# Long–Time Dynamics of Open Quantum Systems

Matthias Westrich

# Long–Time Dynamics of Open Quantum Systems

Matthias Westrich

PhD Dissertation
June 2011

Supervisors:

Volker Bach and Jacob Schach Møller

Institut für Analysis und Algebra
Technische Universität
Braunschweig

Department of Mathematical
Sciences
Aarhus University

**Colophon**

*Long–Time Dynamics of Open Quantum Systems*

A PhD thesis by Matthias Westrich. Written under the supervision of Volker Bach and Jacob Schach Møller at Institut für Analysis und Algebra, Carl–Friedrich–Gauß–Fakultät, Technische Universität Braunschweig and Department of Mathematical Sciences, Faculty of Science, Aarhus University, respectively.

Typeset using LaTeX and the memoir document class. The text is set with the Palatino font at 10.0/12.0pt, and the Pazo Math fonts are used for mathematical formulae.

Among the packages used are the $\mathcal{AMS}$ packages `amsfonts`, `amsmath`, `amssymb` as well as `babel`, `bbm`, `fontenc`, `graphicx`, `hyperref`, `inputenc`, `mathpazo`, `mathtools`, `ntheorem`, `soul` and `url`. Questions and comments are welcome, and can be sent to the author by emailing `westrich@imf.au.dk`.

Printed at SUN–TRYK, Aarhus University.

# Contents

# Preface

The present thesis encompasses three different papers, "Regularity of eigenstates in regular Mourre theory", [MW11], "Characterisation of the quasi-stationary state of an impurity driven by monochromatic light I - The effective theory", [BPW11a], including a chapter on the construction of time dependent $C$–Liouvilleans and "Towards a dynamical renormalisation group", [BMW11], as well as an overview. We refer to the different parts by [MW11], [BPW11a] and [BMW11], respectively.

The overview is organised as follows. We first provide a general context for the three projects [MW11], [BPW11a] and [BMW11] in Chapter 1 and explain their conceptual relations from a wider perspective. Chapter 2 is devoted to the more specific mathematical framework used in the several projects, to present our results and to relate it to the literature. In the Sections 2.1,2.2 and 2.3 we also expand on the conceptual relations between [MW11], [BPW11a] and [BMW11]. For each of the four parts of the present thesis, the references can be found in the last section of the corresponding part.

* * *

A bi–national PhD–programme has certainly many aspects which are not present in a normal PhD–programme. It opens great opportunities, but also demands more of the relevant people. Thus, it is my pleasure to express my deep gratitude to my teachers Volker Bach and Jacob Schach Møller. It has been an inspiration to work with these distinguished supervisors, who opened many opportunities beyond the work of this thesis.

I am grateful for the joint work with Jean-Bernard Bru and Walter de Siqueira Pedra and I learned a lot during the time of this collaboration.

I would like to thank Juliane for her love and support during the time of my PhD studies. My thanks to my parents and my family, in particular my brother Benjamin, for their encouragement.

I am grateful to Hans Knörr for showing me again that the trombone *is* the most beautiful instrument. Morten Grud Rasmussen helped me a lot with administrative issues, for which I am thankful, as well as for discussions with members of the working group in Braunschweig and Mainz. In the process of writing this thesis I have benefited from Rasmus Villemoes' Ph.D. thesis, which I used as a LaTeX template, a lot of TeXnical help by Hans Knörr and from the proofreading on parts of the manuscript performed by Hans Knörr and Edmund Menge. Part of this work has been performed at the Johannes–Gutenberg–Universität Mainz.

Matthias Westrich
Braunschweig, June 29, 2011

# Part I

# Overview

Chapter 1

# Introduction

A classical problem in dynamical systems is the relation between the evolution of semigroups and the behaviour of the resolvents of their generators near critical points. One relation between the two is established by the Laplace transform. Our main interest here is the long time dynamics of quantum systems which are in constant interaction with the environment. These systems are called *open (quantum) systems* and they are said to be *closed* if there is no interaction with the environment. Open systems are usually modelled by closed systems consisting of two parts, a large subsystem, which describes the environment, and a small subsystem encoding the degrees of freedom one is interested in. The open system is then the (effective) evolution of the small subsystem. The long time dynamics for open quantum systems is quite different from the long time dynamics in the context of scattering theory. In scattering theory one considers timescales (or distances), which are large compared to the scale of interaction.

The problems addressed in our work do not take into account the back–reaction of the small subsystem onto the large subsystem, i.e., fluctuations are not considered. Nevertheless, there have been recent results in this direction, [DRM08]. We consider small subsystems with finitely many energy levels. Even though this is a strong simplification as compared to more realistic models for the small subsystem, it does yield important consequences, which are relevant even for physical experiments. For example, the Nd:YAG laser is a crystal doped with neodymium atoms, which correspond to the impurities in [BPW11a]. In such a situation our model is the state–of–the–art model and provides useful insights. The environment is typically modelled by a quantised boson or fermion field.

The three projects [MW11], [BPW11a] and [BMW11], involve a closed or even selfadjoint operator $H$, on a Hilbert space $\mathcal{H}$ and a selfadjoint operator $A$. Depending on the regularity of

$$t \mapsto e^{itA} (z - H)^{-1} e^{-itA}, \tag{1.1}$$

our results provide information on the long time behaviour of the dynamics of the subsystem. The framework in [MW11] is abstract, whereas in [BMW11] we consider a spin boson type model at zero temperature. In

[BPW11a] we study the effective dynamics, which results from a fermion–impurity interaction in presence of an external monochromatic light source. The mechanism we rely on to obtain the long time dynamics is second order perturbation theory. In case of [MW11], we derive abstract, non–perturbative results, which can be used as an input to second order perturbation theory, but these results are of interest beyond second order perturbation theory. In [BPW11a] and [BMW11] we directly analyse the dynamics of specific models.

We first define in Section 1.1 the closed quantum systems underlying the analysis of [MW11] and [BPW11a]. In Section 1.2 we explain the relation between second order perturbation theory and long time dynamics, which is amplified in the more specific discussion of Chapter 2.

## 1.1 Definition of Models

Unlike in classical physical theories, like Newtonian mechanics, not all objects in quantum theory correspond to measurable quantities. For instance, the physicists notion of "wave functions", which are elements of a Hilbert space $\mathcal{H}$, do not have a direct physical meaning in the sense, that it cannot be measured directly in an experiment. On the other hand, the measured quantities in physical experiments are the so–called *observables*. Observables are well described by elements of a $C^*$–algebra, $\mathcal{V}$, which is called *algebra of observables.* The *states* of the physical system are implemented by positive linear functionals on $\mathcal{V}$, with norm one. For any given state $\omega$, one may use the GNS construction to obtain a $*$–representation $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$, consisting of a Hilbert space $\mathcal{H}_\omega$, generated by the *cyclic vector* $\Omega_\omega$, such that

$$\omega\left(A\right) = \left(\Omega_\omega, \pi_\omega\left(A\right)\Omega_\omega\right)_{\mathcal{H}_\omega}, \qquad \forall A \in \mathcal{V}.$$

This construction suggests to consider the algebra of observables to be the central object of the theory and that the Hilbert space is then constructed after specification of the initial state of the system. In systems with infinitely many degrees of freedom this point of view is even necessary. For instance, models involving *boson fields*, to be defined in a moment, turn out to have inequivalent representations for equilibrium states at different temperatures. In the context of relativistic quantum field theory Haag's Theorem, [Haa55], states that the so–called *vacuum representation* of the free field is not unitarily equivalent to the vacuum representation of an interacting theory.

The dynamics of a closed physical system is described by a one–parameter group of $*$–automorphisms, $\{\tau_t\}_{\{t\in\mathbb{R}\}}$, on $\mathcal{V}$. The representation above naturally induces a one–parameter group of $*$–automorphisms, $\{\tau_t^\omega\}_{\{t\in\mathbb{R}\}}$, with

$$\omega\left(\tau_t\left(A\right)\right) = \left(\Omega_\omega, \tau_t^\omega\left(\pi_\omega\left(A\right)\right)\Omega_\omega\right)_{\mathcal{H}_\omega}, \quad \forall t \in \mathbb{R}, \forall A \in \mathcal{V}.$$

The represented dynamics, $\{\tau_t^\omega\}_{\{t\in\mathbb{R}\}}$, is in general only defined on a dense set in the Hilbert space $\mathcal{H}_\omega$, but extends by continuity to the entire space and will be denoted by the same symbol. In order to associate

$\{\tau_t^\omega\}_{\{t\in\mathbb{R}\}}$ with the flow of an equation of motion, one needs to specify the topology in which it is continuous. The two most prominent examples are the $C^*$*–dynamical systems*, which are strongly continuous in the norm–topology of $\mathcal{V}$ and $\pi_\omega(\mathcal{V}) \subseteq \mathfrak{B}(\mathcal{H}_\omega)$, respectively, and the $W^*$*–dynamical systems*, defined on the *von Neumann* algebra $\pi_\omega(\mathcal{V})'' \subseteq \mathfrak{B}(\mathcal{H}_\omega)$, which are continuous in the weak operator topology. We denote with $\pi_\omega(\mathcal{V})''$ the bi–commutant of $\pi_\omega(\mathcal{V})$. In the present work we encounter both situations. The projects [BMW11, MW11] address situations where the dynamics form a $W^*$–dynamical system, but we use the *Fock space representation* at zero temperature, where the group $\{\tau_t^\omega\}_{\{t\in\mathbb{R}\}}$ is unitarily implemented, i.e., there is a strongly continuous unitary one–parameter group, $\{U_\omega(t)\}_{\{t\in\mathbb{R}\}}$, such that

$$\tau_t^\omega(\pi_\omega(A)) = U_\omega^*(t)\,\pi_\omega(A)\,U_\omega(t), \quad \forall t\in\mathbb{R}, \forall A \in \mathcal{V}.$$

Then, we study the object $\{U_\omega(t)\}_{\{t\in\mathbb{R}\}}$ instead of $\{\tau_t^\omega\}_{\{t\in\mathbb{R}\}}$. In [BPW11a] the dynamics of the closed physical system is a $C^*$–dynamical system. We start with the definition of the type of Hamiltonians considered in [BMW11].

### 1.1.1 Spin–Boson Type Models

As already explained, open quantum systems are typically modelled by system composed of a "big" and a "small" subsystem, along with an interaction between the two subsystems. The small system is described as follows. Let $N \in \mathbb{N}$, and define the Hilbert space of the atom as

$$\mathcal{H}_{\mathrm{at}} := \mathbb{C}^N.$$

The Hamiltonian describing the energy levels of the atom is given by a selfadjoint operator,

$$H_{\mathrm{at}} = H_{\mathrm{at}}^* \in \mathfrak{B}(\mathcal{H}_{\mathrm{at}}) = \mathbb{C}^N \times \mathbb{C}^N.$$

The eigenvalues $\{E_1, \ldots, E_N\} \subset \mathbb{R}$, $E_j \leq E_\ell$*, for* $1 \leq j \leq \ell \leq N$, of $H_{\mathrm{at}}$, represent the energy levels of the atom.

We now turn to the definition of the *boson free field* on the Hilbert space of its vacuum representation, the *bosonic Fock space*. These constructions are standard and may for instance be found in [RS80b, DG99, HH08]. Let $\mathfrak{h}$ be a separable complex Hilbert space and denote the $n$–fold tensor product of $\mathfrak{h}$ by

$$\mathfrak{h}^{\otimes n} := \underbrace{\mathfrak{h} \otimes \cdots \otimes \mathfrak{h}}_{n \text{ times}}, \quad n \in \mathbb{N}.$$

The tensor product is to be understood as the closure of the algebraic tensor product with respect to the induced Hilbert space norm on $\mathfrak{h}^{\otimes n}$. Moreover, we set $\mathfrak{h}^{\otimes 0} := \mathbb{C}$.

**Remark 1.1.** We stress that whenever we consider tensor products of Hilbert spaces they will be understood as the closure of the algebraic tensor product, unless one of the Hilbert spaces is the domain of an unbounded closed operator, which is then specified in the text. In the latter case we understand the tensor product as the algebraic tensor product.

For any $n \in \mathbb{N}$ we denote with $\mathcal{S}_n$ the orthogonal projection onto the totally symmetric tensors, i.e. for $\varphi_j \in \mathfrak{h}$, $j = 1, \ldots, n$,

$$\mathcal{S}_n\left(\varphi_1 \otimes \cdots \otimes \varphi_n\right) := \sum_{\sigma \in \mathrm{Sym}(n)} \varphi_{\sigma(1)} \otimes \cdots \otimes \varphi_{\sigma(n)},$$

where $\mathrm{Sym}\,(n)$ denotes the symmetric group of $\{1, \ldots, n\}$.We define the *bosonic Fock space* as

$$\mathcal{F}^+ := \Gamma\left(\mathfrak{h}\right) := \bigoplus_{n=0}^{\infty} \mathcal{F}_n^+, \quad \mathcal{F}_n^+ := \mathcal{S}_n\left(\mathfrak{h}^{\otimes n}\right), \forall n \in \mathbb{N} \cup \{0\} =: \mathbb{N}_0,$$

where $\mathcal{S}_0\left(\mathfrak{h}^{\otimes 0}\right) := \mathbb{C}$, By definition, $\psi \in \mathcal{F}^+$ is a sequence $\left(\psi_{(n)}\right)_{n \in \mathbb{N}}$, with $\psi_{(n)} \in \mathcal{F}_n^+$, such that

$$\sum_{n=0}^{\infty} \left\|\psi_{(n)}\right\|^2 < \infty.$$

The sequence $\Omega := (1, 0, 0, \ldots) \in \mathcal{F}^+$ is called the *vacuum vector* or short *vacuum*. The Fock space renders a situation where the *particle number*, to be defined in a moment, is not a conserved quantity, i.e. creation and annihilation of particles are possible. The Hilbert space $\mathfrak{h}$ is called *one–particle Hilbert space* and for later use we define the *subspace of finitely many particles* as

$$\mathcal{F}_{\mathrm{fin}} := \left\{ \psi \in \mathcal{F}^+ \,\middle|\, \psi_{(n)} = 0 \text{ except for finitely many } n \in \mathbb{N} \right\}.$$

Let $A$ be a densely defined operator on $\mathfrak{h}$ with domain $\mathcal{D}\left(A\right) \subseteq \mathfrak{h}$. Assume, that

$$A \otimes 1 \otimes \cdots \otimes 1 + 1 \otimes A \otimes \cdots \otimes 1 + \cdots + 1 \otimes 1 \otimes \cdots \otimes A$$

defined on $\mathcal{S}_n\left(\otimes^n \mathcal{D}\left(A\right)\right)$ is closable for any $n \in \mathbb{N}$ and denote its closure by $A_{(n)}$. We then define the *second quantisation*, $d\Gamma\left(A\right)$, of $A$ by

$$\left(d\Gamma\left(A\right)\psi\right)_{(n)} := A_{(n)}\psi_{(n)},$$

for all $\psi \in \mathcal{D}\left(d\Gamma\left(A\right)\right)$, where

$$\mathcal{D}\left(d\Gamma\left(A\right)\right) := \left\{ \psi \in \mathcal{F}^+ \,\middle|\, \psi_{(n)} \in \mathcal{D}\left(A_{(n)}\right), \sum_{n=0}^{\infty} \left\|A_{(n)}\psi_{(n)}\right\|^2 < \infty \right\}.$$

If $A$ is selfadjoint on $\mathcal{D}\left(A\right)$, then $d\Gamma\left(A\right)$ is selfadjoint on $\mathcal{D}\left(d\Gamma\left(A\right)\right)$. For $h \in \mathfrak{h}$ define the *annihilation operator* $a\left(h\right)$ by

$$a\left(h\right)\mathcal{S}_n\left(\varphi_1 \otimes \cdots \otimes \varphi_n\right) := n^{-\frac{1}{2}}\mathcal{S}_{n-1}\left(\sum_{\ell=1}^{n}\left(h, \varphi_\ell\right)\varphi_1 \otimes \cdots \otimes \hat{\varphi}_\ell \otimes \cdots \otimes \varphi_n\right), \tag{1.2}$$

where $\hat{\varphi}_\ell$ means that $\varphi_\ell$ is omitted in the product, and extend to a dense set of $\mathcal{F}^+$ by taking the closure, see [RS80b, Chapter X.7]. We set $a\left(h\right)\Omega = 0$. The *creation operator* is its adjoint, $a^*\left(h\right) := \left(a\left(h\right)\right)^*$ and on $\mathcal{F}_{\mathrm{fin}}$ given by

$$\left(a^*\left(h\right)\psi\right)_{(n)} := \left(n+1\right)^{\frac{1}{2}} \mathcal{S}_{n+1}\left(h \otimes \psi_{(n)}\right). \tag{1.3}$$

The creation operator defined on $\mathcal{F}_{\mathrm{fin}}$ is also closable. The annihilation and the creation operator satisfy the *canonical commutation relations* (CCR), i.e. for $f, h \in \mathfrak{h}$

$$\left[a^{\sharp}(f), a^{\sharp}(h)\right] = 0, \ [a(f), a^{*}(h)] = (f, h),$$

$a^{\sharp}(\cdot) = a(\cdot), a^{*}(\cdot)$, as identities on $\mathcal{F}_{\mathrm{fin}}$. The *field operator* is defined as

$$\phi(h) := \frac{1}{\sqrt{2}}\left(a(h) + a^{*}(h)\right), \tag{1.4}$$

on the dense set $\mathcal{F}_{\mathrm{fin}}$. Note, that $\phi(h)$ is symmetric and hence closable. Its closure will also be denoted by $\phi(h)$.

In the sequel we in particular consider semigroups which arise from semigroups on $\mathfrak{h}$. Let $A$ be the generator of the contraction $C_0$–semigroup $\{T(t)\}_{t\in\mathbb{R}^+}$. We use the following convention in this chapter, as well as in [BMW11]:

$$\mathbb{R}_0^+ := [0, \infty), \quad \mathbb{R}_+ := (0, \infty).$$

Then, we lift this contraction semigroup to $\mathcal{F}^+$, by extension of linear combinations of

$$\Gamma(T(t))\,\mathcal{S}_n(\varphi_1 \otimes \cdots \otimes \varphi_n) := \mathcal{S}_n(T(t)\,\varphi_1 \otimes \cdots \otimes T(t)\,\varphi_n),$$

for any $\varphi_\ell \in \mathfrak{h}$, $1 \leq \ell \leq n$. We have

$$\Gamma(T(t)) = e^{td\Gamma(A)}, \ \forall t \in \mathbb{R}^+,$$

and this construction readily carries over to contractive groups, like unitary one–parameter groups.

From now on we choose for this chapter $\mathfrak{h} := L^2\left(\mathbb{R}^d, \mathbb{C}^p\right)$, with $d, p \in \mathbb{N}$. The *number operator* is defined as

$$\mathrm{N} := d\Gamma(1),$$

where 1 is associated with the function $\mathbb{R}^d \ni k \mapsto 1$ and clearly, $(\mathrm{N}\psi)_{(n)} = n\psi_{(n)}$, for any $\psi \in \mathcal{F}_{\mathrm{fin}}$. Let $\omega : \mathbb{R}^d \to \mathbb{R}^+$ be a measurable function, which is non–zero almost everywhere. This function defines a multiplication operator on $\mathfrak{h}$, which we again denote with $\omega$. We define the *free field energy* as

$$H_{\mathrm{f}} := d\Gamma(\omega),$$

which is selfadjoint on $\mathcal{D}(d\Gamma(\omega))$. We occasionally use the Hilbert space

$$\mathfrak{h}_\omega := \left\{ h \in \mathfrak{h} \,\middle|\, \|h\|_\omega^2 := \|h\|^2 + \left\|\omega^{-\frac{1}{2}} h\right\|^2 < \infty \right\}.$$

For $p = 1$, the Hilbert space of the compound system is given by

$$\mathcal{H} := \mathcal{H}_{\mathrm{at}} \otimes \mathcal{F}^+$$

and the *free Hamiltonian* defined as

$$H_0 := H_{\mathrm{at}} \otimes 1 + 1 \otimes H_{\mathrm{f}}. \tag{1.5}$$

Let $G \in L^2\left(\mathbb{R}^d, \mathbb{C}^{N\times N}\right)$ and $g \geq 0$. We define the Hamiltonian of the full system by

$$H_g := H_0 + \phi\,(gG)\,, \tag{1.6}$$

on the set $\mathbb{C}^N \otimes (\mathcal{F}_{\text{fin}} \cap \mathcal{D}\,(H_{\text{f}}))$. Since $\phi\,(h)$ is relatively $H_{\text{f}}^{1/2}$–bounded for any $h \in \mathfrak{h}_\omega$, it follows that it is infinitesimally $H_{\text{f}}$–bounded and hence $H_g$ is selfadjoint for any $g \in \mathbb{R}$, by the Kato–Rellich theorem. Even though "spin" usually refers to models with $N = 2$, we refer to all models of the type (1.6) as *spin-boson models*.

