac{2\pi^2 \|B\|^2}{6\eta^2} \sum_{k \geq 1} \|P_k\psi\|^2 \\
&= \frac{\pi^2 \|B\|^2}{3\eta^2} \|\psi\|^2 .
\end{aligned} \tag{4.19}$$

Hence,

$$\|X\| \leq \frac{\pi}{\sqrt{3}\eta} \|B\| . \tag{4.20}$$

We now derive the bound (4.10). Let $\psi \in D(H)$. Using the explicit expression (4.8) for X, we write:

$$\begin{aligned}
-\mathrm{i}HX\psi &= \sum_{k \neq \ell} \frac{h_k}{h_k - h_\ell} P_k B P_\ell \psi && (4.21) \\
&= \sum_{k \neq \ell} \left(\frac{h_k - h_\ell + h_\ell}{h_k - h_\ell} \right) P_k B P_\ell \psi && (4.22) \\
&= \sum_{k \neq \ell} P_k B P_\ell \psi + \sum_{k \neq \ell} \frac{h_\ell}{h_k - h_\ell} P_k B P_\ell \psi && (4.23) \\
&= \{B\}\psi - \mathrm{i}XH\psi. && (4.24)
\end{aligned}$$

Taking the norm of both sides and applying the triangle inequality gives

$$\|HX\psi\| \leq \|\{B\}\psi\| + \|X\| \, \|H\psi\|. \tag{4.25}$$

[1]Indeed, without loss of generality, assume $k \geq \ell$. Then:

$$\begin{aligned}
|h_k - h_\ell| = h_k - h_\ell &= (h_k - h_{k-1}) + (h_{k-1} - h_{k-2}) + \cdots + (h_{\ell+1} - h_\ell) \\
&\geq \eta + \eta + \cdots + \eta = (k-\ell)\eta = \eta|k-\ell|.
\end{aligned}$$

Since

$$\|\{B\}\| = \|B - [B]\| \leq \|B\| + \|[B]\|, \tag{4.26}$$

and

$$\|[B]\| \leq \sup_k \|P_k B P_k\| \leq \|B\|, \tag{4.27}$$

we obtain

$$\|\{B\}\| \leq 2\|B\|. \tag{4.28}$$

Substituting this bound into (4.25) yields

$$\|HX\psi\| \leq 2\|B\| \, \|\psi\| + \|X\| \, \|H\psi\|. \tag{4.29}$$

Finally, using the estimate (4.20) for $\|X\|$, we conclude:

$$\|HX\psi\| \leq \left(2\|\psi\| + \frac{\pi}{\sqrt{3}\eta}\|H\psi\|\right) \|B\|. \tag{4.30}$$

□

Remark 4.1.1. The homological equation depends only on the off-diagonal part of the operator B. Indeed, one can always replace B with $B + [A]$, for any $A \in B(\mathcal{H})$, without affecting the solution. This freedom allows for an optimization of the norm estimate:

$$\|X\| \leq \frac{\pi}{\sqrt{3}\eta} \inf_{A \in B(\mathcal{H})} \|B + [A]\|. \tag{4.31}$$

The infimum is not necessarily attained by choosing $A = -[B]$, as it may happen that

$$\|B - [B]\| = \|\{B\}\| > \|B\|. \tag{4.32}$$

For instance, consider

$$B = \begin{pmatrix} -\frac{1}{2} & 1 & 1 \\ 1 & -\frac{1}{2} & 1 \\ 1 & 1 & -\frac{1}{2} \end{pmatrix}, \tag{4.33}$$

for which it is straightforward to verify that

$$\|\{B\}\| = 2 > \|B\| = \frac{3}{2}, \tag{4.34}$$

where the off-diagonal decomposition is taken with respect to 1-dimensional blocks, that is,

$$\{B\} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}. \tag{4.35}$$

See [23].

4.2 KAM Iteration

We are now ready to state the main theorem of this chapter. This is a reformulation of Theorem 3.3.2 of the previous chapter, but with explicit quantitative constants. We consider perturbations of the form

$$H(\varepsilon) = H + \varepsilon V(\varepsilon),$$

where $V(\varepsilon)$ is a bounded operator satisfying the uniform estimate

$$\sup_{\varepsilon} \|V(\varepsilon)\| \leq C.$$

Then the following theorem holds.

Theorem 4.2.1. *There exist two families of operators $W(\varepsilon)$ and $\hat{V}(\varepsilon)$ with the following properties:*

1. *$\hat{V}(\varepsilon)$ is self-adjoint and belongs to the commutant of H, i.e. $\hat{V}(\varepsilon) = \hat{V}(\varepsilon)^\dagger \in \{H\}'$.*

2. *$W(\varepsilon)$ is unitary.*

3. *$W(\varepsilon)$ leaves the domain of H invariant: $W(\varepsilon)D(H) \subseteq D(H)$.*

4. *$W(0) = \mathbb{I}$.*

5. *The operators $H + \varepsilon V(\varepsilon)$ and $H + \varepsilon\hat{V}(\varepsilon)$ are unitarily equivalent through $W(\varepsilon)$:*

$$W(\varepsilon)^\dagger (H + \varepsilon V(\varepsilon)) W(\varepsilon)\psi = (H + \varepsilon\hat{V}(\varepsilon))\psi, \tag{4.36}$$

   for all $\psi \in D(H)$.

6. *$W(\varepsilon)$ satisfies the bound*

$$\|W(\varepsilon) - \mathbb{I}\| \leq \beta \frac{C}{\eta} |\varepsilon|, \tag{4.37}$$

   for all ε such that

$$|\varepsilon| \leq \frac{\eta}{C\rho}.$$

   The constants β and ρ are given by

$$\beta := \frac{4\pi}{\sqrt{3}} \alpha \left(\mathrm{e}^{\frac{1}{2\alpha}} - 1 \right), \tag{4.38}$$

$$\rho := \frac{4\pi\alpha}{\sqrt{3}}, \tag{4.39}$$

   where $\alpha \approx 4.79$ is the unique positive solution of the transcendental equation

$$(\alpha + 1) \left(\mathrm{e}^{\frac{2}{\alpha}} - 1 \right) = 3.$$

The idea of the proof is the following. We first construct two operators $W(\varepsilon)$ and $\hat{V}(\varepsilon)$ as formal series in ε, and then establish their convergence.

Condition (v) of Theorem 4.2.1 requires that $W(\varepsilon)$ and $\hat{V}(\varepsilon)$ satisfy

$$W(\varepsilon)^\dagger(H + \varepsilon V(\varepsilon))W(\varepsilon)\psi = (H + \varepsilon\hat{V}(\varepsilon))\psi, \tag{4.40}$$

for all $\psi \in D(H)$. To guarantee unitarity, we parametrize

$$W(\varepsilon) = \mathrm{e}^{\mathrm{i}K(\varepsilon)}, \tag{4.41}$$

where $K(\varepsilon) = K(\varepsilon)^\dagger$ and $K(\varepsilon)D(H) \subseteq D(H)$. With this choice, the above condition is equivalent to

$$\mathrm{e}^{-\mathrm{i}K(\varepsilon)}(H + \varepsilon V(\varepsilon))\mathrm{e}^{\mathrm{i}K(\varepsilon)} = H + \varepsilon\hat{V}(\varepsilon). \tag{4.42}$$

This relation can be rewritten in the form

$$\mathrm{e}^{-\mathrm{i}\tilde{\mathcal{K}}(\varepsilon)}(H + \varepsilon V(\varepsilon)) = H + \varepsilon\hat{V}(\varepsilon), \tag{4.43}$$

where

$$\tilde{\mathcal{K}}(\varepsilon)(Y) := [K(\varepsilon), Y], \qquad \forall Y, \tag{4.44}$$

denotes the adjoint action generated by $K(\varepsilon)$.

We seek $K(\varepsilon)$ and $\hat{V}(\varepsilon)$ in the form of formal power series:

$$K(\varepsilon) = \sum_{s\geq 1} \varepsilon^s K_s(\varepsilon), \tag{4.45}$$

$$\hat{V}(\varepsilon) = \sum_{s\geq 0} \varepsilon^s V_s(\varepsilon), \tag{4.46}$$

with $K(0) = 0$, so that $W(0) = \mathrm{e}^{\mathrm{i}K(0)} = \mathbb{I}$.

Inserting the expansions (4.45)–(4.46) into (4.43) and comparing terms of equal order in ε yields a hierarchy of equations for the coefficients $K_\ell(\varepsilon)$ and $V_s(\varepsilon)$. This recursive scheme is referred to as the *Quantum KAM Iteration*, as it closely mirrors the classical procedure of Kolmogorov–Arnold–Moser. The result is summarized in the following lemma.

Lemma 4.2.1. *Let* $W(\varepsilon) = \mathrm{e}^{\mathrm{i}K(\varepsilon)}$*, and assume that* $K(\varepsilon)$ *and* $\hat{V}(\varepsilon)$ *admit the expansions* (4.45) *and* (4.46)*. Then equation (4.43) holds on* $D(H)$ *if and only if, for all* $s \geq 1$*,*

$$V_{s-1}(\varepsilon) = B_s(\varepsilon) - \mathrm{i}[K_s(\varepsilon), H], \tag{4.47}$$

where $B_s(\varepsilon)$ is defined as

$$B_1(\varepsilon) = V(\varepsilon), \tag{4.48}$$

$$B_s(\varepsilon) = \sum_{n=2}^{s} \frac{(-\mathrm{i})^n}{n!} \sum_{|\boldsymbol{\ell}|=s} \tilde{\mathcal{K}}^{\varepsilon}_{\ell_1} \cdots \tilde{\mathcal{K}}^{\varepsilon}_{\ell_n}(H) + \sum_{n=1}^{s-1} \frac{(-\mathrm{i})^n}{n!} \sum_{|\boldsymbol{\ell}|=s-1} \tilde{\mathcal{K}}^{\varepsilon}_{\ell_1} \cdots \tilde{\mathcal{K}}^{\varepsilon}_{\ell_n}(V(\varepsilon)), \tag{4.49}$$

where $\tilde{\mathcal{K}}^{\varepsilon}_{\ell_1} \cdots \tilde{\mathcal{K}}^{\varepsilon}_{\ell_n}(A) = [K_{\ell_1}(\varepsilon), \cdots, [K_{\ell_n}(\varepsilon), A] \cdots]$ for any suitable linear operator A. We use the multi-index notation $\boldsymbol{\ell} = (\ell_1, \dots, \ell_n) \in \mathbb{N}^n$, and $|\boldsymbol{\ell}| = \ell_1 + \cdots + \ell_n$.

Proof. We insert the expansions (4.45) and (4.46) into equation (4.43), obtaining:

$$\sum_{s\geq 0} \varepsilon^{s+1} V_s(\varepsilon) = \varepsilon V(\varepsilon) + \sum_{s\geq 1} \varepsilon^s \sum_{n=1}^{s} \frac{(-\mathrm{i})^n}{n!} \sum_{|\boldsymbol{\ell}|=s} \tilde{\mathcal{K}}^{\varepsilon}_{\ell_1} \cdots \tilde{\mathcal{K}}^{\varepsilon}_{\ell_n}(H) + \sum_{s\geq 1} \varepsilon^{s+1} \sum_{n=1}^{s} \frac{(-\mathrm{i})^n}{n!} \sum_{|\boldsymbol{\ell}|=s} \tilde{\mathcal{K}}^{\varepsilon}_{\ell_1} \cdots \tilde{\mathcal{K}}^{\varepsilon}_{\ell_n}(V(\varepsilon)). \tag{4.50}$$

Matching the coefficients of each power of ε we find at the first order:

$$\begin{aligned} V_0(\varepsilon) &= V(\varepsilon) - \mathrm{i}\tilde{\mathcal{K}}^{\varepsilon}_1(H) \\ &= V(\varepsilon) - \mathrm{i}[K_1(\varepsilon), H], \end{aligned} \tag{4.51}$$

which coincides with equation (4.47) for $s = 1$. At higher orders $s \geq 2$, we obtain:

$$V_{s-1}(\varepsilon) = \sum_{n=1}^{s} \frac{(-\mathrm{i})^n}{n!} \sum_{|\boldsymbol{\ell}|=s} \tilde{\mathcal{K}}^{\varepsilon}_{\ell_1} \cdots \tilde{\mathcal{K}}^{\varepsilon}_{\ell_n}(H) + \sum_{n=1}^{s-1} \frac{(-\mathrm{i})^n}{n!} \sum_{|\boldsymbol{\ell}|=s-1} \tilde{\mathcal{K}}^{\varepsilon}_{\ell_1} \cdots \tilde{\mathcal{K}}^{\varepsilon}_{\ell_n}(V(\varepsilon)). \tag{4.52}$$

Isolating the term with $n = 1$ in the first sum, we write:

$$-\mathrm{i}[K_s(\varepsilon), H] + \sum_{n=2}^{s} \frac{(-\mathrm{i})^n}{n!} \sum_{|\boldsymbol{\ell}|=s} \tilde{\mathcal{K}}^{\varepsilon}_{\ell_1} \cdots \tilde{\mathcal{K}}^{\varepsilon}_{\ell_n}(H), \tag{4.53}$$

which, substituted into (4.52), yields the recursive identity (4.47). □

We now solve equation (4.47) by imposing the main requirement of the construction: $\hat{V}(\varepsilon) \in \{H\}'$. Imposing this condition order by order leads to explicit expressions for both $V_\ell(\varepsilon)$ and $K_\ell(\varepsilon)$, as stated in the following result.

Lemma 4.2.2. *Equation* (4.47) *admits a unique solution under the constraint* $[K_s(\varepsilon)] = 0$, *given by the self-adjoint operators:*

$$V_{s-1}(\varepsilon) = \sum_{k\geq 1} P_k B_s(\varepsilon) P_k, \tag{4.54}$$

$$K_s(\varepsilon) = \mathrm{i} \sum_{k\neq \ell} \frac{P_k B_s(\varepsilon) P_\ell}{h_k - h_\ell}, \tag{4.55}$$

Proof. Fix $s \geq 1$. According to Lemma 4.2.1, the operators $V_{s-1}(\varepsilon)$ and $K_s(\varepsilon)$ must satisfy

$$V_{s-1}(\varepsilon) = B_s(\varepsilon) - \mathrm{i}[K_s(\varepsilon), H]. \tag{4.56}$$

We impose that $V_{s-1}(\varepsilon) \in \{H\}'$, i.e., that it commutes with H. This is equivalent to requiring

$$V_{s-1}(\varepsilon) = [V_{s-1}(\varepsilon)] := \sum_{k\geq 1} P_k V_{s-1}(\varepsilon) P_k. \tag{4.57}$$

Let us take the block-diagonal part of both sides of (4.56). The block-diagonal component of a commutator with H vanishes. Indeed,

$$P_k[K_s(\varepsilon), H]P_k = (h_k - h_k) P_k K_s(\varepsilon) P_k = 0. \tag{4.58}$$

Hence,

$$V_{s-1}(\varepsilon) = [B_s(\varepsilon)] = \sum_{k\geq 1} P_k B_s(\varepsilon) P_k, \tag{4.59}$$

which proves equation (4.54). Next, we determine $K_s(\varepsilon)$ by taking the off-diagonal part of (4.56):

$$\mathrm{i}[K_s(\varepsilon), H] = \{B_s(\varepsilon)\}. \tag{4.60}$$

This is a homological equation of the type considered in Lemma 4.1.1, whose unique solution under the constraint $[K_s(\varepsilon)] = 0$ is given by

$$K_s(\varepsilon) = \mathrm{i} \sum_{k\neq \ell} \frac{P_k B_s(\varepsilon) P_\ell}{h_k - h_\ell}, \tag{4.61}$$

as stated in (4.55).

It remains to prove that the operators $V_{s-1}(\varepsilon)$ and $K_s(\varepsilon)$ are self-adjoint, in order to complete the argument. It is sufficient to show that $B_s(\varepsilon)$ is self-adjoint. We proceed by induction on s. For $s = 1$, we have

$$B_1(\varepsilon) = V(\varepsilon), \tag{4.62}$$

which is self-adjoint by hypothesis. Suppose now that

$$B_j(\varepsilon) = B_j(\varepsilon)^\dagger \quad \text{for all } j = 1, \ldots, s-1. \tag{4.63}$$

Then, the corresponding operators $K_j(\varepsilon)$ are also self-adjoint for all $j = 1, \ldots, s-1$. Now consider the definition (4.49) of $B_s(\varepsilon)$: it is a linear combination of terms of the form

$$(-\mathrm{i})^n \tilde{\mathcal{K}}^\varepsilon_{\ell_1} \ldots \tilde{\mathcal{K}}^\varepsilon_{\ell_n}(A) = (-\mathrm{i})^n [K_{\ell_1}(\varepsilon), \cdots, [K_{\ell_n}(\varepsilon), A] \cdots]. \tag{4.64}$$

where $A = H$ or V and $\ell_i \leq s-1$ for all $i = 1 \ldots, n$. Hence, all these terms are self-adjoint operators. □

4.2.1 Convergence of the formal expansion

The construction in the previous subsection was purely formal. The operators $B_s(\varepsilon)$, $K_s(\varepsilon)$, and $V_s(\varepsilon)$ were defined through infinite series, and their convergence has not yet been established. Similarly, the operators $K(\varepsilon)$ and $\hat{V}(\varepsilon)$ were introduced by formal expansions in ε, whose convergence still needs to be proved. It is therefore necessary to show that these series converge in a nontrivial neighborhood of $\varepsilon = 0$.

To this end we make use of a well-known combinatorial sequence, the *Catalan numbers*, defined recursively by

$$\begin{aligned} d_1 &= 1, \\ d_s &= \sum_{\ell=1}^{s-1} d_\ell d_{s-\ell}, \quad \text{for } s \geq 2. \end{aligned} \tag{4.65}$$

For background on Catalan numbers and their applications, see Appendix A and [24].

We begin with an explicit estimate for the operators $B_s(\varepsilon)$.

Lemma 4.2.3. *For all $s \geq 1$,*

$$\frac{\pi}{\sqrt{3}\eta} \|B_s(\varepsilon)\| \leq \alpha^{s-1} b^s d_s, \tag{4.66}$$

where

$$b := \frac{\pi}{\sqrt{3}\eta} C, \tag{4.67}$$

and $\alpha \approx 4.79$ is the unique positive solution of the transcendental equation

$$(\alpha + 1)\left(\mathrm{e}^{\frac{2}{\alpha}} - 1\right) = 3. \tag{4.68}$$

Proof. We proceed by induction on s. For $s = 1$, inequality (4.66) holds trivially, since

$$\frac{\pi}{\sqrt{3}\eta} \|B_1(\varepsilon)\| = \frac{\pi}{\sqrt{3}\eta} \|V(\varepsilon)\| \leq \frac{\pi}{\sqrt{3}\eta} C = b = \alpha^0 d_1 b. \tag{4.69}$$

Let $s \geq 2$ and assume that

$$\frac{\pi}{\sqrt{3}\eta}\|B_j(\varepsilon)\| \leq \alpha^{j-1}b^j d_j, \quad \text{for all } j = 1, \dots, s-1. \tag{4.70}$$

We show that the same holds for $j = s$. From the definition (4.49) and the triangle inequality we obtain

$$\begin{aligned}\frac{\pi}{\sqrt{3}\eta}\|B_s(\varepsilon)\| \leq{}& \frac{\pi}{\sqrt{3}\eta}\sum_{n=2}^{s}\frac{1}{n!}\sum_{|\boldsymbol{\ell}|=s}\|\tilde{\mathcal{K}}^{\varepsilon}_{\ell_1}\cdots\tilde{\mathcal{K}}^{\varepsilon}_{\ell_n}(H)\| \\ &+ \frac{\pi}{\sqrt{3}\eta}\sum_{n=1}^{s}\frac{1}{n!}\sum_{|\boldsymbol{\ell}|=s-1}\|\tilde{\mathcal{K}}^{\varepsilon}_{\ell_1}\cdots\tilde{\mathcal{K}}^{\varepsilon}_{\ell_n}(V(\varepsilon))\|.\end{aligned} \tag{4.71}$$

From the homological equation

$$\mathrm{i}[K_s(\varepsilon), H] = \{B_s(\varepsilon)\}, \tag{4.72}$$

together with

$$\|\{B_s(\varepsilon)\}\| \leq 2\|B_s(\varepsilon)\|, \tag{4.73}$$

we deduce

$$\frac{\pi}{\sqrt{3}\eta}\|\tilde{\mathcal{K}}^{\varepsilon}_{\ell_1}\cdots\tilde{\mathcal{K}}^{\varepsilon}_{\ell_n}(H)\| \leq 2^n\prod_{j=1}^{n}\left(\frac{\pi}{\sqrt{3}\eta}\|B_{\ell_j}(\varepsilon)\|\right), \tag{4.74}$$

where we used Lemma 4.1.1 to bound $\|K_{\ell_j}(\varepsilon)\|$. Since $\ell_j \leq s-1$ for all j, we may apply the inductive hypothesis, obtaining

$$\frac{\pi}{\sqrt{3}\eta}\|\tilde{\mathcal{K}}^{\varepsilon}_{\ell_1}\cdots\tilde{\mathcal{K}}^{\varepsilon}_{\ell_n}(H)\| \leq \left(\frac{2}{\alpha}\right)^n \alpha^s b^s d_{\ell_1}\cdots d_{\ell_n}. \tag{4.75}$$

A similar estimate yields

$$\frac{\pi}{\sqrt{3}\eta}\|\tilde{\mathcal{K}}^{\varepsilon}_{\ell_1}\cdots\tilde{\mathcal{K}}^{\varepsilon}_{\ell_n}(V(\varepsilon))\| \leq \left(\frac{2}{\alpha}\right)^n \alpha^{s-1} b^s d_{\ell_1}\cdots d_{\ell_n}. \tag{4.76}$$

Combining the previous bounds, we get

$$\begin{aligned}\frac{\pi}{\sqrt{3}\eta}\|B_s(\varepsilon)\| \leq{}& \left[\alpha\sum_{n=2}^{s}\frac{1}{n!}\left(\frac{2}{\alpha}\right)^n\sum_{|\boldsymbol{\ell}|=s}d_{\ell_1}\cdots d_{\ell_n}\right. \\ &\left.+\sum_{n=1}^{s-1}\frac{1}{n!}\left(\frac{2}{\alpha}\right)^n\sum_{|\boldsymbol{\ell}|=s-1}d_{\ell_1}\cdots d_{\ell_n}\right]\alpha^{s-1}b^s.\end{aligned} \tag{4.77}$$

Using the recursive property (A.2) of Catalan numbers, we have

$$\sum_{|\boldsymbol{\ell}|=s} d_{\ell_1} \cdots d_{\ell_n} \leq d_s. \tag{4.78}$$

Hence, by extending the sum to ∞ yields

$$\frac{\pi}{\sqrt{3}\eta}\|B_s(\varepsilon)\| \leq \left[\alpha \sum_{n=2}^{\infty} \frac{1}{n!}\left(\frac{2}{\alpha}\right)^n d_s + \sum_{n=1}^{\infty} \frac{1}{n!}\left(\frac{2}{\alpha}\right)^n d_{s-1}\right] \alpha^{s-1} b^s. \tag{4.79}$$

Since $d_{s-1} \leq d_s$, this gives

$$\frac{\pi}{\sqrt{3}\eta}\|B_s(\varepsilon)\| \leq \left[(\alpha+1)\left(\mathrm{e}^{\frac{2}{\alpha}}-1\right)-2\right] d_s\, \alpha^{s-1} b^s. \tag{4.80}$$

By the definition (4.68) of α, the bracket equals 1, which proves the desired bound. This completes the induction step, and hence the proof. □

By using the estimates for the operators $B_s(\varepsilon)$ established in Lemma 4.2.3, we can prove that the operators $\hat{V}(\varepsilon)$ and $K(\varepsilon)$ are bounded for sufficiently small values of ε. As a preliminary step, we show that the coefficients appearing in the expansions of these operators can be themselves bounded in terms of the norms of the $B_s(\varepsilon)$.

Lemma 4.2.4. *For all $s \geq 1$, the operators $V_{s-1}(\varepsilon)$ and $K_s(\varepsilon)$ constructed in Lemma 4.2.2 satisfy the bounds:*

$$\|V_{s-1}(\varepsilon)\| \leq \|B_s(\varepsilon)\|, \tag{4.81}$$

$$\|K_s(\varepsilon)\| \leq \frac{\pi}{\sqrt{3}\eta}\|B_s(\varepsilon)\|. \tag{4.82}$$

Proof. To estimate the norm of $V_{s-1}(\varepsilon)$, observe that for any unit vector $\psi \in \mathcal{H}$,

$$\|V_{s-1}(\varepsilon)\psi\|^2 = \left\|\sum_{k\geq 1} P_k B_s(\varepsilon) P_k \psi\right\|^2 \tag{4.83}$$

$$= \sum_{k\geq 1} \|P_k B_s(\varepsilon) P_k \psi\|^2 \tag{4.84}$$

$$\leq \sum_{k\geq 1} \|P_k B_s(\varepsilon) P_k\|^2 \cdot \|P_k \psi\|^2 \tag{4.85}$$

$$\leq \sup_{k\geq 1} \|P_k B_s(\varepsilon) P_k\|^2 \cdot \sum_{k\geq 1} \|P_k \psi\|^2 \tag{4.86}$$

$$\leq \|B_s(\varepsilon)\|^2, \tag{4.87}$$

hence

$$\|V_{s-1}(\varepsilon)\| \leq \|B_s(\varepsilon)\|. \tag{4.88}$$

The bound (4.82) for $\|K_s(\varepsilon)\|$ follows directly from Lemma 4.1.1, since $K_s(\varepsilon)$ is the solution of the Homological Equation. □

Now we are ready to prove the boundedness of the operators $K(\varepsilon)$ and $\hat{V}(\varepsilon)$.

Lemma 4.2.5. *Let $K(\varepsilon)$ and $\hat{V}(\varepsilon)$ be the operators defined by the expansions* (4.45) *and* (4.46). *Then, for all $\varepsilon \in \mathbb{R}$ such that*

$$|\varepsilon| \leq \frac{\eta}{C\rho}, \tag{4.89}$$

the following bounds hold:

$$\|K(\varepsilon)\| \leq |\varepsilon|\, b\, \mathcal{D}(\alpha|\varepsilon|b), \tag{4.90}$$

$$\|\hat{V}(\varepsilon)\| \leq C\, \mathcal{D}(\alpha|\varepsilon|b), \tag{4.91}$$

where the function $\mathcal{D}$ is defined as

$$\mathcal{D}(y) := \frac{1-\sqrt{1-4y}}{2y}, \tag{4.92}$$

that is, the generating function of the Catalan numbers. Finally, we recall the definition (4.39) *of ρ:*

$$\rho = \frac{4\pi\alpha}{\sqrt{3}}. \tag{4.93}$$

Proof. We start by estimating the norm of the operator $K(\varepsilon)$. Using the bound (4.82) and Lemma 4.2.3, we obtain

$$\|K(\varepsilon)\| \leq \sum_{\ell\geq 1} |\varepsilon|^{\ell}\|K_\ell(\varepsilon)\| \leq |\varepsilon| b \sum_{\ell \geq 1} d_\ell (\alpha|\varepsilon|b)^{\ell-1}. \tag{4.94}$$

It can be shown that, for all $|y| \leq \frac{1}{4}$,

$$\sum_{\ell\geq 1} d_\ell y^{\ell-1} = \mathcal{D}(y). \tag{4.95}$$

Hence

$$\|K(\varepsilon)\| \leq |\varepsilon| b\, \mathcal{D}(\alpha|\varepsilon|b), \tag{4.96}$$

provided that

$$|\varepsilon| \leq \frac{1}{4\alpha b} = \frac{\sqrt{3}\eta}{4\pi\alpha C} = \frac{\eta}{\rho C}. \tag{4.97}$$

The bound for $\hat{V}(\varepsilon)$ follows similarly. Using the bound (4.81) we can write

$$\|\hat{V}(\varepsilon)\| \leq \sum_{\ell\geq 0} |\varepsilon|^{\ell}\|V_\ell(\varepsilon)\| \leq \sum_{\ell\geq 0} |\varepsilon|^{\ell}\|B_{\ell+1}(\varepsilon)\|. \tag{4.98}$$

Using the estimate of Lemma 4.2.3

$$\|B_{\ell+1}(\varepsilon)\| \leq \frac{\sqrt{3}\eta}{\pi}\alpha^\ell b^{\ell+1} d_{\ell+1} = C(\alpha b)^\ell d_{\ell+1},$$

we get, after shifting the index of sum

$$\|\hat{V}(\varepsilon)\| \leq C\sum_{\ell\geq 1} d_\ell(\alpha|\varepsilon|b)^{\ell-1} = C\,\mathcal{D}(\alpha|\varepsilon|b), \tag{4.99}$$

again under the same condition $|\varepsilon| \leq \eta/(C\rho)$. □

This concludes the construction of the operators $K(\varepsilon)$ and $\hat{V}(\varepsilon)$.