### 1.1.2 Few Level Atoms and Fermion Fields

Models involving fermion fields instead of boson fields are more regular, and it is possible to construct a dynamics on the level of the algebra of observables as a $C^*$–dynamical system. For this standard construction consult for instance [BR96].

Observables of the reservoir are selfadjoint elements of the fermion $C^*$–algebra $\mathcal{V}_{\text{f}}$, which is defined as follows. Let $\mathfrak{h}$ be a separable and complex Hilbert space, e.g. $L^2\left(\mathbb{R}^d, \mathbb{C}\right)$, $d \in \mathbb{N}$. The *fermionic Fock space* is defined as

$$\mathcal{F}^- := \bigoplus_{n=0}^{\infty} \mathfrak{h}^{\wedge n},$$

where $\wedge$ denotes the *wedge product*, i.e. for $\varphi_\ell \in \mathfrak{h}$, $1 \leq \ell \leq n \in \mathbb{N}$,

$$\varphi_1 \wedge \cdots \wedge \varphi_n := \sum_{\sigma \in \text{Sym}(n)} \text{sgn}\,(\sigma)\, \varphi_{\sigma(1)} \otimes \cdots \otimes \varphi_{\sigma(n)}.$$

$\text{sgn}\,(\sigma)$ denotes the *signum* of the permutation $\sigma$, which is 1 if $\sigma$ is even and $-1$ if it is odd. For any $f \in \mathfrak{h}$, we define the *fermionic annihilation* and *creation operators*, $a(f)$ and $a^*(f) := (a(f))^*$, respectively, by (1.2) and (1.3), with only replacing the symmetric tensor product with the wedge product. These operators implement the canonical anti-commutation relations (CAR):

$$\begin{aligned} a(f)a^*(h) + a^*(h)a(f) &= (f,h)\,, \\ a^\sharp(f)a^\sharp(h) + a^\sharp(h)a^\sharp(f) &= 0, \end{aligned} \tag{1.7}$$

which yield the boundedness of $a(f)$ and $a^*(f)$:

$$\|a^*(f)\|_{\mathfrak{B}(\mathcal{F}^-)} = \|a(f)\|_{\mathfrak{B}(\mathcal{F}^-)} = \|f\|_{\mathfrak{h}}, \quad f \in \mathfrak{h}. \tag{1.8}$$

The algebra of *fermion observables*, $\mathcal{V}_{\text{f}}$, is defined as the $C^*$–algebra generated by annihilation operators $\{a(f)\}_{f\in\mathfrak{h}}$. The free fermion dynamics is implemented by a *Bogoliubov automorphism*,

$$\tau_t^{\text{f}}\,(a\,(f)) := a\left(e^{it\omega} f\right), \quad \forall t \in \mathbb{R}, \forall f \in \mathfrak{h}, \tag{1.9}$$

where $\omega$ is defined as in the previous subsection. Equation (1.8) gives directly the strong continuity of $\left\{\tau_t^{\text{f}}\right\}_{\{t\in\mathbb{R}\}}$ and hence $\left\{\mathcal{V}_{\text{f}}, \tau_t^{\text{f}}\right\}$ is a $C^*$–dynamical system. Its generator, $\delta_{\text{f}}$, is a symmetric derivation, i.e., the domain $\mathcal{D}(\delta_{\mathrm{f}})$ of the generator $\delta_{\mathrm{f}}$ is a dense $*$–sub-algebra of $\mathcal{V}_{\mathrm{f}}$ and for all $A, B \in \mathcal{D}(\delta_{\mathrm{f}})$,

$$\delta_{\mathrm{f}}(A)^* = \delta_{\mathrm{f}}(A^*), \quad \delta_{\mathrm{f}}(AB) = \delta_{\mathrm{f}}(A)B + A\delta_{\mathrm{f}}(B). \tag{1.10}$$

The algebra of observables of the *few level atom* is $\mathfrak{B}(\mathcal{H}_{\mathrm{at}}) = \mathbb{C}^{N\times N}$, with $\mathcal{H}_{\mathrm{at}} := \mathbb{C}^N$. The Hamiltonian of the free atom is some selfadjoint matrix, $0 \neq H_{\mathrm{at}} = H_{\mathrm{at}}^* \in \mathfrak{B}(\mathcal{H}_{\mathrm{at}})$. Its dynamics is the continuous automorphism group

$$\tau_t^{\mathrm{at}}(A) := e^{itH_{\mathrm{at}}} A e^{-itH_{\mathrm{at}}}, \quad \forall A \in \mathfrak{B}(\mathcal{H}_{\mathrm{at}}), \forall t \in \mathbb{R},$$

generated by the symmetric derivation

$$\delta_{\mathrm{at}}(\cdot) := i\,[H_{\mathrm{at}}, \cdot\,].$$

We define the compound system's algebra of observables as

$$\mathcal{V} := \mathfrak{B}(\mathcal{H}_{\mathrm{at}}) \otimes \mathcal{V}_{\mathrm{f}},$$

where the meaning of the tensor product is unambiguous as $\mathcal{V}_{\mathrm{f}}$ is already realised as an operator algebra of the Fock space and $\mathfrak{B}(\mathcal{H}_{\mathrm{at}})$ is finite-dimensional. The induced free dynamics is given by

$$\tau_t := \tau_t^{\mathrm{at}} \otimes \tau_t^{\mathrm{f}}, \forall t \in \mathbb{R}. \tag{1.11}$$

A simple interaction between the fermions and the atom is the bounded symmetric derivation

$$\delta_{\mathrm{int}}(\cdot) := i\,[Q \otimes \Phi(f), \cdot\,],$$

where $f \in \mathfrak{h}$ and $Q = Q^* \in \mathfrak{B}(\mathcal{H}_{\mathrm{at}})$. The dynamics, $\left\{\tau_t^{(\lambda,0)}\right\}_{\{t\in\mathbb{R}\}}$, is generated by the symmetric derivation

$$\delta^{(\lambda,0)}(\cdot) := \delta_{\mathrm{at}}(\cdot) + \delta_{\mathrm{f}}(\cdot) + \lambda\delta_{\mathrm{int}}(\cdot), \, 0 \neq \lambda \in \mathbb{R},$$

with domain $\mathcal{D}\left(\delta^{(\lambda,0)}\right) := \mathcal{H}_{\mathrm{at}} \otimes \mathcal{D}(\delta_{\mathrm{f}})$, is again a $C^*$–dynamical system, see [BR87]. We introduced the *coupling constant* $\lambda$, measuring the interaction between fermions and the atom. In [BPW11a] we consider a situation where the dynamics $\left\{\tau_t^{(\lambda,0)}\right\}_{\{t\in\mathbb{R}\}}$ is perturbed by an external force, acting on the atomic degrees of freedom, only. Mathematically, this is implemented by

$$\delta_{\mathrm{P}}(\cdot) := i\,[H_{\mathrm{P}}, \cdot\,],$$

where $H_P \in \mathfrak{B}(\mathcal{H}_{\mathrm{at}})$ is a selfadjoint matrix, multiplied with $\cos(\varpi t)$, for a certain frequency $\varpi \in \mathbb{R}$. In [BPW11a] we require that $H_{\mathrm{P}}$ maps the eigenspace of the biggest eigenvalue of $H_{\mathrm{at}}$ to the eigenspace of the lowest eigenvalue and vice versa, and is zero otherwise. Moreover, $\varpi$ has to satisfy a *resonance condition*, namely it is assumed to equal the energy difference of the biggest and the lowest eigenvalue. Thus we define the full generator of the dynamics for any $t \in \mathbb{R}$ as

$$\delta_t^{(\lambda,\mu)}(\cdot) := \delta^{(\lambda,0)}(\cdot) + \mu\cos(\varpi t)\,\delta_{\mathrm{P}}(\cdot), \, 0 \neq \mu \in \mathbb{R},$$

which is a closed symmetric derivation on $\mathcal{D}\left(\delta_t^{(\lambda,\mu)}\right) = \mathcal{D}\left(\delta^{(0,0)}\right)$, $\forall t \in \mathbb{R}$. Finally, we specify the initial states of the system.

*Thermal equilibrium states* of the free atom are Gibbs states $\mathfrak{g}_{\mathrm{at}}$ for any inverse temperature $\beta \in (0,\infty)$, given by the density matrix

$$\rho_{\mathfrak{g}} := \frac{e^{-\beta H_{\mathrm{at}}}}{\mathrm{Tr}_{\mathbb{C}^d}\left(e^{-\beta H_{\mathrm{at}}}\right)}. \tag{1.12}$$

However, in presence of interactions with the pump or the reservoir, the state $\omega$ of the atom is generally far from any Gibbs state $\mathfrak{g}_{\mathrm{at}}$. For any state $\omega_{\mathrm{at}}$ on $\mathcal{B}(\mathbb{C}^d)$, there is a unique trace–one positive operator $\rho_{\mathrm{at}}$ on $\mathbb{C}^d$, the so–called density matrix of $\omega_{\mathrm{at}}$, such that

$$\omega_{\mathrm{at}}(A) = \mathrm{Tr}_{\mathbb{C}^d}\left(\rho_{\mathrm{at}}\, A\right), \qquad A \in \mathcal{B}(\mathbb{C}^d).$$

Thermal equilibrium states of the reservoir are defined through the bounded positive operators

$$d_{\mathcal{R}} := \frac{1}{1+e^{\beta h_1}} \tag{1.13}$$

acting on $\mathfrak{h}_1$ for all (inverse temperatures) $\beta \in (0,\infty)$. Indeed, the so–called *symbol* $d_{\mathcal{R}}$ uniquely defines a (faithful) quasi–free state

$$\omega_{\mathcal{R}} := \omega_{d_{\mathcal{R}}} \tag{1.14}$$

on the fermion algebra $\mathcal{V}_{\mathcal{R}}$, by the following well known result:

**Lemma 1.2 (Two-point correlation functions and quasi–free states).**
*Let $d$ be any bounded operator on $\mathfrak{h}_1$ satisfying $0 \leq d \leq 1$. Then the correlation functions*

$$\omega_d(\mathbf{1}_{\mathcal{R}}) := 1 \tag{1.15}$$

$$\omega_d\left(a^*(f_1)\dots a^*(f_m)a(g_1)\dots a(g_n)\right) := \delta_{mn}\det\left([\langle f_j, d g_k\rangle]_{j,k}\right) \tag{1.16}$$

*for all $\{f_j\}_{j=1}^n, \{g_j\}_{j=1}^n \subset \mathfrak{h}_1$ define a functional which is the unique bounded linear extension to the algebra $\mathcal{V}_{\mathcal{R}}$ is a state $\omega_d$. The operator $d$ is called the symbol of $\omega_d$.*

We call $\omega_{\mathcal{R}}$ the thermal state of the reservoir at inverse temperature $\beta$. The *initial state*, $\omega_0$ is defined as

$$\omega_0 := \omega_{\mathrm{at}} \otimes \omega_{\mathcal{R}}, \tag{1.17}$$

for some state $\omega_{\mathrm{at}}$ on $\mathcal{B}(\mathbb{C}^d)$. The evolution of the full system acting on the initial state (1.17) is given by

$$\omega_t := \omega_0 \circ \tau_{t,0}^{(\lambda,\eta)} = (\omega_{\mathrm{at}} \otimes \omega_{\mathcal{R}}) \circ \tau_{t,0}^{(\lambda,\eta)}, \quad t \in \mathbb{R}_0^+.$$

This state reduced to the atomic part only yields a state

$$\omega_{\mathrm{at}}(t)(A) := \omega_t(A \otimes \mathbf{1}_{\mathcal{R}}), \qquad A \in \mathcal{B}(\mathbb{C}^d), \tag{1.18}$$

for any $t \in \mathbb{R}_0^+$.

## 1.2 Long–Time Behaviour of Non-Relativistic Matter Coupled to Quantised Fields

Now, we relate the projects of the present thesis, [BMW11, BPW11a, MW11]. We are interested in the long–time behaviour of quantum systems coupled to quantum fields, which serve as "reservoirs". In [MW11] we establish a result on regularity of eigenstates of an abstract selfadjoint operator $H$, which is useful as an ingredient to prove the existence of *metastable states*, see Section 2.1.3 and estimate their decay in context of *regular Mourre theory*, see Section 2.1.2. Although the analysis of [BMW11, BPW11a] is based on direct estimates of the dynamics, *spectral theory* enters as an important tool. More specifically, the asymptotic behaviour of the dynamics of the full system restricted to the atomic degrees of freedom is linked to the behaviour of the resolvent close to certain parts of the spectrum.

This is related to a classical problem of dynamical systems. Namely consider the *(autonomous) Cauchy problem* (aCP),

$$\text{(aCP)}\ \begin{cases} \frac{d}{dt}u(t) = Au(t) \quad (t \in \mathbb{R}^+), \\ u(0) = x, \end{cases}$$

where $A$ is a closed operator on a Banach space $X$ and $x \in X$. (aCP) is *mildly well posed*, i.e. for any $x \in X$ there is a unique mild solution, if and only if $A$ generates a $C_0$–semigroup, which is equivalent to the resolvent of $A$,

$$R(z, A) := (z - A)^{-1},$$

being a Laplace transform, [ABHN01, Sect. 3.1]. If $u(t)$ converges in an appropriate sense as $t \to \infty$, then $\hat{u}(\lambda)\lambda$ converges as $\lambda \to 0$, where $\hat{u}(\cdot)$ is the Laplace transform of $u(\cdot)$. Results about this implication are known as *Abelian theorems*. Our main interest lies however in the converse implication, i.e. to determine the long time behaviour based on spectral information. These type of results are customarily called *Tauberian theorems*. We analyse the behaviour of $\hat{u}(\cdot)$ close to the real axis to determine the long time behaviour. Theorems of this type are usually referred to as *complex Tauberian theorems*.

### 1.2.1 Long–Time Dynamics and 2nd–Order Perturbation Theory

In this section we discuss the relation of long time behaviour of quantum systems with second order perturbation theory, more specifically with Fermi's golden rule and thereby use [DF06]. Consider, for simplicity, a spin-boson model (1.6), with the $C_0$ unitary group, $Y(t) := \exp(-itH_0)$ on $\mathcal{H}$. Moreover, we define the $C_0$ unitary group,

$$X(t) := e^{-itH_g}, \quad t \in \mathbb{R}^+.$$

For a selfadjoint operator $L$, $x \in \mathbb{R}$ and bounded operators $A, B \in \mathfrak{B}(\mathcal{H})$, we define

$$A(x \pm i0 - L)^{-1} B := \lim_{\epsilon \searrow 0} A(x \pm i\epsilon - L)^{-1} B,$$

provided the right hand side exists in norm. In this case the *principal value of* $(x - L)^{-1}$,

$$A\mathcal{P}\,(x-L)^{-1}\,B := \frac{1}{2}\left(A\,(x+i0-L)^{-1}\,B + A\,(x-i0-L)^{-1}\,B\right),$$

and the *delta function of* $(x - L)^{-1}$,

$$A\delta\,(x-L)\,B := \frac{i}{2\pi}\left(A\,(x+i0-L)^{-1}\,B - A\,(x-i0-L)^{-1}\,B\right)$$

are well defined. Let

$$P_\ell := \mathbf{1}\,[H_{\mathrm{at}} = E_\ell] \otimes \mathbf{1}\,[H_{\mathrm{f}} = 0]\,, \quad \overline{P}_\ell := \mathbb{1} - P_\ell,$$

where $\mathbf{1}\,[\cdot]$ denotes a spectral projection. Note that for these projections $P_\ell\phi\,(G)\,P_\ell = 0$. If

$$\begin{aligned} M_\ell &:= P_\ell\phi\,(G)\,\overline{P}_\ell\left((E_\ell+i0)\,\overline{P}_\ell - H_0\overline{P}_\ell\right)^{-1}\overline{P}_\ell\phi\,(G)\,P_\ell \\ &:= \lim_{\epsilon\searrow 0} P_\ell\phi\,(G)\,\overline{P}_\ell\left((E_\ell+i\epsilon)\,\overline{P}_\ell - H_0\overline{P}_\ell\right)^{-1}\overline{P}_\ell\phi\,(G)\,P_\ell, \end{aligned}$$

exists for $\ell = 1, \ldots, N$, we define the *level shift operator (LSO)*, as

$$M := -i\sum_{\ell=1}^{N} P_\ell\phi\,(G)\,\overline{P}_\ell\left((E_\ell+i0)\,\overline{P}_\ell - H_0\overline{P}_\ell\right)^{-1}\overline{P}_\ell\phi\,(G)\,P_\ell. \tag{1.19}$$

There are several notions of *Fermi golden rule (FGR)*, depending on the problem one has in mind. In the following definition we give a local version of Fermi golden rule. "Local" means that one considers only a spectral region close to a particular spectral value $E_\ell$.

**Definition 1.3 (Fermi golden rule).** The *(local) Fermi golden rule (FGR)* holds iff $M_\ell$ exists for an $\ell \in \{1, \ldots, N\}$ and $\mathrm{Im}\,(M_\ell) \neq 0$.

**Remark 1.4.** If Fermi's golden rule holds, then the eigenvalue $E_\ell$ is unstable if the perturbation is switched on.

Provided FGR holds and the resolvent of $H_g$ is sufficiently regular, see Sections 2.1,2.3.3, then one can determine the evolution of

$$(\psi_\ell, f(H_g)e^{-itH_g}\psi_\ell) = e^{-i\lambda_g t} + o\left(g^2\right),$$

where $f$ is some compactly supported regular function, with support close to $E_\ell$ and $\psi_\ell$ is an eigenstate of $H_0$ corresponding to $E_\ell$. For a discussion of these type of results see Sections 2.1.3,2.3. For open quantum systems however, one is more interested to find an effective evolution for the entire "small system", i.e. the atom. The results of the literature, discussed in Sections 2.1.3,2.3 do not address eigenstates of $H_g$ and in particular not the ground state. Following [DF06], there are three "non–local" types of FGR involving the LSO:

1. **Analytic Fermi golden rule:** $H_0 P + g^2 M$, $P := \sum_{\ell=1}^{N} P_\ell$, predicts up to an error $o\left(g^2\right)$ the location and multiplicity of the resonances and eigenvalues of $H_g$ in a neighbourhood of the spectrum of $H_0$, $\sigma\left(H_0\right)$, for small $|g|$.

2. **Spectral Fermi golden rule:** The intersection
$$\sigma\left(H_0 P + g^2 M\right) \cap \mathbb{R},$$
predicts the possible location of eigenvalues of $H_g$, for small $|g| \neq 0$.

3. **Dynamical Fermi golden rule:** The semigroup
$$\left\{\exp\left(-it\left(H_0 P + g^2 M\right)\right)\right\}_{t \geq 0},$$
describes approximately the reduced dynamics $PX\left(t\right)P$, for small $|g|$.

The dynamical Fermi golden rule has first been rigorously established by Davies, [Dav74, Dav75, Dav76] in form of a *weak coupling limit (WCL)*. Davies proved under mild assumptions

$$\lim_{g \to 0} e^{i\tau g^{-2} H_0 P} P e^{-i\tau g^{-2} H_g} P = e^{-i\tau M}. \tag{1.20}$$

Note, that the time has been subject to a rescaling, i.e. the weak coupling limit refers to a timescale where

$$\tau = tg^2, \tag{1.21}$$

which is sometimes referred to as the *van Hove timescale*. Results beyond this timescale are scarce, but see [Kos00] for the analysis of an explicitly solvable model.

In the context of positive temperature and operators with a high degree of regularity, namely *translation analytic models*, Jaksic and Pillet developed a powerful method to compute the asymptotics as

$$\left(\Psi, e^{-itH_g}\Phi\right) = \left(A\Psi, e^{-it\left(H_{\mathrm{at}} + \sum_{n=1}^{\infty} g^{2n} M^{(2n)}\right)} B\Phi\right) + \mathcal{O}\left(e^{-ct}\right),$$

known as *Jaksic–Pillet glueing*, see [JP96a, Thm. 2.5]. Due to fundamental obstacles, this method cannot extended to the zero temperature case. In this case, one expects that the WCL cannot be extended to the original timescale, but one rather has to find "higher order" LSO's $M^{(n)}$, for a given timescale $\tau_n = tg^{n+\epsilon}$, $\epsilon \in [0,1)$, $n \in \mathbb{N}$, $n \geq 2$. That is the eventual goal of [BMW11].

Chapter 2

# Mathematical Framework and Results

The present chapter is devoted to a discussion of the mathematical framework used in the projects, [BMW11, BPW11a, MW11] and the relation of the results to the literature. We remark, that the notation is chosen in accordance with the notation of the different projects. This naturally leads to a situation where a symbol is used in different meanings in the different Sections 2.1,2.2,2.3, but we prefer this over introducing new notations.

## 2.1 Regularity of Eigenstates

The setup for this section is abstract, i.e. not dependent on a particular model. [MW11] contains results proving a certain regularity of eigenstates, $\Psi$, of an abstract selfadjoint operator $H$. More precisely, there is a second selfadjoint operator $A$, such that $H$ and $A$ have a positive commutator locally around the eigenvalue appertaining to $\Psi$. Then we prove that

$$\mathbb{R} \ni t \mapsto e^{-itA}\Psi$$

is either $C^k(\mathbb{R})$ or extends to an analytic map around the real axis, provided $H$ is in a certain sense regular w.r.t. $A$. Thus we first introduce the class of operators, $C^k(A)$, then positive commutators, also called *Mourre estimate* and finally state our results and relate them to second order perturbation theory, which is based on a work of Cattaneo, Graf, and Hunziker, [CGH06].

### 2.1.1 $C^k$–Regularity

The notions and results presented in this section may be found in [GGM04, Sect. 2], which contains also a refinement of the class $C^1(A)$. For a general account on the subject one may consult [AdMG96]. Let $A$ be a densely defined closed operator on a Hilbert space $\mathcal{H}$. Note that then the adjoint of $A$, denoted by $A^*$, is also a densely defined closed operator. If $B \in \mathfrak{B}(\mathcal{H})$, then we define the sesquilinear form $[B, A]$ by

$$(\varphi, [B, A]\, \psi) := (B^* \varphi, A\psi) - (A^* \varphi, B\psi)\,, \quad \forall \varphi \in \mathcal{D}(A^*)\ \forall \psi \in \mathcal{D}(A)\,. \tag{2.1}$$

**Definition 2.1 (The linear space $C^1(A)$).** An operator $B \in \mathfrak{B}(\mathcal{H})$ is said to be *of class* $C^1(A)$ iff the sesquilinear form $[B, A]$ is continuous in the topology of $\mathcal{H} \times \mathcal{H}$. In this case, we denote the unique bounded operator associated with $[B, A]$ by $\mathrm{ad}_A(B)$ and moreover introduce the linear space

$$C^1(A) := \left\{ B \in \mathfrak{B}(\mathcal{H}) \middle|\ B \text{ is of class } C^1(A) \right\}. \tag{2.2}$$

It can be shown that $B \in \mathfrak{B}(\mathcal{H})$ is in $C^1(A)$ iff $B$ preserves the domain of $A$. For $k \geq 1$ one could define a class $C^k(A)$ by iterating (2.1), i.e. first replacing $B$ with $\mathrm{ad}_A(B)$ and assuming continuity of $[\mathrm{ad}_A(B), A]$ in the topology of $\mathcal{H} \times \mathcal{H}$ to obtain a unique $\mathrm{ad}_A(\mathrm{ad}_A(B)) \in \mathfrak{B}(\mathcal{H})$, associated with $[\mathrm{ad}_A(B), A]$ and proceed iteratively. However, for the applications we have in mind, $A$ is selfadjoint which allows to give a more practical definition of the class $C^k(A)$. From now on we shall assume that $A$ is a selfadjoint operator on $\mathcal{H}$.

**Definition 2.2 ($C^k(A)$ class for selfadjoint $A$).** Let $k \in \mathbb{N}$. A bounded operator $B \in \mathfrak{B}(\mathcal{H})$ is said to be of class $C^k(A)$, in short $B \in C^k(A)$, if

$$\mathbb{R} \ni t \mapsto e^{itA} B e^{-itA} \tag{2.3}$$

is strongly in $C^k(\mathbb{R})$. A (possibly unbounded) self-adjoint operator $S$ is said to be of class $C^k(A)$ iff $(i - S)^{-1} \in C^k(A)$.

As indicated earlier, this notion coincides with Definition 2.1 if $k = 1$. Namely for all $t \in \mathbb{R}$, $B \in \mathfrak{B}(\mathcal{H})$ and $\psi, \varphi \in \mathcal{D}(A)$, holds

$$\begin{aligned} \left(\varphi, e^{itA} B e^{-itA} - B\psi\right) &= \int_0^t ds\, \frac{d}{ds} \left(e^{-isA}\varphi, B e^{-isA}\psi\right) \\ &= -i \int_0^t ds\, \left(e^{-isA}\varphi, [B, A]\, e^{-isA}\psi\right). \end{aligned} \tag{2.4}$$

Thus, if $B \in C^1(A)$ then one observes using (2.4) that $B$ is of class $C^1(A)$ in the sense of Definition 2.2. Conversely, if $B$ is of class $C^1(A)$ in the sense of Definition 2.2, then taking the derivative of (2.4) at $t = 0$ yields $B \in C^1(A)$. Similarly, one observes that $B$ being of class $C^2(A)$ implies $\mathrm{ad}_A(B) \in C^1(A)$. Thus one may construct iteratively

$$\mathrm{ad}_A^k(A) := \mathrm{ad}_A\left(\mathrm{ad}_A^{k-1}(B)\right), \quad \mathrm{ad}_A^0(B) := B, \tag{2.5}$$

if $B$ being of class $C^k(A)$, for $k \in \mathbb{N}$. In concrete situations one has to work with commutators involving two possibly unbounded selfadjoint operators $H$ and $A$. In general they will not extend to bounded operators on $\mathcal{H}$

and the definition of the quadratic form $[H, A]$ requires further restrictions on its domain. Thus we denote by $[H, A]$ the form

$$(\varphi, [H, A]\psi) := (H\varphi, A\psi) - (A\varphi, H\psi), \quad \forall \varphi, \psi \in \mathcal{D}(A) \cap \mathcal{D}(H). \tag{2.6}$$

If $(i - H)^{-1} \in C^1(A)$, then $\mathcal{D}(A) \cap \mathcal{D}(H)$ is dense in $\mathcal{D}(H)$ in the graph norm of $H$ and $[H, A]$ extends to an $H$-form bounded quadratic form, which in turn defines a unique element of $\mathfrak{B}(\mathcal{D}(H), \mathcal{D}(H)^*)$ denoted by

$$\mathrm{ad}_A(H) : \ \mathcal{D}(H) \to \mathcal{D}(H)^*, \tag{2.7}$$

see [GGM04]. The space $\mathcal{D}(H)^*$ is the dual of $\mathcal{D}(H)$ in the sense of rigged Hilbert spaces.

Our result on the analyticity of eigenvectors of $H$ with respect to $A$ requires a construction of multiple commutators of $H$ and $A$ which are bounded as maps from $\mathcal{D}(H)$ to $\mathcal{H}$ in the graph norm of $H$. The construction is as follows: Let $H \in C^1(A)$ and assume $\mathrm{ad}_A(H) \in \mathfrak{B}(\mathcal{D}(H), \mathcal{H})$. Then, $[\mathrm{ad}_A(H), A]$ is defined as

$$(\varphi, [\mathrm{ad}_A(H), A]\psi) := (-\,\mathrm{ad}_A(H)\varphi, A\psi) - (A\varphi, \mathrm{ad}_A(H)\psi), \tag{2.8}$$

for all $\varphi, \psi \in \mathcal{D}(A) \cap \mathcal{D}(H)$. Here we used, that $\mathrm{ad}_A(H)$ is skew-symmetric on the domain $\mathcal{D}(A) \cap \mathcal{D}(H)$. Assume that this form extends in graph norm of $H$ to a form which is implemented by an element $\mathrm{ad}_A^2(H) \in \mathfrak{B}(\mathcal{D}(H), \mathcal{H})$. Proceeding iteratively, we construct $\mathrm{ad}_A^k(H) \in \mathfrak{B}(\mathcal{D}(H), \mathcal{H})$. One may show, [MW11], that if $H \in C^1(A)$ and $\mathrm{ad}_A^j(H) \in \mathfrak{B}(\mathcal{D}(H), \mathcal{H})$ for $0 \leq j \leq k$, then $H \in C^k(A)$.

### 2.1.2 Positive Commutators and Results

Let again $H$ and $A$ be selfadjoint operators on some Hilbert space $\mathcal{H}$. Denote with $I \subseteq \mathbb{R}$ an interval and with $\mathbf{1}_I(H)$ the spectral projections of $H$ onto the the spectral subspace pertaining to $I$. A *positive commutator*, or *Mourre estimate*, is an inequality of the type

$$\mathbf{1}_I(H) i[H, A] \mathbf{1}_I(H) \geq C_0 \mathbf{1}_I(H) - K, \tag{2.9}$$

where $C_0 > 0$ and $K$ is a compact operator. Mourre estimates with $K = 0$ are called *strict Mourre estimates*. The Mourre estimate in the form cast here goes back to a fundamental paper of Mourre, [Mou81], where it has been used to prove absence of singular continuous spectrum in $I$. In the context of *regular Mourre theory*, i.e. where the commutator of $H$ and $A$ is relatively $H$ bounded, these concepts have been developed further by many authors, see for instance [PSS81, Mou83, JMP84, AdMG96, Sah97]. We use a more recent form of the Mourre estimate. Namely, let $\lambda \in \mathbb{R}$ be the eigenvalue w.r.t. the eigenstate $\Psi$ of $H$ and let $h$ be a bounded smooth function with

$$h'(0) = 1, \quad h(0) = 0,$$

and

$$\sup_{t \in \mathbb{R}} \left| h^{(k)}(t) \langle t \rangle^k \right| < \infty.$$

Moreover, assume that $h$ is real analytic in a ball about 0. Set $h_\lambda(s) := h(s-\lambda)$ and assume $h_\lambda(H) \in C^1(A)$ and that there is a $f_{\text{loc}} \in C_0^\infty(\mathbb{R}, [0,1])$, such that

$$f_{\text{loc}}(\lambda) = 1, \text{ and } h'_\lambda(x) > 0, \quad \forall x \in \operatorname{supp}(f_{\text{loc}}).$$

**Definition 2.3 (Smooth Mourre estimate).** We say $H$ and $A$ admit a *smooth Mourre estimate w.r.t.* $\lambda$, if there are $C_0, C_1 > 0$ and a compact operator $K$, such that

$$i \operatorname{ad}_A(h_\lambda(H)) \geq C_0 - C_1 f^2_{\text{loc},\perp}(H) - K, \tag{2.10}$$

where $f_{\text{loc},\perp}$ is defined as $f_{\text{loc},\perp} := 1 - f_{\text{loc}}$.

**Remark 2.4.** If $H$ is of class $C^1(A)$, then the two formulations, (2.9), (2.10), are equivalent in the vicinity of $\lambda$, see [MW11] for details.

We are now prepared to formulate our results.

**Theorem 2.5 (Finite regularity).** *Let $H, A$ be selfadjoint operators on the Hilbert space $\mathcal{H}$ and $\Psi$ be an eigenvector of $H$ with eigenvalue $\lambda$. Assume that $H$ and $A$ admit a smooth Mourre estimate w.r.t. $\lambda$ and $h_\lambda(H) \in C^{k+1}(A)$, for some $k \in \mathbb{N}$. Then $\Psi \in \mathcal{D}\left(A^k\right)$ and there exists $c_k > 0$, only depending on* $\operatorname{supp}(f_{\text{loc}})$, *$C_0$, $C_1$, $K$, $\|\operatorname{ad}_A^\ell(f_{\text{loc}}(H))\|$, $\|\operatorname{ad}_A^j(h_\lambda(H))\|$, $1 \leq \ell \leq k$, $1 \leq j \leq k+1$, such that*

$$\left\|A^k \Psi\right\| \leq c_k \|\Psi\|. \tag{2.11}$$

**Remark 2.6.** If one requires $h_\lambda \in C^k(A)$ only, it is shown in [FMS11a], that the statement of this theorem is false in general. Therefore, the result is optimal concerning integer values of $k$. Above result is intimately related to a result proven in [FMS11a] in the context of singular Mourre theory. In contrast to the result obtained there, the bounds derived in [MW11] are however explicit, which allows to prove that $\Psi$ is an analytic vector of $H$ if a natural growth condition on the multiple commutators is required.

**Theorem 2.7 (Analyticity).** *Let $H, A$ be self-adjoint operators on the Hilbert space $\mathcal{H}$ and $\Psi$ be an eigenvector of $H$ with eigenvalue $\lambda$. Assume that $H$ and $A$ admit a smooth Mourre estimate w.r.t. $\lambda$ and that $H$ is of class $C^1(A)$. If there exists a $v > 0$, such that, for all $k \in \mathbb{N}$,*

$$\|\operatorname{ad}_A^k(H)(i-H)^{-1}\| \leq k! v^{-k}, \tag{2.12}$$

*then the map*

$$\mathbb{R} \ni \theta \mapsto e^{i\theta A}\Psi \in \mathcal{H} \tag{2.13}$$

*extends to an analytic function in a strip around the real axis.*

The applications of Theorem 2.5 and its connection to second order perturbation theory are discussed in Section 2.1.3. Theorem 2.7 reproduces a result due to Balslev and Combes, [BC71, Thm. 1] on non-threshold eigenstates of Schrödinger operators with dilation analytic interaction. Our result is abstract and, as such, allows for new results of the type of Balslev and Combes, [BC71, Thm. 1]. We close this section with an application of Theorem 2.7, which is beyond the scope of [BC71]:

Let $H_g$ be the Hamiltonian of a spin-boson model (1.6). Define the coupling between atom and field by

$$G(k) = Bv(k), \quad \forall k \in \mathbb{R}^d,$$

with a complex $N \times N$ matrix $B$. The function $v$ is given by

$$v(k) := \frac{e^{-\frac{k^2}{\Lambda^2}}}{\omega(k)^{\frac{1}{2}}}, \quad \forall k \in \mathbb{R}^3$$

and

$$\omega(k) := \sqrt{k^2 + m^2}, \quad m > 0,$$

i.e. we assume the model to be *massive*. The constant $\Lambda > 0$ plays the role of an ultraviolet cutoff. Define

$$\alpha := \frac{i}{2}\left(\nabla_k \cdot k + k \cdot \nabla_k\right).$$

This operator is symmetric and densely defined on $L^2(\mathbb{R}^3)$ as it is the well-known generator of the strongly continuous unitary group

$$\left(u(t)\psi\right)(k) := e^{-\frac{3}{2}t}\psi\left(e^{-t}k\right).$$

Then, take $A := d\Gamma(\alpha)$. From [DG99] we may infer a Mourre estimate for our model. Dereziński and Gérard use a different generator of dilations, namely

$$\alpha_\omega := \tfrac{i}{2}\big((\nabla_k\omega)(k) \cdot \nabla_k + \nabla_k \cdot (\nabla_k\omega)(k)\big).$$

It is also possible to prove a Mourre estimate using their techniques if $\omega(k)$ is radially increasing, $\omega(k) > 0$, $\forall k \in \mathbb{R}^3$ and 0 is the only critical point of $\omega$. One can prove, [MW11], that $H_g$ is of class $C^1(A)$ for all $g \in \mathbb{R}$ and that (2.12) is satisfied for all $k \in \mathbb{N}$. Thus, for all $g \in \mathbb{R}$ any eigenvector of $H_g$ pertaining to an embedded non-threshold eigenvalue is an analytic vector with respect to $A$. In the fundamental paper of Balslev and Combes on spectral theory of dilation analytic models [BC71] and an extension due to Simon [Sim72] it is proved that, for $N$-body Schrödinger operators with dilation analytic potentials, there are no excited eigenstates. The proof is based on an indirect argument using the fact that any non–threshold eigenstate would be an analytic vector w.r.t. to the generator of dilations.

### 2.1.3 Resonance Theory based on Mourre Theory

In many physical problems excited eigenvalues which are embedded in the continuous spectrum become unstable when a perturbation is switched on. We refer to such unstable eigenvalues as *resonances*. The corresponding eigenstates are called *metastable states*. Cattaneo, Graf and Hunziker develop in [CGH06] a mathematical theory of resonances based on positive commutators using the following condition.

**Condition 2.8 (CGH).** Let $H_g := H_0 + V$, where $H_0$ is selfadjoint, $\lambda$ is an eigenvalue of $H_0$ with eigenprojection $P$. The interaction $V$ is symmetric and $H_0$-bounded. There is a selfadjoint operator $A$ such that $H_0$ and $V$ are of class $C^1(A)$ and for $\nu \in \mathbb{N}$ the multiple commutators $\mathrm{ad}_A^k(H_0)$, $\mathrm{ad}_A^k(V) \in \mathfrak{B}(\mathcal{D}(H_0), \mathcal{H})$, for $k = 0, \dots \nu$. $H_0$ and $A$ satisfy a Mourre estimate (2.9), with some open interval $I \ni \lambda$.

Using this condition the authors obtain the following result on the regularity of the resolvent, which in particular implies a LAP.

**Theorem 2.9 (CGH '06).** *Let Condition 2.8 be satisfied for $\nu = n+3$ and let $\Delta$ be a compact subset of $I$. For $s > n-1$, $g$ small enough and*

$$z \in \Delta_a^{\pm} := \{x + iy \in \mathbb{R} + i\mathbb{R} |\, x \in \Delta,\ 0 < |y| \leq a\},$$

*define*

$$R(z,g) := (i-A)^{-s}\left(z - \bar{P}H_g\bar{P}\right)^{-1}(i-A)^{-s},$$

*where $\bar{P} := 1 - P$. Then, there a constants $c_1, c_2 > 0$ such that for $k = 0, \dots, n-1$,*

$$\left\| \frac{d^k}{dz^k} R(z,g) \right\| \leq c_1$$

*and*

$$\left\| \frac{d^{n-1}}{dz^{n-1}} R(z,g) - \frac{d^{n-1}}{dz^{n-1}} R(z',g) \right\| \leq c_2 \left|z - z'\right|^{\frac{2s-2n+1}{2s-2n+2sn+1}}.$$

*Moreover, derivatives and boundary value limits, both w.r.t. the operator norm, may be interchanged.*

This result implies a decay of metastable states, which is the content of the next theorem. The regularity of the resolvents of the previous result are directly related to the polynomial decay in time.

**Theorem 2.10 (CGH '06).** *Let Condition 2.8 be satisfied for $\nu = n+5$ and $\lambda$ be a simple eigenvalue of $H_0$. Moreover, assume that the Fermi Golden Rule holds, i.e.,*

$$\frac{\gamma}{2} := \mathrm{Im}\,(\Psi, V(\lambda + i0 - \bar{P}H_0\bar{P})V\Psi) < 0. \tag{2.14}$$

*Then, there is a $f \in C_0^\infty(I)$, with $f(x) \equiv 1$ for $x$ close to $\lambda$, such that*

$$(\Psi, f(H_g)e^{-itH_g}\Psi) = a(g)e^{-i\lambda_g t} + b(t,g),$$

*with $a(g) = 1 + \mathcal{O}(g^2)$,*

$$|b(t,g)| \leq cg^2|\log(g)|(1+t)^{-n}$$

*and*

$$\lambda_g = \lambda + g(\Psi, V\Psi) + g^2(\Psi, V(\lambda + i0 - \bar{P}H_0\bar{P})V\Psi) + o\left(g^2\right).$$

*In particular,* $\mathrm{Im}\left(\lambda_g\right) < 0$.

The two preceding results are a main ingredient for the following result.

**Theorem 2.11 (CGH '06).** *Let Condition 2.8 be satisfied for $\nu = n + 2$, then*

$$\operatorname{ran}(P) \subset \mathcal{D}(A^n).$$

Our result improves on this by reducing the requirement to $\nu = n + 1$, thus improving the Theorems 2.9 and 2.10. The limiting absorption principle can be deduced assuming $H$ is of class $C^2(\bar{P}A\bar{P})$. This implies in particular that $\operatorname{ran}(P) \subseteq \mathcal{D}(A^2)$, i.e. $\psi \in \mathcal{D}(A^2)$. Even by the improvement of our result we would still need $H$ to be of class $C^3(A)$ in order to verify this property. This would for example preclude application to the model considered in [Ras10, Chapt. 2]. In [FMS11b] the authors prove the Fermi Golden Rule (2.14) directly, bypassing the general limiting absorption theorems, assuming only $\psi \in \mathcal{D}(A)$. Combined with Theorem 2.5 this establishes the existence of the limit in the Fermi Golden Rule abstractly under a $C^2(A)$ condition. Moreover, the Theorem 2.11 does neither apply to $\phi_2^4$–models nor to Pauli–Fierz models below the ionisation threshold, [FGS08], whereas our result applies to both.

## 2.2 A Pumping Scheme for Solid State Lasers

Before we start with the precise mathematical description of the framework and our results, we first explain heuristically the phenomenology and the purpose of our work.