4.2.2 Proof of (iii) and (vi) of Theorem 4.2.1

In the previous subsections, we have explicitly constructed the operators $W(\varepsilon) = \mathrm{e}^{\mathrm{i}K(\varepsilon)}$ and $\hat{V}(\varepsilon)$ appearing in Theorem 3.3.2. We now verify that they satisfy the required properties. Properties $(i), (ii), (iv), (v)$ follow directly from the construction. It remains to prove properties (iii) and (vi). We begin with property (iii), namely that for all $\psi \in D(H)$, we have $\|HW(\varepsilon)\psi\| < +\infty$. In fact, we can prove a more quantitative bound in terms of the Catalan generating function.

Lemma 4.2.6. *Let $W(\varepsilon) = \mathrm{e}^{\mathrm{i}K(\varepsilon)}$. Then, for all $\psi \in D(H)$,*

$$\|HW(\varepsilon)\psi\| \leq \mathrm{e}^{|\varepsilon|b\mathcal{D}(\alpha|\varepsilon|b)}\left(\|H\psi\| + \frac{2\sqrt{3}\eta}{\pi}|\varepsilon|b\mathcal{D}(\alpha|\varepsilon|b)\|\psi\|\right), \tag{4.100}$$

for $|\varepsilon| \leq \eta/(\rho C)$.

Proof. Recall the expansion

$$K(\varepsilon) = \sum_{s\geq 1}\varepsilon^s K_s(\varepsilon), \tag{4.101}$$

where the coefficients $K_s(\varepsilon)$ are solutions the homological equations

$$\mathrm{i}[K_s(\varepsilon), H] = \{B_s(\varepsilon)\}. \tag{4.102}$$

By Lemma 4.1.1, they satisfy the bound

$$\|HK_s(\varepsilon)\psi\| \leq \left(2\|\psi\| + \frac{\pi}{\sqrt{3}\eta}\|H\psi\|\right)\|B_s(\varepsilon)\|, \qquad \forall\psi \in D(H). \tag{4.103}$$

This yields

$$\|HK(\varepsilon)\psi\| \leq \left(2\|\psi\| + \frac{\pi}{\sqrt{3}\eta}\|H\psi\|\right)\sum_{s\geq 1}|\varepsilon|^s\|B_s(\varepsilon)\|. \tag{4.104}$$

Using the bound

$$\|B_s(\varepsilon)\| \leq \frac{\sqrt{3}\eta}{\pi}\alpha^{s-1}d_s b^s, \tag{4.105}$$

we find, for $|\varepsilon| < \eta/(C\rho)$

$$\|HK(\varepsilon)\psi\| \leq \left(\|H\psi\| + 2\frac{\sqrt{3}\eta}{\pi}\|\psi\|\right)|\varepsilon|b\mathcal{D}(\alpha|\varepsilon|b), \tag{4.106}$$

where $\mathcal{D}(y)$ is the generating function of Catalan numbers. This shows that $K(\varepsilon)D(H) \subseteq D(H)$. We now prove by induction that, for all $n \geq 1$,

$$\|HK(\varepsilon)^n\psi\| \leq \left(\|H\psi\| + 2n\frac{\sqrt{3}\eta}{\pi}\|\psi\|\right)\left(|\varepsilon|b\mathcal{D}(\alpha|\varepsilon|b)\right)^n. \tag{4.107}$$

We have already shown the case $n = 1$. Suppose the estimate holds for $n = s - 1$:

$$\|HK(\varepsilon)^{s-1}\psi\| \leq \left(\|H\psi\| + 2(s-1)\frac{\sqrt{3}\eta}{\pi}\|\psi\|\right)\left(|\varepsilon|b\mathcal{D}(\alpha|\varepsilon|b)\right)^{s-1}. \tag{4.108}$$

Then, since $K(\varepsilon)\psi \in D(H)$, we can apply (4.108) to $\varphi = K(\varepsilon)\psi$, obtaining:

$$\begin{aligned} \|HK(\varepsilon)^s\psi\| &= \|HK(\varepsilon)^{s-1}K(\varepsilon)\psi\| && (4.109)\\ &\leq \left(\|HK(\varepsilon)\psi\| + 2(s-1)\frac{\sqrt{3}\eta}{\pi}\|K(\varepsilon)\psi\|\right)|\varepsilon|b\mathcal{D}(\alpha|\varepsilon|b) \\ &\leq \left(\|H\psi\| + 2s\frac{\sqrt{3}\eta}{\pi}\|\psi\|\right)\left(|\varepsilon|b\mathcal{D}(\alpha|\varepsilon|b)\right)^s, && (4.110) \end{aligned}$$

where we used Theorem 4.2.5 and (4.106).

We are now ready to estimate $\|HW(\varepsilon)\psi\|$ for all $\psi \in D(H)$:

$$\begin{aligned} \|HW(\varepsilon)\psi\| &= \|H\psi + H(W(\varepsilon) - \mathbb{I})\psi\| && (4.111)\\ &\leq \|H\psi\| + \left\|H\sum_{n\geq 1}\frac{(-\mathrm{i})^n K(\varepsilon)^n}{n!}\psi\right\| && (4.112)\\ &\leq \|H\psi\| + \sum_{n\geq 1}\frac{\|HK(\varepsilon)^n\psi\|}{n!} && (4.113)\\ &\leq \|H\psi\| + \sum_{n\geq 1}\left(\|H\psi\| + 2n\frac{\sqrt{3}\eta}{\pi}\|\psi\|\right)\frac{\left(b|\varepsilon|\mathcal{D}(\alpha|\varepsilon|b)\right)^n}{n!} && (4.114)\\ &= \mathrm{e}^{b|\varepsilon|\mathcal{D}(\alpha|\varepsilon|b)}\left(\|H\psi\| + 2\frac{\sqrt{3}\eta}{\pi}b|\varepsilon|\mathcal{D}(\alpha|\varepsilon|b)\|\psi\|\right), && (4.115) \end{aligned}$$

valid again for $|\varepsilon| \leq \eta/(C\rho)$. □

The last point to verify is property (vi) of Theorem 3.3.2. We first prove the following lemma.

Lemma 4.2.7. *Let* $W(\varepsilon) = \mathrm{e}^{\mathrm{i}K(\varepsilon)}$. *Then*

$$\|W(\varepsilon) - \mathbb{I}\| \leq \mathrm{e}^{|\varepsilon| b\, \mathcal{D}(\alpha|\varepsilon| b)} - 1, \qquad \textit{for } |\varepsilon| \leq \frac{\eta}{C\rho}. \tag{4.116}$$

Proof. We estimate:

$$\begin{aligned}\|W(\varepsilon) - \mathbb{I}\| &= \left\|\mathrm{e}^{\mathrm{i}K(\varepsilon)} - \mathbb{I}\right\| = \left\| \sum_{n\geq 1} \frac{(-\mathrm{i}K(\varepsilon))^n}{n!} \right\| \\ &\leq \sum_{n\geq 1} \frac{\|K(\varepsilon)\|^n}{n!} = \mathrm{e}^{\|K(\varepsilon)\|} - 1 \\ &\leq \mathrm{e}^{|\varepsilon| b\, \mathcal{D}(\alpha|\varepsilon| b)} - 1, \end{aligned} \tag{4.117}$$

for all $|\varepsilon| \leq \eta/(C\rho)$. The last step follows from Theorem 4.2.5. □

Let us define

$$f_\alpha(x) := \mathrm{e}^{x\mathcal{D}(\alpha x)} - 1. \tag{4.118}$$

A direct analysis shows that, for $x < \frac{1}{4\alpha}$,

$$f_\alpha(x) < 4\alpha\big(\mathrm{e}^{\frac{1}{2\alpha}} - 1\big)x. \tag{4.119}$$

Setting $x = |\varepsilon| b$, we obtain

$$\|W(\varepsilon) - \mathbb{I}\| \leq \beta \frac{C}{\eta}|\varepsilon|, \qquad \text{for } |\varepsilon| \leq \frac{\eta}{C\rho}, \tag{4.120}$$

where

$$\beta := \frac{4\pi\alpha}{\sqrt{3}}\big(\mathrm{e}^{\frac{1}{2\alpha}} - 1\big). \tag{4.121}$$

This completes the proof of property (vi).

Alternatively, $f_\alpha(x)$ may be approximated by a quadratic upper bound,

$$f_\alpha(x) < x + cx^2, \tag{4.122}$$

where

$$c := (4\alpha)^2\big(\mathrm{e}^{\frac{1}{2\alpha}} - 1\big) - 4\alpha. \tag{4.123}$$

A comparison between $f_\alpha(x)$, its optimal linear bound (4.120), and the quadratic upper bound (4.122) is shown in Fig. 4.1.

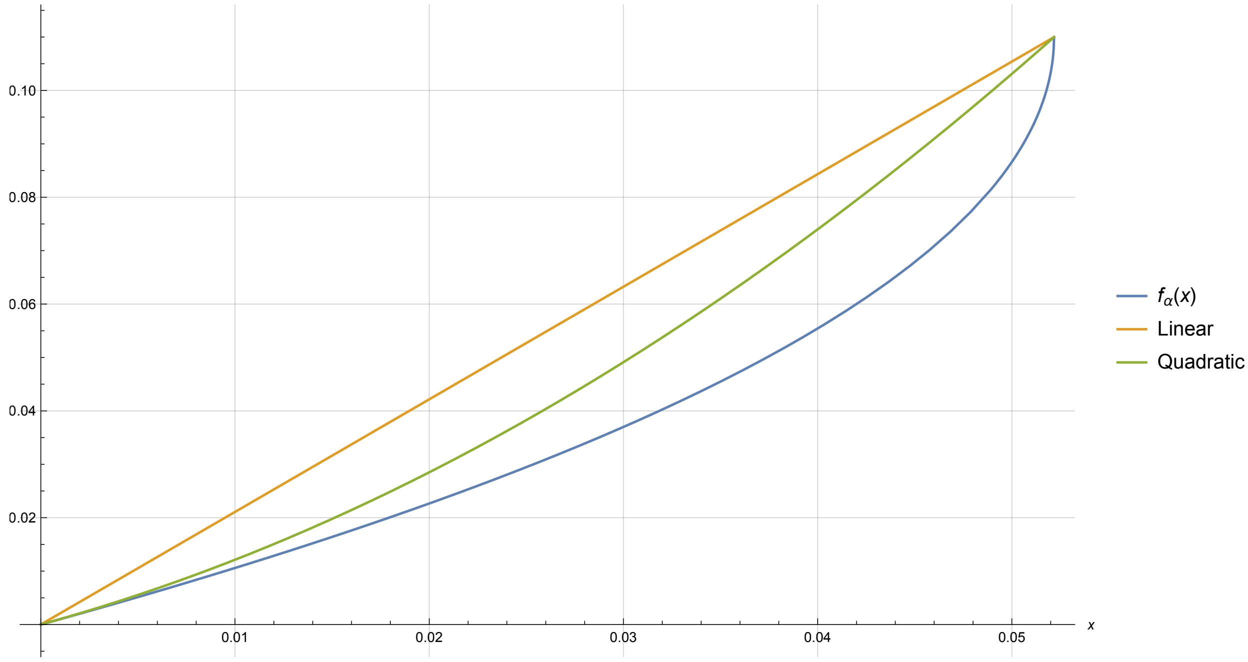

Figure 4.1: Comparison of $f_\alpha(x) = \mathrm{e}^{x\mathcal{D}(\alpha x)} - 1$ with its linear bound (4.120) and quadratic upper bound (4.122), as a function of $x = |\varepsilon|\, b$, with $b = \pi C/(\sqrt{3}\eta)$.

Chapter 5

Trotter Product Method

In the previous chapter, we constructed the unitary operator $W(\varepsilon)$ as the exponential of an imaginary bounded self-adjoint operator $K(\varepsilon)$, itself defined as a convergent power series. In this chapter, we adopt an alternative strategy inspired by the *Trotter product formula*. This formula is widely used in quantum physics to approximate the exponential of a sum of two or more non-commuting operators by a product of exponentials [3–5]. Following this idea, we replace the single exponential representation (the power-series definition of $K(\varepsilon)$) with an infinite product of unitary factors of the kind $\mathrm{e}^{\mathrm{i}\varepsilon^\ell K_\ell}$, where each K_ℓ is a bounded self-adjoint operator. This construction automatically guarantees the unitarity of $W(\varepsilon)$ and provides a framework that is particularly advantageous from a numerical perspective, as will be discussed at the end of this chapter.

5.1 Trotter KAM Iteration

Let us again consider the conjugation equation

$$H + \varepsilon\hat{V}(\varepsilon) = W(\varepsilon)^\dagger \left(H + \varepsilon V(\varepsilon)\right) W(\varepsilon), \tag{5.1}$$

where we use for $\hat{V}(\varepsilon)$ the same expansion as in the previous chapters:

$$\hat{V}(\varepsilon) = \sum_{s\geq 1} \varepsilon^s V_s(\varepsilon), \tag{5.2}$$

and require it to be block-diagonal in the spectral representation of H.

In the previous chapters, we parametrized $W(\varepsilon)$ through the ansatz

$$W(\varepsilon) = \mathrm{e}^{\mathrm{i}K(\varepsilon)}, \tag{5.3}$$

and expanded $K(\varepsilon)$ in powers of ε. We now adopt a different strategy, inspired by the Trotter product formula: we express $W(\varepsilon)$ as an ordered product of exponentials,

$$W(\varepsilon) = \overrightarrow{\prod_{\ell \geq 1}} \mathrm{e}^{\mathrm{i}\varepsilon^\ell K_\ell}, \tag{5.4}$$

where the arrow indicates that factors with smaller indices appear on the left. With this approach, we can state the following theorem.

Theorem 5.1.1. *Let H be a Hamiltonian with purely point spectrum $\{h_k\}_{k\geq 1}$ and non-vanishing minimal spectral gap*

$$\eta = \inf_{k \neq \ell} |h_k - h_\ell| > 0. \tag{5.5}$$

Then, there exist two families of operators $W(\varepsilon)$ and $\hat{V}(\varepsilon)$ satisfying the following properties:

1. *$\hat{V}(\varepsilon)$ is self-adjoint and belongs to the commutant of H, i.e. $\hat{V}(\varepsilon) = \hat{V}(\varepsilon)^\dagger \in \{H\}'$.*
2. *$W(\varepsilon)$ is unitary.*
3. *$W(\varepsilon)$ leaves the domain of H invariant: $W(\varepsilon)D(H) \subseteq D(H)$.*
4. *$W(0) = \mathbb{I}$.*
5. *The operators $H + \varepsilon V(\varepsilon)$ and $H + \varepsilon\hat{V}(\varepsilon)$ are unitarily equivalent through $W(\varepsilon)$:*

$$W(\varepsilon)^\dagger (H + \varepsilon V(\varepsilon)) W(\varepsilon)\psi = (H + \varepsilon\hat{V}(\varepsilon))\psi, \qquad \forall\, \psi \in D(H). \tag{5.6}$$

6. *$W(\varepsilon)$ satisfies the bound*

$$\|W(\varepsilon) - \mathbb{I}\| \leq \beta \frac{C}{\eta} |\varepsilon|, \tag{5.7}$$

for all ε such that

$$|\varepsilon| \leq \frac{\eta}{C\rho}.$$

The constants β and ρ are given by

$$\beta := \frac{2\pi}{\sqrt{3}} \alpha \left(\mathrm{e}^{\frac{1}{\alpha}} - 1 \right), \tag{5.8}$$

$$\rho := \frac{2\pi\alpha}{\sqrt{3}}, \tag{5.9}$$

where $\alpha \approx 4.79$ is the unique positive solution of the transcendental equation

$$(\alpha + 1) \left(\mathrm{e}^{\frac{2}{\alpha}} - 1 \right) = 3.$$

In order to prove the theorem, we proceed as in the previous chapter: we first construct the operators $\hat{V}(\varepsilon)$ and $W(\varepsilon)$ formally, and then establish their convergence and corresponding bounds.

5.1.1 Formal construction

Since the operators K_ℓ do not commute in general, expression (5.4) is not equivalent to (5.3). Nevertheless, (5.4) always defines a unitary operator whenever the K_ℓ are self–adjoint, and therefore it can be consistently inserted into equation (5.1):

$$\left(\overleftarrow{\prod_{\ell\geq 1}} \mathrm{e}^{-\mathrm{i}\varepsilon^\ell K_\ell}\right)(H+\varepsilon V(\varepsilon))\left(\overrightarrow{\prod_{\ell\geq 1}} \mathrm{e}^{\mathrm{i}\varepsilon^\ell K_\ell}\right), \tag{5.10}$$

where $\overleftarrow{\prod}_{\ell\geq 1}$ denotes a product ordered from right to left.

Using the definition of the adjoint action, the above expression can be rewritten as

$$H+\varepsilon\hat{V}(\varepsilon)=\overleftarrow{\prod_{\ell\geq 1}} \mathrm{e}^{-\mathrm{i}\varepsilon^\ell \tilde{\mathcal{K}}_\ell}(H+\varepsilon V(\varepsilon)), \tag{5.11}$$

where $\tilde{\mathcal{K}}_\ell$ denotes the adjoint action of K_ℓ.

The infinite product in (5.11) is to be interpreted in a formal sense. At any finite order in ε, only finitely many factors contribute. More precisely, to determine all terms up to order ε^s, it is sufficient to truncate the product to its first s factors. Indeed, each exponential factor satisfies

$$\mathrm{e}^{-\mathrm{i}\varepsilon^\ell K_\ell(\varepsilon)}=\mathbb{I}+O(\varepsilon^\ell), \qquad \ell\geq 2,$$

and therefore affects the expansion only starting from order ε^ℓ. This observation will be crucial for deriving the recursive relations below.

Lemma 5.1.1. *Assume that $\hat{V}(\varepsilon)$ admits the expansion* (5.2)*. Then equation* (5.11) *holds on $D(H)$ if and only if, for all $s\geq 1$,*

$$V_{s-1}(\varepsilon)=B_s(\varepsilon)-\mathrm{i}[K_s(\varepsilon),H], \tag{5.12}$$

where $B_s(\varepsilon)$ is defined as

$$B_1(\varepsilon)=V(\varepsilon), \tag{5.13}$$

$$B_s(\varepsilon)=\sum_{\substack{\boldsymbol{n}\in\mathbb{N}^{s-1}\\ \boldsymbol{s}\cdot\boldsymbol{n}=s}}\frac{(-\mathrm{i})^{|\boldsymbol{n}|}}{\boldsymbol{n}!}\tilde{K}_{s-1}^{n_{s-1}}\cdots\tilde{K}_1^{n_1}(H) \tag{5.14}$$

$$+\sum_{\substack{\boldsymbol{n}\in\mathbb{N}^{s-1}\\ \boldsymbol{s}\cdot\boldsymbol{n}=s-1}}\frac{(-\mathrm{i})^{|\boldsymbol{n}|}}{\boldsymbol{n}!}\tilde{K}_{s-1}^{n_{s-1}}\cdots\tilde{K}_1^{n_1}\big(V(\varepsilon)\big), \tag{5.15}$$

with the multi-index notation $\boldsymbol{n}=(n_1,\dots,n_{s-1})\in\mathbb{N}^{s-1}$, $|\boldsymbol{n}|=n_1+\cdots+n_{s-1}$ and $\boldsymbol{s}\cdot\boldsymbol{n}=n_1+2n_2+\cdots+(s-1)n_{s-1}$.

Proof. As noted above, it suffices to consider only the first factor in the product defining $W(\varepsilon)$ to determine the first order of equation (5.12). Hence, to fix the operator $V_0(\varepsilon)$, it is enough to study

$$\mathrm{e}^{-\mathrm{i}\varepsilon\tilde{\mathcal{K}}_1}(H+\varepsilon V(\varepsilon)) = H + \varepsilon V_0(\varepsilon) + O(\varepsilon^2), \tag{5.16}$$

where $V_0(\varepsilon)$ coincides with the first term of the expansion (5.2).

Expanding the left-hand side of (5.16), we find

$$\begin{aligned}\mathrm{e}^{-\mathrm{i}\varepsilon\tilde{\mathcal{K}}_1}(H+\varepsilon V(\varepsilon)) &= H + \varepsilon V(\varepsilon) + \sum_{n\geq 1}\frac{(-\mathrm{i})^n}{n!}\varepsilon^n\tilde{\mathcal{K}}_1(H) + \sum_{n\geq 1}\frac{(-\mathrm{i})^n}{n!}\varepsilon^{n+1}\tilde{\mathcal{K}}_1(V(\varepsilon)) && (5.17)\\ &= H + \varepsilon\big(V(\varepsilon) - \mathrm{i}[K_1(\varepsilon), H]\big) + O(\varepsilon^2). && (5.18)\end{aligned}$$

By imposing equality in (5.16) at order ε, we obtain

$$V_0(\varepsilon) = V(\varepsilon) - \mathrm{i}[K_1(\varepsilon), H], \tag{5.19}$$

which coincides with equation (5.12) for $s = 1$.

To derive the generic order s, we consider the first s factors of the operator $W(\varepsilon)$. The operator $V_{s-1}(\varepsilon)$ will then correspond to the coefficient of order ε^s. Expanding the exponentials, we obtain

$$\begin{aligned}\mathrm{e}^{-\mathrm{i}\varepsilon^s\tilde{\mathcal{K}}_s}\dots\mathrm{e}^{-\mathrm{i}\varepsilon\tilde{\mathcal{K}}_1}(H+\varepsilon V(\varepsilon)) &= \sum_{n_s\geq 0}\cdots\sum_{n_1\geq 0}\frac{(-\mathrm{i})^{n_s+\cdots+n_1}}{n_s!\cdots n_1!}\,\varepsilon^{sn_s+\cdots+n_1}\tilde{\mathcal{K}}_s^{n_s}\cdots\tilde{\mathcal{K}}_1^{n_1}(H+\varepsilon V(\varepsilon))\\ &= \sum_{\boldsymbol{n}\in\mathbb{N}^s}\frac{(-\mathrm{i})^{|\boldsymbol{n}|}}{\boldsymbol{n}!}\,\varepsilon^{\boldsymbol{s}\cdot\boldsymbol{n}}\,\tilde{\mathcal{K}}_s^{n_s}\cdots\tilde{\mathcal{K}}_1^{n_1}(H+\varepsilon V(\varepsilon)). && (5.20)\end{aligned}$$

where we have introduced the notation

$$\boldsymbol{n} = (n_1,\dots,n_s), \tag{5.21}$$

$$\boldsymbol{s} = (1,2,\dots,s), \tag{5.22}$$

$$|\boldsymbol{n}| = n_1 + \cdots + n_s, \tag{5.23}$$

$$\boldsymbol{n}! = n_1!\cdots n_s!, \tag{5.24}$$

$$\boldsymbol{s}\cdot\boldsymbol{n} = n_1 + 2n_2 + \cdots + sn_s. \tag{5.25}$$

Expanding each power of ε, we get

$$\mathrm{e}^{-\mathrm{i}\varepsilon^s\tilde{\mathcal{K}}_s}\cdots\mathrm{e}^{-\mathrm{i}\varepsilon\tilde{\mathcal{K}}_1}(H+\varepsilon V(\varepsilon)) = H+\varepsilon V(\varepsilon)+\sum_{\ell\geq 1}\varepsilon^\ell\sum_{\substack{\boldsymbol{n}\in\mathbb{N}^s\\ \boldsymbol{s}\cdot\boldsymbol{n}=\ell}}\frac{(-\mathrm{i})^{|\boldsymbol{n}|}}{\boldsymbol{n}!}\tilde{\mathcal{K}}_s^{n_s}\cdots\tilde{\mathcal{K}}_1^{n_1}(H+\varepsilon V(\varepsilon)) \tag{5.26}$$

$$= H+\varepsilon V(\varepsilon)+\sum_{\ell\geq 1}\varepsilon^\ell\sum_{\substack{\boldsymbol{n}\in\mathbb{N}^s\\ \boldsymbol{s}\cdot\boldsymbol{n}=\ell}}\frac{(-\mathrm{i})^{|\boldsymbol{n}|}}{\boldsymbol{n}!}\tilde{\mathcal{K}}_s^{n_s}\cdots\tilde{\mathcal{K}}_1^{n_1}(H) \tag{5.27}$$

$$+\sum_{\ell\geq 1}\varepsilon^{\ell+1}\sum_{\substack{\boldsymbol{n}\in\mathbb{N}^s\\ \boldsymbol{s}\cdot\boldsymbol{n}=\ell}}\frac{(-\mathrm{i})^{|\boldsymbol{n}|}}{\boldsymbol{n}!}\tilde{\mathcal{K}}_s^{n_s}\cdots\tilde{\mathcal{K}}_1^{n_1}(V(\varepsilon)). \tag{5.28}$$

We then identify $V_{s-1}(\varepsilon)$ with the coefficient of ε^s in the expansion above, namely

$$V_{s-1}(\varepsilon)=\sum_{\substack{\boldsymbol{n}\in\mathbb{N}^s\\ \boldsymbol{s}\cdot\boldsymbol{n}=s}}\frac{(-\mathrm{i})^{|\boldsymbol{n}|}}{\boldsymbol{n}!}\tilde{\mathcal{K}}_s^{n_s}\cdots\tilde{\mathcal{K}}_1^{n_1}(H)+\sum_{\substack{\boldsymbol{n}\in\mathbb{N}^s\\ \boldsymbol{s}\cdot\boldsymbol{n}=s-1}}\frac{(-\mathrm{i})^{|\boldsymbol{n}|}}{\boldsymbol{n}!}\tilde{\mathcal{K}}_s^{n_s}\cdots\tilde{\mathcal{K}}_1^{n_1}(V(\varepsilon)). \tag{5.29}$$

In the first sum we separate the contribution of the multi-index $\boldsymbol{n}=(0,\dots,0,1)$. Indeed, this is the *only* multi-index with $n_s\geq 1$ compatible with the constraint $\boldsymbol{s}\cdot\boldsymbol{n}=s$: if $n_s\geq 1$ and some $n_j>0$ with $j<s$, then $\boldsymbol{s}\cdot\boldsymbol{n}\geq s+1$. Thus we can write

$$V_{s-1}(\varepsilon)=-\mathrm{i}[K_s(\varepsilon),H]+\sum_{\substack{\boldsymbol{n}\in\mathbb{N}^s\\ \boldsymbol{s}\cdot\boldsymbol{n}=s,\ n_s=0}}\frac{(-\mathrm{i})^{|\boldsymbol{n}|}}{\boldsymbol{n}!}\tilde{\mathcal{K}}_s^{0}\cdots\tilde{\mathcal{K}}_1^{n_1}(H) \tag{5.30}$$

$$+\sum_{\substack{\boldsymbol{n}\in\mathbb{N}^s\\ \boldsymbol{s}\cdot\boldsymbol{n}=s-1,\ n_s=0}}\frac{(-\mathrm{i})^{|\boldsymbol{n}|}}{\boldsymbol{n}!}\tilde{\mathcal{K}}_s^{0}\cdots\tilde{\mathcal{K}}_1^{n_1}(V(\varepsilon)). \tag{5.31}$$

The condition $\boldsymbol{s}\cdot\boldsymbol{n}=s-1$ in the second sum forces $n_s=0$ as well, since otherwise $sn_s\leq s-1$ would be violated. Hence in both sums we have $n_s=0$, so that $\tilde{\mathcal{K}}_s^0=\mathbb{I}$ and the multi-indices can be identified with elements of $\mathbb{N}^{s-1}$. Renaming $\boldsymbol{n}=(n_1,\dots,n_{s-1})$, we obtain

$$V_{s-1}(\varepsilon)=B_s(\varepsilon)-\mathrm{i}[K_s(\varepsilon),H], \tag{5.32}$$

where

$$B_s(\varepsilon):=\sum_{\substack{\boldsymbol{n}\in\mathbb{N}^{s-1}\\ \boldsymbol{s}\cdot\boldsymbol{n}=s}}\frac{(-\mathrm{i})^{|\boldsymbol{n}|}}{\boldsymbol{n}!}\tilde{\mathcal{K}}_{s-1}^{n_{s-1}}\cdots\tilde{\mathcal{K}}_1^{n_1}(H) \tag{5.33}$$

$$+\sum_{\substack{\boldsymbol{n}\in\mathbb{N}^{s-1}\\ \boldsymbol{s}\cdot\boldsymbol{n}=s-1}}\frac{(-\mathrm{i})^{|\boldsymbol{n}|}}{\boldsymbol{n}!}\tilde{\mathcal{K}}_{s-1}^{n_{s-1}}\cdots\tilde{\mathcal{K}}_1^{n_1}(V(\varepsilon)). \tag{5.34}$$

This is precisely equation (5.12) for $s\geq 1$, and the proof is complete. □

We now solve equation (5.12) by imposing the main requirement of the construction:

$\hat{V}(\varepsilon) \in \{H\}'$. Imposing this condition order by order leads to explicit expressions for both $V_{s-1}(\varepsilon)$ and $K_s(\varepsilon)$, as stated in the following result.