For a pumping scheme we have in mind a setup consisting of an atom, a reservoir and an external light source, we call also pump. In solid state lasers, the atom is an impurity in a crystal, where the electrons of the latter serve as the reservoir. The pump is tuned such that it is resonant with respect to the largest difference of energy levels of the impurity. If there is no pump, then the atom evolves to its thermal equilibrium, which is effectively given by the Gibbs state. In this state, excited energy levels become strictly monotonously decreasingly populated as one goes from lower to higher energy levels. Thus for long times, a higher energy level less populated than a lower one. Therefore it cannot be used as a source for the creation of a coherent light beam, which is the laser. As soon as the pump is switched on, it pumps electrons from the lowest level to the highest. If the pump is strong enough to compensate for the relaxation to the thermal equilibrium due to the interaction with the reservoir, one may obtain even for long times a higher population of an excited level than for instance in the ground state. This effect is called *inversion of population*. If the pump becomes much stronger than the reservoir–impurity interaction, the system starts oscillating. These oscillations are customarily called *Rabi oscillations*. We aim at a situation where Rabi oscillations are not dominant.

The evolution of the population of the energy levels is phenomenologically described by a differential equation, called *Pauli Equation*, [AL07],

$$\frac{d}{dt} n(t) = (A + B)\, n(t), \tag{2.15}$$

where $A$ and $B$ are generators of *completely positive semigroups*, and $n(t) := (n_1(t), \ldots, n_N(t))$ consists of the populations, $n_\ell(t)$, $\ell = 1, \ldots, N$, appertaining to the energy level $E_\ell$. The operator$A$ encodes the transition rates between the different energy levels due to the interaction with the reservoir. The Markov chain generated by $A$ is called *spontaneous process*. The operator $B$ encodes the transition rates due to the pump and the generated Markov chain is called *stimulated process*. It is known that $B$ is proportional to the intensity of the pump. Note that (2.15) is an autonomous differential equation. We prove in [BPW11a] the following:

1. The phenomenological Pauli Equation can be rigorously be derived from an evolution generated by a time–dependent *Lindbladian*, which in turn is associated to a microscopic Hamiltonian dynamics. The derivation is not restricted to certain timescales, but holds uniformly in $t$.

2. Under certain conditions, most importantly the requirement that the Lindbladian satisfies a non–commutative analogue of the *irreducibility of Markov chains*, there is a unique *stationary population*, $n(\infty)$, such that $n(t) \to n(\infty)$ as $t \to \infty$. The evolution described by (2.15) is not the physical one. Our derivation of the effective dynamics of the population leads to an integro–differential equation which generates an evolution that converges to $n(\infty)$. However, as memory effects are important, this state is attained in a different way than predicted by (2.15).

3. We analyse the structure of $A$ and $B$ and find necessary conditions for $A, B$ to be satisfied. As $(A+B)\, n(\infty) = 0$, this implies necessary conditions on the stationary population $n(\infty)$.

We proceed now as follows. First we establish in Section 2.2.1 a link between the algebraic dynamics and a non–autonomous evolution family on a GNS Hilbert space which is well–suited for our purpose. This evolution family can be reformulated as a semigroup on a larger Hilbert space, e.g. $L^2\left(\mathbb{R}_0^+, \mathfrak{H}\right)$, see Section 2.2.2. Then, we introduce the notions of complete positivity and detailed balance condition, Section 2.2.3. Finally, we present in Section 2.2.4 a simplified version of our results in [BPW11a].

### 2.2.1 Algebraic Dynamics and Tomita–Takesaki Modular Theory

We are interested in the dynamics of the atom originating from the microscopic automorphic evolution of the full system and intend to explain how this is related to objects which may be analysed by spectral theory. It is expected that this dynamics is described by an effective (generally dissipative) completely positive (CP) semigroup whose generator, the so–called Lindbladian, is given by second order perturbation theory.

To this end, the GNS representation of the initial state $\omega_0$ of the system is the natural framework to use because it provides a Hilbert space structure which enables powerful tools of spectral analysis. This observation is well–known, see, e.g., [BFS00, JP02]. The present section is an extract of the chapter about time dependent $C$–Liouvilleans, [BPW11b], to which we refer for the details.

Assume that the initial state $\omega_0$ is of the form

$$\omega_0 = \mathfrak{g}_{\mathrm{at}} \otimes \omega_{\mathcal{R}}, \tag{2.16}$$

i.e., $\omega_{\mathrm{at}} = \mathfrak{g}_{\mathrm{at}}$ is the Gibbs state. Let $(\mathfrak{H}, \pi, \Omega_{\mathfrak{g}})$ be its GNS representation. Note that $\mathfrak{H} := \mathfrak{H}_{\mathrm{at}} \otimes \mathfrak{H}_{\mathcal{R}}$, $\pi := \pi_{\mathrm{at}} \otimes \pi_{\mathcal{R}}$ and $\Omega_{\mathfrak{g}} := \Omega_{\mathrm{at},\mathfrak{g}} \otimes \Omega_{\mathcal{R}}$, where $(\mathfrak{H}_{\mathrm{at}}, \pi_{\mathrm{at}}, \Omega_{\mathrm{at},\mathfrak{g}})$ and $(\mathfrak{H}_{\mathcal{R}}, \pi_{\mathcal{R}}, \Omega_{\mathcal{R}})$ are the GNS representation of $\mathfrak{g}_{\mathrm{at}}$ and $\omega_{\mathcal{R}}$, respectively. An important property of the initial state is that $\omega_0$ is faithful. In particular, $\pi$ is injective.

For simplicity, $\pi(A)$ and $\pi(\mathcal{V})$ are denoted by $A$ and $\mathcal{V}$, respectively. Moreover, the cyclic vector $\Omega_{\mathfrak{g}}$ of the GNS representation is in this case separating for $\mathfrak{M}$, i.e., $A\Omega_{\mathfrak{g}} = 0$ implies $A = 0$. Indeed, $\omega_0$ is a $(\beta, \tau)$–KMS state, where $\{\tau_t\}_{t\in\mathbb{R}}$ is the one–parameter group of $*$–automorphisms on $\mathcal{V}$ defined by (1.11), see also [BR87, Corollary 5.3.9]. The weak closure of the $C^*$–algebra $\pi(\mathcal{V})$ is a von Neumann algebra denoted by $\mathfrak{M} := \mathcal{V}''$. The state $\omega_0$ on $\mathcal{V}$ uniquely extends to a normal state on the von Neumann algebra $\mathfrak{M}$ and $\{\tau_t\}_{t\in\mathbb{R}}$ also extends uniquely to a $\sigma$–weakly continuous $*$–automorphism group on $\mathfrak{M}$, see [BR87, Corollary 5.3.4]. Both extensions are again denoted by $\omega_0$ and $\{\tau_t\}_{t\in\mathbb{R}}$, respectively. Because $\omega_0$ is, in this case, invariant with respect to $\{\tau_t\}_{t\in\mathbb{R}}$, there is a unique unitary representation $\{U_t\}_{t\in\mathbb{R}}$ of $\{\tau_t\}_{t\in\mathbb{R}}$, i.e.,

$$\forall t \in \mathbb{R},\ A \in \mathfrak{M} : \qquad \tau_t(A) = U_t A U_t^*,$$

such that $U_t\Omega_{\mathfrak{g}} = \Omega_{\mathfrak{g}}$. As $t \mapsto \tau_t$ is $\sigma$–weakly continuous, the map $t \mapsto U_t$ is strongly continuous. Therefore, the unitary group $\{U_t\}_{t\in\mathbb{R}}$ is generated by a selfadjoint operator $L$, $U_t = \mathrm{e}^{itL}$. In particular, $\Omega_{\mathfrak{g}} \in \mathrm{Dom}(L)$ and $L$ annihilates $\Omega_{\mathfrak{g}}$, i.e. $L\Omega_{\mathfrak{g}} = 0$. Moreover, $L$ is related to the generator $\delta$ of the group $\{\tau_t\}_{t\in\mathbb{R}}$ by the following relations: We have

$$\{A\Omega : A \in \mathrm{Dom}(\delta)\} \subset \mathrm{Dom}(L) \subset \mathfrak{H} \tag{2.17}$$

and

$$\forall A \in \mathrm{Dom}(\delta) : \qquad L(A\Omega) = \delta(A)\,\Omega. \tag{2.18}$$

Now, if the faithful state $\omega_{\mathrm{at}}$ is not the Gibbs state $\mathfrak{g}_{\mathrm{at}}$ in (2.16) then the GNS representation of $\omega_0$ is also given by $(\mathfrak{H}, \pi, \Omega)$ where $\Omega = \Omega_{\mathrm{at}} \otimes \Omega_{\mathcal{R}}$ for some $\Omega_{\mathrm{at}} \in \mathfrak{H}_{\mathrm{at}}$. In other words, the von Neumann algebra $\mathfrak{M}$, the corresponding extension of the $*$–automorphism group $\{\tau_t\}_{t\in\mathbb{R}}$ does not depend on the initial state $\omega_{\mathrm{at}}$ of the atom. So, we assume from now on that

$$\omega_0 := \omega_{\mathrm{at}} \otimes \omega_{\mathcal{R}}$$

for any faithful state $\omega_{\mathrm{at}}$.

The (Tomita–Takesaki) modular objects of the pair $(\mathfrak{M}, \Omega_{\mathfrak{g}})$ are important for our further analysis. We write $\Delta$, $J$, and

$$\mathcal{P} := \overline{\{AJA\Omega_{\mathfrak{g}} \ :\ A \in \mathfrak{M}\}}$$

respectively for the modular operator, the modular conjugation and the natural positive cone of the pair $(\mathfrak{M}, \Omega_{\mathfrak{g}})$. Observe that $\Omega = AJA\Omega_{\mathfrak{g}} \in \mathcal{P}$ with

$$A = \rho_{\mathrm{at}}^{1/4} \rho_{\mathfrak{g}}^{-1/4} \otimes \mathbf{1}_{\mathfrak{H}_{\mathcal{R}}},$$

where $\rho_{\mathfrak{g}}$ is the density matrix (1.12) of the Gibbs state $\mathfrak{g}_{\mathrm{at}}$. Additionally, $\Omega$ is a cyclic vector for any faithful initial state $\omega_{\mathrm{at}}$ of the atom and hence, by [BR87, Proposition 2.5.30], it is also separating for $\mathfrak{M}$.

Standard results from Tomita–Takesaki theory (cf. [BR87, Corollary 2.5.32] and [BR96, Chapt. 5]) show that the generator $L$ of the unitary group $\{U_t\}_{t\in\mathbb{R}}$ satisfies

$$\forall t \in \mathbb{R}: \qquad LJ + JL = 0, \qquad \mathrm{e}^{itL}\mathcal{P} \subset \mathcal{P}, \qquad \Delta = \mathrm{e}^{-\beta L}. \tag{2.19}$$

Here, $L$ refers to as the *standard Liouvillean* of the $*$–automorphism group $\{\tau_t\}_{t\in\mathbb{R}}$.

In our setting, however, the free dynamics is perturbed by the pump and the atom–reservoir interaction. Altogether, this leads to a perturbation $W_t$ of the standard Liouvillean $L$. For time independent perturbations of the generator $\delta$ of the dynamics $\{\tau_t\}_{t\in\mathbb{R}}$ (on $\mathcal{V}$) of the form $i[W,\cdot]$ with some bounded selfadjoint $W \in \mathcal{V}$, one has

$$\forall t \in \mathbb{R}: \qquad \tau_t^W(A) = \mathrm{e}^{it(L+W)}A\mathrm{e}^{-it(L+W)} \in \mathfrak{M}, \qquad A \in \mathcal{V}, \tag{2.20}$$

where $\{\tau_t^W\}_{t\in\mathbb{R}}$ is the strongly continuous $*$–automorphism group on $\mathcal{V}$ generated by $\delta + i[W,\cdot]$. Analogously as above, $\{\tau_t^W\}_{t\in\mathbb{R}}$ defines a $\sigma$–weakly continuous group on whole $\mathfrak{M}$. In general, the operator $L+W$ neither annihilates $\Omega_{\mathfrak{g}}$ nor satisfies

$$(L+W)\,J + J\,(L+W) = WJ + JW = 0.$$

It is known, [BR87, Corollary 2.5.32], that there is an operator $L_W$, the standard Liouvillean of the dynamics $\{\tau_t^W\}_{t\in\mathbb{R}}$, satisfying $[L_W, J] = 0$ together with

$$\forall t \in \mathbb{R}: \qquad \tau_t^W(A) = \mathrm{e}^{itL_W}A\mathrm{e}^{-itL_W}, \qquad A \in \mathfrak{M},$$

use [BR87, Corollary 2.5.32] and the $\sigma$–weakly continuity of the map $t \mapsto \tau_t^W$. Indeed, $L_W$ equals $L+W$ up to an element of the commutant $\mathfrak{M}' = J\mathfrak{M}J$ of the von Neumann algebra $\mathfrak{M}$. To determine it explicitly, it suffices to solve the equation

$$[W + JAJ, J] = 0 \tag{2.21}$$

for $A \in \mathfrak{M}$. Straightforward computations show that $A = W$ is a solution of (2.21). Additionally using the uniqueness of the standard Liouvillean $L_W$, one concludes that

$$L_W = L + W - JWJ,$$

is the only solution of (2.21).

The operator $L_W$ does not necessarily annihilate $\Omega_{\mathfrak{g}}$ or some prescribed vector $\Omega \in \mathcal{P}$. In general, $L_W$ only annihilates $\Omega_W \in \mathcal{P}$, the vector representing the unique $(\beta, \tau^W)$–KMS state normal to $\omega_0$. In other words, the standard Liouvillean $L_W$ anti-commutes with the modular conjugation $J$, but has the drawback of not having $\Omega_{\mathfrak{g}}$ in its kernel. A way to bypass this problem is presented in [JP02, Section 2.2] where the notion of $C$–Liouvilleans, $\mathcal{L}$, is introduced. It is constructed such that $\mathcal{L}\Omega = 0$ for any fixed $\Omega \in \mathcal{P}$. In our case, we face the problem that the dynamics is non–autonomous and the standard Liouvillean $L_{W_t}$ is time dependent. Using the $C$–Liouvilleans construction of [JP02, Section 2.2] we can design the time depending Liouvillean of the non-autonomous dynamics such that $\mathcal{L}_t\Omega = 0$. This is a very useful property for the analysis of the dynamics.

Therefore, we now extend the definition of $C$–Liouvilleans [JP02, Section 2.2] to non-autonomous evolutions. First, the time dependent, bounded, selfadjoint perturbation $\{W_t\}_{t\in\mathbb{R}} \subset \mathcal{V}$ should define a family of symmetric derivations

$$\delta_{W_t} := \delta + i[W_t, \cdot]$$

for all $t \in \mathbb{R}$, which generates a strongly continuous two–parameter family $\{\tau_{t,s}\}_{t\geq s}$ of automorphisms of $\mathcal{V}$, similar to the autonomous case (2.20).

The time dependent $C$–Liouvillean is defined by

$$\mathcal{L}_t := L + W_t - J\Delta^{1/2}W_t\Delta^{-1/2}J \tag{2.22}$$

for any $t \in \mathbb{R}$.
Note that the term

$$V_t := W_t - J\Delta^{1/2}W_t\Delta^{-1/2}J \tag{2.23}$$

implements the commutator $[W_t, \cdot]$ for any $t \in \mathbb{R}$, i.e. for any $A \in \mathcal{V}$,

$$[W_t, A]\,\Omega = W_tA\Omega - (W_tA^*)^*\,\Omega \tag{2.24}$$

and using $J\Delta^{1/2}A\Omega = A^*\Omega$ we also deduce that

$$J\Delta^{1/2}W_t\Delta^{-1/2}JA\Omega = (W_tA^*)^*\,\Omega.$$

In particular,

$$\forall t \in \mathbb{R}: \quad \mathcal{L}_t\Omega = 0. \tag{2.25}$$

We have the following result.

**Proposition 2.12 (Time-dependent $C$–Liouvilleans).**
*Assume that $\{W_t\}_{t\geq 0} \in C^1(\mathbb{R},\mathcal{V})$ and $\{V_t\}_{t\geq 0} \in C^1(\mathbb{R},\mathcal{B}(\mathfrak{H}))$. Then, there is an evolution family $\{U_{t,s}\}_{t\geq s} \subset \mathcal{B}(\mathfrak{H})$ solving on* Dom $(L)$ *the non–autonomous evolution equations*

$$\forall t > s: \quad \partial_t U_{t,s} = i\mathcal{L}_t U_{t,s}\,, \quad \partial_s U_{t,s} = -iU_{t,s}\mathcal{L}_s\,, \quad U_{s,s} := \mathbf{1}.$$

*Moreover, for any $t \geq s$, $U_{t,s}$ possesses a bounded inverse $U_{t,s}^{-1}$. If $\{W_t\}_{t\in\mathbb{R}}$ is periodic with period $T > 0$, then*

$$\forall t \geq s,\ k \in \mathbb{Z}: \quad U_{t,s} = U_{t+kT,s+kT}.$$

*The evolution family satisfies $U_{t,s}\Omega = \Omega$ and*

$$\forall t \geq s,\ A \in \mathcal{V}: \quad \tau_{t,s}(A) = U_{t,s}AU_{t,s}^{-1}$$

*In particular, $\{\tau_{t,s}\}_{t\in\mathbb{R}}$ also extends uniquely to a $\sigma$–weakly continuous $*$–automorphism evolution family on $\mathfrak{M}$.*

The use of $C$–Liouvilleans is advantageous because of the presence of only one evolution family in the dynamics described by

$$\forall A \in \mathfrak{M}: \quad U_{t,s}AU_{s,t}\Omega = U_{t,s}A\Omega.$$

In particular, it establishes a direct relation to the *Lindbladian*, which is an operator defined on the von Neumann algebra $\mathfrak{M}$. Observe also that $\mathcal{L}_t$ is not selfadjoint anymore and may thus be dissipative.

### 2.2.2 Evolution Semigroups

In the previous section we identified an evolution family, $\{U_{t,s}\}_{t\geq s}$, which implements the algebraic dynamics. In the present section we explain how this is related to objects which may be analysed by spectral theory. To this end, we represent this non–autonomous evolution as an *autonomous* dynamics on an enlarged Hilbert space emerging through an additional degree of freedom, which is a new time variable denoted by $\alpha$. This method enables a long–time analysis of the non-autonomous dynamics via a spectral analysis of the generator of the associated evolution semigroup.

The enlarged Hilbert space is defined as

$$\mathfrak{H}_{\mathrm{evo}} := L^2(\mathbb{T}_\varpi, \mathfrak{H}_{\mathrm{at}}), \quad \mathbb{T}_\varpi := \mathbb{R}/_{\frac{2\pi}{\varpi}\mathbb{Z}}, \tag{2.26}$$

of time–dependent $2\pi\varpi^{-1}$–*periodic* functions with images in $\mathfrak{H}$. The scalar product on $\mathfrak{H}_{\mathrm{evo}}$ is naturally defined, for all $f, g \in \mathfrak{H}_{\mathrm{evo}}$, by

$$\langle f, g\rangle_{\mathrm{evo}} := \frac{\varpi}{2\pi}\int_0^{\frac{2\pi}{\varpi}} \langle f(t), g(t)\rangle_{\mathfrak{H}}\, \mathrm{d}t.$$

Then, there is a strongly continuous one–parameter semigroup $\{\mathcal{T}_\alpha\}_{\alpha\geq 0}$, called *evolution semigroup*, such that, for all $\alpha \geq 0$ and $f \in \mathfrak{H}_{\mathrm{evo}}$,

$$\forall t \in \mathbb{T}_\varpi \text{ a.e.} : \qquad \mathcal{T}_\alpha(f)(t) = U_{t,t-\alpha} f(t-\alpha).$$

The evolution semigroup is generated by

$$\mathfrak{G} := -\frac{d}{dt} + \mathfrak{L}_{\mathrm{evo}}, \;\; \mathcal{D}(\mathfrak{G}), \tag{2.27}$$

where $\mathfrak{L}_{\mathrm{evo}}$ is the bounded operator defined, for all $f \in \mathfrak{H}_{\mathrm{evo}}$, by

$$\forall t \in \mathbb{T}_\varpi \text{ a.e.} : \qquad \mathfrak{L}_{\mathrm{evo}}(f)(t) := \mathfrak{L}_t(f(t)).$$

In [BPW11a] we analyse an effective dynamics, which approximates the two–parameter family $\{U_{t,s}\}_{t\geq s}$ in a certain sense uniformly in time. This dynamics gives also rise to an evolution semigroup, but the operator $\mathfrak{L}_{\mathrm{evo}}$ is bounded, see Section 2.2.4, and hence $\mathcal{D}(\mathfrak{G}) = \mathcal{D}\left(\frac{d}{dt}\right)$ in this case.

### 2.2.3 Completely Positive Markov Semigroups and Balance Conditions

In open quantum systems, one usually studies the restricted dynamics on the small quantum system of the time evolution of the full, composite system that typically is a small quantum object in interaction with macroscopic systems, i.e., reservoirs. This restriction on the time evolution formally defines at any fixed time a map $\mathcal{C}$ within the set of density matrices of the small system. This is pedagogically explained in [AL07, Section 1.2.1]. As explained in [AL07, Section 1.2.2], such maps usually share similar mathematical properties, which refer to *completely positive maps* defined below. In some situations, for instance if the system evolves to a thermal equilibrium, there is a balance condition for the generator of the effective dynamics of the small subsystem, namely the *(quantum) detailed balance condition*. We start with the definition CP maps and semigroups.

**Definition 2.13 (Completely positive maps).**
A positive map $\mathcal{C} \in \mathcal{B}(\mathcal{B}(\mathcal{X}))$ acting on the set $\mathcal{B}(\mathcal{X})$ of bounded operators on a Hilbert space $\mathcal{X}$ is called *completely positive (CP)* if the extended map $\mathcal{C} \otimes \mathbf{1}_{\mathcal{B}(\mathbb{C}^n)}$ is positive for any $n \in \mathbb{N}$. If $\mathcal{C}$ is unital, i.e., $\mathcal{C}(\mathbf{1}_{\mathcal{X}}) = \mathbf{1}_{\mathcal{X}}$, then the operator $\mathcal{C}$ is called a *Markov map*.

Completely positive semigroups are simply semigroups which are CP maps for all times.

**Definition 2.14 (Completely positive semigroups).**
A semigroup $\{\mathcal{C}_t\}_{t\geq 0} \subset \mathcal{B}(\mathcal{B}(\mathcal{X}))$, with $\mathcal{X}$ being a Hilbert space, is *CP* if the map $\mathcal{C}_t$ is CP for any $t \in \mathbb{R}^+$. If $\mathcal{C}_t$ is unital for any $t \in \mathbb{R}^+$, then $\{\mathcal{C}_t\}_{t\geq 0}$ is called *Markov*.

From now on until the end of this section, $\mathcal{X}$ is always a $n$–dimensional Hilbert space. We denote by $\mathcal{B}_2(\mathcal{X}) \equiv \mathcal{B}(\mathcal{X})$ the Hilbert space of Hilbert–Schmidt operators with scalar product

$$\langle A, B\rangle_{\mathcal{B}_2(\mathcal{X})} := \mathrm{Tr}_{\mathcal{X}}(A^*B), \qquad A, B \in \mathcal{B}_2(\mathcal{X}).$$

In the special case where a semigroup $\{\mathcal{C}_t\}_{t\geq 0} \subset \mathcal{B}(\mathcal{B}_2(\mathcal{X}))$ acts on $\mathcal{B}_2(\mathcal{X})$, we can define the (unique) *adjoint semigroup* $\{\mathcal{C}_t^\dagger\}_{t\geq 0} \subset \mathcal{B}(\mathcal{B}_2(\mathcal{X}))$ via the equations

$$\forall t \geq 0: \quad \langle \mathcal{C}_t^\dagger(A), B\rangle_{\mathcal{B}_2(\mathcal{X})} = \langle A, \mathcal{C}_t(B)\rangle_{\mathcal{B}_2(\mathcal{X})}, \qquad A, B \in \mathcal{B}_2(\mathcal{X}).$$

Note that a Markov CP and $C_0$ semigroup $\{\mathcal{C}_t\}_{t\geq 0}$ defines a $C_0$ semigroup $\{\mathcal{C}_t^\dagger\}_{t\geq 0}$ which *preserves the trace*. In this case, $\{\mathcal{C}_t^\dagger\}_{t\geq 0}$ is also called a Markov CP and $C_0$ semigroup. Generators of Markov CP and $C_0$ semigroups $\{\mathcal{C}_t\}_{t\geq 0}$ and $\{\mathcal{C}_t^\dagger\}_{t\geq 0}$ can then be characterised in the finite dimensional case (cf. [DF06, Sect. 4.3]):

**Theorem 2.15 (Generators of (CP) Markov semigroups, dim $\mathcal{X} = n$).**
*An operator $M \in \mathcal{B}(\mathcal{B}(\mathcal{X}))$ is the generator of a CP semigroup iff there is a completely positive map $\Xi \in \mathcal{B}(\mathcal{B}(\mathcal{X}))$ and an operator $\Delta \in \mathcal{B}(\mathcal{X})$ such that*

$$M = \underset{\longrightarrow}{\Delta} + \underset{\longleftarrow}{\Delta^*} + \Xi. \tag{2.28}$$

*$M \in \mathcal{B}(\mathcal{B}(\mathcal{X}))$ the generator of a CP Markov semigroup iff it is the generator of a CP semigroup and*

$$M = i\left[\frac{1}{2}(\Delta + \Delta^*), \cdot\right] - \frac{1}{2}\left(\underset{\longrightarrow}{\Xi(1)} + \underset{\longleftarrow}{\Xi(1)}\right) + \Xi. \tag{2.29}$$

**Remark 2.16.** We use in Theorem2.15 the left and right multiplication, $\underset{\longrightarrow}{\Delta}A := \Delta A$ and $\underset{\longleftarrow}{\Delta^*}A := A\Delta^*$, $\forall A \in \mathcal{B}(\mathcal{X})$, respectively. Operators of the form (2.28) are usually called *Lindblad-*, *Lindblad–Kossakowski generator*, or short *Lindbladian*, [GKS76, Lin76]. We will use Lindbladian.

Let $\{\Gamma_t\}_{t\in\mathbb{R}^+}$ , $\Gamma_t \in \mathcal{B}(\mathcal{B}(\mathcal{H}))$ be a continuous Markov CP semigroup and $\omega$ be a stationary state, i.e. $\omega = \omega \circ \Gamma_t$, $\forall t \in \mathbb{R}^+$, w.r.t. $\{\Gamma_t\}_{t\in\mathbb{R}^+}$. Assume that $\omega$ is a faithful state of the $C^*$-algebra $\mathcal{B}(\mathcal{H})$ and denote the corresponding GNS representation with $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$. There exists a continuous contraction semigroup $\{e^{-itL}\}_{t\in\mathbb{R}^+}$ on $\mathcal{H}_\omega$ such that

$$\pi_\omega\left(\Gamma_t\left(A\right)\right)\Omega_\omega = e^{itL}\pi_\omega\left(A\right)\Omega_\omega.$$

The following definition of the *detailed balance condition* is due to [FGKV77, FGKV78], but we formulate it as presented in [Ali76].

**Definition 2.17 (Detailed Balance Condition).** We say that $L$ satisfies the *detailed balance condition (DBC)* iff it is a normal operator w.r.t. the scalar product of $\mathcal{H}_\omega$.

**Remark 2.18.** Let $L = L_{\mathrm{Re}} + iL_{\mathrm{Im}}$ be the unique decomposition with respect to the scalar product of $\mathcal{H}_\omega$, such that $L_{\mathrm{Re}}, L_{\mathrm{Im}}$ are self-adjoint operators. If $L$ satisfies the DBC one can show, [Ali76, Lemma 4], that $L\Omega_\omega = 0$. Define by

$$\pi_\omega\left(\alpha_t\left(A\right)\right)\Omega_\omega = e^{itL_{\mathrm{Re}}}\pi_\omega\left(A\right)\Omega_\omega$$

a continuous group $\{\alpha_t\}_{t\in\mathbb{R}}$ of automorphisms of the $C^*$-algebra $\mathcal{B}\left(\mathcal{H}\right)$. Moreover, the detailed balance condition implies that

$$\pi_\omega\left(\zeta_t\left(A\right)\right)\Omega_\omega = e^{-tL_{\mathrm{Im}}}\pi_\omega\left(A\right)\Omega_\omega$$

defines a Markov CP continous semigroup $\{\zeta_t\}_{t\in\mathbb{R}_0^+}$, [FGKV77], and

$$L_{\mathrm{Re}}\left(\Omega_\omega\right) = 0 = L_{\mathrm{Im}}\left(\Omega_\omega\right).$$

We conclude this section with a short illustration of the DBC for Markov chains with some finite state space which is not necessarily related to $\mathcal{H}_\omega$. Consider

$$\frac{d}{dt}n_j\left(t\right) = \sum_{\ell=1}^{N}\Big(A_{j\ell}n_\ell\left(t\right) - A_{\ell j}n_j\left(t\right)\Big), \quad A_{j,\ell} \geq 0,\ j,\ell = 1,\ldots,N. \tag{2.30}$$

This Markov chain satisfies the DBC w.r.t. $\tilde{n} = (\tilde{n}_1, \ldots, \tilde{n}_N)$, if

$$A_{j\ell}\tilde{n}_\ell = A_{\ell j}\tilde{n}_j, \qquad j,\ell = 1,\ldots,N.$$

In case of thermal equilibrium, when $n_\ell$ is associated to the population of the $\ell^{\text{th}}$ atomic energy level, the relation between $A_{j\ell}$ and $A_{\ell j}$ is given by the *Boltzmann factor* $\exp\left(-\beta\left(E_\ell - E_j\right)\right)$.

### 2.2.4 Results

In the present section we present a simplified version of the results of [BPW11a]. We analyse the atomic dynamics resulting from the restriction on $\mathcal{B}(\mathbb{C}^d)$ of the full dynamics generated by the symmetric derivation $\delta_t^{(\lambda,\eta)}$. This corresponds to study the family of states $\{\omega_{\mathrm{at}}\left(t\right)\}_{t\in\mathbb{R}_0^+}$ defined by (1.18) or, equivalently, to study the corresponding family $\{\rho_{\mathrm{at}}\left(t\right)\}_{t\in\mathbb{R}_0^+}$ of density matrices. We are more precisely interested in the time behaviour of observables related to atomic levels only, and not to correlations between different levels. Mathematically, this amounts to study the orthogonal projection $P_{\mathfrak{D}}(\rho_{\text{at}}(t))$ of the density matrix $\rho_{\text{at}}(t)$ on the subspace

$$\mathfrak{D} = \mathfrak{D}(H_{\text{at}}) := \mathcal{B}(\mathcal{H}_1) \oplus \cdots \oplus \mathcal{B}(\mathcal{H}_{\text{N}}) \subset \mathfrak{H}_{\text{at}}. \tag{2.31}$$

In other words, we analyse the density matrix

$$P_{\mathfrak{D}}(\rho_{\text{at}}(t)) = \sum_{k=1}^{N} \mathbf{1}[H_{\text{at}} = E_k]\ \rho_{\text{at}}(t)\ \mathbf{1}[H_{\text{at}} = E_k]$$

for any $t \in \mathbb{R}_0^+$. The density matrix $\rho_{\text{at}}(t)$ is approximated by the solution of an effective non-autonomous initial value problem in $\mathcal{B}(\mathbb{C}^d)$ called the *effective atomic master equation*, see [BPW11a, BPW11b]. Its generator is a time–dependent Lindbladian $\mathfrak{L}_t^{(\lambda,\eta)}$, i.e. it generates for any $t \in \mathbb{R}$ a completely positive group. This Lindbladian $\mathfrak{L}_t^{(\lambda,\eta)} \in \mathcal{B}(\mathfrak{H}_{\text{at}})$ is defined by the following sum:

$$\mathfrak{L}_t^{(\lambda,\eta)}(\rho) := \mathfrak{L}_{\text{at}}(\rho) + \eta\cos(\varpi t)\mathfrak{L}_{\text{p}}(\rho) + \lambda^2\mathfrak{L}_{\mathcal{R}}(\rho), \qquad \rho \in \mathfrak{H}_{\text{at}}. \tag{2.32}$$

The first term is the Lindbladian of the free atomic dynamics which is the anti–selfadjoint operator defined by

$$\mathfrak{L}_{\text{at}}(\rho) := -i[H_{\text{at}},\rho] = -\mathfrak{L}_{\text{at}}^*(\rho), \qquad \rho \in \mathfrak{H}_{\text{at}}. \tag{2.33}$$

Similarly, the second term of (2.32) corresponds to the Lindbladian

$$\mathfrak{L}_{\text{p}}(\rho) := -i[H_{\text{p}},\rho] = -\mathfrak{L}_{\text{p}}^*(\rho), \qquad \rho \in \mathfrak{H}_{\text{at}}. \tag{2.34}$$

The third term includes a dissipative part $\mathfrak{L}_d \in \mathcal{B}(\mathfrak{H}_{\text{at}})$, i.e., $\mathfrak{L}_{\mathcal{R}} \in \mathcal{B}(\mathfrak{H}_{\text{at}})$ is not anti–selfadjoint, which results from the Markov approximation of atom–reservoir interaction. More precisely, the Lindbladian $\mathfrak{L}_{\mathcal{R}}$ equals

$$\mathfrak{L}_{\mathcal{R}}(\rho) := -i[H_{\text{Lamb}},\rho] + \mathfrak{L}_d(\rho), \qquad \rho \in \mathfrak{H}_{\text{at}}. \tag{2.35}$$

The so–called *atomic Lamb shift* $H_{\text{Lamb}}$ and *effective atomic dissipation* $\mathfrak{L}_d$ encode the influence of the electron field-impurity interaction on the dynamics. For the explicit form of $\mathfrak{L}_d$ and $H_{\text{Lamb}}$ in terms of quantities of the underlying microscopic dynamics, we refer to [BPW11a]. Here, we focus on the structural properties.

We define now the effective atomic master equation as the initial value problem

$$\forall t \geq 0: \qquad \frac{d}{dt}\rho(t) = \mathfrak{L}_t^{(\lambda,\eta)}(\rho(t)), \qquad \rho(0) = \rho_{\text{at}}(0) \equiv \rho_{\text{at}}. \tag{2.36}$$

This evolution equation has a unique solution, since $\mathfrak{H}_{\text{at}}$ is finite dimensional. We denote the two parameter family solving (2.36) by $\{\hat{\tau}_{t,s}^{(\lambda,\eta)}\}_{t\geq s}$. Let $\{\mathcal{T}_\alpha\}_{\alpha\geq 0}$ be the evolution semigroup on $\mathfrak{H}_{\text{evo}} := L^2(\mathbb{T}_\varpi, \mathfrak{H}_{\text{at}})$ associated to $\{\hat{\tau}_{t,s}^{(\lambda,\eta)}\}_{t\geq s}$. The generator of $\{\mathcal{T}_\alpha\}_{\alpha\geq 0}$ is given by

$$G^{(\lambda,\eta)} := -\frac{d}{dt} + \mathfrak{L}_{\text{evo}}^{(\lambda,\eta)}, \ \mathcal{D}\left(G^{(\lambda,\mu)}\right) = \mathcal{D}\left(\frac{d}{dt}\right),$$

where $\mathfrak{L}_{\mathrm{evo}}^{(\lambda,\eta)}$ is the bounded operator defined for any $f \in \mathfrak{H}_{\mathrm{evo}}$ as

$$\forall t \in \mathbb{T}_{\varpi} \text{ a.e.}: \qquad \mathfrak{L}_{\mathrm{evo}}^{(\lambda,\eta)}(f)(t) := \mathfrak{L}_{t}^{(\lambda,\eta)}(f(t)).$$

For each $\epsilon \in \sigma(i[H_{\mathrm{at}},\cdot])$,

$$\mathfrak{H}_{\epsilon}^{(\lambda,\eta)} := P_{\epsilon}^{(\lambda,\eta)}\mathfrak{H}_{\mathrm{evo}}$$

is an invariant, finite dimensional subspace (see [Kat76, Chapter II]) of the evolution semigroup $\{\mathcal{T}_{\alpha}\}_{\alpha\geq 0}$ and

$$P_{\epsilon}^{(\lambda,\eta)} := \frac{1}{2\pi i} \oint_{|z-\epsilon|=\frac{R}{4}} \left(z - G^{(\lambda,\eta)}\right)^{-1} \mathrm{d}z \tag{2.37}$$

is the Kato projection. Here, we choose $R$ and $\lambda$ small enough to ensure that the Kato projection, $P_{\epsilon}^{(\lambda,\eta)}$, is well–defined. The restriction of $G^{(\lambda,\eta)}$ onto the space $\mathfrak{H}_{0}^{(0,0)}$ is denoted by

$$\Lambda^{(\lambda,\eta)} := P_{0}^{(0,0)} G^{(\lambda,\eta)} P_{0}^{(0,0)}. \tag{2.38}$$

In [BPW11a] we construct a unitary operator

$$U: \mathfrak{H}_{0}^{(0,0)} \to \widetilde{\mathfrak{H}}_{0}^{(0,0)},$$

such that, for

$$\tilde{\Lambda}^{(\lambda,\eta)}(\rho) := \frac{\eta}{2}\mathfrak{L}_{\mathrm{p}}(\rho) + \lambda^{2}\mathfrak{L}_{\mathcal{R}}(\rho),$$

we find

$$\tilde{\Lambda}^{(\lambda,\eta)} = U\Lambda^{(\lambda,\eta)}U^{*}.$$

Under certain technical assumptions, we prove the following result.

**Theorem 2.19 (Bru–Pedra–W. '11).**
(i) *For any $\varepsilon \in (0,1)$, any state $\rho \in \mathfrak{D} \subset \mathfrak{H}_{\mathrm{at}}$, with $\rho = \rho(0)$, and any observable $A \in \mathcal{B}(\mathbb{C}^{d}) \equiv \mathfrak{H}_{\mathrm{at}}$, the unique solution $\{\rho(t)\}_{t\geq 0}$ of the effective atomic master equation (2.36) satisfies the bound*

$$\begin{aligned} &\left| \langle P_{\mathfrak{D}}(\rho(\alpha)), A\rangle_{\mathrm{at}} - \left\langle \exp\left(\alpha\Lambda^{(\lambda,\eta)}\right)\rho, A\right\rangle_{\mathrm{evo}} \right| \\ \leq\ & C\,\|A\| \left(|\lambda|^{2(1-\varepsilon)} + \frac{|\lambda|(1+|\lambda|)}{\varpi}\right). \end{aligned}$$

*Here $C$ is a finite constant independent of $\rho$, $A$, $\lambda$, $\eta$, $\varpi$, and $\alpha$.*
(ii) *There is a unique density matrix $\tilde{\rho}_{\infty} \in \tilde{\mathfrak{H}}_{0}^{(0,0)}$ such that $\tilde{\Lambda}^{(\lambda,\eta)}(\tilde{\rho}_{\infty}) = 0$. Moreover, for all $\rho \in \mathfrak{H}_{\mathrm{at}}$ and any $\varepsilon \in (0,1)$,*

$$\limsup_{\alpha\to\infty} \|P_{\mathfrak{D}}(\rho(\alpha)) - P_{\mathfrak{D}}(\tilde{\rho}_{\infty})\| \leq C\left(|\lambda|^{2(1-\varepsilon)} + \frac{|\lambda|(1+|\lambda|)}{\varpi}\right), \tag{2.39}$$

*where $C$ is a finite constant independent of $\rho$, $A$, $\lambda$, $\eta$, $\varpi$, and $\alpha$.*

**Remark 2.20.** We stress, that our analysis does note require a *rotating wave approximation (RWA)*, which would amount to replacing $H_{\mathrm{P}} \cos(\varpi t)$ by a matrix of the type

$$\begin{pmatrix} 0 & \cdots & 0 & a e^{it\varpi} \\ \vdots & \ddots & \ddots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \bar{a} e^{-it\varpi} & 0 & \cdots & 0 \end{pmatrix}.$$

The RWA suppresses certain "rapidly oscillating" terms in the "interaction picture" of the equation (2.36), i.e. the evolution equation obtained by conjugating $\left\{\hat{\tau}_{t,s}^{(\lambda,\mu)}\right\}_{t\geq s}$ with the one parameter group $\left\{\hat{\tau}_{t,0}^{(0,0)}\right\}_{t\in\mathbb{R}}$. This approximation is physically meaningful if the *detuning*, $\Delta$, is small compared to the sum of the frequencies of the external light source, $\varpi$, and the energy difference of the atomic levels which are coupled i.e. $\Delta := |\varpi - (E_N - E_1)| \ll \varpi + (E_N - E_1)$. In our setting, we even have $\Delta = 0$, i.e. a resonant pump.