Lemma 5.1.2. *Equation* (5.12) *admits a unique solution under the constraint* $[K_s(\varepsilon)] = 0$, *given by the self-adjoint operators:*

$$V_{s-1}(\varepsilon) = \sum_{k\geq 1} P_k B_s(\varepsilon) P_k, \tag{5.35}$$

$$K_s(\varepsilon) = \mathrm{i} \sum_{k\neq \ell} \frac{P_k B_s(\varepsilon) P_\ell}{h_k - h_\ell}, \tag{5.36}$$

Proof. Equation (5.12) has the same structure of equation (4.47) (with $B_s(\varepsilon)$ defined differently). Then, we can follow the same steps of the proof of Lemma 4.2.2 in order to get the thesis. Notice that also in such a case $K_s(\varepsilon)$ is the solution of the homological equation

$$\mathrm{i}[K_s(\varepsilon), H] = \{B_s(\varepsilon)\} \tag{5.37}$$

and then satisfies the estimate

$$\|K_s(\varepsilon)\| \leq \frac{\pi}{\sqrt{3}\eta} \|B_s(\varepsilon)\| \,. \tag{5.38}$$

□

5.1.2 Estimates

The construction in the previous subsection was purely formal. The operators $B_s(\varepsilon)$, $K_s(\varepsilon)$, and $V_s(\varepsilon)$ were defined through infinite series, and their convergence has not yet been established. Similarly, the operators $W(\varepsilon)$ and $\hat{V}(\varepsilon)$ were introduced, respectively, as an infinite product and an infinite sum, whose convergence still needs to be proved. It is therefore necessary to show that these series converge in a nontrivial neighborhood of $\varepsilon = 0$.

As in the previous analysis, we will use the *Catalan numbers*, defined recursively by

$$\begin{aligned} d_1 &= 1, \\ d_s &= \sum_{\ell=1}^{s-1} d_\ell \, d_{s-\ell}, \qquad \text{for } s \geq 2. \end{aligned} \tag{5.39}$$

In order to perform the forthcoming estimates, it is convenient to rewrite the operators $B_s(\varepsilon)$ in a form that makes explicit their combinatorial structure. This representation will allow us to count and bound systematically all contributions appearing at each order in ε.

Let us compute their explicit expression for the first few orders:

$$B_1(\varepsilon) = V(\varepsilon), \tag{5.40}$$
$$B_2(\varepsilon) = \frac{(-\mathrm{i})^2}{2}\,\tilde{\mathcal{K}}_1^2(H) - \mathrm{i}\,\tilde{\mathcal{K}}_1(V(\varepsilon))\,, \tag{5.41}$$
$$B_3(\varepsilon) = \frac{(-\mathrm{i})^3}{3!}\,\tilde{\mathcal{K}}_1^3(H) + \frac{(-\mathrm{i})^3}{2!1!}\,\tilde{\mathcal{K}}_2\tilde{\mathcal{K}}_1(H) + \frac{(-\mathrm{i})^2}{2}\,\tilde{\mathcal{K}}_1^2(V(\varepsilon)) - \mathrm{i}\,\tilde{\mathcal{K}}_2(V(\varepsilon))\,. \tag{5.42}$$

From these examples, one sees that every term in $B_s(\varepsilon)$, with $s \geq 2$, in which H appears, has the general structure

$$\frac{(-\mathrm{i})^n}{\boldsymbol{m_\ell}!}\,\tilde{\mathcal{K}}_{\ell_n}\cdots\tilde{\mathcal{K}}_{\ell_1}(H), \tag{5.43}$$

where $|\boldsymbol{\ell}| = s$, $1 \leq \ell_1 \leq \cdots \leq \ell_n$, $2 \leq n \leq s$, and $\boldsymbol{m_\ell}$ is a multiplicity vector defined as follows. If $\boldsymbol{\ell}$ is an ordered multi–index, it can be written as

$$\boldsymbol{\ell} = (\underbrace{a_1, \ldots, a_1}_{m_1 \text{ times}}, \underbrace{a_2, \ldots, a_2}_{m_2 \text{ times}}, \ldots, \underbrace{a_r, \ldots, a_r}_{m_r \text{ times}}), \tag{5.44}$$

where $1 \leq a_1 < a_2 < \cdots < a_r$. Then we define

$$\boldsymbol{m_\ell} = (m_1, \ldots, m_r), \tag{5.45}$$

that is, the multiplicity vector describing how many times each distinct index appears in $\boldsymbol{\ell}$. Accordingly, we set

$$\boldsymbol{m_\ell}! := \prod_{i=1}^{r} m_i!, \tag{5.46}$$

which compensates for the overcounting due to identical indices, in complete analogy with the multinomial coefficients. Similarly, the terms in $B_s(\varepsilon)$ which contain $V(\varepsilon)$ have the form

$$\frac{(-\mathrm{i})^n}{\boldsymbol{m_\ell}!}\,\tilde{\mathcal{K}}_{\ell_n}\cdots\tilde{\mathcal{K}}_{\ell_1}(V(\varepsilon)), \tag{5.47}$$

with $|\boldsymbol{\ell}| = s-1$, $\ell_1 \leq \cdots \leq \ell_n$, and $n \geq 1$.

As a result, we can write

$$B_1(\varepsilon) = V(\varepsilon), \tag{5.48}$$

$$B_s(\varepsilon) = \sum_{n=2}^{s} \sum_{\substack{|\boldsymbol{\ell}|=s \\ \ell_1\le\cdots\le\ell_n}} \frac{(-\mathrm{i})^n}{\boldsymbol{m}_{\boldsymbol{\ell}}!} \tilde{\mathcal{K}}_{\ell_n}\cdots\tilde{\mathcal{K}}_{\ell_1}(H) + \sum_{n=1}^{s-1} \sum_{\substack{|\boldsymbol{\ell}|=s-1 \\ \ell_1\le\cdots\le\ell_n}} \frac{(-\mathrm{i})^n}{\boldsymbol{m}_{\boldsymbol{\ell}}!} \tilde{\mathcal{K}}_{\ell_n}\cdots\tilde{\mathcal{K}}_{\ell_1}(V(\varepsilon)), \qquad \forall s \ge 2, \tag{5.49}$$

where $\boldsymbol{\ell} = (\ell_1, \dots, \ell_n)$ with $\ell_i \ge 1$. As in the previous chapter, the Catalan numbers will naturally arise in bounding the total number of admissible operator products in (5.49). They provide a recursive control of the combinatorial growth of terms at each order s. We now derive an estimate of the operators $B_s(\varepsilon)$ in terms of the Catalan numbers.

Lemma 5.1.3. *For all $s \ge 1$,*

$$\frac{\pi}{\sqrt{3}\eta}\|B_s(\varepsilon)\| \le \alpha^{s-1} b^s d_s, \tag{5.50}$$

where

$$b := \frac{\pi}{\sqrt{3}\eta} C, \tag{5.51}$$

and $\alpha \approx 4.79$ is the unique positive solution of the transcendental equation

$$(\alpha+1)\left(\mathrm{e}^{\frac{2}{\alpha}} - 1\right) = 3. \tag{5.52}$$

Proof. We proceed by induction on s. For $s = 1$, inequality (5.50) holds trivially, since

$$\frac{\pi}{\sqrt{3}\eta}\|B_1(\varepsilon)\| = \frac{\pi}{\sqrt{3}\eta}\|V(\varepsilon)\| \le \frac{\pi}{\sqrt{3}\eta} C = b = \alpha^0 d_1 b. \tag{5.53}$$

Let $s \ge 2$ and assume that

$$\frac{\pi}{\sqrt{3}\eta}\|B_j(\varepsilon)\| \le \alpha^{j-1} b^j d_j, \quad \text{for all } j = 1, \dots, s-1. \tag{5.54}$$

We show that the same holds for $j = s$. From the definition (5.49) and the triangle inequality we obtain

$$\frac{\pi}{\sqrt{3}\eta}\|B_s(\varepsilon)\| \le \frac{\pi}{\sqrt{3}\eta} \sum_{n=2}^{s} \sum_{\substack{|\boldsymbol{\ell}|=s \\ \ell_1\le\cdots\le\ell_n}} \frac{1}{\boldsymbol{m}_{\boldsymbol{\ell}}!} \|\tilde{\mathcal{K}}_{\ell_n}\cdots\tilde{\mathcal{K}}_{\ell_1}(H)\| + \sum_{n=1}^{s-1} \sum_{\substack{|\boldsymbol{\ell}|=s-1 \\ \ell_1\le\cdots\le\ell_n}} \frac{1}{\boldsymbol{m}_{\boldsymbol{\ell}}!} \|\tilde{\mathcal{K}}_{\ell_n}\cdots\tilde{\mathcal{K}}_{\ell_1}(V(\varepsilon))\|. \tag{5.55}$$

From the homological equation

$$i[K_s(\varepsilon), H] = \{B_s(\varepsilon)\}, \tag{5.56}$$

together with

$$\|\{B_s(\varepsilon)\}\| \leq 2\|B_s(\varepsilon)\|, \tag{5.57}$$

we deduce, using Lemma 4.1.1 to bound $\|K_{\ell_j}(\varepsilon)\|$,

$$\frac{\pi}{\sqrt{3}\eta}\big\|\tilde{\mathcal{K}}^\varepsilon_{\ell_n}\cdots\tilde{\mathcal{K}}^\varepsilon_{\ell_1}(H)\big\| \leq 2^n \prod_{j=1}^{n}\left(\frac{\pi}{\sqrt{3}\eta}\big\|B_{\ell_j}(\varepsilon)\big\|\right). \tag{5.58}$$

Since $\ell_j \leq s-1$ for all j, we may apply the inductive hypothesis, obtaining

$$\frac{\pi}{\sqrt{3}\eta}\big\|\tilde{\mathcal{K}}^\varepsilon_{\ell_1}\cdots\tilde{\mathcal{K}}^\varepsilon_{\ell_n}(H)\big\| \leq \left(\frac{2}{\alpha}\right)^n \alpha^s b^s d_{\ell_1}\cdots d_{\ell_n}. \tag{5.59}$$

A similar estimate yields

$$\frac{\pi}{\sqrt{3}\eta}\big\|\tilde{\mathcal{K}}^\varepsilon_{\ell_1}\cdots\tilde{\mathcal{K}}^\varepsilon_{\ell_n}(V(\varepsilon))\big\| \leq \left(\frac{2}{\alpha}\right)^n \alpha^{s-1} b^s d_{\ell_1}\cdots d_{\ell_n}. \tag{5.60}$$

Combining the previous bounds, we get

$$\begin{aligned}\frac{\pi}{\sqrt{3}\eta}\|B_s(\varepsilon)\| \leq \Bigg[&\alpha\sum_{n=2}^{s}\left(\frac{2}{\alpha}\right)^n \sum_{\substack{|\boldsymbol{\ell}|=s\\ \ell_1\leq\cdots\leq\ell_n}} \frac{1}{\boldsymbol{m_\ell}!} d_{\ell_1}\cdots d_{\ell_n}\\ &+\sum_{n=1}^{s-1}\left(\frac{2}{\alpha}\right)^n \sum_{\substack{|\boldsymbol{\ell}|=s-1\\ \ell_1\leq\cdots\leq\ell_n}} \frac{1}{\boldsymbol{m_\ell}!}\, d_{\ell_1}\cdots d_{\ell_n}\Bigg]\alpha^{s-1}b^s.\end{aligned} \tag{5.61}$$

Consider the sum

$$\sum_{\substack{|\boldsymbol{\ell}|=s\\ \ell_1\leq\cdots\leq\ell_n}} \frac{1}{\boldsymbol{m_\ell}!}\, d_{\ell_1}\cdots d_{\ell_n}. \tag{5.62}$$

The product $d_{\ell_1}\cdots d_{\ell_n}$ is invariant under permutations of the indices. Extending the sum to all (not necessarily ordered) multi–indices produces an overcounting by a factor $n!/\boldsymbol{m_\ell}!$. Therefore,

$$\begin{aligned}\frac{\pi}{\sqrt{3}\eta}\|B_s(\varepsilon)\| \leq \Bigg[&\alpha\sum_{n=2}^{s}\frac{1}{n!}\left(\frac{2}{\alpha}\right)^n \sum_{|\boldsymbol{\ell}|=s} d_{\ell_1}\cdots d_{\ell_n}\\ &+\sum_{n=1}^{s-1}\frac{1}{n!}\left(\frac{2}{\alpha}\right)^n \sum_{|\boldsymbol{\ell}|=s-1} d_{\ell_1}\cdots d_{\ell_n}\Bigg]\alpha^{s-1}b^s.\end{aligned} \tag{5.63}$$

Using the recursive property of Catalan numbers,

$$\sum_{|\boldsymbol{\ell}|=s} d_{\ell_1} \cdots d_{\ell_n} \le d_s, \tag{5.64}$$

and $d_{s-1} \le d_s$, we get

$$\frac{\pi}{\sqrt{3}\eta} \|B_s(\varepsilon)\| \le \left[(\alpha+1)\left(\mathrm{e}^{\frac{2}{\alpha}}-1\right)-2\right] d_s\, \alpha^{s-1} b^s. \tag{5.65}$$

By definition of α, the bracket equals 1, which proves the desired bound. This completes the induction step, and hence the proof. □

As a direct consequence of the previous lemma and of (5.56), we have that

$$\|K_s(\varepsilon)\| \le \alpha^{s-1} d_s b^s, \tag{5.66}$$

for all $s \ge 1$.

5.1.3 Proof of (vi) of Theorem 5.1.1

Using this result, we can bound $W(\varepsilon) - \mathbb{I}$. This is the content of the next lemma.

Lemma 5.1.4. *Let $W(\varepsilon)$ be defined as the infinite product*

$$W(\varepsilon) = \overrightarrow{\prod_{\ell\ge 1}} \mathrm{e}^{\mathrm{i}\,\varepsilon^\ell K_\ell}. \tag{5.67}$$

Then

$$\|W(\varepsilon) - \mathbb{I}\| \le \alpha(\mathrm{e}^{\frac{1}{\alpha}} - 1)\, |\varepsilon|\, b\, \mathcal{D}(\alpha|\varepsilon|\, b)\,, \quad \textit{for } |\varepsilon| \le \frac{\eta}{C\rho}, \tag{5.68}$$

where $\mathcal{D}(x)$ is the generating function of the Catalan numbers:

$$\mathcal{D}(x) = \frac{1-\sqrt{1-4x}}{2x}\,, \tag{5.69}$$

defined for $|x| \le 1/4$ and

$$\rho := \frac{2\pi\alpha}{\sqrt{3}}. \tag{5.70}$$

Proof. It is convenient to expand each exponential in the product as a power series:

$$W(\varepsilon) = \left(\sum_{n_1\ge 0} \frac{(\mathrm{i}\varepsilon)^{n_1}}{n_1!} K_1^{n_1}\right) \cdots \left(\sum_{n_\ell \ge 0} \frac{(\mathrm{i}\varepsilon^\ell)^{n_\ell}}{n_\ell!} K_\ell^{n_\ell}\right) \cdots \tag{5.71}$$

Repeating the same combinatorial reordering used above, we obtain

$$W(\varepsilon) - \mathbb{I} = \sum_{s \geq 1} \varepsilon^s \sum_{n=1}^{s} \sum_{\substack{|\boldsymbol{\ell}|=s \\ \ell_1 \geq \cdots \geq \ell_n}} \frac{\mathrm{i}^n}{\boldsymbol{m}_{\boldsymbol{\ell}}!} K_{\ell_n} \cdots K_{\ell_1} \;=:\; \sum_{s \geq 1} \varepsilon^s A_s. \tag{5.72}$$

Here we defined

$$A_s := \sum_{n=1}^{s} \sum_{\substack{|\boldsymbol{\ell}|=s \\ \ell_1 \geq \cdots \geq \ell_n}} \frac{\mathrm{i}^n}{\boldsymbol{m}_{\boldsymbol{\ell}}!} K_{\ell_n} \cdots K_{\ell_1}. \tag{5.73}$$

By the triangle inequality,

$$\|A_s\| \leq \sum_{n=1}^{s} \sum_{\substack{|\boldsymbol{\ell}|=s \\ \ell_1 \geq \cdots \geq \ell_n}} \frac{1}{\boldsymbol{m}_{\boldsymbol{\ell}}!} \|K_{\ell_n}\| \cdots \|K_{\ell_1}\|. \tag{5.74}$$

As before, extending the sum to non–ordered multi–indices and dividing by $n!/\boldsymbol{m}_{\boldsymbol{\ell}}!$ to avoid overcounting yields

$$\|A_s\| \leq \sum_{n=1}^{s} \frac{1}{n!} \sum_{|\boldsymbol{\ell}|=s} \|K_{\ell_n}\| \cdots \|K_{\ell_1}\|. \tag{5.75}$$

Using (5.66),

$$\|A_s\| \leq (\alpha b)^s \sum_{n=1}^{s} \frac{1}{n!} \left(\frac{1}{\alpha}\right)^n \sum_{|\boldsymbol{\ell}|=s} d_{\ell_n} \cdots d_{\ell_1}. \tag{5.76}$$

By the property

$$\sum_{|\boldsymbol{\ell}|=s} d_{\ell_1} \cdots d_{\ell_n} \leq d_s, \tag{5.77}$$

and extending the outer sum to infinity (all terms are nonnegative), we get

$$\|A_s\| \leq (\mathrm{e}^{\frac{1}{\alpha}} - 1)\, d_s\, (\alpha b)^s. \tag{5.78}$$

Therefore,

$$\|W(\varepsilon) - \mathbb{I}\| \leq \sum_{s \geq 1} |\varepsilon|^s \|A_s\| \leq (\mathrm{e}^{\frac{1}{\alpha}} - 1) \sum_{s \geq 1} d_s (\alpha|\varepsilon|\, b)^s \tag{5.79}$$

$$= (\mathrm{e}^{\frac{1}{\alpha}} - 1)\, \mathcal{D}(\alpha|\varepsilon|\, b)\, \alpha|\varepsilon| b, \tag{5.80}$$

where we have used that

$$\mathcal{D}(x) = \sum_{s \geq 1} d_s x^{s-1}, \tag{5.81}$$

for $|x| \leq 1/4$. □

In Fig. 5.1 we compare this bound with the corresponding bound obtained in the previous chapter.

We can use this lemma in order to prove the point (vi) of the Theorem 5.1.1. Since $\mathcal{D}(x) < 2$ for all $x \leq 1/4$, we obtain

$$\|W(\varepsilon) - \mathbb{I}\| \leq 2\,\alpha\big(\mathrm{e}^{\frac{1}{\alpha}} - 1\big)\,|\varepsilon|\,b, \tag{5.82}$$

for $|\varepsilon|\,b \leq 1/(4\alpha)$. Recalling $b = \dfrac{\pi}{\sqrt{3}\eta}\,C$, we arrive at

$$\|W(\varepsilon) - \mathbb{I}\| \leq \frac{2\pi\alpha}{\sqrt{3}}\left(\mathrm{e}^{\frac{1}{\alpha}} - 1\right)\frac{C}{\eta}\,|\varepsilon|, \tag{5.83}$$

for all ε such that

$$|\varepsilon| \leq \frac{\sqrt{3}\,\eta}{4\pi\alpha\,C}. \tag{5.84}$$

This concludes the proof.

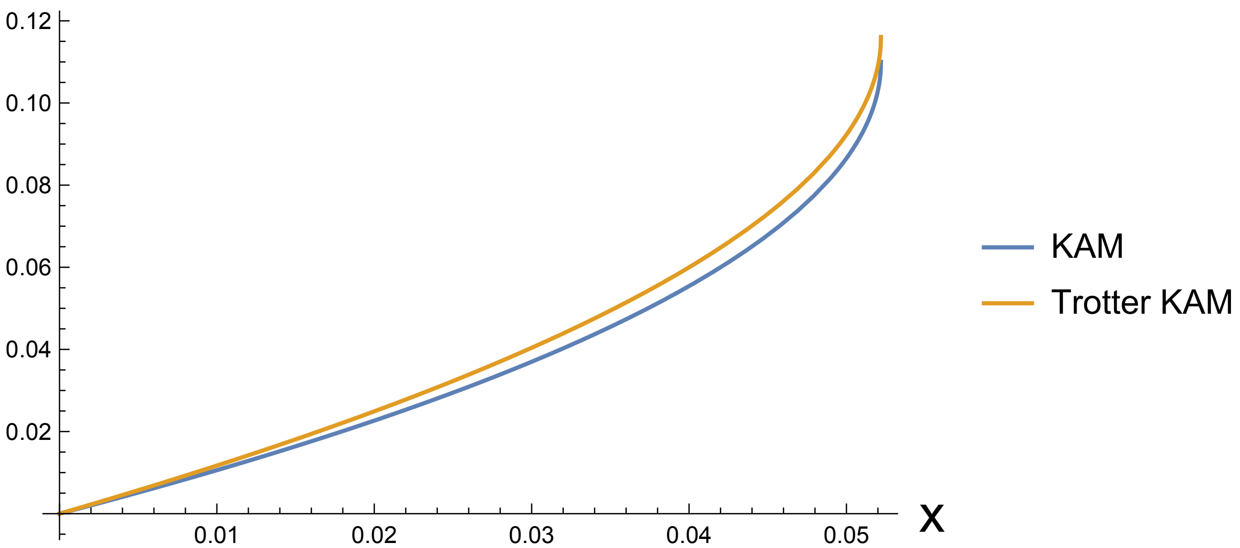

Figure 5.1: Comparison between the bounds (4.116) and (5.68) on $\|W(\varepsilon) - \mathbb{I}\|$, obtained via the KAM and Trotter–KAM schemes, respectively. The horizontal axis is $x = \varepsilon b$, with $b = \pi C/(\sqrt{3}\eta)$.

5.1.4 Proof of (iii) of Theorem 5.1.1

It remains to prove properties (iii), namely that for all $\psi \in D(H)$, we have $\|HW(\varepsilon)\psi\| < +\infty$. In fact, we can prove a more quantitative bound in terms of the Catalan generating function.

Lemma 5.1.5. *For all* $\psi \in D(H)$,

$$\|HW(\varepsilon)\psi\| \le \mathrm{e}^{b|\varepsilon|\mathcal{D}(\alpha|\varepsilon|b)} \left(\|H\psi\| + \frac{2\sqrt{3}\eta b}{\pi} |\varepsilon| \mathcal{D}(\alpha|\varepsilon|b) \|\psi\| \right), \tag{5.85}$$

for $|\varepsilon| \, \|V(\varepsilon)\| \le \eta/\rho$.

Proof. In the previous paragraph we have seen that

$$W(\varepsilon) - \mathbb{I} = \sum_{s \ge 1} \varepsilon^s \sum_{n=1}^{s} \sum_{\substack{|\boldsymbol{\ell}|=s \\ \ell_1 \ge \dots \ge \ell_n}} \frac{\mathrm{i}^n}{\boldsymbol{m_\ell}!} K_{\ell_n} \cdots K_{\ell_1} =: \sum_{s \ge 1} \varepsilon^s A_s. \tag{5.86}$$

where the coefficients $K_\ell(\varepsilon)$ are solutions the homological equations. By Lemma 4.1.1, they satisfy the bound

$$\|HK_s(\varepsilon)\psi\| \le \left(2\|\psi\| + \frac{\pi}{\sqrt{3}\eta} \|H\psi\| \right) \|B_s(\varepsilon)\|, \qquad \forall \psi \in D(H), \tag{5.87}$$

which can be put in the form

$$\|HK_s(\varepsilon)\psi\| \le \left(\|H\psi\| + 2\frac{\sqrt{3}\eta}{\pi} \|\psi\| \right) \frac{\pi}{\sqrt{3}\eta} \|B_s(\varepsilon)\|, \qquad \forall \psi \in D(H), \tag{5.88}$$

We now prove by induction that, for all $n \ge 1$,

$$\|HK_{\ell_n}(\varepsilon) \cdots K_{\ell_1}(\varepsilon)\psi\| \le \left(\|H\psi\| + 2n\frac{\sqrt{3}\eta}{\pi} \|\psi\| \right) d_{\ell_1} \dots d_{\ell_n} \alpha^{\ell_1 + \dots + \ell_n - n} b^{\ell_1 + \dots + \ell_n}, \tag{5.89}$$

for all the multi-indices $\boldsymbol{\ell}$.