Having established the existence of a stationary state, we still need to derive a Pauli equation, for which $n(\infty) = P_{\mathfrak{D}}(\tilde{\rho}_{\infty})$. Denoting $P_{\mathfrak{D}}^{\perp} := \mathbf{1} - P_{\mathfrak{D}}$ we find the following integro–differential equation:

**Theorem 2.21 (The pre–master equation).**
*The family $\{\rho_{\mathfrak{D}}(\alpha)\}_{\alpha\geq 0}$ of density matrices defined by*

$$\rho_{\mathfrak{D}}(\alpha) := P_{\mathfrak{D}}\left(\exp\left(\alpha \Lambda^{(\lambda,\eta)}\right)\rho\right),$$

*for any initial density matrix $\rho \in \mathfrak{H}_{\mathrm{at}}$, obeys the integro–differential equation*

$$\begin{aligned} \frac{d}{d\alpha}\rho_{\mathfrak{D}}(\alpha) &= \lambda^2 \mathfrak{L}_{\mathcal{R}}(\rho_{\mathfrak{D}}(\alpha)) \\ &\quad + \frac{\eta^2}{4\lambda^2}\int_0^{\alpha\lambda^{-2}} P_{\mathfrak{D}}\mathfrak{L}_{\mathrm{p}}P_{\mathfrak{D}}^{\perp} e^{s\mathfrak{L}_{\mathcal{R}}} P_{\mathfrak{D}}^{\perp}\mathfrak{L}_{\mathrm{p}}P_{\mathfrak{D}}\left(\rho_{\mathfrak{D}}\left(\alpha - s\lambda^{-2}\right)\right) \mathrm{d}s, \end{aligned}$$

*called here the* pre–master equation. *Moreover,*

$$\mathfrak{B} := \int_0^{\infty} P_{\mathfrak{D}}\mathfrak{L}_{\mathrm{p}}P_{\mathfrak{D}}^{\perp} e^{s\mathfrak{L}_{\mathcal{R}}} P_{\mathfrak{D}}^{\perp}\mathfrak{L}_{\mathrm{p}}P_{\mathfrak{D}} \mathrm{d}s \in \mathcal{B}(\mathfrak{H}_{\mathrm{at}}),$$

*where the integral exists in norm.*

Now we introduce

$$B := \frac{\eta^2}{4\lambda^2}\mathfrak{B}$$

and

$$A := \lambda^2 \mathfrak{L}_{\mathcal{R}} P_{\mathfrak{D}}.$$

Since $\mathfrak{D}$ is an invariant space of $\mathfrak{L}_{\mathcal{R}}$ and $\mathfrak{B}$, we can define the Pauli Equation

$$\forall t \in \mathbb{R}_+ : \quad \frac{d}{dt} n(t) := (A + B)\, n(t), \quad n(0) \in \mathfrak{D}.$$

It has a unique solution which converges to $n(\infty) := P_{\mathfrak{D}}(\tilde{\rho}_\infty)$. Note, the following two facts:

1. The generator of the stimulated process, $B$, is indeed proportional to $\eta^2$, which measures the strength of the pump, i.e., its intensity.

2. The operator $B$ is a depends on $\mathfrak{L}_{\mathcal{R}}$, whose "diagonal entries", i.e., the part of $\mathfrak{L}_{\mathcal{R}}$ which acts non–trivially on $\mathfrak{D}$, defining the spontaneous process generated by $A$.

We refer to [BPW11a] for a discussion of the relation of $A$ and $B$ to the well-known "Einstein coefficients". Those coefficients are known to satisfy several restrictions and we derive analogues for the present setup.

## 2.3 Towards a Dynamical Renormalisation Group

In [BMW11], we study the long time dynamics of an open quantum system consisting of a two–level atom which is weakly coupled to the environment. The environment is modelled by a massless boson field at zero temperature. Assuming dilation analyticity of the Hamiltonian, we derive an effective generator for the evolution of the atomic- and low energy photon degrees of freedom and provide quantitative errors in the coupling constant. In the weak coupling limit our result reproduces the well known results of Davies, [Dav74, Dav75, Dav76], for our model. As already explained in Section 1.2, one expects for the type of model we investigate, that the weak coupling limit in the sense of Davies cannot be extended to times beyond the van Hove timescale. Our approach is a first step to develop a renormalisation group analysis that provides for a given timescale $\tau_n = tg^n$ an effective generator $H_{\mathrm{at}} + \mathfrak{T}_g^{(n)}(H_{\mathrm{f}})$ for the evolution of atomic- and low energy field degrees of freedom, as well as quantitative error bounds. The effective operator is obtained as the unique solution of an implicit equation.

We explain in Section 2.3.1 the isospectral Feshbach map, which is an important tool in our analysis. In Section 2.3.2, we present a standard result on $C_0$–semigroups, which expresses a $C_0$–semigroups in terms of the resolvent of its generator. This is the starting point for our analysis in [BMW11]. Then, deformation analyticity and in particular dilation analyticity are defined in Section 2.3.3. Finally, our main result is presented in Section 2.3.4. In Section 2.3.4 we also discuss the relation of our work to results on resonances and metastable states.

### 2.3.1 The Isospectral Feshbach Map

We present here a new variant of the the Feshbach map for matrices, which has been introduced in [BCFS03], namely the *smooth Feshbach map*. In [BMW11] we use in fact the conventional Feshbach map, but as smooth

Feshbach map can easily be related to the conventional one, and has proven to provide significant simplifications in the renormalisation group analysis of singular perturbation theory, [BFS98b, BCFS03], we believe it is of interest for the reader. We also use [GH08], where some assumptions of [BCFS03] connected to the isospectrality could be generalised. Let $\mathcal{H}$ be a separable Hilbert space and $\chi$ and $\overline{\chi}$ be commuting, non–zero bounded operators on $\mathcal{H}$ and satisfying

$$\chi^2 + \overline{\chi}^2 = 1. \tag{2.40}$$

Let

$$H, T : \mathcal{D}(H) = \mathcal{D}(T) \to \mathcal{H},$$

be closed operators and set $W := H - T$. Moreover, we use the abbreviations

$$\begin{aligned} W_\chi &:= \chi W \chi, & W_{\overline{\chi}} &:= \overline{\chi} W \overline{\chi}, \\ H_\chi &:= T + W_\chi, & H_{\overline{\chi}} &:= T + W_{\overline{\chi}}, \end{aligned}$$

where all operators are defined on $\mathcal{D}(T)$. Then, we have the following definition.

**Definition 2.22 (Feshbach pair).** The pair of operators $(H, T)$ is called *Feshbach pair for $\chi, \overline{\chi}$*, or short *Feshbach pair*, iff
(i) $\chi T \subseteq T\chi$ and $\overline{\chi} T \subseteq T\overline{\chi}$,
(ii) $T, H_{\overline{\chi}} : \mathcal{D}(T) \cap \operatorname{ran}(\overline{\chi}) \to \operatorname{ran}(\overline{\chi})$ are bijections with bounded inverse
(iii) $\overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi} W \chi : \mathcal{D}(T) \to \mathcal{H}$ is a bounded operator.

At several stages inverse operators on subspaces are considered. We say $A : \mathcal{D}(A) \to \mathcal{H}$ is *bounded invertible on a subspace $V$*, if its restriction to $V$ is bounded invertible. Note that

$$\chi W \overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi} = \chi H \overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi} - \chi T \overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi}$$

is bounded by (i) and (ii).

**Definition 2.23 (Smooth Feshbach map).** Let $\chi$ and $\overline{\chi}$ be commuting, non–zero bounded operators on $\mathcal{H}$ and satisfying (2.40) and $(H, T)$ be a Feshbach pair. The *Feshbach map* is defined as

$$F_\chi(H, T) := H_\chi - \chi W \overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi} W \chi.$$

It is also useful to introduce the following auxiliary operators

$$\begin{aligned} Q_\chi &:= \chi - \overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi} W \chi \\ Q_\chi^\sharp &:= \chi - \chi W \overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi}. \end{aligned}$$

With these prerequisites, we have the following theorem.

**Theorem 2.24 (Feshbach isospectrality).** *Let $\chi$ and $\overline{\chi}$ be commuting, non–zero bounded operators on $\mathcal{H}$ and satisfying (2.40) and $(H, T)$ be a Feshbach pair.*

*Then, the following holds:*
*(i) Let $V$ be a subspace with* $\mathrm{ran}\,(\chi) \subseteq V$ *and* $T : \mathcal{D}(T) \cap V \to V$, $\overline{\chi} T^{-1} \overline{\chi} V \subseteq V$, *then $H$ is bounded invertible iff* $F_\chi (H, T) : \mathcal{D}(T) \cap V \to V$ *is bounded invertible in $V$. Moreover,*

$$\begin{aligned} H^{-1} &= Q_\chi F_\chi (H, T)^{-1} Q_\chi^\sharp + \overline{\chi} H_{\overline{\chi}}^{-1} \overline{\chi}, \\ F_\chi (H, T)^{-1} &= \chi H^{-1} \chi + \overline{\chi} T^{-1} \overline{\chi}. \end{aligned}$$

*(ii)* $\chi \ker (H) \subseteq \ker (F_\chi (H, T))$ *and* $Q_\chi \ker (F_\chi (H, T)) \subseteq \ker (H)$. *Moreover,*

$$\begin{aligned} \chi : \ker (H) &\to \ker (F_\chi (H, T)), \\ Q_\chi : \ker (F_\chi (H, T)) &\to \ker (H), \end{aligned}$$

*are linear isomorphisms and inverse to each other.*

It remains to relate the smooth Feshbach map to the original Feshbach map, [BFS98a, BFS98b], where $\chi = P$ and $P$ is an orthogonal projection, i.e. $P^2 = P$ and $P^* = P$. In this case, we may set $T := PHP + \overline{P} H \overline{P}$, where $\overline{P} := 1 - P$, and obtain

$$PF_P (H, T) P = PHP - PH\overline{P} \left( \overline{P} H \overline{P} \right)^{-1} \overline{P} HP =: F_P (H),$$

where $F_P (H)$ is the original Feshbach map.

### 2.3.2 An Inverse Laplace Transform

The starting point of our analysis in [BMW11] is the following result on $C_0$–semigroups. It is in fact the inverse Laplace transform of the resolvent of the generator, [ABHN01, Thm. 3.12.2].

**Theorem 2.25.** *Let $\mathfrak{X}$ be a Hilbert space and* $\{\mathcal{T}(t)\}_{t \in \mathbb{R}_0^+}$ *be a $C_0$–semigroup with generator $A$ and*

$$\|\mathcal{T}(t)\| \le M e^{\omega(\mathcal{T}) t}, \quad M > 0,\ \omega(\mathcal{T}) \in \mathbb{R}.$$

*Then, for all $t > 0$, $x \in \mathfrak{X}$, $\omega > \omega(\mathcal{T})$, we have*

$$\mathcal{T}(t)\, x = \lim_{k \to \infty} \frac{1}{2\pi} \int_{-k}^{k} e^{(\omega + is)} (\omega + is - A)^{-1} x. \tag{2.41}$$

**Remark 2.26.** (i) The preceding theorem is not valid for general Banach spaces. However, if one replaces the assumption $x \in \mathfrak{X}$ by $x \in \mathcal{D}(A)$, then an analogue statement is true for Banach spaces.

(ii) Even though (2.41) is an expression for positive $t$, a representation for unitary groups can be obtained by means of Stone's Formula, [RS80a, Thm. VII.13].

(iii) If the spectrum of $A$ is contained in a sector of angle $< \pi$, the integration (2.41) can be deformed to an appropriately chosen contour. This has the advantage, that one can get rid of the "symmetric limit", $\lim_{k \to \infty} \frac{1}{2\pi} \int_{-k}^{k} \dots$, and several parts of the contour may be discussed separately. In [BMW11] we just do that in order to obtain Theorem 2.30.

### 2.3.3 Dilation Analyticity

Complex deformation techniques have first been used by Balslev and Combes in the context of $N$-body Schrödinger operators, [BC71]. The interaction is usually assumed to be relatively compact with respect to the free Hamiltonian, which is not the case for our model. I.e. let

$$H = H_0 + V,$$

where $H_0$ is selfadjoint and $V$is relatively compact. If the complex deformed $V$, $V_\xi$ is relatively compact w.r.t. the complex deformed $H_0$, denoted by $H_{0,\xi}$, then one can conclude by Weyl's Theorem, [RS78, Thm. XIII.14], that the essential spectrum of the deformed Hamiltonian $H_\xi = H_{0,\xi} + V_\xi$ equals the essential spectrum of the deformed "free" Hamiltonian, i.e.

$$\sigma_{\text{ess}}\left(H_\xi\right) = \sigma_{\text{ess}}\left(H_{0,\xi}\right).$$

In particular, if the essential spectrum of $H_{0,\xi}$ is only in one half plane, then this also holds for $H_\xi$. In our model, the interaction $\phi(G)$ of the quantised boson field is not relatively compact with respect to the free energy. Therefore, the essential spectrum can in general be spread in the lower and upper half plane. In view of (2.41) this means that we pick up exponential growth in those regions.

Next we define the complex deformation relevant for our application. It is useful to introduce the following notion.

**Definition 2.27 (Type A families).** For some open subset $\mathcal{B} \subseteq \mathbb{C}$, a family $\left\{H_\xi\right\}_{\xi\in\mathcal{B}}$ of closed operators defined on a Banach space $\mathfrak{X}$ is of said to be of *type A* iff $\mathcal{D}\left(A_\xi\right) = \mathfrak{Y} \subseteq \mathfrak{X}$ for all $\xi \in \mathcal{B}$ and the map

$$\mathcal{B} \ni \xi \mapsto H_\xi x$$

is analytic for all $x \in \mathfrak{Y}$.

We have the following well-known result on type A families, see [Kat76, Sect. VII.2, Thm. 1.3].

**Lemma 2.28 (Resolvents of type A families).** *Let $\left\{H_\xi\right\}_{\xi\in\mathcal{B}}$ be a type A family and $z \in \varrho\left(H_{\xi_0}\right)$, where $\varrho\left(H_{\xi_0}\right)$ is the resolvent set of $H_{\xi_0}$ and $\xi_0 \in \mathcal{B}$. Then,*

$$\xi \mapsto \left(z - H_\xi\right)^{-1} \tag{2.42}$$

*is analytic in some neighbourhood of $\xi_0$.*

Lemma 2.28 implies that the resolvent set of $H_{\xi_0}$ is preserved in the vicinity of the given $\xi_0$. In applications, we usually have a–priori knowledge on the resolvent set for the free Hamiltonian for any $\xi_0 \in \mathcal{B}$. In our situation, we are lead to stronger statements than Lemma 2.28, where analyticity of (2.42) is even true for some strip around the real axis.

Let now $H_g$ be defined as in (1.6), $N = 2$, $d = 3$, and $\omega(k) := |k|$, $\forall k \in \mathbb{R}^3$. Let $f \in \mathfrak{h}$ and define the unitary strongly continuous one-parameter group of dilations, $u(\cdot)$, on the space $\mathfrak{h}$ by $(u(\alpha)f)(r,\Omega) :=$

$e^{-\frac{3}{2}\alpha} f\left(e^{-\alpha} r, \Omega\right)$, using *polar coordinates*, $(r, \Omega)$. Its second quantised analogue is denoted by $U(\alpha) := \Gamma(u(\alpha))$. $U$ leaves the domain of $H_0$, $\mathcal{D}(H_0)$, invariant and one easily computes

$$H_{0,\alpha} = H_{\mathrm{at}} + e^{-\alpha} H_{\mathrm{f}}, \ \forall \alpha \in \mathbb{R}. \tag{2.43}$$

For any $\xi \in \mathbb{C}$,

$$H_{0,\xi} = H_{\mathrm{at}} + e^{-\xi} H_{\mathrm{f}},$$

is a closed and even normal operator on $\mathcal{H}_{\mathrm{at}} \otimes \mathcal{D}(H_{\mathrm{f}})$, as $\mathcal{H}_{\mathrm{at}}$ is finite dimensional. Moreover, $\left\{H_{0,\xi}\right\}_{\xi \in \mathbb{C}}$ is a family of type A. From

$$\frac{1}{\left(z - e^{-\xi} x - E_\ell\right)} = \frac{e^{\xi}}{\left(e^{\xi} z - x - e^{\xi} E_\ell\right)},$$

it follows by functional calculus of the selfadjoint operator $H_{\mathrm{f}}$, that $z \in \varrho\left(H_{0,\xi}\right)$ iff

$$e^{\xi} z \in \mathbb{C} \setminus \left(e^{\xi}\left\{E_0, E_1\right\} + \mathbb{R}_0^+\right),$$

and hence

$$\sigma\left(H_{0,\xi}\right) = \left\{E_0, E_1\right\} + e^{\xi} \mathbb{R}_0^+.$$

We introduce now a condition on the coupling functions, which insures that the full Hamiltonian gives rise to a family of type A. For matrix–valued functions, we use the convention that the norm is the operator norm on $\mathfrak{B}\left(\mathbb{C}^2\right)$ and we write again $\|G\|_{\mathfrak{h}_\omega}$ instead of $\|G\|_{\mathfrak{h}_\omega \otimes \mathbb{C}^{2\times 2}}$ if $G$ is matrix–valued.

**Condition 2.29 (Coupling functions).** Let $\xi_0 \in \left(0, \frac{\pi}{2}\right)$ and the *coupling function*, $G$, be an element of $L^2\left(\mathbb{R}^3, \mathfrak{B}\left(\mathcal{H}_{\mathrm{at}}\right)\right)$. The map $\mathbb{R} \ni \alpha \mapsto G_\alpha := u(\alpha) G$ extends to an analytic function in the strip $I\left(\xi_0\right) := \mathbb{R} + i(-\xi_0, \xi_0)$ and

$$\sup_{|\theta| < \xi_0} \left\|G_{\alpha + i\theta}\right\|_{\mathfrak{h}_\omega} < \infty. \tag{2.44}$$

Moreover,

$$G(k) = G(|k|), \quad (G(k))_{\ell\ell} = 0, \quad \forall k \in \mathbb{R}^3, \ \ell = 0, 1. \tag{2.45}$$

There is a $c_{2.29} \in \mathbb{R}_+$, such that

$$\|G(k)\| \leq \frac{c_{2.29}}{\sqrt{|k|}}, \quad \forall k \in \mathbb{R}^3. \tag{2.46}$$

Finally, assume that $\|G(k)\| \to 0$ sufficiently rapid, as $|k| \to \infty$. We refer to the sufficiently fast convergence $\|G(k)\| \to 0$ as the *ultraviolet cutoff.*

Finally, on the domain $\mathcal{H}_{\mathrm{at}} \otimes \mathcal{F}_{\mathrm{fin}}$ we define for $\xi \in I\left(\xi_0\right)$,

$$\check{\phi}\left(G_\xi\right) := \frac{1}{\sqrt{2}}\left(a\left(G_{\bar{\xi}}\right) + a^\dagger\left(G_\xi\right)\right). \tag{2.47}$$

Note, that we used $\bar{\xi}$ for the annihilation operator, $a(\cdot)$, since it is antilinear in the argument. On the domain $\mathcal{H}_{\mathrm{at}} \otimes \mathcal{D}(H_{\mathrm{f}})$, we define the closed operator

$$H_{g,\xi} := H_{0,\xi} + \check{\phi}\left(g G_\xi\right). \tag{2.48}$$

As $\check{\phi}\left(G_\xi\right)$ is infinitesimally $H_{\mathrm{f}}$ bounded, it follows that $H_{g,\xi}$ is a family of type A.

### 2.3.4 Main Result and Resonance Theory

We distinguish two different problems of perturbation theory of eigenvalues, the *regular perturbation theory*, where the eigenvalue to be localised is an element of the discrete spectrum of the unperturbed operator and the *singular perturbation theory*, where the eigenvalue is in the essential spectrum. More specifically, let

$$H_g := H_0 + gW,$$

where $H_0$ is assumed to be selfadjoint, $W$ is a relatively $H_0$–bounded perturbation of $H_0$. Then, assume that $\lambda$ is an eigenvalue of $H_0$ with multiplicity $m \in \mathbb{N}$. If $\lambda \in \sigma_{\text{disc}}(H_0)$, or if there is a *complex deformation*[1] $H_{0,\xi}$, of $H_0$, such that $\lambda \in \sigma_{\text{disc}}\left(H_{0,\xi}\right)$ one can analyse the spectrum by means of the Riesz projection,

$$P(\lambda) := \frac{-1}{2\pi i} \oint_{\gamma} dz \, \left(H_{g,\xi} - z\right)^{-1}, \tag{2.49}$$

for sufficiently small $g$. Here, $\gamma$ is a contour in the resolvent set of $H_{0,\xi}$ which encloses $\lambda$ as the only spectral point of $H_{0,\xi}$ and $H_{g,\xi}$ is the "complex deformed" $H_g$. We have already seen in Section 2.1.3 that excited eigenvalues may be unstable and it is possible to estimate the decay of matrix elements

$$\begin{aligned} (\psi, f(H_g)e^{-itH_g}\psi) &= \left(1 + \mathcal{O}\left(g^2\right)\right) e^{-it\lambda(g)} + b(t,g), \, \mathrm{Im}(\lambda(g)) > 0, \\ |b(t,g)| &\leq o\left(g^2\right)(1+t)^{-N}, \quad \forall N \in \mathbb{N}, \, t \geq 0, \end{aligned} \tag{2.50}$$

provided Fermi Golden Rule holds and the resolvent, $\left(H_g - z\right)^{-1}$, is sufficiently regular with respect to some auxiliary operator $A$. In Section 2.3.3 we consider the case where $A$ is selfadjoint and the resolvent is even analytic in a strip around the real axis with respect to the conjugation with the group generated by $A$. In the context of regular perturbation theory there are strong results on the decay rate of the resonances. These results do usually assume a deformation analyticity of the Hamiltonian $H_g$, in order to separate the essential form the discrete spectrum, but they to not require a Mourre estimate. The first result which provided rigorous estimates on the decay law of resonances states is due to Hunziker, [Hun90]. He proves a result with the same consequences as in Theorem 2.10, but the error term $b(t,g)$ decays as $(1+t)^{-n}$ for any $n \in \mathbb{N}$, instead of some fixed $n$ related to the regularity of the resolvent. Both results, [CGH06] and [Hun90], depend on the function $f(\cdot)$, which localises the group $e^{-itH_g}$ to a small interval around the eigenvalue $\lambda$. For a different choice of $f$, namely assuming that $f$ is of Gevrey class, Rama and Klein proved recently, [KR10], that for an abstract dilation analytic model that $b(t,g)$ is almost exponentially decaying,

$$|b(t,g)| \leq o\left(g^2\right) e^{-Ct^{\frac{1}{a}}}, \quad C \leq ac^{\frac{1}{a}},$$

[1] See Section 2.3.3.

for any $a > 1$, $c > 0$ and $g$ sufficiently small. Finally, in the case of finite temperature, Jaksic and Pillet developed in [JP95, JP96a, JP96b] a complex deformation technique, a complex translation, which allows to deform Liouvilleans such that the discrete spectrum is separated from the essential spectrum, even if the reservoir arises from a massless field. In this vein the problem becomes tractable by regular perturbation theory, whereas this is not possible for the generator of dilations.

In the context of singular perturbation theory, more specifically in massless quantum field theoretic models, resonances have first been analysed by Bach, Fröhlich and Sigal, [BFS98a]. Their analysis is based on the *isospectral Feshbach map*. The Feshbach map has as an intrinsic feature a reduction of state space. An iteration based on an repeated decimation of the state space lead to the construction of a *renormalisation group analysis*, which provides an algorithm to localise the resonance to arbitrary precision, [BFS98b, BCFS03]. The first result to determine the decay rate of (2.50) for dilation analytic, massless, quantum field theoretic models has been established in [BFS99], using a single step Feshbach map analysis. The result proved there is of the same type than the result by Hunziker, [Hun90]. In a more recent paper Hasler, Herbst and Huber proved also a lower bound on the decay rate of (2.50). Their analysis is also based on the Feshbach map, see [HHH08].

In [BMW11] we provide a detailed analysis of the dynamics generated by a two level spin boson model, with a dispersion relation $\omega(k) = |k|$, restricted to low field energies. More precisely, let $H_g$ be defined by (1.6), with $N = 2$ and eigenvalues of $H_{\mathrm{at}}$, $E_1 > E_0$. We prove for the complex deformed operator, $H_{g,\xi}$, see Section 2.3.3, a result, which we present here in a simplified version.

**Theorem 2.30 (Bach–Møller–W. '11).** *Let*

$$X_{g,\xi}(t) := e^{-itH_{g,\xi}}$$

*and* $\rho = g^{\mu}$, $\mu \in (0,2)$, *and pick* $\nu \in \left(0, \min\left(1, \mu^{-1} - \frac{1}{2}\right)\right)$. *There is a bounded operator,* $\Xi_{g,\xi}(H_{\mathrm{f}})$, *with* $\left[\Xi_{g,\xi}(H_{\mathrm{f}}), H_{0,\xi}\right] = 0$, *such that for any* $t \in \mathbb{R}_+$,

$$\begin{aligned}&\left\| \boldsymbol{1}[H_{\mathrm{f}} < \rho]\, X_{g,\xi}(t)\, \boldsymbol{1}[H_{\mathrm{f}} < \rho] - e^{-it\Xi_{g,\xi}(H_{\mathrm{f}})} \right\| \\ &\leq C\left(e^{-tc_2} + e^{c_1 g^2 \rho^{\nu} t}\left(\rho^{\frac{1-\nu}{2}} + g^{\frac{1}{2}} \rho^{-\frac{1}{2}\left(\nu + \frac{1}{2}\right)}\right)\right),\end{aligned}$$

*for some* $C, c_0, c_1, c_2 \in \mathbb{R}_+$, *which are independent of* $g$. *Moreover, for* $\ell = 0, 1$, $r \in [0, \rho]$ *and* $P_{\mathrm{at},\ell} := \boldsymbol{1}[H_{\mathrm{at}} = E_\ell] \otimes \boldsymbol{1}[H_{\mathrm{f}} < \rho]$,

$$\Xi_{g,\xi}(r)\, P_{\mathrm{at},\ell} = \left(E_\ell + e^{-\xi} r - g^2 \widetilde{\Lambda}_{\ell\ell}(0, E_\ell)\right) P_{\mathrm{at},\ell} + \mathcal{O}\left(g^2 \rho\right).$$

*Here, we used for* $\ell = 0, 1$ *the abbreviation*

$$\widetilde{\Lambda}_{\ell\ell}(0, E_\ell) := \int_0^\infty dk\, \frac{e^{-3\xi} k^2 \left|(G)_{(1-\ell)\ell}\left(e^{-\xi} k\right)\right|^2}{E_{1-\ell} - E_\ell + e^{-\xi} k}.$$

**Remark 2.31.** (i) It is possible to relate $\widetilde{\Lambda}_{\ell\ell}(0, E_\ell)$ to objects which are $\xi$ independent. For the ground state, $\ell = 0$, this yields a correction in second order of $g$ with vanishing imaginary part $= 0$. For the excited state, $\ell = 1$, the obtained correction has a negative imaginary part, provided Fermi Golden Rule holds.
(ii) To our knowledge, the evolution of the ground state has previously not been addressed in singular perturbation theory. Note, that the error contains an exponentially growing factor, $e^{c_1 g^2 \rho^\nu t}$, which is due to contributions of the ground state. This exponential growth is however of a mild type, as it becomes constant on the van Hove timescale, where $tg^2 = \text{const.}$ as $g \to 0$.
(iii) The optimal choice of $\mu$ depends on the value of $t$. If one chooses $\mu = \frac{2}{3}$, then $\rho^{\frac{1-\nu}{2}} = g^{\frac{1}{2}} \rho^{-\frac{1}{2}(\nu+\frac{1}{2})}$.
(iv) Our result reproduces Davies results in the weak coupling limit, but also provides quantitative bounds.

## 2.4 Bibliography


[ABHN01] W. Arendt, C. J. K. Batty, M. Hieber, and F. Neubrander, *Vector–valued laplace transforms and cauchy problems*, Monographs in Mathematics, vol. 96, Birkhäuser Verlag, 2001.

[AdMG96] W. Amrein, A. Boutet de Monvel, and V. Georgescu, *$c_0$-groups, commutator methods, and spectral theory of n-body Hamiltonians*, Birkhäuser, 1996.

[AL07] R. Alicki and K. Lendi, *Quantum dynamical semigroups and applications*, Lecture Notes in Phys., vol. 286, Springer, 2007.

[Ali76] R. Alicki, *On the detailed balance condition for non-Hamiltonian systems*, Rep. on Math. Phys. **2** (1976), 249–258.

[BC71] E. Balslev and J. M. Combes, *Spectral properties of Schrödinger operators with dilatation analytic potentials*, Commun. Math. Phys. **22** (1971), 280–294.

[BCFS03] V. Bach, T. Chen, J. Fröhlich, and I. M. Sigal, *Smooth Feshbach map and operator-theoretic renormalization group methods*, J. Funct. Anal. **203** (2003), no. 1, 44–92.

[BFS98a] V. Bach, J. Fröhlich, and I. M. Sigal, *Quantum electrodynamics of confined non-relativistic particles*, Adv. in Math. **137** (1998), 299–395.

[BFS98b] ———, *Renormalization group analysis of spectral problems in quantum field theory*, Adv. in Math. **137** (1998), 205–298.

[BFS99] V. Bach, J. Fröhlich, and I. M. Sigal, *Spectral analysis for systems of atoms and molecules coupled to the quantized radiation field*, Commun. Math. Phys. **207** (1999), no. 2, 249–290.

[BFS00] ———, *Return to equilibrium*, J. Math. Phys. **41** (2000), no. 6, 3985–4060.

[BMW11] V. Bach, J. Møller, and M. Westrich, *Towards a dynamical renormalisation group*, in preparation (2011).

[BPW11a] J.-B. Bru, W. Pedra, and M. Westrich, *Characterisation of the quasi-stationary state of an impurity driven by monochromatic light I - The effective theory*, in preparation (2011).

[BPW11b] ______, *Characterisation of the quasi-stationary state of an impurity driven by monochromatic light II - Microscopic foundations*, in preparation (2011).

[BR87] O. Bratteli and D. Robinson, *Operator algebras and quantum statistical mechanics 1*, 2 ed., Text and Monographs in Physics, Springer-Verlag, Berlin, 1987.

[BR96] ______, *Operator algebras and quantum statistical mechanics 2*, 2 ed., Text and Monographs in Physics, Springer-Verlag, Berlin, 1996.

[CGH06] L. Cattaneo, G.M. Graf, and W. Hunziker, *A general resonance theory based on Mourre's inequality*, Ann. Henri Poincaré **7** (2006), no. 3, 583–601.

[Dav74] E. B. Davies, *Markovian master equations*, Commun. Math. Phys. **39** (1974), 91–110.

[Dav75] ______, *Markovian master equations III*, Markovian Master Equations III **XI** (1975), 265–273.

[Dav76] ______, *Markovian master equations II*, Math. Ann. **219** (1976), 147–158.

[DF06] J. Derezinski and R. Früboes, *Fermi Golden Rule and Open Quantum Systems*, Open Quantum Systems III, vol. 1882, Springer Verlag, 2006, pp. 67–116.

[DG99] J. Derezinski and C. Gérard, *Asymptotic completeness in quantum field theory. massive Pauli-Fierz Hamiltonians*, Rev. Math. Phys. **11** (1999), no. 4, 383–450.

[DRM08] J. Derezinski, W. De Roeck, and C. Maes, *Fluctuations of quantum currents and unravelings of master equations*, J. Stat. Phys. **131** (2008), 341–356.

[FGKV77] A. Frigerio, V. Gorini, A. Kossakowski, and M. Verri, *Quantum detailed balance and kms condition*, Comm. Math. Phys. **57** (1977), 97–110.

[FGKV78] ______, *Erratum: Quantum detailed balance and KMS condition*, Comm. Math. Phys. **60** (1978), 96.

[FGS08] J. Fröhlich, M. Griesemer, and I.M. Sigal, *Commun. math. phys.*, Spectral Theory for the Standard Model of Non-Relativistic QED **283** (2008), 613–646.

[FMS11a] J. Faupin, J. S. Møller, and E. Skibsted, *Regularity of bound states*, Rev. in Math. Phys. (2011).

[FMS11b] ———, *Second order perturbation theory for embedded eigenvalues*, Comm. Math. Phys. (2011).

[GGM04] V. Georgescu, C. Gerard, and J. Moeller, *Commutators, $C_0$−semigroups and resolvent estimates*, J. Funct. Anal. **216** (2004), 303–361.

[GH08] M. Griesemer and D. Hasler, *On the smooth Feshbach–Schur map*, J. of Funct. Anal. **254** (2008), 2329–2335.

[GKS76] V. Gorini, A. Kossakowski, and E.C.G. Sudarshan, *Completely positive dynamical semigroups of n-level systems*, J. of Math. Phys. **17** (1976), 821–825.

[Haa55] R. Haag, *On quantum field theories*, Matematiske-fysiske Meddelelser **29** (1955), 1–37.

[HH08] D. Hasler and I. Herbst, *On the self–adjointness and domain of Pauli-Fierz type hamiltonians*, Rev. in Math. Phys. **20** (2008), 787–800.

[HHH08] D. Hasler, I. Herbst, and M. Huber, *On the lifetime of quasi-stationary states in non-relativistic QED*, Ann. Henri Poincaré **9** (2008), 1005–1028.

[Hun90] W. Hunziker, *Resonances, metastable states and exponential decay laws in perturbation theory*, Commun. Math. Phys. **132** (1990), 177–188.

[JMP84] A. Jensen, E. Mourre, and P. Perry, *Multiple commutator estimates and resolvent smoothness in quantum scattering theory*, Ann. Inst. Henri Poincaré **41** (1984), 207–225.

[JP95] V. Jakšić and C. A. Pillet, *On a model for quantum friction. I: Fermi's golden rule and dynamics at zero temperature*, Ann. Inst. H. Poincaré **62** (1995), 47–68.

[JP96a] ———, *On a model for quantum friction. II: Fermi's golden rule and dynamics at positive temperature*, Commun. Math. Phys. **176** (1996), no. 3, 619–643.

[JP96b] ———, *On a model for quantum friction III: Ergodic properties of the spin-boson system*, Commun. Math. Phys. **178** (1996), no. 3, 627–651.

[JP02] ———, *Non-equilibrium steady states of finite quantum systems coupled to thermal reservoirs*, Comm. Math. Phys. **226** (2002), 131–162.

[Kat76] T. Kato, *Perturbation theory of linear operators*, 2 ed., Grundlehren der mathematischen Wissenschaften, vol. 132, Springer-Verlag, 1976.

[KR10] M. Klein and J. Rama, *Almost exponential decay of quantum resonance states and Paley-Wiener type estimates in Gevrey spaces*, Ann. Henri Poincaré **11** (2010), 499–537.

[Kos00] Andrzej Kossakowski, *On higher order weak coupling limits i*, Open Systems and Information Dynamics **7** (2000), 201–208.

[Lin76] G. Lindblad, *On the generators of quantum dynamical semigroups*, Commun. Math. Phys. **2** (1976), 119–130.

[Mou81] E. Mourre, *Absence of singular continuous spectrum for certain self-adjoint operators*, Comm. Math. Phys. **78** (1981), 391–408.

[Mou83] ______, *Opérateurs conjugués et propriétés de propagation*, Comm. Math. Phys. **91** (1983), 279–300.

[MW11] J. S. Møller and M. Westrich, *Regularity of Eigenstates in Regular Mourre-Theory*, Journal of Funct. Anal. **260** (2011), 852–878.

[PSS81] P. Perry, I. M. Sigal, and B. Simon, *Spectral analysis of n-body Schrödinger operators*, Annals Math. **114** (1981), 519–567.

[Ras10] M. G. Rasmussen, *Spectral and scattering theory for translation invariant models in quantum field theory*, Ph.D. thesis, Aarhus University, June 2010.

[RS78] M. Reed and B. Simon, *Methods of modern mathematical physics: Analysis of operators*, 1 ed., vol. 4, Academic Press, San Diego, 1978.

[RS80a] ______, *Methods of modern mathematical physics: I. Functional analysis*, 2 ed., vol. 1, Academic Press, San Diego, 1980.

[RS80b] ______, *Methods of modern mathematical physics: II. Fourier analysis and self-adjointness*, 2 ed., vol. 2, Academic Press, San Diego, 1980.

[Sah97] J. Sahbani, *The conjugate operator method for locally regular Hamiltonians*, J. Operator Theory **38** (1997), 297–322.

[Sim72] B. Simon, *Quadratic form techniques and the Balslev-Combes theorem*, Commun. math. Phys. **27** (1972), 1–9.

# Part II

# Regularity of Eigenstates in Regular Mourre Theory

CHAPTER 3

# Regularity of Eigenstates in Regular Mourre Theory

J. S. MØLLER AND M. WESTRICH

**Abstract**

The present paper gives an abstract method to prove that possibly embedded eigenstates of a self-adjoint operator $H$ lie in the domain of the $k$th power of a conjugate operator $A$. Conjugate means here that $H$ and $A$ have a positive commutator locally near the relevant eigenvalue in the sense of Mourre. The only requirement is $C^{k+1}(A)$ regularity of $H$. Regarding integer $k$, our result is optimal. Under a natural boundedness assumption of the multiple commutators we prove that the eigenstate 'dilated' by $\exp(i\theta A)$ is analytic in a strip around the real axis. In particular, the eigenstate is an analytic vector with respect to $A$. Natural applications are 'dilation analytic' systems satisfying a Mourre estimate, where our result can be viewed as an abstract version of a theorem due to Balslev and Combes, [BC71]. As a new application we consider the massive Spin-Boson Model.

## 3.1 Introduction and main results

In this paper we study regularity of eigenstates $\psi$ of a self-adjoint operator $H$, with respect to an auxiliary operator $A$ for which $i[H,A]$ satisfies a so-called Mourre estimate near the associated eigenvalue $\lambda$. Our results are partly an extract of a recent work of Faupin, Skibsted and one of us [FlS10a], and partly an improvement of a result of Cattaneo, Graf and Hunziker [CGH06]. We consider in the present work the case of regular Mourre theory, where the derivation of the bounds on $A^k\psi$ is simpler compared to [FlS10a]. In fact we derive explicit bounds which are independent of proof technical constructions. The bounds are good enough to formulate a natural condition on the growth of norms of multiple commutators which ensures that eigenstates are analytic vectors with respect to A. We discuss how these growth conditions may be checked in concrete examples and illustrate this for dilation analytic $N$-body Hamiltonians and the massive Spin-Boson Model.

The general strategy in this paper, as well as in [CGH06] and [FlS10a], is to implement a Froese-Herbst type argument, [FH82], in an abstract setting. In a formal computation the Mourre estimate suffices to extract results of the type presented here but to make the argument rigorous one has to impose enough conditions on the pair of operators $H$ and $A$ to enable a calculus of operators. This is usually done by requiring a number of iterated commutators between $H$ and $A$ to exist and be controlled by operators already present in the calculus. The type of conditions imposed is typically guided by a set of applications that the authors have in mind. Most examples, like many-body quantum systems with or without external classical fields, have been possible to treat using natural extensions of conditions originally introduced by Mourre in [Mou81]. The same goes for a number of models in non-relativistic QED like confined massive Pauli-Fierz models and massless models, with $A$ being the generator of dilations. These are the type of conditions used in [CGH06].

Over the last 10 years a number of models that fall outside the scope of Mourre's original conditions, and hence not covered by [CGH06], have appeared. We split them into two types. The first type are models that, while not covered by Mourre type conditions on iterated commutators, still satisfy weaker conditions developed over some years by Amrein, Boutet de Monvel, Georgescu and Sahbani [AdMG96, Sah97]. These conditions play the same role as Mourre's original conditions in that they enable the same type of calculus of the operators $H$ and $A$. We call this setting for *regular Mourre theory*. Examples of models that fall in this category but are not covered by Mourre type conditions as in [CGH06], are: $P(\phi)_2$-models [DG00] (with $P(\varphi) \neq \varphi^4$), the renormalised massive Nelson model [Amm00], Pauli-Fierz type models without confining potential [FGS01], the standard model of non-relativistic QED near the ground state energy, where only local $C^k$ conditions are available [FGS08], and the translation invariant massive Nelson model [MR10].

The second type of models we wish to highlight are those for which the commutator $H' = i[H, A]$ is not comparable to $H$ (or $A$). Here one views the commutator as a new operator in the calculus and impose assumptions of mixed iterated commutators between the three possibly unbounded operators $H, A$ and $H'$. This type of analysis goes back to [Ski98] and was further developed in [MS04] and [GGM04a]. This situation we call *singular Mourre theory* and is the topic considered in [FlS10a]. There are two examples where this type of analysis is natural. The first is massless Pauli-Fierz models with $A$ being the generator of radial translations [DJ01, GGM04b, FlS10a, FlS10b, Ski98, Gol09] and the second is many-body systems with time-periodic pair-potentials, in particular AC-Stark Hamiltonians [MS04, FlS10a]. The technical complications arising from having to deal with a calculus of three unbounded operators are significant.

Part of the motivation of this work is to extract the essence of [FlS10a] in the context of regular Mourre theory, where the technical overhead is more manageable.