The case $n = 1$ is a direct consequence of (5.88) together with the bound

$$\frac{\pi}{\sqrt{3}\eta} \|B_{\ell_1}(\varepsilon)\| \le \alpha^{\ell_1 - 1} d_{\ell_1} b^{\ell_1}. \tag{5.90}$$

Suppose the estimate holds for $n = j - 1$:

$$\|HK_{\ell_1}(\varepsilon) \cdots K_{\ell_{j-1}}(\varepsilon)\psi\| \le \left(\|H\psi\| + 2(j-1)\frac{\sqrt{3}\eta}{\pi} \|\psi\| \right) d_{\ell_1} \cdots d_{\ell_{j-1}} \alpha^{\ell_1 + \dots + \ell_{j-1} - j + 1} b^{\ell_1 + \dots + \ell_{j-1}}. \tag{5.91}$$

Then, since $K_{\ell_j}(\varepsilon)\psi \in D(H)$, we can apply (5.91) to $\varphi = K_{\ell_j}(\varepsilon)\psi$, obtaining:

$$\|HK_{\ell_1}(\varepsilon)\cdots K_{\ell_j}(\varepsilon)\psi\| = \|HK_{\ell_1}(\varepsilon)\cdots K_{\ell_{j-1}}(\varepsilon)K_{\ell_j}(\varepsilon)\psi\| \tag{5.92}$$
$$\leq \left(\|HK_{\ell_j}(\varepsilon)\psi\| + 2(s-1)\frac{\sqrt{3}\eta}{\pi}\|K_{\ell_j}(\varepsilon)\psi\|\right) d_{\ell_1}\cdots d_{\ell_{j-1}}\alpha^{\ell_1+\cdots+\ell_{j-1}-j+1}b^{\ell_1+\cdots+\ell_{j-1}}$$
$$\leq \left(\|H\psi\| + 2j\frac{\sqrt{3}\eta}{\pi}\|\psi\|\right) d_{\ell_1}\cdots d_{\ell_j}\alpha^{\ell_1+\cdots+\ell_j-j}b^{\ell_1+\cdots+\ell_j}, \tag{5.93}$$

where we used that

$$\left\|K_{\ell_j}\right\| \leq \frac{\pi}{\sqrt{3}\eta}\left\|B_{\ell_j}\right\| \tag{5.94}$$

and the inequality (5.90). Let us estimate now $\|H(W(\varepsilon)-\mathbb{I})\|$. By applying the triangular inequality and the inequality (5.89), we get, for all $\psi \in D(H)$,

$$\|H(W(\varepsilon)-\mathbb{I})\psi\| \leq \sum_{s\geq 1}\varepsilon^s\sum_{n=1}^{s}\sum_{\substack{|\boldsymbol{\ell}|=s\\ \ell_1\geq\cdots\geq\ell_n}}\frac{1}{\boldsymbol{m}_{\boldsymbol{\ell}}!}\,\|HK_{\ell_n}\cdots K_{\ell_1}\| \tag{5.95}$$
$$\leq \sum_{s\geq 1}(\alpha\,|\varepsilon|\,b)^s\sum_{n=1}^{s}\left(\frac{1}{\alpha}\right)^n\sum_{\substack{|\boldsymbol{\ell}|=s\\ \ell_1\geq\cdots\geq\ell_n}}\frac{1}{\boldsymbol{m}_{\boldsymbol{\ell}}!}\,d_{\ell_1}\cdots d_{\ell_n}. \tag{5.96}$$

Following a similar procedure to the one used in the previous sections, we can extend the previous sum to the non ordered multi-indices if we divide for $\frac{\boldsymbol{m}_{\boldsymbol{\ell}}!}{n!}$. We get

$$\|H(W(\varepsilon)-\mathbb{I})\psi\| \leq \sum_{s\geq 1}(\alpha\,|\varepsilon|\,b)^s\sum_{n=1}^{s}\left(\frac{1}{\alpha}\right)^n\frac{1}{n!}\left(\|H\psi\| + 2n\frac{\sqrt{3}\eta}{\pi}\|\psi\|\right)\sum_{|\boldsymbol{\ell}|=s}d_{\ell_1}\cdots d_{\ell_n}. \tag{5.97}$$

By using the property of Catalan numbers

$$\sum_{|\boldsymbol{\ell}|=s}d_{\ell_1}\cdots d_{\ell_n} \leq d_s \tag{5.98}$$

and by extending the sum in n to $+\infty$, we get

$$\|H(W(\varepsilon)-\mathbb{I})\psi\| \leq \sum_{s\geq 1}(\alpha\,|\varepsilon|\,b)^s d_s \sum_{n\geq 1}\left(\frac{1}{\alpha}\right)^n \frac{1}{n!}\left(\|H\psi\| + 2n\frac{\sqrt{3}\eta}{\pi}\|\psi\|\right) \tag{5.99}$$

$$= \alpha\,|\varepsilon|\,b\,\mathcal{D}\,(\alpha\,|\varepsilon|\,b)\left(\|H\psi\|\,(\mathrm{e}^{\frac{1}{\alpha}}-1) + 2\frac{\sqrt{3}\eta}{\pi}\,\|\psi\|\,\frac{1}{\alpha}\sum_{n\geq 1}\frac{1}{(n-1)!}\left(\frac{1}{\alpha}\right)^{n-1}\right) \tag{5.100}$$

$$= \alpha\,|\varepsilon|\,b\,\mathcal{D}\,(\alpha\,|\varepsilon|\,b)\left(\|H\psi\|\,(\mathrm{e}^{\frac{1}{\alpha}}-1) + 2\frac{\sqrt{3}\eta}{\pi}\,\|\psi\|\,\frac{1}{\alpha}\mathrm{e}^{\frac{1}{\alpha}}\right) \tag{5.101}$$

We are now ready to estimate $\|HW(\varepsilon)\psi\|$ for all $\psi \in D(H)$:

$$\|HW(\varepsilon)\psi\| = \|H\psi + H(W(\varepsilon)-\mathbb{I})\psi\| \tag{5.102}$$

$$\leq \|H\psi\| + \|H(W(\varepsilon)-\mathbb{I})\psi\| \tag{5.103}$$

$$\leq \|H\psi\| + \alpha\,|\varepsilon|\,b\,\mathcal{D}\,(\alpha\,|\varepsilon|\,b)\left(\|H\psi\|\,(\mathrm{e}^{\frac{1}{\alpha}}-1) + 2\frac{\sqrt{3}\eta}{\pi}\,\|\psi\|\,\frac{1}{\alpha}\mathrm{e}^{\frac{1}{\alpha}}\right) \tag{5.104}$$

$$\leq (1+\alpha\,|\varepsilon|\,b\,\mathcal{D}\,(\alpha\,|\varepsilon|\,b))\,(\mathrm{e}^{\frac{1}{\alpha}}-1)\,\|H\psi\| + 2\,|\varepsilon|\,b\frac{\sqrt{3}\eta}{\pi}\mathrm{e}^{\frac{1}{\alpha}}\,\|\psi\|\,, \tag{5.105}$$

valid again for $|\varepsilon| \leq \eta/(C\rho)$. □

5.1.5 Advantages of the Trotter formulation

The Trotter formulation yields bounds analogous to those obtained with the single–exponential method. However, it offers a crucial numerical advantage: it produces a hierarchy of block–diagonal dynamics that are not eternal, but remain accurate over progressively longer time scales.

Previously, we considered the operator $W(\varepsilon)$ defined in (5.4),

$$W(\varepsilon) = \overrightarrow{\prod_{\ell\geq 1}} \mathrm{e}^{\mathrm{i}\varepsilon^\ell K_\ell(\varepsilon)} = \overrightarrow{\prod_{\ell\geq 1}} W_{\varepsilon,\ell}, \tag{5.106}$$

and searched for a block–diagonal operator $\hat{V}(\varepsilon)$ such that

$$H + \varepsilon\hat{V}(\varepsilon) = W(\varepsilon)^\dagger(H+\varepsilon V(\varepsilon))W(\varepsilon). \tag{5.107}$$

We then introduced a series expansion for $\hat{V}(\varepsilon)$,

$$\hat{V}(\varepsilon) = \sum_{\ell\geq 0}\varepsilon^\ell V_\ell(\varepsilon), \tag{5.108}$$

and obtained an iterative solution for each $V_\ell(\varepsilon)$.

Let us now consider only the first factor of $W(\varepsilon)$ and analyze its action on $H + \varepsilon V(\varepsilon)$:

$$W_{\varepsilon,1}^{\dagger}\big(H + \varepsilon V(\varepsilon)\big)W_{\varepsilon,1} = H + \varepsilon V_0(\varepsilon) + O(\varepsilon^2). \tag{5.109}$$

The subsequent factors $W_{\varepsilon,\ell}$, for all $\ell \geq 2$, cannot modify the order–ε contribution in (5.109), since

$$W_{\varepsilon,\ell} = \mathbb{I} + O(\varepsilon^{\ell}), \tag{5.110}$$

and thus contain no terms of order ε. Therefore, the operator $V_0(\varepsilon)$ appearing in (5.109) coincides with the one in (5.108).

This procedure can be generalized as follows:

$$\left(\overleftarrow{\prod_{1\leq\ell\leq n}} W_{\varepsilon,\ell}^{\dagger}\right)\big(H + \varepsilon V(\varepsilon)\big)\left(\overrightarrow{\prod_{1\leq\ell\leq n}} W_{\varepsilon,\ell}\right) = H + \sum_{\ell=0}^{n-1} \varepsilon^{\ell+1} V_{\ell}(\varepsilon) + O(\varepsilon^{n+1}). \tag{5.111}$$

Defining

$$\overline{H}_n(\varepsilon) := \left(\overleftarrow{\prod_{1\leq\ell\leq n}} W_{\varepsilon,\ell}^{\dagger}\right)\big(H + \varepsilon V(\varepsilon)\big)\left(\overrightarrow{\prod_{1\leq\ell\leq n}} W_{\varepsilon,\ell}\right), \tag{5.112}$$

we can write

$$H + \varepsilon \hat{V}(\varepsilon) = \overline{H}_n(\varepsilon) + O(\varepsilon^{n+1}). \tag{5.113}$$

We now show that the evolution generated by $\overline{H}_n(\varepsilon)$ provides a good approximation of the one generated by $H + \varepsilon V(\varepsilon)$. Consider their difference:

$$\big\|\mathrm{e}^{\mathrm{i}t(H+\varepsilon V(\varepsilon))} - \mathrm{e}^{\mathrm{i}t\overline{H}_n(\varepsilon)}\big\| \leq \big\|\mathrm{e}^{\mathrm{i}t(H+\varepsilon V(\varepsilon))} - \mathrm{e}^{\mathrm{i}t(H+\varepsilon\hat{V}(\varepsilon))}\big\| + \big\|\mathrm{e}^{\mathrm{i}t(H+\varepsilon\hat{V}(\varepsilon))} - \mathrm{e}^{\mathrm{i}t\overline{H}_n(\varepsilon)}\big\|. \tag{5.114}$$

For the first term, using the unitary equivalence

$$H + \varepsilon \hat{V}(\varepsilon) = W(\varepsilon)^{\dagger}\big(H + \varepsilon V(\varepsilon)\big)W(\varepsilon), \tag{5.115}$$

we obtain

$$\begin{aligned}
\big\|\mathrm{e}^{\mathrm{i}t(H+\varepsilon V(\varepsilon))} - \mathrm{e}^{\mathrm{i}t(H+\varepsilon\hat{V}(\varepsilon))}\big\| &= \big\|\mathrm{e}^{\mathrm{i}t(H+\varepsilon V(\varepsilon))} - W(\varepsilon)^{\dagger}\mathrm{e}^{\mathrm{i}t(H+\varepsilon V(\varepsilon))}W(\varepsilon)\big\| &(5.116)\\
&= \big\|\,[W(\varepsilon) - \mathbb{I},\, \mathrm{e}^{\mathrm{i}t(H+\varepsilon V(\varepsilon))}]\,\big\| &(5.117)\\
&\leq 2\,\|W(\varepsilon) - \mathbb{I}\| = O(\varepsilon), &(5.118)
\end{aligned}$$

where in the last step we used (5.68).

For the second term in (5.114), we write:

$$e^{it(H+\varepsilon\hat{V}(\varepsilon))} - e^{it\overline{H}_n(\varepsilon)} = - e^{i(t-s)(H+\varepsilon\hat{V}(\varepsilon))} e^{is\overline{H}_n(\varepsilon)}\Big|_{s=0}^{s=t} \tag{5.119}$$

$$= - \int_0^t \frac{\partial}{\partial s}\left(e^{i(t-s)(H+\varepsilon\hat{V}(\varepsilon))} e^{is\overline{H}_n(\varepsilon)}\right) ds \tag{5.120}$$

$$= i \int_0^t e^{i(t-s)(H+\varepsilon\hat{V}(\varepsilon))} \left(H + \varepsilon\hat{V}(\varepsilon) - \overline{H}_n(\varepsilon)\right) e^{is\overline{H}_n(\varepsilon)} ds. \tag{5.121}$$

Therefore,

$$\left\|e^{it(H+\varepsilon\hat{V}(\varepsilon))} - e^{it\overline{H}_n(\varepsilon)}\right\| \leq t\left\|H + \varepsilon\hat{V}(\varepsilon) - \overline{H}_n(\varepsilon)\right\| = O(t\,\varepsilon^{n+1}), \tag{5.122}$$

where we used (5.113). Combining this with (5.118), we conclude

$$\left\|e^{it(H+\varepsilon V(\varepsilon))} - e^{it\overline{H}_n(\varepsilon)}\right\| = O(\varepsilon) + O(t\,\varepsilon^{n+1}). \tag{5.123}$$

Thus, the dynamics generated by $\overline{H}_n(\varepsilon)$ approximates the evolution under $H + \varepsilon V(\varepsilon)$ with $O(\varepsilon)$ accuracy up to times $t = O(\varepsilon^{-n})$, as shown in Fig. 5.2.

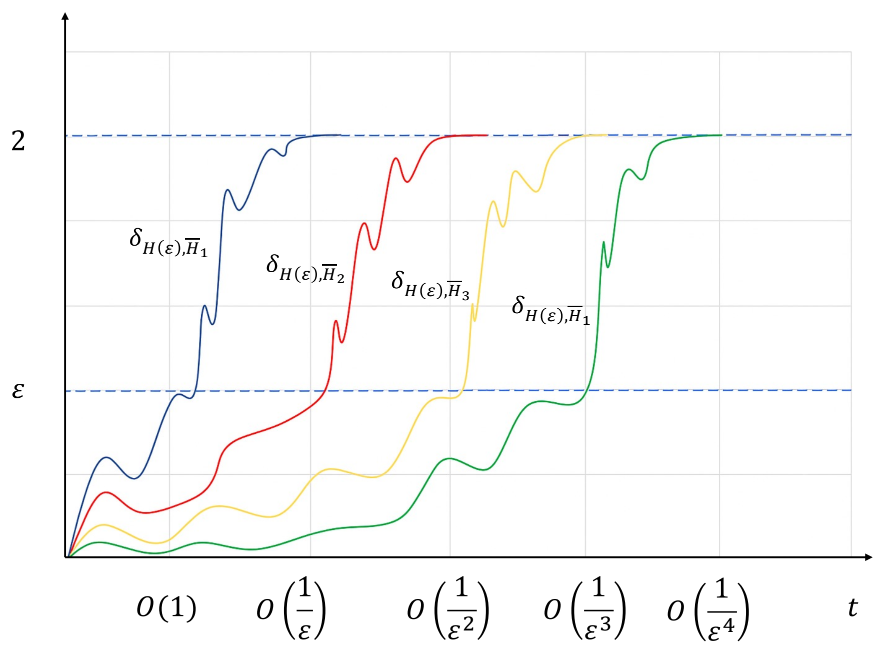

Figure 5.2: Comparison between the dynamics generated by $H+\varepsilon V$ and its Trotter approximations $\overline{H}_n$. The deviation $\delta_{H(\varepsilon),\overline{H}_n}$ remains of order $O(\varepsilon)$ up to times $t = O(\varepsilon^{-n})$. The horizontal axis is in logarithmic scale.

Chapter 6

Quantum KAM Iteration Beyond Discrete Spectrum: The Band Case

The results obtained so far rely on the assumption that the Hamiltonian has purely point spectrum with a strictly positive spectral gap. This setting allowed us to characterize completely robust symmetries as elements of the bicommutant $\{H\}''$ and to establish uniform bounds on their wandering range under bounded perturbations.

It is natural to ask whether these conclusions extend to more general situations, in which the spectrum of the Hamiltonian is not purely discrete but organized in bands, as is often the case in condensed matter physics. In such a scenario, the complete characterization of robust symmetries no longer applies, and additional difficulties arise from the continuous structure of the bands.

Nevertheless, we shall demonstrate that a distinguished subclass of symmetries, namely those belonging to the bicommutant of the band projections, retain robustness under bounded perturbations. In fact, the Quantum KAM Iteration admits a natural extension to the setting of Hamiltonians with band structure, which will be developed in this chapter [15, 25].

6.1 Hamiltonians with band structure

We begin with a rigorous definition of the band decomposition of a Hamiltonian.

Definition 6.1.1 (Band decomposition). *Let $H = H^\dagger$ be a self-adjoint operator on a Hilbert space $\mathcal{H}$. A* band decomposition *of H is a partition of its spectrum*

$$\sigma(H) = \bigcup_{k\geq 1} \sigma_k, \tag{6.1}$$

into closed, pairwise disjoint subsets $\{\sigma_k\}_{k\geq 1}$, called bands. *For each band σ_k, the associated spectral projection is*

$$\widehat{P}_k := P_H(\sigma_k), \tag{6.2}$$

where $P_H(\cdot)$ is the spectral measure of H. These projections satisfy

$$\widehat{P}_k\widehat{P}_\ell = \delta_{k\ell}\,\widehat{P}_k, \qquad \widehat{P}_k^\dagger = \widehat{P}_k, \qquad \sum_{k\geq 1}\widehat{P}_k = \mathbb{I} \quad \textit{(strongly)}. \tag{6.3}$$

Accordingly,

$$H = \sum_{k\geq 1}\widehat{P}_k H\widehat{P}_k = \sum_{k\geq 1} H_k, \qquad H_k := \widehat{P}_k H\widehat{P}_k, \tag{6.4}$$

with $\sigma(H_k) = \sigma_k$.

We do not impose any restriction on the spectral type of each H_k: it may contain point, continuous, or even singular components. In particular, a spectrum consisting of continuous bands is the typical situation encountered in solid-state physics. We will assume that there exists a minimal gap between the bands. More explicitly,

$$\widehat{\eta} := \inf_{j\neq j'} \operatorname{dist}(\sigma_j, \sigma_{j'}) > 0. \tag{6.5}$$

As is clear from the following example, every Hamiltonian with purely point spectrum and strictly positive spectral gap satisfies these hypotheses.

Example 6.1.1 (From pure point spectrum to arbitrary band decompositions). Assume that H has purely point spectrum with spectral resolution

$$H = \sum_{k\geq 1} h_k P_k, \qquad \eta := \inf_{k\neq\ell} |h_k - h_\ell| > 0,$$

where $\{P_k\}_{k\geq 1}$ are the spectral projections onto the eigenspaces of H. Let $\{I_j\}_{j\in J}$ be any partition of $\mathbb{N}$ into disjoint (finite or countable) index sets (indexed by a countable set J). Define the *band projections*

$$\widehat{P}_j := \sum_{k\in I_j} P_k \quad \text{(strong operator convergence)}, \qquad H_j := \widehat{P}_j H\widehat{P}_j = \sum_{k\in I_j} h_k P_k.$$

Then $\{\widehat{P}_j\}_{j\in J} \subset \{H\}'$ is a family of pairwise orthogonal projections with

$$\widehat{P}_j^\dagger = \widehat{P}_j, \qquad \widehat{P}_j\widehat{P}_{j'} = \delta_{jj'}\,\widehat{P}_j, \qquad \sum_{j\in J}\widehat{P}_j = \mathbb{I},$$

and gives a band decomposition

$$H = \sum_{j\in J} H_j, \qquad \sigma(H) = \bigcup_{j\in J}\sigma(H_j) = \bigcup_{j\in J}\{h_k : k\in I_j\}.$$

Moreover, the inter–band separation is strictly positive and bounded below by the global gap:

$$\widehat{\eta} \;:=\; \inf_{j\neq j'} \operatorname{dist}\big(\sigma(H_j),\sigma(H_{j'})\big) \;=\; \inf_{\substack{k\in I_j,\,\ell\in I_{j'}\\ j\neq j'}} |h_k-h_\ell| \;\geq\; \eta \;>\; 0.$$

In particular, *any* finite or countable regrouping of eigenvalues yields a valid band structure with uniform inter–band gap at least η.

This class of Hamiltonians is more general than the one considered in the previous chapter. In this case it is no longer possible to provide a precise algebraic characterization of robust symmetries. However, we shall prove that those symmetries belonging to the bicommutant of the band projections remain robust against bounded perturbations, and that their wandering range is linear in the perturbation strength.

Theorem 6.1.1 (Robust symmetries for band Hamiltonians). *Let $H=H^\dagger$ be a self-adjoint operator admitting a band decomposition $\{\sigma_k\}_{k\geq 1}$ with non-vanishing interband separation*

$$\hat{\eta} := \inf_{k\neq\ell} \operatorname{dist}(\sigma_k,\sigma_\ell) > 0. \tag{6.6}$$

Let $H(\varepsilon)=H+\varepsilon V(\varepsilon)$ be a uniformly bounded perturbation, i.e.

$$\sup_{\varepsilon\in I} \|V(\varepsilon)\| \leq C. \tag{6.7}$$

Then, for every symmetry S in the bicommutant of the band projections,

$$S\in\{\widehat{P}_k\}'' = \{A\in B(\mathcal{H}) : [A,B]=0 \;\; \forall B\in\{\widehat{P}_k\}'\}, \tag{6.8}$$

the following bound holds uniformly in $t\in\mathbb{R}$:

$$\sup_{t\in\mathbb{R}} \big\|\mathrm{e}^{\mathrm{i}tH(\varepsilon)}S\mathrm{e}^{-\mathrm{i}tH(\varepsilon)}-S\big\| \;\leq\; \frac{4C\,\hat{\beta}\,\|S\|}{\hat{\eta}}\,|\varepsilon|, \tag{6.9}$$

for $|\varepsilon|\leq\hat{\eta}/(C\hat{\rho})$.

The constants $\hat{\beta}$ and $\hat{\rho}$ are defined as follows

$$\hat{\beta} := 4\pi\alpha\left(\mathrm{e}^{\frac{1}{2\alpha}}-1\right) \tag{6.10}$$

$$\hat{\rho} := 4\pi\alpha, \tag{6.11}$$

where $\alpha\approx 4.79$ is the unique solution of the transcendental equation

$$(\alpha+1)\left(\mathrm{e}^{\frac{2}{\alpha}}-1\right)=3. \tag{6.12}$$

This theorem proves that the symmetries belonging to the bicommutant of the band projections are robust, and that their wandering range is linear in the strength of the perturbation. The strategy for proving this theorem is very similar to the discrete case. It is based on the following generalization of Theorem 3.3.2.

Theorem 6.1.2. *There exist two families of operators $W(\varepsilon)$ and $\hat{V}(\varepsilon)$ with the following properties:*

1. $\hat{V}(\varepsilon) = \hat{V}(\varepsilon)^\dagger \in \{\widehat{P}_k\}'$.
2. $W(\varepsilon)$ *unitary*
3. $W(\varepsilon)D(H) \subseteq D(H)$.
4. $W(0) = \mathbb{I}$
5. *The operators* $H + \varepsilon V(\varepsilon)$ *and* $H + \varepsilon\hat{V}(\varepsilon)$ *are unitarily equivalent through* $W(\varepsilon)$*:*

$$W(\varepsilon)^\dagger (H + \varepsilon V(\varepsilon)) W(\varepsilon)\psi = (H + \varepsilon\hat{V}(\varepsilon))\psi, \tag{6.13}$$

   for all $\psi \in D(H)$.

6. $W(\varepsilon)$ *satisfies the following inequality:*

$$\|W(\varepsilon) - \mathbb{I}\| \leq \hat{\beta}\frac{C}{\hat{\eta}}|\varepsilon|, \tag{6.14}$$

   for all ε *such that*

$$|\varepsilon| \leq \frac{\hat{\eta}}{C\hat{\rho}}. \tag{6.15}$$

   The constants $\hat{\beta}$ *and* $\hat{\rho}$ *are defined in Eqs.* (6.10) *and* (6.11).

As in the discrete case, we postpone the proof of the previous theorem to the next section (See Subsections 6.2.2 and 6.2.3).

Proof of Theorem 6.1.1. Let $S \in \{\widehat{P}_k\}''$, we have

$$\begin{aligned}
\left\|e^{it(H+\varepsilon V(\varepsilon))} S e^{-it(H+\varepsilon V(\varepsilon))} - S\right\| &= \left\|\left[e^{it(H+\varepsilon V(\varepsilon))}, S\right]\right\| && (6.16)\\
&= \left\|\left[e^{it(H+\varepsilon V(\varepsilon))} - e^{it(H+\varepsilon\hat{V}(\varepsilon))}, S\right]\right\| && (6.17)\\
&\leq 2\|S\| \left\|e^{it(H+\varepsilon V(\varepsilon))} - e^{it(H+\varepsilon\hat{V}(\varepsilon))}\right\|,
\end{aligned}$$

where in step (6.17) we used that $S \in \{\widehat{P}_k\}''$, i.e. S commutes with all the operators in $\{\widehat{P}_k\}'$, and then with $\hat{V}(\varepsilon)$.

By using the unitary equivalence above, we obtain

$$\begin{aligned}
\left\|e^{it(H+\varepsilon V(\varepsilon))} S e^{-it(H+\varepsilon V(\varepsilon))} - S\right\| &\leq 2\|S\| \left\|e^{it(H+\varepsilon V(\varepsilon))} - W(\varepsilon) e^{it(H+\varepsilon V(\varepsilon))} W(\varepsilon)^\dagger\right\| && (6.18)\\
&= 2\|S\| \left\|\left[e^{it(H+\varepsilon V(\varepsilon))}, W(\varepsilon) - \mathbb{I}\right]\right\| && (6.19)\\
&\leq 4\|S\| \|W(\varepsilon) - \mathbb{I}\| && (6.20)\\
&\leq 4\|S\| \hat{\beta}\frac{C}{\hat{\eta}}|\varepsilon|,
\end{aligned}$$

□

where in step (6.20) we used (6.14).

Remark 6.1.1. Theorem 6.1.1 shows that a special class of symmetries — those in the bi-commutant of the band projections — are robust even in the band spectrum case, with a linear wandering range. The structure of the proof is essentially the same as in the discrete case, though the constants differ slightly. This result highlights a genuine extension of the notion of robust symmetries beyond the purely point spectrum setting.

6.2 Band spectrum: homological equation and Quantum KAM Iteration

In this section we extend the construction of the families $W(\varepsilon)$ and $\hat{V}(\varepsilon)$ to Hamiltonians whose spectrum is organized in *bands*. The key input is a band–version of the homological equation with sharp bounds; once this is available, the Quantum KAM iteration follows the discrete case, with constants adapted to the band gap $\hat{\eta}$.

6.2.1 The Homological Equation for Band Hamiltonians

Given $A \in B(\mathcal{H})$, we write its block–diagonal and off–diagonal parts with respect to $\{\widehat{P}_k\}$ as

$$[A] := \sum_{k\geq 1} \widehat{P}_k A \widehat{P}_k, \qquad \{A\} := A - [A] = \sum_{k\neq \ell} \widehat{P}_k A \widehat{P}_\ell. \tag{6.21}$$

In the previous sections we proved, for Hamiltonians with purely point spectrum and a non-vanishing spectral gap, the existence of the families $W(\varepsilon)$ and $\hat{V}(\varepsilon)$ via the Quantum KAM Iteration, whose key ingredient is the solution of the homological equation (Lemma 4.1.1). We now show that the homological equation admits a band-version with analogous sharp bounds.

Lemma 6.2.1 (Homological Equation)**.** *Let H be an unbounded self-adjoint operator with band decomposition $\{\sigma_k\}_{k\geq 1}$ and non-vanishing minimal interband gap $\hat{\eta} > 0$. Let $B \in B(\mathcal{H})$ be a bounded operator. Then, there is a unique operator $X \in B(\mathcal{H})$ satisfying the following conditions:*

(i) $XD(H) \subseteq D(H)$*;*

(ii) For all $\psi \in D(H)$*,*

$$\mathrm{i}[X, H]\psi = \{B\}\psi; \tag{6.22}$$

(iii) The block-diagonal part of X vanishes, i.e.,

$$[X] = 0; \tag{6.23}$$

and it is given by

$$X = \mathrm{i} \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}tH} \{B\} \mathrm{e}^{\mathrm{i}tH} f(t) \mathrm{d}t, \tag{6.24}$$

where f is any real function in $L^1(\mathbb{R})$ such that its Fourier transform is given by

$$\hat{f}(s) := \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}ts} f(t) \mathrm{d}t = \frac{1}{s}, \tag{6.25}$$

for all $|s| \geq \hat{\eta}$. Moreover, if B is self-adjoint then X is self-adjoint. Finally, the following estimates hold:

$$\|X\| \leq \frac{\pi}{\hat{\eta}} \|B\|, \tag{6.26}$$

$$\|HX\psi\| \leq \left(2\|\psi\| + \frac{\pi}{\hat{\eta}} \|H\psi\|\right) \|B\|, \qquad \forall\, \psi \in D(H). \tag{6.27}$$

Proof. Let $\psi \in \mathcal{H}$. Since equation (4.6) must hold for all $\phi \in D(H)$, it must in particular hold for $\phi = \psi_\ell := P_\ell \psi$, for any $\ell \geq 1$. In this case, multiplying from the left by $\widehat{P}_k$ and removing the dependence on ψ, we obtain

$$H_k \widehat{P}_k X \widehat{P}_\ell - \widehat{P}_k X \widehat{P}_\ell H_\ell = \mathrm{i}\, \widehat{P}_k B \widehat{P}_\ell. \tag{6.28}$$

For $k = \ell$ we obtain

$$\left[\widehat{P}_k X \widehat{P}_k, H_k\right] = 0. \tag{6.29}$$

Since, by hypothesis, $[X] = 0$, we have $\widehat{P}_k X \widehat{P}_k = 0$, and therefore the previous equation is automatically satisfied.

For $k \neq \ell$, we obtain

$$H_k \widehat{P}_k X \widehat{P}_\ell - \widehat{P}_k X \widehat{P}_\ell H_\ell = \mathrm{i}\, \widehat{P}_k B \widehat{P}_\ell. \tag{6.30}$$

Thus, $\widehat{P}_k X \widehat{P}_\ell$ (for $k \neq \ell$) satisfies an equation of the form

$$AZ - ZB = Y, \tag{6.31}$$

in the unknown Z, with $A = H_k$, $B = H_\ell$ and $Y = \mathrm{i}\widehat{P}_k B \widehat{P}_\ell$. This equation is known in the literature as the *Sylvester equation.* It admits a unique solution provided that $\mathrm{dist}(\sigma(A), \sigma(B)) > 0$, i.e. if the spectra of A and B are disjoint (See Theorem B.2.1). This condition is satisfied here by assumption, since

$$\hat{\eta} := \inf_{k \neq \ell} \mathrm{dist}(\sigma_k, \sigma_\ell) > 0. \tag{6.32}$$

The solution can then be written in the following way:

$$\widehat{P}_k X \widehat{P}_\ell = \mathrm{i} \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}tH_k} \widehat{P}_k B \widehat{P}_\ell \mathrm{e}^{\mathrm{i}tH_\ell} f(t) \mathrm{d}t \tag{6.33}$$

$$= \mathrm{i} \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}tH} \widehat{P}_k B \widehat{P}_\ell \mathrm{e}^{\mathrm{i}tH} f(t) \mathrm{d}t, \tag{6.34}$$

where in the last step we have used the identity

$$\mathrm{e}^{\pm \mathrm{i}tH} \widehat{P}_m = \mathrm{e}^{\pm \mathrm{i}tH_m} \widehat{P}_m \tag{6.35}$$

and f is any real function in $L^1(\mathbb{R})$ such that its Fourier transform is given by

$$\hat{f}(s) := \int_{\mathbb{R}} f(t) \mathrm{e}^{-\mathrm{i}st} \mathrm{d}t = \frac{1}{s}. \tag{6.36}$$

Finally, summing over $k \neq \ell$, we obtain

$$\{X\} = X = \mathrm{i} \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}tH} \{B\} \, \mathrm{e}^{\mathrm{i}tH} f(t) \mathrm{d}t, \tag{6.37}$$

where again we have used the fact that $[X] = 0$. Then, at least formally, the solution holds. We now have to show that the integral is convergent. Taking the operator norm of the previous expression, we obtain

$$\|X\| \leq 2 \|B\| \, \|f\|_{L^1(\mathbb{R})}, \tag{6.38}$$

for all $f \in \mathcal{F}_{\hat{\eta}}$, where

$$\mathcal{F}_{\hat{\eta}} := \Big\{ f \in L^1(\mathbb{R}) : \hat{f}(s) = \frac{1}{s} \;\; \forall |s| \geq \hat{\eta} \Big\}. \tag{6.39}$$

Optimizing over $f \in \mathcal{F}_{\hat{\eta}}$, we deduce

$$\|X\| \leq 2 \|B\| \inf_{f \in \mathcal{F}_{\hat{\eta}}} \|f\|_{L^1(\mathbb{R})}. \tag{6.40}$$

It is known (see [26]) that

$$\inf_{f \in \mathcal{F}_{\hat{\eta}}} \|f\|_{L^1(\mathbb{R})} = \frac{\pi}{2\hat{\eta}}. \tag{6.41}$$

Therefore,

$$\|X\| \leq \frac{\pi}{\hat{\eta}} \|B\|. \tag{6.42}$$

Moreover, we have to prove the bound

$$\|HX\psi\| \leq \Big(2 \|\psi\| + \frac{\pi}{\hat{\eta}} \|H\psi\| \Big) \|B\|, \qquad \psi \in D(H). \tag{6.43}$$

Take $\psi \in D(H)$. Using the explicit expression of X, we can write

$$\begin{aligned} -\mathrm{i}HX &= \int_{\mathbb{R}} H\, \mathrm{e}^{-\mathrm{i}tH}\{B\}\mathrm{e}^{\mathrm{i}tH} f(t)\,\mathrm{d}t \\ &= \sum_{k\neq\ell} \int_{\mathbb{R}} H_k \mathrm{e}^{-\mathrm{i}tH_k}\widehat{P}_k B \widehat{P}_\ell \mathrm{e}^{\mathrm{i}tH_\ell} f(t)\,\mathrm{d}t, \end{aligned}$$

where in the last step we have use the decomposition

$$H = \sum_{k\geq 1} H_k. \tag{6.44}$$

The operators H_k can be regarded as operators on $P_k\mathcal{H}$. Since they are self adjoint, we can consider their spectral decomposition

$$H_m = \int_{\sigma_m} \lambda \mathrm{d}P_m(\lambda), \tag{6.45}$$

where $\{P_m(\lambda)\}$ is the projection-valued measure canonically associated with H_m, which satisfies

$$\widehat{P}_m = \int_{\sigma_m} \mathrm{d}P_m(\lambda). \tag{6.46}$$

By inserting this decomposition in the previous expression, we get

$$\begin{aligned} -\mathrm{i}HX &= \sum_{k\neq\ell} \int_{\mathbb{R}} \int_{\sigma_k} \int_{\sigma_\ell} \lambda\, \mathrm{e}^{-\mathrm{i}t\lambda}\, dP_k(\lambda)\, B\, dP_\ell(\mu)\, \mathrm{e}^{\mathrm{i}t\mu} f(t)\,\mathrm{d}t \\ &= \sum_{k\neq\ell} \int_{\sigma_k} \int_{\sigma_\ell} \lambda\, dP_k(\lambda)\, B\, dP_\ell(\mu) \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}t(\lambda-\mu)} f(t)\,\mathrm{d}t \\ &= \sum_{k\neq\ell} \int_{\sigma_k} \int_{\sigma_\ell} \lambda\, dP_k(\lambda)\, B\, dP_\ell(\mu) \hat{f}(\lambda-\mu) \\ &= \sum_{k\neq\ell} \int_{\sigma_k} \int_{\sigma_\ell} \frac{\lambda}{\lambda-\mu}\, dP_k(\lambda)\, B\, dP_\ell(\mu) \end{aligned}$$

where we have used the definition of f and that, in particular,

$$\hat{f}(s) = \frac{1}{s}, \tag{6.47}$$

for $|s| \geq \hat{\eta}$. By summing and subtracting μ at the numerator, we get

$$
\begin{aligned}
-\mathrm{i}HX &= \sum_{k\neq\ell}\int_{\sigma_k}\int_{\sigma_\ell}\frac{\lambda-\mu+\mu}{\lambda-\mu}\,dP_k(\lambda)\,B\,dP_\ell(\mu)\\
&= \sum_{k\neq\ell}\int_{\sigma_k}\int_{\sigma_\ell}dP_k(\lambda)\,B\,dP_\ell(\mu) + \sum_{k\neq\ell}\int_{\sigma_k}\int_{\sigma_\ell}\frac{\mu}{\lambda-\mu}dP_k(\lambda)\,B\,dP_\ell(\mu)\\
&= \sum_{k\neq\ell}\widehat{P}_k B\widehat{P}_\ell + \sum_{k\neq\ell}\int_{\sigma_k}dP_k(\lambda)\,B\int_{\sigma_\ell}\mu dP_\ell(\mu)\hat{f}(\lambda-\mu)\\
&= \{B\} + \sum_{k\neq\ell}\int_{\mathbb{R}}\int_{\sigma_k}\int_{\sigma_\ell}\mathrm{e}^{-\mathrm{i}t\lambda}dP_k(\lambda)\,B\,dP_\ell(\mu)\,\mu\,\mathrm{e}^{\mathrm{i}t\mu}f(t)\,\mathrm{d}t\\
&= \{B\} + \int_{\mathbb{R}}\sum_{k\neq\ell}\mathrm{e}^{-\mathrm{i}tH_k}\widehat{P}_k B\widehat{P}_\ell H_\ell \mathrm{e}^{\mathrm{i}tH_\ell}f(t)\,\mathrm{d}t\\
&= \{B\} + \int_{\mathbb{R}}\mathrm{e}^{-\mathrm{i}tH}\{B\}\mathrm{e}^{\mathrm{i}tH}f(t)H\,\mathrm{d}t\\
&= \{B\} - \mathrm{i}XH.
\end{aligned}
$$

Applying the triangle inequality and using the previous norm estimate for X, we obtain, for $\psi \in D(H)$,

$$
\begin{aligned}
\|HX\psi\| &\leq 2\,\|B\|\;\|\psi\| + \|X\|\;\|H\psi\| &(6.48)\\
&\leq \left(2\,\|\psi\| + \frac{\pi}{\hat{\eta}}\,\|H\psi\|\right)\|B\|\,. &(6.49)
\end{aligned}
$$

This proves that, also in this case, $XD(H) \subseteq D(H)$, and therefore the commutator $[X,H]$ is well defined on $D(H)$. □

6.2.2 Formal construction: KAM Iteration

We are now ready to prove Theorem 6.1.2. We aim to construct two operators $W(\varepsilon)$ and $\hat{V}(\varepsilon) \in \{\widehat{P}_k\}'$ satisfying the properties of Theorem 6.1.2. In particular, we require that for all $\psi \in D(H)$,

$$W(\varepsilon)^\dagger(H+\varepsilon V(\varepsilon))W(\varepsilon)\psi = (H+\varepsilon\hat{V}(\varepsilon))\psi. \tag{6.50}$$

We seek $W(\varepsilon)$ in the form

$$W(\varepsilon) = \mathrm{e}^{\mathrm{i}K(\varepsilon)}, \tag{6.51}$$

where $K(\varepsilon) = K(\varepsilon)^\dagger$ and $K(\varepsilon)D(H) \subseteq D(H)$. In this case, the equation above can be rewritten as

$$\mathrm{e}^{-\mathrm{i}K(\varepsilon)}(H+\varepsilon V(\varepsilon))\mathrm{e}^{\mathrm{i}K(\varepsilon)} = H + \varepsilon\hat{V}(\varepsilon). \tag{6.52}$$

As in the discrete case, we look for $K(\varepsilon)$ and $\hat{V}(\varepsilon)$ as formal power series in ε:

$$K(\varepsilon) = \sum_{s\geq 1} \varepsilon^s K_s(\varepsilon), \tag{6.53}$$

$$\hat{V}(\varepsilon) = \sum_{s\geq 0} \varepsilon^s V_s(\varepsilon), \tag{6.54}$$

with $K(0) = 0$ to ensure that $W(0) = \mathrm{e}^{\mathrm{i}K(0)} = \mathbb{I}$.

From now on the strategy is very similar to the discrete case.

Lemma 6.2.2. *Let $W(\varepsilon) = \mathrm{e}^{\mathrm{i}K(\varepsilon)}$, and assume that $K(\varepsilon)$ and $\hat{V}(\varepsilon)$ admit the expansions* (6.53) *and* (6.54)*. Then equation (6.52) holds on $D(H)$ if and only if, for all $s \geq 1$,*

$$V_{s-1}(\varepsilon) = B_s(\varepsilon) - \mathrm{i}[K_s(\varepsilon), H], \tag{6.55}$$

where $B_s(\varepsilon)$ is defined as

$$B_1(\varepsilon) = V(\varepsilon), \tag{6.56}$$

$$B_s(\varepsilon) = \sum_{n=2}^{s} \frac{(-\mathrm{i})^n}{n!} \sum_{|\boldsymbol{\ell}|=s} \tilde{\mathcal{K}}^{\varepsilon}_{\ell_1} \cdots \tilde{\mathcal{K}}^{\varepsilon}_{\ell_n}(H)$$
$$+ \sum_{n=1}^{s-1} \frac{(-\mathrm{i})^n}{n!} \sum_{|\boldsymbol{\ell}|=s-1} \tilde{\mathcal{K}}^{\varepsilon}_{\ell_1} \cdots \tilde{\mathcal{K}}^{\varepsilon}_{\ell_n}(V(\varepsilon)), \tag{6.57}$$

where $\tilde{\mathcal{K}}^{\varepsilon}_{\ell_1} \cdots \tilde{\mathcal{K}}^{\varepsilon}_{\ell_n}(A) = [K_{\ell_1}(\varepsilon), \cdots, [K_{\ell_n}(\varepsilon), A] \cdots]$ for any suitable linear operator A. We use the multi-index notation $\boldsymbol{\ell} = (\ell_1, \dots, \ell_n) \in \mathbb{N}^n$, and $|\boldsymbol{\ell}| = \ell_1 + \cdots + \ell_n$.

Proof. See proof of lemma 4.2.1. □

We now solve equation (6.55) by imposing the main requirement of the construction: $\hat{V}(\varepsilon) \in \{\widehat{P}_k\}'$. Imposing this condition order by order leads to explicit expressions for both $V_\ell(\varepsilon)$ and $K_\ell(\varepsilon)$, as stated in the following result.

Lemma 6.2.3. *Equation* (4.47) *admits a unique solution under the constraint* $[K_s(\varepsilon)] = 0$, *given by the self-adjoint operators:*

$$V_{s-1}(\varepsilon) = \sum_{k\geq 1} \widehat{P}_k B_s(\varepsilon) \widehat{P}_k, \tag{6.58}$$

$$K_s(\varepsilon) = \mathrm{i} \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}tH} \{B_s(\varepsilon)\} \mathrm{e}^{\mathrm{i}tH} f(t) \mathrm{d}t, \tag{6.59}$$

where $f(t)$ is any $L^1(\mathbb{R})$ real function such that

$$\hat{f}(s) := \int_{\mathbb{R}} f(t) \mathrm{e}^{-\mathrm{i}st} \mathrm{d}t = \frac{1}{s}, \tag{6.60}$$

for $|s| \geq \hat{\eta}$.

Proof. Fix $s \geq 1$. According to Lemma 6.2.2, the operators $V_{s-1}(\varepsilon)$ and $K_s(\varepsilon)$ must satisfy

$$V_{s-1}(\varepsilon) = B_s(\varepsilon) - \mathrm{i}[K_s(\varepsilon), H]. \tag{6.61}$$

We impose that $V_{s-1}(\varepsilon) \in \{P_k\}'$. This is equivalent to requiring

$$V_{s-1}(\varepsilon) = [V_{s-1}(\varepsilon)] := \sum_{k\geq 1} \widehat{P}_k V_{s-1}(\varepsilon) \widehat{P}_k. \tag{6.62}$$

Let us take the block-diagonal part of Equation (6.61). As in the discrete case, the block-diagonal part of the commutator vanishes. Indeed,

$$\widehat{P}_k [K_s(\varepsilon), H] \widehat{P}_k = [\widehat{P}_k K_s(\varepsilon) \widehat{P}_k, H_k] = 0, \tag{6.63}$$

since $\widehat{P}_k K_s(\varepsilon) \widehat{P}_k = 0$. Then, we find

$$V_{s-1}(\varepsilon) = [B_s(\varepsilon)] = \sum_{k\geq 1} \widehat{P}_k B_s(\varepsilon) \widehat{P}_k, \tag{6.64}$$

which proves equation (6.58). Next, we determine $K_s(\varepsilon)$ by taking the off-diagonal part of (4.56):

$$\mathrm{i}[K_s(\varepsilon), H] = \{B_s(\varepsilon)\}. \tag{6.65}$$

This is a homological equation of the type considered in Lemma 6.2.1, whose unique solution under the constraint $[K_s(\varepsilon)] = 0$ is given by

$$K_s(\varepsilon) = \mathrm{i} \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}tH} \{B_s(\varepsilon)\} \mathrm{e}^{\mathrm{i}tH} f(t) \mathrm{d}t, \tag{6.66}$$

as stated in (6.59). The proof of the self-adjointness of $V_{s-1}(\varepsilon)$ and $K_s(\varepsilon)$ is identical to the one of lemma 4.2.2. □

6.2.3 Convergence of the formal expansion

The construction presented in the previous subsection is purely formal. The operators $B_s(\varepsilon)$, $K_s(\varepsilon)$, and $V_s(\varepsilon)$ are defined through infinite series, and their convergence must still be proved. The proof of the convergence is exactly the same as in the discrete case. The only difference is in the bound of the homological equation. We have shown in the previous paragraph that $K_s(\varepsilon)$, for $s \geq 1$ is the solution of the homological equation

$$\mathrm{i}[K_s(\varepsilon), H] = \{B_s(\varepsilon)\}. \tag{6.67}$$

In the fine-grained case, we have shown that

$$\|K_s(\varepsilon)\| \leq \frac{\pi}{\sqrt{3}\eta} \|B_s(\varepsilon)\|, \tag{6.68}$$

where η is the fine-grained spectral gap. On the other hand, in the coarse grained case, we have

$$\|K_s(\varepsilon)\| \leq \frac{\pi}{\hat{\eta}} \|B_s(\varepsilon)\|, \tag{6.69}$$

where $\hat{\eta}$ is the inter-bands minimal spectral gap.

Then, the bounds found in the fine-grained case are still valid in the coarse grained case, if we make the replacement

$$\frac{1}{\sqrt{3}\eta} \to \frac{1}{\hat{\eta}}. \tag{6.70}$$

According to this observation, we can enunciate the generalizations of the lemmas 4.2.3,4.2.4,4.2.5 to the bands case. The proofs are identical to the discrete case.

Lemma 6.2.4. *For all $s \geq 1$,*

$$\frac{\pi}{\hat{\eta}}\|B_s(\varepsilon)\| \leq \alpha^{s-1}\hat{b}^s d_s, \tag{6.71}$$

where

$$\hat{b} := \frac{\pi}{\hat{\eta}}C, \tag{6.72}$$

and $\alpha \approx 4.79$ is the solution of the transcendental equation

$$(\alpha+1)\left(\mathrm{e}^{\frac{2}{\alpha}} - 1\right) = 3. \tag{6.73}$$

Lemma 6.2.5. *For all $s \geq 1$, the operators $V_{s-1}(\varepsilon)$ and $K_s(\varepsilon)$ constructed in Lemma 6.2.3 satisfy the bounds:*

$$\|V_{s-1}(\varepsilon)\| \leq \|B_s(\varepsilon)\|, \tag{6.74}$$

$$\|K_s(\varepsilon)\| \leq \frac{\pi}{\hat{\eta}}\|B_s(\varepsilon)\|. \tag{6.75}$$

Lemma 6.2.6. *Let $K(\varepsilon)$ and $\hat{V}(\varepsilon)$ be the operators defined by the expansions* (4.45) *and* (4.46)*. Then, for all $\varepsilon \in \mathbb{R}$ such that*

$$|\varepsilon| \leq \frac{\hat{\eta}}{C\hat{\rho}}, \tag{6.76}$$

the following bounds hold:

$$\|K(\varepsilon)\| \leq |\varepsilon|\hat{b}\,\mathcal{D}(\alpha|\varepsilon|\hat{b}), \tag{6.77}$$

$$\|\hat{V}(\varepsilon)\| \leq C\,\mathcal{D}(\alpha|\varepsilon|\hat{b}), \tag{6.78}$$

where the function $\mathcal{D}$ is defined as

$$\mathcal{D}(y) := \frac{1-\sqrt{1-4y}}{2y}, \tag{6.79}$$

the generating function of the Catalan numbers.

As direct consequence of the previous lemmas, one can prove, following the same steps of the fine grained case, the following theorem.

Theorem 6.2.1. *Let* $W(\varepsilon) = \mathrm{e}^{\mathrm{i}K(\varepsilon)}$ *and* $\hat{V}(\varepsilon)$ *defined before. Then*

$$\|W(\varepsilon) - \mathbb{I}\| \leq \hat{\beta}\frac{C}{\hat{\eta}}|\varepsilon|, \quad \textit{for } |\varepsilon| \leq \frac{\hat{\eta}}{C\hat{\rho}}, \tag{6.80}$$

$$\|HW(\varepsilon)\psi\| \leq \mathrm{e}^{\hat{b}|\varepsilon|\mathcal{D}(\alpha|\varepsilon|\hat{b})}\left(\|H\psi\| + \frac{2\hat{\eta}\hat{b}}{\pi}|\varepsilon|\mathcal{D}(\alpha|\varepsilon|\hat{b})\|\psi\|\right) \tag{6.81}$$

$$\|\hat{V}(\varepsilon)\| \leq C\,\mathcal{D}(\alpha|\varepsilon|\hat{b}) \tag{6.82}$$

This theorem concludes the proof of Theorem 6.1.2. Indeed, properties (*i*), (*ii*), (*iv*) and (*v*) hold by construction. Estimate (6.81) establishes property (*iii*), while estimate (6.80) yields property (*vi*).

Chapter 7

Differential Approach

In the previous chapter, we constructed the operators $W(\varepsilon)$ and $\hat{V}(\varepsilon)$ so that

$$W(\varepsilon)^\dagger\big(H + \varepsilon V(\varepsilon)\big)W(\varepsilon) = H + \varepsilon\hat{V}(\varepsilon), \tag{7.1}$$

with $\hat{V}(\varepsilon) \in \{H\}'$, by means of the Quantum KAM iteration. As already noted in Chapter 3, however, the definition of these operators is not unique, and alternative strategies can be employed to obtain the same result.

In this chapter we develop a differential approach, based on Kato's perturbation theory [20]. The central idea is to formulate a differential equation for the operator $W(\varepsilon)$, solve it as a formal power series, and then prove its convergence. The resulting transformation will again satisfy the requirements of Theorem 3.3.2.

Unlike the Quantum KAM scheme, which is discrete and combinatorial, the differential approach offers a continuous analytic framework based on the perturbation theory of spectral projections. We begin by recalling the relevant aspects of Kato's perturbation theory, and then apply this framework to construct the unitary transformation $W(\varepsilon)$ and establish its convergence.

7.1 Kato's Perturbation Theory

Let $\mathcal{H}$ be a separable Hilbert space, and let $H = H^\dagger$ be a self-adjoint operator. Suppose that H has purely discrete spectrum. Then, the spectral decomposition of H reads

$$H = \sum_{k\geq 1} h_k P_k, \tag{7.2}$$

where $\{h_k\}_{k\geq 1}$ are the distinct (increasingly ordered) eigenvalues of H, and $\{P_k\}_{k\geq 1}$ are the corresponding orthogonal spectral projections.

We assume that the Hamiltonian has a non-vanishing minimal spectral gap, i.e.,

$$\eta = \inf_{k\neq \ell} |h_k - h_\ell| > 0. \tag{7.3}$$

We now investigate how the resolvent operator of such a Hamiltonian is modified when the Hamiltonian is subjected to a perturbation.

7.1.1 Perturbation of the Resolvent Operator

We start by recalling the definition of the resolvent operator $R_\zeta(H)$. For every $\zeta \notin \{h_k\}_{k\geq 1}$, we set

$$R_\zeta(H) = (H - \zeta\mathbb{I})^{-1}, \tag{7.4}$$

which defines a bounded operator on the Hilbert space. Throughout this chapter, for brevity, we will adopt the shorthand notation

$$R_\zeta(H) \equiv R(\zeta), \tag{7.5}$$

omitting the explicit dependence on H when no confusion arises.

We aim to study how the resolvent operator is modified when the Hamiltonian is subjected to a perturbation of the form

$$H(\varepsilon) = H + \varepsilon V(\varepsilon), \tag{7.6}$$

where $V(\varepsilon) = V(\varepsilon)^\dagger \in B(\mathcal{H})$ is a generic bounded self-adjoint operator, uniformly bounded in ε, i.e.

$$\sup_{\varepsilon\in I} \|V(\varepsilon)\| \leq C < \infty,$$

and $\varepsilon \in I \subseteq \mathbb{R}$.

In order to use Kato's perturbation theory, it is convenient to consider a broader family of perturbations, parametrized by a complex variable $z \in \mathbb{C}$:

$$H(z;\varepsilon) = H + zV(\varepsilon). \tag{7.7}$$

Here $V(\varepsilon)$ is kept fixed, while the dependence on z allows us to exploit analyticity in the complex parameter. The original perturbed Hamiltonian is recovered by setting $z = \varepsilon \in \mathbb{R}$. In the following, to simplify notation, we shall often write $H(z)$ instead of $H(z;\varepsilon)$, and V instead of $V(\varepsilon)$, tacitly keeping in mind the underlying dependence on ε.

For all $z \in \mathbb{C}$, we define the perturbed resolvent operator as

$$R(\zeta, z) = (H(z) - \zeta\mathbb{I})^{-1}. \tag{7.8}$$

We now prove that $R(\zeta, z)$ is analytic in a neighborhood of $z = 0$.

Theorem 7.1.1. *Let $R(\zeta, z)$ be the resolvent operator of the perturbed Hamiltonian $H(z) = H + zV$. Then $R(\zeta, z)$ is analytic in a neighborhood of $z = 0$. In particular, it admits the* *expansion*

$$R(\zeta, z) = \sum_{n\geq 0} z^n R^{(n)}(\zeta), \tag{7.9}$$

where

$$R^{(n)}(\zeta) = R(\zeta)(-VR(\zeta))^n, \qquad n \geq 0. \tag{7.10}$$

Proof. Let ζ belong to the resolvent set of H, so that $R(\zeta) = (H - \zeta\mathbb{I})^{-1} \in B(\mathcal{H})$. Then,

$$H(z) - \zeta\mathbb{I} = H - \zeta\mathbb{I} + zV = (\mathbb{I} + zVR(\zeta))(H - \zeta\mathbb{I}), \tag{7.11}$$

where we have used the identity $(H - \zeta\mathbb{I})R(\zeta) = \mathbb{I}$.

Taking the inverse, we obtain

$$R(\zeta, z) = R(\zeta)[\mathbb{I} + zVR(\zeta)]^{-1}. \tag{7.12}$$

We now expand the inverse operator on the right-hand side of (7.12) using the Neumann series:

$$(\mathbb{I} - A)^{-1} = \sum_{n\geq 0} A^n, \tag{7.13}$$

which is valid whenever $\|A\| < 1$. Applying it to $A = -zVR(\zeta)$, we get

$$[\mathbb{I} + zVR(\zeta)]^{-1} = \sum_{n\geq 0} (-zVR(\zeta))^n. \tag{7.14}$$

This series converges for all $z \in \mathbb{C}$ such that

$$|z| < \|VR(\zeta)\|^{-1}, \tag{7.15}$$

which holds for $|z|$ sufficiently small.

Substituting the expansion (7.14) into (7.12), we find

$$R(\zeta, z) = R(\zeta) \sum_{n\geq 0} (-zVR(\zeta))^n = \sum_{n\geq 0} z^n R(\zeta)(-VR(\zeta))^n, \tag{7.16}$$

which concludes the proof. □

In the following section, we study how the perturbation of the Hamiltonian affects its spectral projections. In particular, the expansion (7.9) will be the key tool to derive perturbative formulas for the spectral projectors.

7.1.2 Perturbation of the Spectral Projections

Let h_k be an isolated eigenvalue of the unperturbed Hamiltonian H, with multiplicity $m \in \mathbb{N} \cup \{+\infty\}$. The associated spectral projection can be written as

$$P_k = -\frac{1}{2\pi \mathrm{i}} \int_{\Gamma_k} R(\zeta) \mathrm{d}\zeta, \tag{7.17}$$

where Γ_k is a positively oriented, closed curve (e.g., a circle) in the resolvent set of H enclosing h_k and no other eigenvalues.

Let us now define the perturbed projection operator

$$P_k(z) = -\frac{1}{2\pi \mathrm{i}} \int_{\Gamma_k} R(\zeta, z) \mathrm{d}\zeta, \tag{7.18}$$

where $P_k(z)$ projects onto the part of the spectrum of $H(z) = H + zV$ enclosed by Γ_k.[1]

The analyticity and boundedness of the resolvent $R(\zeta, z)$ for $|z|$ sufficiently small (as proved in the previous section) ensure that no spectral points of $H(z)$ lie on Γ_k, so the definition is well posed.

Expanding the resolvent operator using Theorem 7.1.1 and integrating term by term yields the Taylor expansion

$$P_k(z) = P_k + \sum_{n=1}^{\infty} z^n P_k^{(n)}, \tag{7.20}$$

with coefficients

$$P_k^{(n)} = -\frac{1}{2\pi \mathrm{i}} \int_{\Gamma_k} R^{(n)}(\zeta) \mathrm{d}\zeta. \tag{7.21}$$

Using Theorem 7.1.1, we now compute an explicit formula for the coefficients $P_k^{(n)}$.

Theorem 7.1.2. *Let $P_k(z)$ be the family of spectral projections with Taylor expansion given by* (7.20)*. Then, for all $n \geq 1$,*

$$P_k^{(n)} = (-1)^{n+1} \sum_{\substack{\mu_1 + \cdots + \mu_{n+1} = n \\ \mu_j \geq 0}} S_k^{(\mu_1)} V S_k^{(\mu_2)} V \cdots V S_k^{(\mu_{n+1})}, \tag{7.22}$$

[1] Note that $H(z)$ is not self-adjoint for general $z \in \mathbb{C}$, hence $P_k(z)$ is not Hermitian. However, since $H(z)^\dagger = H(z^*)$, the same symmetry holds for the projections:

$$P_k(z)^\dagger = P_k(z^*). \tag{7.19}$$

For real z, in particular, $P_k(z)$ reduces to an orthogonal projection.

where

$$S_k^{(0)} = -P_k, \tag{7.23}$$
$$S_k^{(\mu)} = S_k^{\mu} \quad \textit{for } \mu \geq 1, \tag{7.24}$$

and

$$S_k = \sum_{\ell \neq k} \frac{P_\ell}{h_\ell - h_k} \tag{7.25}$$

is the reduced resolvent *of H with respect to the eigenvalue h_k.*

Proof. From (7.10) and (7.21), we obtain

$$P_k^{(n)} = (-1)^{n+1} \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_k} R(\zeta)[VR(\zeta)]^n \mathrm{d}\zeta. \tag{7.26}$$

Since h_k is an isolated eigenvalue, the resolvent $R(\zeta)$ has a Laurent expansion around $\zeta = h_k$. In the Appendix C, we show that this expansion reads

$$R(\zeta) = \sum_{\mu \geq -1} (\zeta - h_k)^{\mu} S_k^{(\mu+1)}, \tag{7.27}$$

with $S_k^{(\mu+1)}$ as defined in (7.23) and (7.24).

Inserting (7.27) into (7.26) and expanding the product yields

$$P_k^{(n)} = (-1)^{n+1} \frac{1}{2\pi \mathrm{i}} \sum_{\mu_1, \dots, \mu_{n+1} \geq -1} \int_{\Gamma_k} (\zeta - h_k)^{\mu_1 + \cdots + \mu_{n+1}} S_k^{(\mu_1+1)} V S_k^{(\mu_2+1)} \cdots V S_k^{(\mu_{n+1}+1)} \mathrm{d}\zeta. \tag{7.28}$$

Let us now evaluate the integral

$$I_k^{(p)} := \int_{\Gamma_k} (\zeta - h_k)^p \mathrm{d}\zeta\,, \quad p \in \mathbb{Z}. \tag{7.29}$$

Case $p \geq 0$: the integrand is holomorphic inside Γ_k, so by Cauchy's theorem,

$$I_k^{(p)} = 0.$$

Case $p < 0$: the integrand has a pole of order $-p$ at $\zeta = h_k$. By the Cauchy Residue Theorem, it is easy to show that

$$I_k^{(p)} = 2\pi \mathrm{i}\, \delta_{p,-1}. \tag{7.30}$$

Then, from (7.28), only the terms with $\mu_1 + \cdots + \mu_{n+1} = -1$ contribute. We obtain

$$P_k^{(n)} = (-1)^{n+1} \sum_{\mu_1 + \cdots + \mu_{n+1} = -1} S_k^{(\mu_1+1)} V S_k^{(\mu_2+1)} \cdots V S_k^{(\mu_{n+1}+1)}. \tag{7.31}$$

Finally, we shift the summation indices $\mu_j \mapsto \mu_j - 1$, yielding the claimed result:

$$P_k^{(n)} = (-1)^{n+1} \sum_{\substack{\mu_1+\cdots+\mu_{n+1}=n \\ \mu_j \geq 0}} S_k^{(\mu_1)} V S_k^{(\mu_2)} \cdots V S_k^{(\mu_{n+1})}. \tag{7.32}$$

□

We now introduce the multi-index notation:

$$\boldsymbol{\mu}_m = (\mu_1, \ldots, \mu_m), \tag{7.33}$$

$$|\boldsymbol{\mu}_m| = \mu_1 + \cdots + \mu_m. \tag{7.34}$$

Then the coefficients can be written compactly as

$$P_k^{(n)} = (-1)^{n+1} \sum_{|\boldsymbol{\mu}_{n+1}|=n} S_k^{(\mu_1)} V S_k^{(\mu_2)} \cdots V S_k^{(\mu_{n+1})}. \tag{7.35}$$

Let us now compute explicitly the first two coefficients:

First-order term:

$$P_k^{(1)} = \sum_{\mu_1+\mu_2=1} S_k^{(\mu_1)} V S_k^{(\mu_2)} \tag{7.36}$$

$$= S_k^{(0)} V S_k^{(1)} + S_k^{(1)} V S_k^{(0)} \tag{7.37}$$

$$= -\left(P_k V S_k + S_k V P_k\right). \tag{7.38}$$

Second-order term:

$$P_k^{(2)} = -\sum_{\mu_1+\mu_2+\mu_3=2} S_k^{(\mu_1)} V S_k^{(\mu_2)} V S_k^{(\mu_3)} \tag{7.39}$$

$$= -\big(S_k^2 V P_k V P_k + P_k V S_k^2 V P_k + P_k V P_k V S_k^2 \tag{7.40}$$

$$+ S_k V S_k V P_k + S_k V P_k V S_k + P_k V S_k V S_k\big). \tag{7.41}$$

In the next section, we construct a similarity transformation that maps the unperturbed projection P_k to the perturbed one $P_k(z)$.

7.2 Similarity transformations of spectral projections

This section follows the classical strategy of Kato's perturbation theory. The central idea is to construct an operator family $U(z)$ that intertwines the perturbed and unperturbed spectral projections. In particular, for all $k \geq 1$,

- $U(z)$ is invertible, and its inverse $U(z)^{-1}$ is holomorphic;

- $U(z)P_k(0)U(z)^{-1} = P_k(z)$.

We start by introducing a lemma about the differential properties of the spectral projections $P_k(z)$.

Lemma 7.2.1. *Let $P_k(z)$ be the spectral projections defined in the previous section. Then*

$$P_k'(z) = [Q(z), P_k(z)], \tag{7.42}$$

where $P_k'(z)$ denotes the derivative of $P_k(z)$, and

$$Q(z) = \sum_{k\geq 1} P_k'(z)P_k(z). \tag{7.43}$$

Proof. Since $P_k(z)$ is a projection, it satisfies $P_k(z)^2 = P_k(z)$. Differentiating both sides and using the Leibniz rule, we obtain

$$P_k(z)P_k'(z) + P_k'(z)P_k(z) = P_k'(z). \tag{7.44}$$

Summing over $k \geq 1$, we have

$$\sum_{k\geq 1} (P_k(z)P_k'(z) + P_k'(z)P_k(z)) = \left(\sum_{k\geq 1} P_k(z)\right)' = 0, \tag{7.45}$$

since the projections form a resolution of the identity. Thus,

$$Q(z) = \sum_{k\geq 1} P_k'(z)P_k(z) = -\sum_{k\geq 1} P_k(z)P_k'(z). \tag{7.46}$$

Let us now compute the commutator of $Q(z)$ with $P_k(z)$. Using (7.46), we obtain:

$$\begin{aligned}[Q(z), P_k(z)] &= Q(z)P_k(z) - P_k(z)Q(z) \\ &= P_k'(z)P_k(z) + P_k(z)P_k'(z) = P_k'(z),\end{aligned}$$

where the last equality follows from (7.44). □

We are now ready to address the problem of finding the operator family $U(z)$. In particular, we will formulate a differential equation that $U(z)$ must satisfy, and in the next section we will solve it.

Theorem 7.2.1. *The operator $U(z)$ is the unique solution of the differential equation*

$$X'(z) = Q(z)X(z), \tag{7.47}$$

with initial condition $X(0) = \mathbb{I}$. Furthermore,

$$U(z)^{-1} = U(z^*)^\dagger, \tag{7.48}$$

meaning that for $z \in \mathbb{R}$, the operator $U(z)$ is unitary.

Proof. The differential equation (7.47) is linear, and thus has a unique holomorphic solution (in a simply connected domain) for a given initial condition $X(0)$. Let $U(z)$ denote the solution with $X(0) = \mathbb{I}$. Then the solution with a generic initial condition $X(0)$ is given by

$$X(z) = U(z)X(0). \tag{7.49}$$

Consider now the following differential equation:

$$Y'(z) = -Y(z)Q(z). \tag{7.50}$$

This also admits a unique holomorphic solution with given initial condition. Let $W(z)$ denote the solution with $Y(0) = \mathbb{I}$.

We now prove that $U(z)$ and $W(z)$ are inverse to each other. Indeed:

$$(W(z)U(z))' = W'(z)U(z) + W(z)U'(z) \tag{7.51}$$

$$= -W(z)Q(z)U(z) + W(z)Q(z)U(z) = 0. \tag{7.52}$$

Thus, $W(z)U(z)$ is constant and

$$W(z)U(z) = W(0)U(0) = \mathbb{I}. \tag{7.53}$$

To prove $U(z)W(z) = \mathbb{I}$, consider:

$$(U(z)W(z))' = U'(z)W(z) + U(z)W'(z) \tag{7.54}$$

$$= Q(z)U(z)W(z) - U(z)W(z)Q(z) = [Q(z), U(z)W(z)]. \tag{7.55}$$

So $R(z) := U(z)W(z)$ satisfies:

$$R'(z) = [Q(z), R(z)], \qquad R(0) = \mathbb{I}. \tag{7.56}$$

Since the identity operator solves this Cauchy problem, and the solution is unique, it follows that

$$U(z)W(z) = \mathbb{I}. \tag{7.57}$$

Hence, $W(z) = U(z)^{-1}$.

Let us now prove that $U(z)$ satisfies the intertwining property for the projections:

$$P_k(z)U(z) = U(z)P_k(0), \quad \forall z. \tag{7.58}$$

Differentiating the left hand side of the previous expression, we get

$$
\begin{aligned}
(P_k(z)U(z))' &= P_k'(z)U(z) + P_k(z)U'(z) && (7.59)\\
&= [Q(z), P_k(z)]U(z) + P_k(z)Q(z)U(z) && (7.60)\\
&= Q(z)P_k(z)U(z) = Q(z)(P_k(z)U(z)). && (7.61)
\end{aligned}
$$

This implies that $R(z) := P_k(z)U(z)$ satisfies:

$$R'(z) = Q(z)R(z), \quad R(0) = P_k(0), \tag{7.62}$$

and by formula (7.49) and uniqueness of the solution,

$$P_k(z)U(z) = U(z)P_k(0). \tag{7.63}$$

Multiplying both sides on the right by $U(z)^{-1}$ yields:

$$P_k(z) = U(z)P_k(0)U(z)^{-1}. \tag{7.64}$$

We now prove that $U(z^*)^\dagger = U(z)^{-1}$. From the differential equation

$$U'(z^*) = Q(z^*)U(z^*), \tag{7.65}$$

taking the adjoint gives:

$$\big(U(z^*)^\dagger\big)' = U(z^*)^\dagger Q(z^*)^\dagger. \tag{7.66}$$

We now compute $Q(z^*)^\dagger$. Using the identity $P_k(z^*)^\dagger = P_k(z)$ (from (7.19)), we obtain:

$$
\begin{aligned}
Q(z^*)^\dagger &= \left(\sum_{k\geq 1} P_k'(z^*)P_k(z^*)\right)^\dagger = \sum_{k\geq 1} P_k(z)P_k'(z)^\dagger && (7.67)\\
&= -Q(z), && (7.68)
\end{aligned}
$$

so $Q(z)$ is skew-Hermitian. Therefore,

$$\big(U(z^*)^\dagger\big)' = -U(z^*)^\dagger Q(z), \tag{7.69}$$

which is the same equation (7.50) satisfied by $U(z)^{-1}$, and both satisfy the same initial condition at $z = 0$. Hence, by uniqueness,

$$U(z^*)^\dagger = U(z)^{-1}. \tag{7.70}$$

□

This concludes the proof of the existence of the operator $U(z)$. In the next section, we will find its explicit form via a formal expansion, and subsequently study its convergence.

7.2.1 Formal series expansion of $U(z)$

Rather than solving directly the differential equation for $U(z)$, we consider the family of operators $U_k(z) := U(z)P_k(0)$, for each $k \in \mathbb{N}$. The full operator $U(z)$ can then be reconstructed via the resolution of the identity:

$$U(z) = \sum_{k\geq 1} U_k(z). \tag{7.71}$$

Let us now derive the differential equation satisfied by $U_k(z)$. Taking the derivative, we obtain:

$$\begin{aligned} U_k'(z) &= U'(z)P_k(0) = Q(z)U(z)P_k(0) && (7.72)\\ &= Q(z)P_k(z)U(z)P_k(0) = P_k'(z)U_k(z), && (7.73) \end{aligned}$$

where we used the definition of $Q(z)$ from (7.46). Thus, each block $U_k(z)$ satisfies the differential equation:

$$U_k'(z) = P_k'(z)U_k(z), \tag{7.74}$$

with initial condition

$$U_k(0) = P_k. \tag{7.75}$$

Theorem 7.2.2. *The solution of the equation* (7.74) *admits a formal series expansion*

$$U_k(z) = \sum_{n\geq 0} z^n U_k^{(n)}, \tag{7.76}$$

where the coefficients satisfy

$$\begin{aligned} U_k^{(0)} &= P_k, && (7.77)\\ U_k^{(n)} &= \sum_{m=1}^{n} (-1)^{m-1}\frac{m}{n} \sum_{|\boldsymbol{\mu}|=m} S_k^{(\mu_1)} V S_k^{(\mu_2)} V \cdots V S_k^{(\mu_{m+1})} U_k^{(n-m)}. && (7.78) \end{aligned}$$

Proof. Recall the expansion of $P_k(z)$:

$$P_k(z) = \sum_{n=0}^{\infty} z^n P_k^{(n)}, \tag{7.79}$$

with

$$\begin{aligned} P_k^{(0)} &= P_k, && (7.80)\\ P_k^{(n)} &= (-1)^{n+1} \sum_{|\boldsymbol{\mu}_{n+1}|=n} S_k^{(\mu_1)} V S_k^{(\mu_2)} V \cdots V S_k^{(\mu_{n+1})}. && (7.81) \end{aligned}$$

Differentiating term-by-term,

$$P_k'(z) = \sum_{n=0}^{\infty} (n+1) z^n P_k^{(n+1)}. \tag{7.82}$$

Seeking $U_k(z)$ in series form

$$U_k(z) = P_k + \sum_{n=1}^{\infty} z^n U_k^{(n)}, \tag{7.83}$$

and substituting into (7.74), we get

$$\sum_{n\geq 0} (n+1) z^n U_k^{(n+1)} = \sum_{m,\ell} (m+1) z^{m+\ell} P_k^{(m+1)} U_k^{(\ell)} \tag{7.84}$$

$$= \sum_{n\geq 0} z^n \sum_{m=0}^{n} (m+1) P_k^{(m+1)} U_k^{(n-m)}. \tag{7.85}$$

Equating coefficients term-by-term for each $n \geq 0$, and shifting index $n+1 \to n$,

$$nU_k^{(n)} = \sum_{m=0}^{n-1} (m+1) P_k^{(m+1)} U_k^{(n-1-m)}. \tag{7.86}$$

Replacing $P_k^{(n)}$ by their explicit expressions,

$$U_k^{(n)} = \sum_{m=0}^{n-1} (-1)^m \frac{m+1}{n} \sum_{|\boldsymbol{\mu}_{m+2}|=m+1} S_k^{(\mu_1)} V S_k^{(\mu_2)} V \cdots V S_k^{(\mu_{m+2})} U_k^{(n-1-m)} \tag{7.87}$$

$$= \sum_{m=1}^{n} (-1)^{m-1} \frac{m}{n} \sum_{|\boldsymbol{\mu}_{m+1}|=m} S_k^{(\mu_1)} V S_k^{(\mu_2)} V \cdots V S_k^{(\mu_{m+1})} U_k^{(n-m)}. \tag{7.88}$$

□

As a direct consequence of (7.71), the full operator $U(z)$ admits the formal expansion

$$U(z) = \sum_{n\geq 0} z^n U^{(n)}, \quad \text{where} \quad U^{(n)} = \sum_{k\geq 1} U_k^{(n)}. \tag{7.89}$$

Although convergence has not yet been established, the operator $U(z)$ is formally unitary for real values $z = \varepsilon$. When restricted to $z = \varepsilon \in \mathbb{R}$, we shall denote it by $W(\varepsilon)$, in agreement with the notation introduced in the previous chapters. In the next section, we shall prove convergence and show that $W(\varepsilon)$ satisfies all the properties of Theorem 3.3.2.

7.3 Unitary Equivalence in Kato's Framework

We now state the main result of Kato's method, which guarantees the existence of a unitary operator $W(\varepsilon)$ reducing the perturbed Hamiltonian to a block–diagonal form commuting with H, together with quantitative bounds.

Theorem 7.3.1. *There exist two families of operators $W(\varepsilon)$ and $\hat{V}(\varepsilon)$ with the following properties:*

(i) $\hat{V}(\varepsilon)$ *is self–adjoint and commutes with* H.

(ii) $W(\varepsilon)$ *is unitary.*

(iii) $W(\varepsilon)$ *leaves the domain of* H *invariant:*

$$W(\varepsilon)D(H) \subseteq D(H).$$

(iv) $W(0) = \mathbb{I}$.

(v) The operators $H + \varepsilon V(\varepsilon)$ *and* $H + \varepsilon\hat{V}(\varepsilon)$ *are unitarily equivalent through* $W(\varepsilon)$*:*

$$W(\varepsilon)^\dagger (H + \varepsilon V(\varepsilon))W(\varepsilon)\psi = (H + \varepsilon\hat{V}(\varepsilon))\psi, \tag{7.90}$$

for all $\psi \in D(H)$.

(vi) $W(\varepsilon)$ *satisfies the bound*

$$\|W(\varepsilon) - \mathbb{I}\| \leq \beta \frac{C}{\eta} |\varepsilon|, \tag{7.91}$$

for all $\varepsilon \in \mathbb{R}$*, where*

$$\beta := \frac{2\left[1 + \log\left(\dfrac{2\sqrt{3}+\pi}{\sqrt{3}+\pi}\right)\right]^2}{\left[1 + \log\left(\dfrac{2\sqrt{3}+\pi}{\sqrt{3}+\pi}\right)\right]^2 - 1}. \tag{7.92}$$

7.3.1 Block-diagonalization via $W(\varepsilon)$

The operator $W(\varepsilon)$, constructed in the previous section, intertwines the spectral projections of the perturbed Hamiltonian $H(\varepsilon) = H + \varepsilon V$ with those of the unperturbed one. As a consequence, it transforms the full Hamiltonian $H(\varepsilon)$ into a new operator $H + \varepsilon\hat{V}(\varepsilon)$ commuting with H. We define

$$H + \varepsilon\hat{V}(\varepsilon) := W(\varepsilon)^\dagger H(\varepsilon)W(\varepsilon). \tag{7.93}$$

We claim that $H + \varepsilon\hat{V}(\varepsilon)$ is block–diagonal in the spectral decomposition of H. Indeed,

$$\sum_{k\geq 1} P_k(H + \varepsilon\hat{V}(\varepsilon))P_k = \sum_{k\geq 1} P_k W(\varepsilon)^\dagger H(\varepsilon) W(\varepsilon) P_k \tag{7.94}$$

$$= \sum_{k\geq 1} W(\varepsilon)^\dagger P_k(\varepsilon) H(\varepsilon) P_k(\varepsilon) W(\varepsilon) \tag{7.95}$$

$$= W(\varepsilon)^\dagger H(\varepsilon) \left(\sum_{k\geq 1} P_k(\varepsilon) \right) W(\varepsilon) \tag{7.96}$$

$$= W(\varepsilon)^\dagger H(\varepsilon) W(\varepsilon) = H + \varepsilon\hat{V}(\varepsilon), \tag{7.97}$$

where we have used the intertwining property $W(\varepsilon)P_k = P_k(\varepsilon)W(\varepsilon)$, together with the completeness relation $\sum_k P_k(\varepsilon) = \mathbb{I}$.

Hence, $H+\varepsilon\hat{V}(\varepsilon)$ commutes with all spectral projections of H. It follows that $\hat{V}(\varepsilon)$ itself commutes with all spectral projections of H, and therefore with H. This establishes point (i) and (v) of Theorem 7.3.1. Properties (ii), and (iv) follow directly from the construction of the operator $W(\varepsilon)$.

7.3.2 Proof of point (vi)

To prove the convergence of the series constructed in the previous sections, we introduce a sequence of rational numbers closely related to the Catalan numbers. Their recursive definition reads

$$c_0 = 1, \tag{7.98}$$

$$c_n = \sum_{m=1}^{n} \binom{2m}{m} \frac{m}{n} c_{n-m}. \tag{7.99}$$

We refer to these as the *modified Catalan numbers.* Further details on this sequence can be found in Appendix A.

Let us consider again the formal expansion of the operator $W(\varepsilon)$:

$$W(\varepsilon) = 1 + \sum_{n\geq 1}\sum_{k\geq 1} \varepsilon^n W_k^{(n)} = 1 + \sum_{n\geq 1} \varepsilon^n W^{(n)}, \tag{7.100}$$

where we have introduced the notation

$$W^{(n)} = \sum_{k\geq 1} W_k^{(n)}. \tag{7.101}$$

To prove convergence we estimate each coefficient in the expansion, both at the block level $W_k^{(n)}$ and in the full operator $W^{(n)}$. We now present a lemma giving such estimates.

Lemma 7.3.1. *For all $n \geq 0$,*

$$\left\| W_k^{(n)} \right\| \leq c_n b^n, \tag{7.102}$$

$$\left\| W^{(n)} \right\| \leq \frac{1}{2}\left(1 + \frac{\pi}{\sqrt{3}}\right) c_n b^n, \tag{7.103}$$

where

$$b = \frac{\|V\|}{\eta}. \tag{7.104}$$

Proof. Let us proceed by induction. For $n = 0$, recall that

$$W_k^{(0)} = P_k, \tag{7.105}$$

and then

$$\left\| W_k^{(0)} \right\| = \|P_k\| = 1 = c_0 b^0. \tag{7.106}$$

Now suppose that for all $m = 1, \ldots, n-1$,

$$\left\| W_k^{(m)} \right\| \leq c_m b^m. \tag{7.107}$$

Using the recursive definition of $W_k^{(n)}$, we obtain

$$\left\| W_k^{(n)} \right\| \leq \sum_{m=1}^{n} \frac{m}{n} \sum_{|\boldsymbol{\mu}_{m+1}|=m} \left\| S_k^{(\mu_1)} V S_k^{(\mu_2)} V \cdots V S_k^{(\mu_{m+1})} W_k^{(n-m)} \right\| \tag{7.108}$$

$$\leq \sum_{m=1}^{n} \frac{m}{n} \sum_{|\boldsymbol{\mu}_{m+1}|=m} \|S_k\|^{\mu_1+\cdots+\mu_{m+1}} \|V\|^m \left\| W_k^{(n-m)} \right\| \tag{7.109}$$

$$\leq \sum_{m=1}^{n} \frac{m}{n} \|S_k\|^m \|V\|^m c_{n-m} b^{n-m} \sum_{|\boldsymbol{\mu}_{m+1}|=m} 1 \tag{7.110}$$

$$\leq b^n \sum_{m=1}^{n} \frac{m}{n} \binom{2m}{m} = c_n b^n, \tag{7.111}$$

where we used the identity

$$\sum_{|\boldsymbol{\mu}_{m+1}|=m} 1 = \binom{2m}{m}. \tag{7.112}$$

Let us now estimate $W^{(n)}$. By the triangle inequality,

$$\left\|W^{(n)}\right\| \leq \sum_{m=1}^{n} \frac{m}{n} \sum_{|\boldsymbol{\mu}_{m+1}|=m} \left\| \sum_{k\geq 1} S_k^{(\mu_1)} V S_k^{(\mu_2)} V \cdots V S_k^{(\mu_{m+1})} W_k^{(n-m)} P_k \right\| \tag{7.113}$$

$$= \sum_{m=1}^{n} \frac{m}{n} \sum_{|\boldsymbol{\mu}_{m+1}|=m} \left\| \sum_{k\geq 1} P_k \left(W_k^{(n-m)}\right)^{\dagger} S_k^{(\mu_{m+1})} V \cdots V S_k^{(\mu_1)} \right\| \tag{7.114}$$

$$:= \sum_{m=1}^{n} \frac{m}{n} \sum_{|\boldsymbol{\mu}_{m+1}|=m} \left\| Z_{n,m}^{(\boldsymbol{\mu})} \right\|, \tag{7.115}$$

where

$$Z_{n,m}^{(\boldsymbol{\mu})} := \sum_{k\geq 1} P_k \left(W_k^{(n-m)}\right)^{\dagger} S_k^{(\mu_{m+1})} V \cdots V S_k^{(\mu_1)}. \tag{7.116}$$

Let $\psi \in \mathcal{H}$. Then

$$\left\| Z_{n,m}^{(\boldsymbol{\mu})} \psi \right\|^2 = \sum_{k\geq 1} \left\| P_k \left(W_k^{(n-m)}\right)^{\dagger} S_k^{(\mu_{m+1})} V \cdots V S_k^{(\mu_1)} \psi \right\|^2 \tag{7.117}$$

$$\leq \sum_{k\geq 1} \left\| W_k^{(n-m)} \right\|^2 \|V\|^{2m} \|S_k\|^{2(m-\mu_1)} \left\| S_k^{(\mu_1)} \psi \right\|^2 \tag{7.118}$$

$$\leq \frac{\|V\|^{2m} \left(c_{n-m} b^{n-m}\right)^2}{\eta^{2(m-\mu_1)}} \sum_{k\geq 1} \left\| S_k^{(\mu_1)} \psi \right\|^2. \tag{7.119}$$

If $\mu_1 = 0$, then $S_k^{(\mu_1)} = -P_k$ and

$$\sum_{k\geq 1} \|P_k \psi\|^2 = \|\psi\|^2. \tag{7.120}$$

If $\mu_1 > 0$, then $S_k^{(\mu_1)} = S_k^{\mu_1}$, and

$$\sum_{k\geq 1} \|S_k^{\mu_1} \psi\|^2 \leq \frac{1}{\eta^{2(\mu_1 - 1)}} \sum_{k\geq 1} \|S_k \psi\|^2 \leq \frac{\pi^2}{3\eta^{2\mu_1}} \|\psi\|^2. \tag{7.121}$$

Thus,

$$\left\| Z_{n,m}^{(\boldsymbol{\mu})} \psi \right\|^2 \leq \left(c_{n-m} b^{n-m}\right)^2 \left[\frac{\|V\|^{2m}}{\eta^{2m}} \delta_{\mu_1,0} + \frac{\|V\|^{2m}}{\eta^{2(m-\mu_1)}} (1 - \delta_{\mu_1,0}) \frac{\pi^2}{3\eta^{2\mu_1}} \right] \|\psi\|^2 \tag{7.122}$$

$$= \left[\delta_{\mu_1,0} + \frac{\pi^2}{3\eta^2} (1 - \delta_{\mu_1,0}) \right] c_{n-m}^2 b^{2n} \|\psi\|^2. \tag{7.123}$$

Taking the supremum over $\|\psi\| = 1$ and then the square root, we obtain

$$\left\| Z_{n,m}^{(\boldsymbol{\mu})} \right\| \leq \left[\left(1 - \frac{\pi}{\sqrt{3}}\right) \delta_{\mu_1,0} + \frac{\pi}{\sqrt{3}} \right] c_{n-m} b^n. \tag{7.124}$$

Inserting this into (7.115), we get

$$\|W^{(n)}\| \leq \sum_{m=1}^{n} \frac{m}{n} \sum_{|\boldsymbol{\mu}_{m+1}|=m} \left[\left(1-\frac{\pi}{\sqrt{3}}\right)\delta_{\mu_1,0} + \frac{\pi}{\sqrt{3}}\right] c_{n-m} b^n \tag{7.125}$$

$$\leq \left(1-\frac{\pi}{\sqrt{3}}\right) b^n \sum_{m=1}^{n} \frac{m}{n} c_{n-m} \sum_{|\boldsymbol{\mu}_m|=m} + \frac{\pi}{\sqrt{3}} b^n \sum_{m=1}^{n} \frac{m}{n} c_{n-m} \sum_{|\boldsymbol{\mu}_{m+1}|=m} 1. \tag{7.126}$$

Since

$$\sum_{|\boldsymbol{\mu}_m|=m} 1 = \binom{2m-1}{m-1} = \frac{1}{2}\binom{2m}{m}, \tag{7.127}$$

$$\sum_{|\boldsymbol{\mu}_{m+1}|=m} 1 = \binom{2m}{m}, \tag{7.128}$$

we have

$$\|W^{(n)}\| \leq \left[\frac{1}{2}\left(1-\frac{\pi}{\sqrt{3}}\right) + \frac{\pi}{\sqrt{3}}\right] b^n \sum_{m=1}^{n} \frac{m}{n} c_{n-m} \binom{2m}{m} = \frac{1}{2}\left(1+\frac{\pi}{\sqrt{3}}\right) c_n b^n. \tag{7.129}$$

□

We are now ready to provide an estimate for $W(\varepsilon) - \mathbb{I}$.

Theorem 7.3.2. *Let $W(\varepsilon)$ be the operator defined above. Then*

$$\|W(\varepsilon) - \mathbb{I}\| \leq \frac{1}{2}\left(1+\frac{\pi}{\sqrt{3}}\right)\big(\mathcal{C}(\varepsilon b) - 1\big), \tag{7.130}$$

where

$$\mathcal{C}(x) = \exp\left(\frac{1}{\sqrt{1-4x}} - 1\right), \tag{7.131}$$

is the generating function of the sequence $\{c_n\}_{n\geq 0}$, and

$$b := \frac{\|V\|}{\eta}, \tag{7.132}$$

with $\eta = \inf_{k\neq\ell} |h_k - h_\ell| > 0$ the minimal spectral gap of H.

Proof. We have

$$\|W(\varepsilon) - \mathbb{I}\| \leq \sum_{n\geq 1} \varepsilon^n \|W^{(n)}\| \leq \sum_{n\geq 1} \frac{1}{2}\left(1+\frac{\pi}{\sqrt{3}}\right) c_n (\varepsilon b)^n \tag{7.133}$$

$$= \frac{1}{2}\left(1+\frac{\pi}{\sqrt{3}}\right)\big(\mathcal{C}(\varepsilon b) - 1\big). \tag{7.134}$$

□

A comparison with the bounds obtained in the previous chapters is shown in Fig. 7.1. We are now ready to complete the proof of point (vi) of Theorem 7.3.1.

Recall that we are interested (See Remark 3.3.5) only in values of ε such that

$$\|W(\varepsilon) - \mathbb{I}\| \leq \frac{1}{2}. \tag{7.135}$$

The function

$$f(x) = \frac{1}{2}\left(1 + \frac{\pi}{\sqrt{3}}\right)\big(\mathcal{C}(x) - 1\big), \tag{7.136}$$

is continuous and strictly increasing for $x \geq 0$, with $f(0) = 0$. Condition (7.135) is saturated at a unique positive value

$$x^* = \frac{\left[1 + \log\left(\frac{2\sqrt{3}+\pi}{\sqrt{3}+\pi}\right)\right]^2 - 1}{4\left[1 + \log\left(\frac{2\sqrt{3}+\pi}{\sqrt{3}+\pi}\right)\right]^2}.$$

By monotonicity of $f(x)$, we have

$$f(x) \leq f(x^*) \cdot \frac{x}{x^*}, \qquad \forall\, x \in [0, x^*].$$

On the interval $[0, x^*]$, the graph of $f(x)$ lies below the chord joining the points $(0,0)$ and $(x^*, f(x^*)) = (x^*, 1/2)$. Therefore,

$$f(x) \leq \frac{1/2}{x^*}\, x = \beta x, \qquad \forall\, x \in [0, x^*]. \tag{7.137}$$

Finally, recalling that $x = \varepsilon b = \varepsilon \|V\|/\eta$, we obtain

$$\|W(\varepsilon) - \mathbb{I}\| \leq \beta\, \frac{\|V\|}{\eta}\, |\varepsilon|, \tag{7.138}$$

where

$$\beta = \frac{2\left[1 + \log\left(\frac{2\sqrt{3}+\pi}{\sqrt{3}+\pi}\right)\right]^2}{\left[1 + \log\left(\frac{2\sqrt{3}+\pi}{\sqrt{3}+\pi}\right)\right]^2 - 1} \approx 4.85. \tag{7.139}$$

This establishes the desired linear bound.

7.3.3 Domain preservation of $W(\varepsilon)$

The last step is to verify that the transformation $W(\varepsilon)$ is well-defined on the domain of H, i.e. the point (iii) of the Theorem 7.3.1. As in the previous chapter, we want to prove that

$$W(\varepsilon)D(H) \subseteq D(H).$$

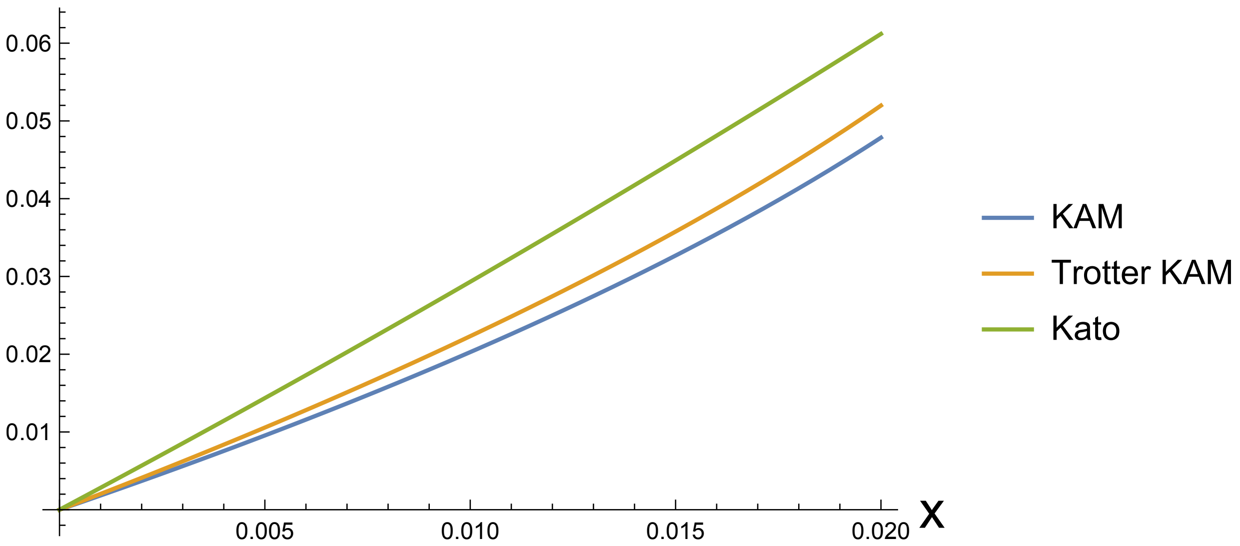

Figure 7.1: Comparison between the bounds on $\|W(\varepsilon) - \mathbb{I}\|$ obtained via the Quantum KAM Iteration, the Trotter–KAM scheme, and Kato's perturbative construction. The horizontal axis is labeled by x, where $x = \varepsilon b$ (with $b = \|V\|/\eta$).

To this end, we provide an explicit bound for $HW(\varepsilon)\psi$, with $\psi \in D(H)$. The following technical lemma will be needed.

Lemma 7.3.2. *For all $\mu \geq 0$, the following identity holds:*

$$HS_k^{(\mu)} = h_k S_k^{(\mu)} + (\mathbb{I} - P_k)\,\delta_{\mu,1} + S_k^{\mu-1}\,(1 - \delta_{\mu,0})(1 - \delta_{\mu,1}). \tag{7.140}$$

Proof. We check the cases separately.

If $\mu = 0$, then

$$HS_k^{(0)} = -HP_k = -h_k P_k = h_k S_k^{(0)}. \tag{7.141}$$

If $\mu = 1$, then

$$HS_k^{(1)} = HS_k = (H - h_k\mathbb{I})S_k + h_k S_k = (\mathbb{I} - P_k) + h_k S_k. \tag{7.142}$$

If $\mu > 1$, then

$$HS_k^{(\mu)} = HS_k^{\mu} = (H - h_k\mathbb{I})S_k^{\mu} + h_k S_k^{\mu} = (\mathbb{I} - P_k)S_k^{\mu-1} + h_k S_k^{\mu} = S_k^{\mu-1} + h_k S_k^{(\mu)}. \tag{7.143}$$

This proves the stated identity for all $\mu \geq 0$. □

We can now apply the lemma to estimate $HW(\varepsilon)\psi$, for $\psi \in D(H)$.

Theorem 7.3.3. *For all $\psi \in D(H)$,*

$$\|HW(\varepsilon)\psi\| \leq \|H\psi\| + \left[\frac{1}{2}\left(1 + \frac{\pi}{\sqrt{3}}\right)\|H\psi\| + \eta\left(\frac{1}{2} + \frac{\pi}{\sqrt{3}}\right)\|\psi\|\right](\mathcal{C}(\varepsilon b) - 1). \tag{7.144}$$

Proof. Let $\psi \in D(H)$. We start by expanding $HW^{(n)}$:

$$HW^{(n)} = \sum_{m=1}^{n} (-1)^{m-1} \frac{m}{n} \sum_{|\boldsymbol{\mu}_{m+1}|=m} \sum_{k\geq 1} HS^{(\mu_1)} V \cdots V S_k^{(\mu_{m+1})} W_k^{(n-m)} P_k. \tag{7.145}$$

Using the lemma, we decompose:

$$HW^{(n)} = \sum_{m=1}^{n} (-1)^{m-1} \frac{m}{n} \sum_{|\boldsymbol{\mu}_{m+1}|=m} \sum_{k\geq 1} h_k S_k^{(\mu_1)} V \cdots V S_k^{(\mu_{m+1})} W_k^{(n-m)} P_k \tag{7.146}$$

$$+ \sum_{m=1}^{n} (-1)^{m-1} \frac{m}{n} \sum_{|\boldsymbol{\mu}_{m+1}|=m} \sum_{k\geq 1} (\mathbb{I} - P_k) \delta_{\mu_1,1} V \cdots V S_k^{(\mu_{m+1})} W_k^{(n-m)} P_k \tag{7.147}$$

$$+ \sum_{m=1}^{n} (-1)^{m-1} \frac{m}{n} \sum_{\substack{|\boldsymbol{\mu}_{m+1}|=m, \\ \mu_1>1}} \sum_{k\geq 1} S_k^{\mu_1 - 1} V \cdots V S_k^{(\mu_{m+1})} W_k^{(n-m)} P_k. \tag{7.148}$$

The first line can be rewritten as

$$\sum_{m=1}^{n} (-1)^{m-1} \frac{m}{n} \sum_{|\boldsymbol{\mu}_{m+1}|=m} \sum_{k\geq 1} S_k^{(\mu_1)} V \cdots V S_k^{(\mu_{m+1})} W_k^{(n-m)} P_k H. \tag{7.149}$$

In the second line, notice that

$$\sum_{|\boldsymbol{\mu}_{m+1}|=m} \delta_{\mu_1,1} = \sum_{\mu_2+\cdots+\mu_{m+1}=m-1} 1 = \sum_{|\boldsymbol{\mu}_m|=m-1} 1, \tag{7.150}$$

so we can rewrite it as

$$\sum_{m=1}^{n} (-1)^{m-1} \frac{m}{n} \sum_{|\boldsymbol{\mu}_m|=m-1} \sum_{k\geq 1} (\mathbb{I} - P_k) V S_k^{(\mu_1)} \cdots V S_k^{(\mu_m)} W_k^{(n-m)} P_k. \tag{7.151}$$

Altogether, we obtain

$$HW^{(n)} = W^{(n)} H \tag{7.152}$$

$$+ V \sum_{m=1}^{n} (-1)^{m-1} \frac{m}{n} \sum_{|\boldsymbol{\mu}_m|=m-1} \sum_{k\geq 1} S_k^{(\mu_1)} V \cdots V S_k^{(\mu_m)} W_k^{(n-m)} P_k \tag{7.153}$$

$$- \sum_{m=1}^{n} (-1)^{m-1} \frac{m}{n} \sum_{|\boldsymbol{\mu}_m|=m-1} \sum_{k\geq 1} P_k V S_k^{(\mu_1)} V \cdots V S_k^{(\mu_m)} W_k^{(n-m)} P_k \tag{7.154}$$

$$+ \sum_{m=1}^{n} (-1)^{m-1} \frac{m}{n} \sum_{\substack{|\boldsymbol{\mu}_{m+1}|=m \\ \mu_1>1}} \sum_{k\geq 1} S_k^{\mu_1 - 1} V \cdots V S_k^{(\mu_{m+1})} W_k^{(n-m)} P_k. \tag{7.155}$$

For convenience, let us denote

$$A_{n,m}^{(\boldsymbol{\mu}_m)} = \sum_{k\geq 1} S_k^{(\mu_1)} V \cdots V S_k^{(\mu_m)} W_k^{(n-m)} P_k, \tag{7.156}$$

$$B_{n,m}^{(\boldsymbol{\mu}_m)} = -\sum_{k\geq 1} P_k V S_k^{(\mu_1)} V \cdots V S_k^{(\mu_m)} W_k^{(n-m)} P_k, \tag{7.157}$$

$$C_{n,m}^{(\boldsymbol{\mu}_{m+1})} = \sum_{k\geq 1} S_k^{\mu_1 - 1} V \cdots V S_k^{(\mu_{m+1})} W_k^{(n-m)} P_k. \tag{7.158}$$

Thus,

$$HW^{(n)} = W^{(n)} H + \sum_{m=1}^{n} (-1)^{m-1} \frac{m}{n} \left(\sum_{|\boldsymbol{\mu}_m| = m-1} \left(V A_{n,m}^{(\boldsymbol{\mu}_m)} + B_{n,m}^{(\boldsymbol{\mu}_m)} \right) + \sum_{\substack{|\boldsymbol{\mu}_{m+1}| = m \\ \mu_1 > 1}} C_{n,m}^{(\boldsymbol{\mu}_{m+1})} \right). \tag{7.159}$$

Taking norms, we find

$$\left\| HW^{(n)} \psi \right\| \leq \left\| W^{(n)} \right\| \|H\psi\| \tag{7.160}$$

$$+ \sum_{m=1}^{n} \frac{m}{n} \left(\sum_{|\boldsymbol{\mu}_m| = m-1} \left(\|V\| \left\| A_{n,m}^{(\boldsymbol{\mu}_m)} \right\| + \left\| B_{n,m}^{(\boldsymbol{\mu}_m)} \right\| \right) + \sum_{\substack{|\boldsymbol{\mu}_{m+1}| = m \\ \mu_1 > 1}} \left\| C_{n,m}^{(\boldsymbol{\mu}_{m+1})} \right\| \right) \|\psi\| \tag{7.161}$$

$$:= \left\| W^{(n)} \right\| \|H\psi\| + D^{(n)} \|\psi\|, \tag{7.162}$$

where

$$D^{(n)} := \sum_{m=1}^{n} \frac{m}{n} \left(\sum_{|\boldsymbol{\mu}_m| = m-1} \left(\|V\| \|A_{n,m}^{(\boldsymbol{\mu}_m)}\| + \|B_{n,m}^{(\boldsymbol{\mu}_m)}\| \right) + \sum_{\substack{|\boldsymbol{\mu}_{m+1}| = m \\ \mu_1 > 1}} \|C_{n,m}^{(\boldsymbol{\mu}_{m+1})}\| \right). \tag{7.163}$$

At this point, we need to estimate the contribution $D^{(n)}$ that appears in the bound for $\|HW^{(n)}\psi\|$. To this end, we proceed in three steps:

Step 1 we estimate separately the norms of the operators $A_{n,m}^{(\boldsymbol{\mu}_m)}$, $B_{n,m}^{(\boldsymbol{\mu}_m)}$ and $C_{n,m}^{(\boldsymbol{\mu}_{m+1})}$;

Step 2 we combine these estimates to obtain an explicit bound for $D^{(n)}$;

Step 3 we plug the resulting estimate into the series expansion of $HW(\varepsilon)\psi$, thus completing the proof.

Step 1: Estimates of A, B, C.

Take $\psi \in \mathcal{H}$. Then

$$\left\| A_{n,m}^{(\boldsymbol{\mu}_m)\dagger} \psi \right\|^2 = \sum_{k\geq 1} \left\| P_k (W_k^{(n-m)})^\dagger S_k^{(\mu_m)} V \cdots V S_k^{(\mu_1)} \psi \right\|^2. \tag{7.164}$$

Using

$$\left\|W_k^{(s)}\right\| \leq c_s b^s, \quad \left\|S_k^{(\mu)}\right\| \leq \frac{1}{\eta^\mu}, \quad \mu_1 + \cdots + \mu_m = m - 1, \tag{7.165}$$

we get

$$\left\|A_{n,m}^{(\boldsymbol{\mu}_m)\dagger}\psi\right\|^2 \leq \left(\frac{\|V\|^{m-1}}{\eta^{m-1-\mu_1}} c_{n-m} b^{n-m}\right)^2 \sum_{k\geq 1} \left\|S_k^{(\mu_1)}\psi\right\|^2. \tag{7.166}$$

From the previous section,

$$\sum_{k\geq 1} \left\|S_k^{(\mu_1)}\psi\right\|^2 \leq \frac{\pi^2}{3\eta^{2\mu_1}} \|\psi\|^2. \tag{7.167}$$

Hence,

$$\left\|A_{n,m}^{(\boldsymbol{\mu}_m)\dagger}\psi\right\|^2 \leq \frac{\pi^2}{3} \left(c_{n-m} b^{n-1}\right)^2 \|\psi\|^2, \tag{7.168}$$

so

$$\left\|A_{n,m}^{(\boldsymbol{\mu}_m)}\right\| \leq \frac{\pi}{\sqrt{3}} c_{n-m} b^{n-1}. \tag{7.169}$$

Similarly,

$$\left\|B_{n,m}^{(\boldsymbol{\mu}_m)}\right\| \leq \|V\| c_{n-m} b^{n-1}, \tag{7.170}$$

$$\left\|C_{n,m}^{(\boldsymbol{\mu}_{m+1})}\right\| \leq \frac{\pi}{\sqrt{3}} \|V\| c_{n-m} b^{n-1}. \tag{7.171}$$

Step 2: Bound for $D^{(n)}$.

Plugging these estimates into the definition, we find

$$D^{(n)} \leq \|V\| \sum_{m=1}^{n} \frac{m}{n} \left(\sum_{|\boldsymbol{\mu}_m|=m-1} \left(\frac{\pi}{\sqrt{3}} c_{n-m} b^{n-1} + c_{n-m} b^{n-1} \right) + \sum_{\substack{|\boldsymbol{\mu}_{m+1}|=m \\ \mu_1 > 1}} \frac{\pi}{\sqrt{3}} c_{n-m} b^{n-1} \right). \tag{7.172}$$

This can be rewritten as

$$D^{(n)} = \|V\| b^{n-1} \sum_{m=1}^{n} \frac{m}{n} c_{n-m} \left[\frac{\pi}{\sqrt{3}} \left(\sum_{|\boldsymbol{\mu}_m|=m-1} 1 + \sum_{\substack{|\boldsymbol{\mu}_{m+1}|=m \\ \mu_1 > 1}} 1 \right) + \sum_{|\boldsymbol{\mu}_m|=m-1} 1 \right]. \tag{7.173}$$

Now observe that

$$\sum_{|\boldsymbol{\mu}_m|=m-1} 1 = \binom{2(m-1)}{m-1} < \frac{1}{2}\binom{2m}{m}, \tag{7.174}$$

$$\sum_{\substack{|\boldsymbol{\mu}_{m+1}|=m \\ \mu_1>1}} 1 < \sum_{\substack{|\boldsymbol{\mu}_{m+1}|=m \\ \mu_1>0}} 1 = \frac{1}{2}\binom{2m}{m}. \tag{7.175}$$

Therefore,

$$D^{(n)} < \eta\left(\frac{1}{2} + \frac{\pi}{\sqrt{3}}\right) c_n b^n. \tag{7.176}$$

Step 3: Conclusion.
Recalling

$$\left\|W^{(n)}\right\| \le \frac{1}{2}\left(1 + \frac{\pi}{\sqrt{3}}\right) c_n b^n, \tag{7.177}$$

we finally obtain

$$\left\|HW^{(n)}\psi\right\| \le \left[\frac{1}{2}\left(1 + \frac{\pi}{\sqrt{3}}\right)\|H\psi\| + \eta\left(\frac{1}{2} + \frac{\pi}{\sqrt{3}}\right)\|\psi\|\right] c_n b^n. \tag{7.178}$$

Summing over $n \ge 1$,

$$\begin{aligned}
\|HW(\varepsilon)\psi\| &\le \|H\psi\| + \sum_{n\ge 1} \varepsilon^n \left\|HW^{(n)}\psi\right\| && (7.179)\\
&\le \|H\psi\| + \left[\frac{1}{2}\left(1 + \frac{\pi}{\sqrt{3}}\right)\|H\psi\| + \eta\left(\frac{1}{2} + \frac{\pi}{\sqrt{3}}\right)\|\psi\|\right] \sum_{n\ge 1} c_n (\varepsilon b)^n && (7.180)\\
&= \|H\psi\| + \left[\frac{1}{2}\left(1 + \frac{\pi}{\sqrt{3}}\right)\|H\psi\| + \eta\left(\frac{1}{2} + \frac{\pi}{\sqrt{3}}\right)\|\psi\|\right] (\mathcal{C}(\varepsilon b) - 1). && (7.181)
\end{aligned}$$

Thus, $W(\varepsilon)\psi \in D(H)$, and the transformation $W(\varepsilon)$ is well-defined on $D(H)$. □

Conclusions and outlook

In this thesis we have investigated the stability of quantum symmetries against perturbations of the system's Hamiltonian. We first focused on Hamiltonians with compact resolvent, such as the harmonic oscillator, characterized by a purely point spectrum and a non-vanishing spectral gap. Under these assumptions, we obtained a precise algebraic characterization of the symmetries that remain robust under a fixed perturbation [12]. We showed that every relatively bounded perturbation induces a family of subprojections of the unperturbed Hamiltonian, and that the robust symmetries are exactly those operators that commute with this family of subprojections. We then extended our analysis to the set of symmetries that are robust with respect to an arbitrary collection of perturbations $\mathcal{P}$. A key result is that this set always forms a von Neumann algebra of bounded operators, independently of the specific structure of $\mathcal{P}$. In particular, when $\mathcal{P}$ coincides with the commutant of a symmetry of the unperturbed Hamiltonian, the resulting algebra of robust symmetries exhibits a well-defined and elegant algebraic structure. Finally, we proved that the completely robust symmetries—those stable against all possible perturbations—are precisely the bounded functions of the Hamiltonian, forming the von Neumann algebra generated by H, that is, its bicommutant. This result generalizes to unbounded Hamiltonians with discrete spectrum a theorem previously known only for finite-dimensional Hilbert spaces [11].

Subsequently, we analyzed in detail the wandering range of robust symmetries, namely the quantitative measure of their deviation induced by a perturbation of the Hamiltonian. In particular, we studied the scaling behavior of the wandering range with respect to the perturbation strength ε. We proved that, in general, the wandering range does not scale linearly with ε, and we provided explicit examples in which this linear dependence does hold. A particularly interesting case is that of completely robust symmetries under bounded perturbations. In this setting, we showed not only that the wandering range is of order ε, but also that it admits an explicit bound in terms of the spectral gap of the Hamiltonian [14]. A remarkable result is that this deviation depends only on the energy gaps and is completely independent of the system size. This independence of the system size is what we call scalability. It means that results established for small systems continue to hold as the system becomes larger, which is a necessary requirement for the practical development of quantum technologies [27]. We presented two alternative proofs of this result: one based on an iterative procedure known as the Quantum KAM Iteration (Chapters 4 and 5), and the other on Kato's perturbation theory (Chapter 7).

Furthermore, we showed that the Quantum KAM Iteration admits a natural extension to the case in which the Hamiltonian has a band spectrum [15]. As a consequence, we proved that all bounded operators belonging to the bicommutant of the band projections are completely robust, with a linear wandering range that depends on the interband gap. This allows us to identify a nontrivial class of completely robust symmetries in the more general setting of Hamiltonians with band spectrum [15]. However, this result does not yet provide a complete algebraic characterization of robust symmetries within the general framework of band-structured Hamiltonians. It would be interesting to determine, also in this context, all possible robust symmetries against an arbitrary family of relatively bounded perturbations.

A second possible direction for generalization concerns the role of the spectral gap. In all the quantum systems analyzed throughout this thesis, the existence of a nonvanishing gap—between energy levels or between spectral bands—in the spectrum of the Hamiltonian plays a crucial role. However, there are physically relevant situations in which this assumption is not satisfied. For instance, many atomic and molecular systems are characterized by a purely point spectrum that possesses an accumulation point, as in the paradigmatic case of the hydrogen atom.

In such cases, one can certainly apply the results of the Quantum KAM Iteration for band Hamiltonians by grouping the energy levels into uniformly separated bands. However, as already mentioned, this construction does *not* provide a complete algebraic characterization of the robust symmetries [15]. It would therefore be interesting to investigate the stability properties of such *gapless* spectra under relatively bounded perturbations. In this direction, Ref. [28] studies the stability of a gapless Hamiltonian with a spectrum consisting of simple eigenvalues accumulating at a point, providing a promising starting point for further analysis.

Furthermore, the Quantum KAM Iteration is not only a powerful tool for estimating the wandering range of completely robust symmetries, but also proves to be highly valuable in the context of the Quantum Adiabatic Theorem [13, 29]. The extension of the Quantum KAM Iteration to unbounded Hamiltonians with band spectrum, developed in this thesis, provides a natural framework for generalizing the Quantum Adiabatic Theorem to this setting [30]. Beyond its conceptual relevance, the Adiabatic Theorem plays a central role in several quantum technologies, most notably in Quantum Adiabatic Computation [31] and in adiabatic quantum state preparation [32].

A further line of research concerns the connection between robustness and quantum control. The stability results developed in this work naturally suggest the possibility of actively *stabilizing* fragile symmetries through suitable modifications of the Hamiltonian [33]. For example, one may analyze control strategies such as dynamical decoupling, where appropriately designed sequences of pulses effectively average out undesired perturbations [4, 5, 34]. By combining the algebraic classification of robust and fragile symmetries with such control protocols, it may be possible to derive rigorous criteria for when the stabilization of fragile symmetries is achievable and to quantify the degree of robustness that can be reached. Beyond the theoretical interest, this analysis has clear relevance for quantum technologies, where maintaining selected symmetries is essential for error suppression and coherence protection.

Finally, an important open direction concerns the generalization of the present analysis to *open quantum systems*, in the presence of environmental interactions [35]. All the results presented in this thesis rely on the fundamental assumption of unitary evolution, which holds for closed quantum systems but generally fails in open ones. Since every real physical system is inherently open, it becomes crucial to investigate how the notions of robustness of symmetries [36, 37] and adiabaticity [38] can be extended to this broader, non-unitary setting. Several works have explored adiabatic behavior in finite-dimensional open systems (see, e.g., Refs. [13]), but the extension of such results to unbounded generators acting on infinite-dimensional Hilbert spaces remains an open challenge of both conceptual and practical importance. Indeed, as in the case of closed quantum systems, one would like to obtain results that are independent of the system size, thereby ensuring scalability.

Appendix A

Catalan numbers

This appendix collects the definitions and properties of the Catalan numbers used in the Quantum KAM estimates, together with a related modified sequence appearing in Kato's perturbative construction.

A.1 Catalan numbers

We define the Catalan numbers in the following way [24]:

$$\begin{aligned} d_1 &= 1, \\ d_s &= \sum_{\ell=1}^{s-1} d_\ell \, d_{s-\ell}, \qquad s \geq 2. \end{aligned} \tag{A.1}$$

This is the standard recursive definition of the Catalan sequence. In the following, we collect the main properties of the numbers $\{d_s\}_{s\geq 1}$, which play a central role in our estimates.

The following lemma provides a bound that is repeatedly used in the estimates of the iterative schemes developed in this thesis.

Lemma A.1.1. *For all $n \geq 1$ and all $s \geq 1$, the Catalan numbers satisfy*

$$\sum_{|\boldsymbol{\ell}|=s} d_{\ell_1} \cdots d_{\ell_n} \leq d_s. \tag{A.2}$$

Proof. The proof is by induction on n. For $n = 1$, the condition $|\boldsymbol{\ell}| = s$ implies $\ell_1 = s$, hence

$$\sum_{|\boldsymbol{\ell}|=s} d_{\ell_1} = d_s. \tag{A.3}$$

Assume now that (A.2) holds for $n = m$ and let us prove it for $n = m + 1$:

$$\sum_{|\boldsymbol{\ell}|=s} d_{\ell_1} \cdots d_{\ell_{m+1}} = \sum_{\ell_{m+1}=1}^{s-m} d_{\ell_{m+1}} \sum_{|\boldsymbol{\ell}|=s-\ell_{m+1}} d_{\ell_1} \cdots d_{\ell_m} \tag{A.4}$$

$$\leq \sum_{\ell_{m+1}=1}^{s-m} d_{\ell_{m+1}}\, d_{s-\ell_{m+1}} \tag{A.5}$$

$$\leq \sum_{\ell_{m+1}=1}^{s-1} d_{\ell_{m+1}}\, d_{s-\ell_{m+1}} = d_s. \tag{A.6}$$

□

We now compute the generating function associated with the sequence $\{d_s\}_{s\geq 1}$, which is used to express the bounds obtained in the main text in a compact analytical form.

Lemma A.1.2 (Generating function of the Catalan numbers)**.** *Let* $\{d_s\}_{s\geq 1}$ *be the Catalan numbers defined by* (A.1)*. The generating function, defined by the power expansion*

$$\mathcal{D}(x) = \sum_{s\geq 1} d_s\, x^{s-1}, \tag{A.7}$$

is given by

$$\mathcal{D}(x) = \frac{1-\sqrt{1-4x}}{2x}, \tag{A.8}$$

for $|x| \leq \frac{1}{4}$*.*

Proof. Starting from the definition (A.7), we compute the square of the generating function:

$$\mathcal{D}^2(x) = \sum_{s_1,s_2\geq 1} d_{s_1} d_{s_2}\, x^{(s_1+s_2)-2}. \tag{A.9}$$

Introducing the variable $s = s_1 + s_2$, we obtain

$$\mathcal{D}^2(x) = \sum_{s\geq 2} x^{s-2} \sum_{s_1=1}^{s-1} d_{s_1} d_{s-s_1} \tag{A.10}$$

$$= \frac{1}{x} \sum_{s\geq 2} d_s\, x^{s-1} \tag{A.11}$$

$$= \frac{\mathcal{D}(x)-1}{x}. \tag{A.12}$$

Hence $\mathcal{D}(x)$ satisfies the quadratic equation

$$x\mathcal{D}^2(x) - \mathcal{D}(x) + 1 = 0, \tag{A.13}$$

whose solution compatible with $\mathcal{D}(0) = 1$ is

$$\mathcal{D}(x) = \frac{1 - \sqrt{1 - 4x}}{2x}. \tag{A.14}$$

□

A.2 Modified Catalan numbers

In the context of Kato's strategy, a sequence of rational numbers naturally arises, which is closely related to the classical Catalan numbers. We refer to this sequence as the *modified Catalan numbers.*

Definition A.2.1 (Modified Catalan numbers)**.** *The* modified Catalan numbers $\{c_n\}_{n\geq 0}$ *are defined recursively by*

$$c_0 = 1, \tag{A.15}$$

$$c_n = \sum_{m=1}^{n} \binom{2m}{m} \frac{m}{n}\, c_{n-m}, \qquad n \geq 1. \tag{A.16}$$

The terminology *modified Catalan numbers* is motivated by the fact that their definition explicitly involves the central binomial coefficients $\binom{2m}{m}$, which also appear in one of the standard definitions of the classical Catalan numbers, namely

$$d_{m+1} = \frac{1}{m+1}\binom{2m}{m}. \tag{A.17}$$

In this sense, the sequence $\{c_n\}_{n\geq 0}$ can be regarded as a modification of the classical Catalan numbers.

We now compute the generating function associated with this sequence.

Lemma A.2.1 (Generating function of the modified Catalan numbers)**.** *Let* $\{c_n\}_{n\geq 0}$ *be the modified Catalan numbers defined above, and let* $\mathcal{C}(x)$ *denote their generating function. Then*

$$\mathcal{C}(x) = \exp\left(\frac{1}{\sqrt{1-4x}} - 1\right). \tag{A.18}$$

Proof. The generating function of the sequence $\{c_n\}_{n\geq 0}$ is defined by the formal power series

$$\mathcal{C}(x) = \sum_{n\geq 0} c_n x^n = 1 + \sum_{n\geq 1} c_n x^n. \tag{A.19}$$

Differentiating term by term and using the recursive definition of the coefficients c_n, we obtain

$$\mathcal{C}'(x) = \sum_{n\geq 1} n c_n x^{n-1} \tag{A.20}$$

$$= \sum_{n\geq 1} \sum_{m=1}^{n} m \binom{2m}{m} c_{n-m} x^{n-1} \tag{A.21}$$

$$= \sum_{m\geq 1} m \binom{2m}{m} \sum_{n\geq m} c_{n-m} x^{n-1}, \tag{A.22}$$

where in the last step we have exchanged the order of summation.

Recall that one of the standard definitions of the Catalan numbers is

$$d_n = \frac{1}{n}\binom{2(n-1)}{n-1}, \qquad n \geq 1. \tag{A.23}$$

Using this identity, we can rewrite the previous expression as

$$\mathcal{C}'(x) = \sum_{m\geq 1} m(m+1)\, d_{m+1}\, x^{m-1} \sum_{n\geq m} c_{n-m} x^{n-m}. \tag{A.24}$$

The inner sum coincides with $\mathcal{C}(x)$, so that

$$\mathcal{C}'(x) = \mathcal{C}(x) \left(x \sum_{m\geq 1} d_{m+1} x^m \right)''. \tag{A.25}$$

Since

$$\sum_{m\geq 1} d_{m+1} x^m = \mathcal{D}(x) - 1, \tag{A.26}$$

where

$$\mathcal{D}(x) = \frac{1-\sqrt{1-4x}}{2x} \tag{A.27}$$

is the generating function of the classical Catalan numbers, it follows that $\mathcal{C}(x)$ satisfies the differential equation

$$\frac{\mathcal{C}'(x)}{\mathcal{C}(x)} = \big(x\mathcal{D}(x)\big)''. \tag{A.28}$$

Together with the initial condition $\mathcal{C}(0) = 1$, this equation admits the unique solution

$$\mathcal{C}(x) = \exp\left(\frac{1}{\sqrt{1-4x}} - 1 \right), \tag{A.29}$$

which concludes the proof. □

Appendix B

Sylvester Equation

In this appendix we recall some basic facts about the Sylvester equation, a classical operator equation of the form

$$AX - XB = Y,$$

whose solutions play an important role in many areas of analysis and mathematical physics. Its connection with the homological equation was emphasized in the proof of Lemma 6.2.3, where it appeared naturally in the block–decomposition of operators with respect to a band structure. For completeness, we present here a short discussion of existence, uniqueness, and norm estimates of its solutions, generalizing the approach of Bhatia [23] to infinite dimensional Hilbert spaces.

B.1 Formulation of the problem

Let $\mathcal{H}$ be a separable Hilbert space. Let A and B be two self–adjoint operators on the domains $D(A)$ and $D(B)$, respectively. Let $Y \in B(\mathcal{H})$ be a bounded operator. We look for a bounded operator $X \in B(\mathcal{H})$ such that

- $XD(B) \subseteq D(A)$;
- for all $\psi \in D(B)$,
$$(AX - XB)\psi = Y\psi. \tag{B.1}$$

Furthermore, we are interested in obtaining an explicit estimate of $\|X\|$ in terms of $\|Y\|$.

The key condition ensuring the existence of a solution is that the spectra of A and B are disjoint,

$$\mathrm{dist}(\sigma(A), \sigma(B)) > 0.$$

Under this assumption, the solution can be written explicitly, and its norm can be controlled. These two aspects are presented in the next sections: first we establish an integral representation, then we derive quantitative norm estimates.

B.2 Integral representation and basic estimates

Under the assumptions stated in the previous section (self–adjoint A, B with disjoint spectra and bounded $Y \in B(\mathcal{H})$), the Sylvester equation

$$AX - XB = Y$$

admits a unique bounded solution. The next theorem provides an explicit integral formula together with a first norm estimate.

Theorem B.2.1. *Let A and B be self–adjoint operators on $\mathcal{H}$ with disjoint spectra. Then the Sylvester equation, understood on $D(B)$,*

$$AX - XB = Y, \qquad Y \in B(\mathcal{H}),$$

admits a unique solution $X \in B(\mathcal{H})$ given by

$$X = \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}tA}\, Y\, \mathrm{e}^{\mathrm{i}tB} f(t)\, \mathrm{d}t, \tag{B.2}$$

where $f \in L^1(\mathbb{R})$ is any function such that

$$\hat{f}(s) := \int_{\mathbb{R}} f(t)\, \mathrm{e}^{-ist}\, \mathrm{d}t = \frac{1}{s}, \tag{B.3}$$

for all $s \in \sigma(A) - \sigma(B)$. Moreover, the solution satisfies the estimates

$$\|X\| \le \|Y\|\, \|f\|_{L^1(\mathbb{R})}, \tag{B.4}$$

$$\|AX\psi\| \le \|Y\| \left(\|f\|_{L^1(\mathbb{R})} \|B\psi\| + \|\psi\| \right), \quad \forall \psi \in D(B), \tag{B.5}$$

where

$$\|f\|_{L^1(\mathbb{R})} = \int_{\mathbb{R}} |f(t)|\, \mathrm{d}t. \tag{B.6}$$

Proof. A and B are self-adjoint operators. Then, they both admit a spectral decomposition

$$A\psi = \int_{\sigma(A)} a\, \mathrm{d}P_A(a)\psi, \qquad \psi \in D(A), \tag{B.7}$$

$$B\psi = \int_{\sigma(B)} b\, \mathrm{d}P_B(b)\psi, \qquad \psi \in D(B). \tag{B.8}$$

We prove that (B.2) is the solution by a direct substitution in the Sylvester equation. Take $\psi \in D(B)$ and any function f such that

$$\hat{f}(s) = \frac{1}{s}, \tag{B.9}$$

for all $s \in \sigma(A) - \sigma(B)$.

$$AX\psi = \int_{\sigma(A)} \mathrm{d}P_A(a) \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}tA}\, Y\, \mathrm{e}^{\mathrm{i}tB} f(t)\, \mathrm{d}t\, \psi \tag{B.10}$$

$$= \int_{\sigma(A)} \int_{\sigma(B)} \mathrm{d}P_A(a) Y \mathrm{d}P_B(b)\, a \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}t(a-b)} f(t) \mathrm{d}t\, \psi \tag{B.11}$$

$$= \int_{\sigma(A)} \int_{\sigma(B)} \mathrm{d}P_A(a) Y \mathrm{d}P_B(b)\, a\, \hat{f}(a-b)\, \psi. \tag{B.12}$$

Since $a \in \sigma(A)$ and $b \in \sigma(B)$, $a - b \in \sigma(A) - \sigma(B)$ and then

$$\hat{f}(a-b) = \frac{1}{a-b}. \tag{B.13}$$

We have

$$AX\psi = \int_{\sigma(A)} \int_{\sigma(B)} \mathrm{d}P_A(a) Y \mathrm{d}P_B(b) \frac{a}{a-b}\, \psi \tag{B.14}$$

$$= \int_{\sigma(A)} \int_{\sigma(B)} \mathrm{d}P_A(a) Y \mathrm{d}P_B(b)\, \psi + \int_{\sigma(A)} \int_{\sigma(B)} \mathrm{d}P_A(a) Y \mathrm{d}P_B(b) \frac{b}{a-b}\, \psi \tag{B.15}$$

$$= \int_{\sigma(A)} \mathrm{d}P_A(a) Y \int_{\sigma(B)} \mathrm{d}P_B(b) \psi + \int_{\sigma(A)} \mathrm{d}P_A(a) Y \mathrm{d}P_B(b) \frac{1}{a-b} B\psi \tag{B.16}$$

$$= Y\psi + \int_{\sigma(A)} \mathrm{d}P_A(a) Y \mathrm{d}P_B(b) \hat{f}(a-b)\, B\psi \tag{B.17}$$

$$= Y\psi + \int_{\mathbb{R}} f(t)\, \mathrm{d}t \int_{\sigma(A)} \mathrm{e}^{-\mathrm{i}ta} \mathrm{d}P_A(a) Y \int_{\sigma(B)} \mathrm{e}^{\mathrm{i}tb} \mathrm{d}P_B(b)\, \psi \tag{B.18}$$

$$= Y\psi + \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}tA} Y \mathrm{e}^{\mathrm{i}tB} f(t) \mathrm{d}t\, \psi \tag{B.19}$$

$$= Y\psi + XB\psi, \tag{B.20}$$

which shows that $(AX - XB)\psi = Y\psi$ for all $\psi \in D(B)$. This concludes the proof that (B.2) is indeed the solution. The norm estimates follow directly from the integral representations. □

Remark B.2.1. The second bound ensures that the solution X preserves the domains in the sense that $XD(B) \subseteq D(A)$. Indeed, for any $\psi \in D(B)$, the estimate

$$\|AX\psi\| \leq \|Y\| \big(\|f\|_{L^1(\mathbb{R})} \|B\psi\| + \|\psi\| \big)$$

shows that $X\psi \in D(A)$ whenever $\psi \in D(B)$. Hence the Sylvester equation is well posed on $D(B)$.

B.3 Optimization of the constant

The bounds obtained in the previous section depend on the particular choice of the function f appearing in the integral representation. Let

$$\eta := \mathrm{dist}(\sigma(A), \sigma(B))$$

be the spectral separation between A and B. We denote by $\mathcal{F}_\eta$ the class of functions $f \in L^1(\mathbb{R})$ such that

$$\hat{f}(s) = \frac{1}{s}, \qquad \forall\, |s| \geq \eta. \tag{B.21}$$

For any such f, the estimate of Theorem B.2.1 gives

$$\|X\| \leq \|f\|_{L^1(\mathbb{R})}\, \|Y\|. \tag{B.22}$$

Hence the optimal constant is obtained by minimizing $\|f\|_{L^1(\mathbb{R})}$ over the whole class $\mathcal{F}_\eta$:

$$\|X\| \leq \inf_{f \in \mathcal{F}_\eta} \|f\|_{L^1(\mathbb{R})}\, \|Y\|. \tag{B.23}$$

It can be shown that the minimum value of $\|f\|_{L^1(\mathbb{R})}$ is attained, and that

$$\inf_{f \in \mathcal{F}_\eta} \|f\|_{L^1(\mathbb{R})} = \frac{\pi}{2\eta}. \tag{B.24}$$

For further details we refer to Chapter VII.6 of [23].

Appendix C

Resolvent Operator

In this appendix we study the properties of the resolvent of a self-adjoint operator with purely point spectrum. We will focus on its analytic structure and, in particular, derive a series expansion around its singularities, namely the isolated eigenvalues. We follow the classical approach of Kato [20].

C.1 The Resolvent

Let $T = T^\dagger$ be a (possibly unbounded) self-adjoint operator on a separable Hilbert space $\mathcal{H}$, with purely point spectrum

$$\sigma(T) = \{\lambda_k\}_{k\geq 1}, \tag{C.1}$$

and associated family of orthogonal spectral projections $\{P_k\}_{k\geq 1}$, such that

$$T = \sum_{k\geq 1} \lambda_k P_k, \qquad \mathbb{I} = \sum_{k\geq 1} P_k. \tag{C.2}$$

For $\zeta \in \mathbb{C}$, we say that ζ belongs to the *resolvent set* of T, denoted by $\rho(T)$, if the operator $T - \zeta$ is bijective from $D(T)$ onto $\mathcal{H}$, and its inverse

$$R_\zeta(T) := (T - \zeta)^{-1} \in B(\mathcal{H}) \tag{C.3}$$

is bounded. The complementary set $\sigma(T) := \mathbb{C}\backslash\rho(T)$ is called the *spectrum* of T. It contains, in particular, the *point spectrum*, i.e. the eigenvalues of T.

The resolvent operator $R_\zeta(T)$ is a bounded operator-valued holomorphic function on $\rho(T)$.

C.2 Singularities of the Resolvent

The singularities of the resolvent $R_\zeta(T)$ coincide with the points of the spectrum. If $\lambda_k \in \sigma(T)$ is an *isolated eigenvalue*, then $R_\zeta(T)$ has a pole at $\zeta = \lambda_k$. In a punctured neighborhood of λ_k one can write the Laurent expansion

$$R_\zeta(T) = \sum_{n=-\infty}^{\infty} A_n\,(\zeta - \lambda_k)^n, \qquad \zeta \in U \setminus \{\lambda_k\}, \tag{C.4}$$

where the coefficients are given by

$$A_n = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_k} (\zeta - \lambda_k)^{-n-1}\, R_\zeta(T)\,\mathrm{d}\zeta, \tag{C.5}$$

and Γ_k is a small positively oriented contour enclosing only λ_k [39].

We now compute the coefficients A_n explicitly for a self-adjoint operator T with purely point spectrum.

Theorem C.2.1. *Let $T = T^\dagger$ be a self-adjoint operator with purely point spectrum $\sigma(T) = \{\lambda_k\}_{k\geq 1}$ and spectral projections $\{P_k\}_{k\geq 1}$. Then the coefficients A_n in the Laurent expansion of $R_\zeta(T)$ around an isolated eigenvalue λ_k are given by*

$$A_n = \begin{cases} 0, & n \leq -2, \\ -P_k, & n = -1, \\ S_k^{n+1}, & n \geq 0, \end{cases} \tag{C.6}$$

where P_k is the projection onto the eigenspace of λ_k, and

$$S_k = \sum_{\ell:\,\ell\neq k} \frac{P_\ell}{\lambda_\ell - \lambda_k} \tag{C.7}$$

is the reduced resolvent*.*

Proof. By the spectral theorem, the resolvent of a self-adjoint operator with pure point spectrum admits the expansion

$$R_\zeta(T) = \sum_{k\geq 1} \frac{P_k}{\lambda_k - \zeta}. \tag{C.8}$$

Substituting this expression into the definition of A_n, we obtain

$$\begin{aligned} A_n &= \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_k} (\zeta - \lambda_k)^{-n-1} R_\zeta(T)\, \mathrm{d}\zeta \\ &= -\frac{1}{2\pi \mathrm{i}} \sum_{\ell \geq 1} P_\ell \int_{\Gamma_k} \frac{(\zeta - \lambda_k)^{-n-1}}{\zeta - \lambda_\ell}\, \mathrm{d}\zeta \\ &= \sum_{\ell \geq 1} I_{k,\ell}^{(n)} P_\ell, \end{aligned} \tag{C.9}$$

where we define

$$I_{k,\ell}^{(n)} := -\frac{1}{2\pi \mathrm{i}} \int_{\Gamma_k} \frac{(\zeta - \lambda_k)^{-n-1}}{\zeta - \lambda_\ell}\, \mathrm{d}\zeta. \tag{C.10}$$

Case 1: $n \leq -2$. The integrand takes the form

$$\frac{(\zeta - \lambda_k)^{-n-1}}{\zeta - \lambda_\ell} = \begin{cases} (\zeta - \lambda_k)^{-n-2}, & k = \ell, \\ \dfrac{(\zeta - \lambda_k)^{-n-1}}{\zeta - \lambda_\ell}, & k \neq \ell, \end{cases}$$

which is holomorphic inside Γ_k, since all possible poles lie outside the contour. Hence $I_{k,\ell}^{(n)} = 0$ for all $n \leq -2$, and therefore $A_n = 0$ for $n \leq -2$.

Case 2: $n = -1$. For $n = -1$, the integrand becomes

$$\frac{1}{\zeta - \lambda_\ell},$$

which has a simple pole inside Γ_k only when $k = \ell$. In that case,

$$I_{k,\ell}^{(-1)} = -\delta_{k\ell}, \qquad A_{-1} = \sum_{\ell \geq 1} I_{k,\ell}^{(-1)} P_\ell = -P_k.$$

Case 3: $n \geq 0$. We now distinguish again between $k = \ell$ and $k \neq \ell$.

(a) Case $k = \ell$: The integrand becomes

$$\frac{1}{(\zeta - \lambda_k)^{n+2}},$$

which has a pole of order $n + 2$ at $\zeta = \lambda_k$. By the residue theorem,

$$I_{k,k}^{(n)} = -\operatorname{Res}_{\zeta = \lambda_k} \frac{1}{(\zeta - \lambda_k)^{n+2}} = -\frac{1}{(n+1)!} \lim_{\zeta \to \lambda_k} \frac{d^{n+1}}{d\zeta^{n+1}}(1) = 0.$$

(b) Case $k \neq \ell$: Here the integrand is

$$\frac{1}{(\zeta - \lambda_\ell)(\zeta - \lambda_k)^{n+1}},$$

which has a pole of order $n+1$ at $\zeta = \lambda_k$. Using the residue theorem, we find

$$\begin{aligned} I_{k,\ell}^{(n)} &= -\operatorname{Res}_{\zeta=\lambda_k} \frac{1}{(\zeta - \lambda_\ell)(\zeta - \lambda_k)^{n+1}} \\ &= -\frac{1}{n!} \frac{d^n}{d\zeta^n} \frac{1}{\zeta - \lambda_\ell}\bigg|_{\zeta=\lambda_k} \\ &= \frac{1}{(\lambda_\ell - \lambda_k)^{n+1}}. \end{aligned} \tag{C.11}$$

Collecting all terms, for $n \geq 0$ we obtain

$$A_n = \sum_{\ell \geq 1} I_{k,\ell}^{(n)} P_\ell = \sum_{\ell : \ell \neq k} \frac{P_\ell}{(\lambda_\ell - \lambda_k)^{n+1}} = S_k^{n+1}, \tag{C.12}$$

where in the last equality we have used the definition of the reduced resolvent S_k. □

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