A second motivating factor is drawn from the paper [FlS10b], which is in fact intimately connected to [FlS10a]. We remind the reader of the Fermi Golden Rule (FGR) which we now formulate. Let $P$ denote the orthogonal projection onto the span of the eigenvector $\psi$, and abbreviate $\bar{P} = I - P$. The FGR states that a, for simplicity isolated and simple, embedded eigenvalue is unstable under a perturbation $W$ provided

$$\mathrm{Im}\Big(\lim_{\epsilon\to 0+}\langle W\psi, \bar{P}(\bar{H}-\lambda-i\epsilon)^{-1}\bar{P}W\psi\rangle\Big) \neq 0. \tag{3.1}$$

Here $\bar{H} = \bar{P}H\bar{P}$ is an operator on the range of $\bar{P}$. In the above statement the existence of the limit is of course implicitly assumed. Due to the presence of the projection $\bar{P}$, the operator $\bar{H}$ has purely continuous spectrum near the eigenvalue $\lambda$, and the existence of the limit can thus be inferred from the *limiting absorption principle* (LAP). The LAP can be deduced using positive commutator estimates, see e.g. [AdMG96], provided there exists an auxiliary operator $A$ such that $H$ and $A$ satisfy a Mourre estimate near $\lambda$ and $(\bar{H}-i)^{-1}$ admits two bounded commutators with $A$, or more precisely $H$ is of class $C^2(\bar{P}A\bar{P})$ (see the next subsection). This implies in particular that $\mathrm{ran}(P) \subseteq \mathcal{D}(A^2)$, i.e. $\psi \in \mathcal{D}(A^2)$. Even by the improvement of [FlS10a], and in turn this paper, we would still need $H$ to be of class $C^3(A)$ in order to verify this property. This would for example preclude application to the model considered in [MR10]. In [FlS10b] the authors study the limit in (3.1) directly, bypassing the general limiting absorption theorems, albeit applying the same differential inequality technique, and prove existence of the limit assuming only $\psi \in \mathcal{D}(A)$. Combined with [FlS10a] (or this paper) this establishes the existence of the limit in the Fermi Golden Rule [FlS10b] abstractly under a $C^2(A)$ condition. The price to pay is that one needs a priori control of the norm $\|A\psi\|$ locally uniformly in possibly existing perturbed eigenstates. While it is clear that such a locally uniform bound does hold, provided all the input in [FlS10a] is controlled locally uniformly in the perturbation, it is however impractical due to the complexity of the setup to extract such bounds in closed form. In this paper we do just that in the simpler context of regular Mourre theory.

As a last motivation, we had in mind a consequence of having good explicit bounds on the norms $\|A^k\psi\|$. Namely, provided one imposes natural conditions on the norms of all iterated commutators, we show as a consequence of our explicit bounds on $\|A^k\psi\|$ that the power series $\sum_{k=1}\frac{(i\theta A)^k}{k!}\psi$ has a positive radius of convergence, thus establishing that $\psi$ is an analytic vector for $A$. Here however, we have to work with conditions of the type considered in [CGH06]. Having established analyticity of the map $\theta \mapsto \exp(i\theta A)\psi$ in a ball around 0 one may observe that this map is actually analytic in a strip around the real axis, and thus this result reproduces a result of Balslev and Combes [BC71, Thm.1] on analyticity of dilated non-threshold eigenstates. As an example of a new result, we prove for the massive Spin-Boson Model that non-threshold eigenstates are analytic vectors with respect to the second quantised generator of dilations.

### 3.1.1 Commutator Calculus

We pause to introduce the commutator calculus of [AdMG96] before formulating our main results. Let $A$ be a self-adjoint operator with domain $\mathcal{D}(A)$ in a Hilbert space $\mathcal{H}$. We denote with $\mathfrak{B}(X,Y)$ the set of bounded operators on the normed space $X$ with images in the normed space $Y$ and $\mathfrak{B}(X) := \mathfrak{B}(X,X)$.

**Definition 3.1.** A bounded operator $B \in \mathfrak{B}(\mathcal{H})$ is said to be of class $C^k(A)$, in short $B \in C^k(A)$, if

$$\mathbb{R} \ni t \mapsto e^{itA} B e^{-itA} \tag{3.2}$$

is strongly in $C^k(\mathbb{R})$. A possibly unbounded self-adjoint operator $S$ is said to be of class $C^k(A)$ if $(i-S)^{-1} \in C^k(A)$.

The property, that $B \in \mathfrak{B}(\mathcal{H})$ is of class $C^1(A)$ is equivalent to the statement that

$$(\phi, [B,A]\chi) := (B^*\phi, A\chi) - (A\phi, B\chi), \quad \forall \phi, \chi \in \mathcal{D}(A)$$

extends to a bounded form on $\mathcal{H} \times \mathcal{H}$, which in turn is implemented by a bounded operator, $\mathrm{ad}_A(B)$, see e.g. [GGM04b]. If $B \in C^2(A)$, then an argument using Duhamel's formula shows $\mathrm{ad}_A(B) \in C^1(A)$ and thus there exists a bounded extension of the form $[\mathrm{ad}_A(B), A]$. This allows to construct iteratively the bounded operator $\mathrm{ad}_A^k(B) := \mathrm{ad}_A(\mathrm{ad}_A^{(k-1)}(B))$, for $B \in C^k(A)$. We set $\mathrm{ad}_A^0(B) := B$.

Commutators involving two possibly unbounded self-adjoint operators $H$ and $A$ will in general not extend to bounded operators on $\mathcal{H}$ and the definition of the quadratic form $[H,A]$ requires further restrictions on its domain. Thus we denote by $[H,A]$ the form

$$(\phi, [H,A]\chi) := (H\phi, A\chi) - (A\phi, H\chi), \quad \forall \phi, \chi \in \mathcal{D}(A) \cap \mathcal{D}(H).$$

If $H \in C^1(A)$, then $\mathcal{D}(A) \cap \mathcal{D}(H)$ is dense in $\mathcal{D}(H)$ in the graph norm of $H$ and $[H,A]$ extends to an $H$-form bounded quadratic form, which in turn defines a unique element of $\mathfrak{B}(\mathcal{D}(H), \mathcal{D}(H)^*)$ denoted by

$$\mathrm{ad}_A(H) : \mathcal{D}(H) \to \mathcal{D}(H)^*,$$

see [GGM04a]. The space $\mathcal{D}(H)^*$ is the dual of $\mathcal{D}(H)$ in the sense of rigged Hilbert spaces.

Our result on the analyticity of eigenvectors of $H$ with respect to $A$ requires a construction of multiple commutators of $H$ and $A$ which are bounded as maps from $\mathcal{D}(H)$ to $\mathcal{H}$ in the graph norm of $H$. The construction is as follows: Let $H \in C^1(A)$. We assume that $\mathrm{ad}_A(H) \in \mathfrak{B}(\mathcal{D}(H), \mathcal{H})$. Then, $[\mathrm{ad}_A(H), A]$ is defined as

$$(\psi, [\mathrm{ad}_A(H), A]\phi) := (-\mathrm{ad}_A(H)\psi, A\phi) - (A\psi, \mathrm{ad}_A(H)\phi), \tag{3.3}$$

for all $\psi, \phi \in \mathcal{D}(A) \cap \mathcal{D}(H)$. Here we used, that $\mathrm{ad}_A(H)$ is skew-symmetric on the domain $\mathcal{D}(A) \cap \mathcal{D}(H)$. Assume that this form extends in graph norm of $H$ to a form which is implemented by an element $\mathrm{ad}_A^2(H) \in$

$\mathfrak{B}(\mathcal{D}(H),\mathcal{H})$. Proceeding iteratively, we construct $\mathrm{ad}_A^k(H) \in \mathfrak{B}(\mathcal{D}(H),\mathcal{H})$.

**Lemma 3.2.** *Let $H, A$ be self-adjoint operators on the Hilbert space $\mathcal{H}$ and assume $H \in C^1(A)$. If $\mathrm{ad}_A^j(H) \in \mathfrak{B}(\mathcal{D}(H),\mathcal{H})$ for $0 \leq j \leq k$, then $H \in C^k(A)$.*

The proof of this lemma may be found in Section 3.5.

In several places we need an appropriate class of functions to regularise the self-adjoint operators $H, A$, defined on $\mathcal{D}(H), \mathcal{D}(A)$ respectively, and enable a calculus for them.

**Definition 3.3.** Define $\mathcal{B} := \{r \in C_b^\infty(\mathbb{R},\mathbb{R}) | r'(0) = 1,\ r(0) = 0,\ \forall k \in \mathbb{N} : \sup_{t\in\mathbb{R}} |r^k(t)\langle t\rangle^k| < \infty,\ r$ is real analytic in some ball around $0\}$.

Let $h \in \mathcal{B}$. For $\lambda \neq 0$ redefine $h_\lambda(x) := h(x-\lambda)$. In the following we will drop the index $\lambda$ as well as the argument of $h_\lambda(H)$ and other regularisations of $H$ and $A$, if the context is clear. The following condition is a local $C^1(A)$ condition, as in [Sah97], plus a Mourre estimate.

**Condition 3.4.** Let $H, A$ be self-adjoint operators on $\mathcal{H}$ and $\lambda \in \mathbb{R}$. There exist an $h \in \mathcal{B}$, $h_\lambda(s) := h(s-\lambda)$, with $h_\lambda(H) \in C^1(A)$ and an $f_{\mathrm{loc}} \in C_0^\infty(\mathbb{R},[0,1])$, such that $f_{\mathrm{loc}}(\lambda) = 1$ and $h'_\lambda(x) > 0$ for all $x \in \mathrm{supp}(f_{\mathrm{loc}})$. Assume there is a *smooth Mourre estimate*, i.e. $\exists C_0, C_1 > 0$ and a compact operator $K$, such that

$$i\,\mathrm{ad}_A(h_\lambda(H)) \geq C_0 - C_1 f^2_{\mathrm{loc},\perp}(H) - K. \tag{3.4}$$

$f_{\mathrm{loc},\perp}$ is defined as $f_{\mathrm{loc},\perp} := 1 - f_{\mathrm{loc}}$.

**Remark 3.5.**
1. The requirement $h'_\lambda(x) > 0$, $\forall x \in \mathrm{supp}(f_{\mathrm{loc}})$, implies $f_{\mathrm{loc}} \in C^k(A)$ if $h_\lambda \in C^k(A)$ for $k \in \mathbb{N}$, since $h_\lambda$ is smoothly invertible (on each connected component of $\mathrm{supp}(f_{\mathrm{loc}})$) and $f_{\mathrm{loc}}$ may be written as a smooth function of $h_\lambda$.
2. The assumption of $K$ being compact is not necessary. In fact we could replace this by the requirement that $\mathbf{1}_{|A|\geq\Lambda}K$, where $\mathbf{1}_{|A|\geq\Lambda}$ denotes the spectral projection on $[\Lambda,\infty)$, can be made arbitrarily small.
3. For a comparison of the 'local' Mourre estimate (3.4) with the standard form of the Mourre estimate see Section 3.6.

**Theorem 3.6 (Finite regularity).** *Let $H, A$ be self-adjoint operators on the Hilbert space $\mathcal{H}$ and $\psi$ be an eigenvector of $H$ with eigenvalue $\lambda$. Assume Condition 3.4 to be satisfied with respect to $\lambda$ and $h_\lambda(H) \in C^{k+1}(A)$ for some $k \in \mathbb{N}$. There exists $c_k > 0$, only depending on* $\mathrm{supp}(f_{\mathrm{loc}})$, $C_0$, $C_1$, $K$, $\|\mathrm{ad}_A^\ell(f_{\mathrm{loc}}(H))\|$, $\|\mathrm{ad}_A^j(h_\lambda(H))\|$, $1 \leq \ell \leq k$, $1 \leq j \leq k+1$, *such that*

$$\left\| A^k\psi \right\| \leq c_k \|\psi\|. \tag{3.5}$$

**Remark 3.7.** In [FlS10a, Ex. 1.4] it is shown, that the statement of Theorem 3.6 is false in general if one requires $h_\lambda \in C^k(A)$ only. Therefore, the result is optimal concerning integer values of $k$.

**Condition 3.8.** The self-adjoint operator $H$ is of class $C^1(A)$ and there exists a $v > 0$, such that for all $k \in \mathbb{N}$

$$\| \mathrm{ad}_A^k(H)(i - H)^{-1} \| \leq k! v^{-k}. \tag{3.6}$$

**Theorem 3.9 (Analyticity).** *Let $H, A$ be self-adjoint operators on the Hilbert space $\mathcal{H}$ and $\psi$ be an eigenvector of $H$ with eigenvalue $\lambda$. Assume Condition 3.4 to be satisfied with respect to $\lambda$ and that Condition 3.8 holds. Then, the map*

$$\mathbb{R} \ni \theta \mapsto e^{i\theta A}\psi \in \mathcal{H} \tag{3.7}$$

*extends to an analytic function in a strip around the real axis.*

## 3.2 Applications

The applications of our result on 'finite regularity of eigenstates' are well known and discussed in the literature [SAS89, CGH06, HS00, MS04, FlS10b]. In contrast results on the analyticity of eigenvalues in regular Mourre theory are to our knowledge unknown. Even though the condition under which our result holds appears difficult to verify in concrete situations, we will illustrate for some deformation analytic models that it is strikingly simple to check the assumptions of Theorem 3.9.

Let $H$ be a self-adjoint operator on the Hilbert space $\mathcal{H}$ and $U(t) := \exp(itA)$ a strongly continuous one parameter group of unitary operators $U(t)$. The self-adjoint operator $A$ is the generator of this group. Assume that $U(t)$ *b-preserves* $\mathcal{D}(H)$, i.e.

$$U(t)\mathcal{D}(H) \subseteq \mathcal{D}(H), \quad \forall t \in \mathbb{R} \text{ and } \sup_{t\in[-1,1]} \|U(t)\phi\|_{\mathcal{D}(H)} < \infty, \quad \forall \phi \in \mathcal{D}(H),$$

where $\|\psi\|_{\mathcal{D}(H)}$ denotes the graph norm of $H$.

**Remark 3.10.** Observe that the following are equivalent:

- $U(t)$ b-preserves $\mathcal{D}(H)$.
- There exist $\mu_0 > 0$ and $C > 0$ such that for all $\mu \in \mathbb{R}$ with $|\mu| \geq \mu_0$, we have $(A - i\mu)^{-1} : \mathcal{D}(H) \to \mathcal{D}(H)$ and

$$\|(A - i\mu)^{-1}\|_{\mathfrak{B}(\mathcal{D}(H),\mathcal{H})} \leq C|\mu|^{-1}.$$

By [GGM04a, Lemma 2.33] one observes that $U^\circ(\cdot) := U(\cdot) \restriction_{\mathcal{D}(H)}$ is a $C_0$-group in the topology of $\mathcal{D}(H)$.

**Proposition 3.11.** *Let $H, A$ be self-adjoint operators and $U(t) := \exp(itA)$. Assume that $U(\cdot)$ b-preserves $\mathcal{D}(H)$. Then for any $k \in \mathbb{N}$ the following statements are equivalent.*

1. *$H$ admits $k$ $H$-bounded commutators with $A$, denoted by $\mathrm{ad}_A^j(H)$, $j = 1, \ldots, k$.*

2. *The map* $t \mapsto I(t) = (\varphi, U(t)HU(t)^*\psi) \in C^k([-1,1])$, *for all* $\psi, \varphi \in \mathcal{D}(H) \cap \mathcal{D}(A)$. *There exist* $H$*-bounded operators* $H^{(j)}(0)$, $j = 1, \dots, k$, *such that* $\frac{d^j}{dt^j} I(t)_{|t=0} = (\varphi, H^{(j)}(0)\psi)$, *for* $j = 1, \dots, k$ *and all* $\psi, \varphi \in \mathcal{D}(H) \cap \mathcal{D}(A)$.

3. $t \mapsto \psi(t) := U(t)HU(t)^*\psi \in C^k([-1,1]; \mathcal{H})$ *for all* $\psi \in \mathcal{D}(H)$, *and there exist* $H$*-bounded operators* $H^{(j)}(0)$, $j = 1, \dots, k$, *with the property that* $\frac{d^j}{dt^j} \psi(t)_{|t=0} = H^{(j)}(0)\psi$, *for all* $j = 1, \dots, k$ *and* $\psi \in \mathcal{D}(H)$.

*If one of the three statements holds, then the pertaining* $H$*-bounded operators are uniquely determined and we have*

$$i^j \operatorname{ad}_A^j(H) = (-1)^j H^{(j)}(0), \quad j = 1, \dots, k. \tag{3.8}$$

*Proof.* Assume the commutator form $[H, A]$ has an extension from $\mathcal{D}(H) \cap \mathcal{D}(A)$ to an $H$-bounded operator. Then an argument of Mourre [Mou81, Prop.II.2], keeping Remark 3.10 in mind, implies that $(H+i)^{-1} : \mathcal{D}(A) \to \mathcal{D}(A)$. Hence, it follows that $(H+i)^{-1}$ is of class $C^1(A)$. A consequence of this is that $\mathcal{D}(A) \cap \mathcal{D}(H)$ is dense in $\mathcal{D}(H)$ (as well as in $\mathcal{D}(A)$). (Alternatively use Remark 3.10 backwards in conjunction with Nelson's theorem [RS75, Thm. X.49].) This remark implies that any extension of the commutator form $[H, A]$ to an $H$-bounded operator is necessarily unique.

(1) $\Rightarrow$ (2): A consequence of the above observation is that $\operatorname{ad}_A^j(H)$, for $j = 1, \dots, k$, is symmetric for $j$ even and anti-symmetric for $j$ odd. Compute first for $\varphi, \psi \in \mathcal{D}(H) \cap \mathcal{D}(A)$

$$\frac{d}{dt} I(t) = -(\varphi, U(t) i [H, A] U(t)^* \psi) = -(\varphi, U(t) i \operatorname{ad}_A(H) U(t)^* \psi).$$

If we evaluate at $t = 0$ we observe that $H^{(1)}(0) = -i \operatorname{ad}_A(H)$ can be used as a weak derivative on $\mathcal{D}(H) \cap \mathcal{D}(A)$. Iteratively we now conclude that

$$\begin{aligned} \frac{d^k}{dt^k} I(t) &= (-1)^k (\varphi, U(t) i^k [\operatorname{ad}_A^{k-1}(H), A] U(t)^* \psi) \\ &= (-1)^k (\varphi, U(t) i^k \operatorname{ad}_A^k(H) U(t)^* \psi). \end{aligned}$$

Taking $t = 0$ implies (2). The computation here also establishes the formula connecting $\operatorname{ad}_A^j(H)$ and $H^{(j)}(0)$.

(2) $\Rightarrow$ (3): From the computation of $I$'s first derivative above, evaluated at 0, we observe that $[H, A]$ extends from the intersection domain to an $H$-bounded operator. Hence this extension is unique, and indeed all the derivatives $H^{(j)}(0)$, $j = 1, \dots, k$ are unique extensions by continuity. In particular $H^{(j)}(0)$ are symmetric operators on $\mathcal{D}(H)$ and, for $j = 1, \dots, k$ and $\varphi, \psi \in \mathcal{D}(H) \cap \mathcal{D}(A)$,

$$\frac{d^j}{dt^j} I(t) = (\varphi, U(t) i [A, H^{(j-1)}(0)] U(t)^* \psi) = (\varphi, U(t) H^{(j)}(0) U(t)^* \psi).$$

That $\psi(t) := U(t)HU(t)^*\psi$ is itself continuous is a consequence of $U^\circ$ being a $C_0$-group on $\mathcal{D}(H)$. We assume inductively that $\psi(t)$ is an element of $C^{k-1}([-1,1];\mathcal{H})$ and

$$\frac{d^{k-1}}{dt^{k-1}}\psi(t) = U(t)H^{(k-1)}(0)U(t)^*\psi.$$

Assume now $\psi, \varphi \in \mathcal{D}(A) \cap \mathcal{D}(H)$ and compute

$$\begin{aligned}\frac{1}{t-s}\Big((\varphi, \frac{d^{k-1}}{dt^{k-1}}\psi(t)) - (\varphi, \frac{d^{k-1}}{dt^{k-1}}\psi(s))\Big) - (\varphi, U(t)H^{(k)}(0)U(t)^*\psi)\\ = \frac{1}{t-s}\int_s^t \big(\varphi, (U(r)H^{(k)}(0)U(r)^* - U(t)H^{(k)}(0)U(t)^*)\psi\big)dr.\end{aligned}$$

This identity now extends by continuity to $\varphi \in \mathcal{H}$ and $\psi \in \mathcal{D}(H)$. We can furthermore estimate (for $s < t$)

$$\begin{aligned}\Big\|\frac{1}{t-s}\Big(\frac{d^{k-1}}{dt^{k-1}}\psi(t) - \frac{d^{k-1}}{dt^{k-1}}\psi(s)\Big) - U(t)H^{(k)}(0)U(t)^*\psi\Big\|\\ \leq \frac{1}{t-s}\int_s^t \big\|\big(U(r)H^{(k)}(0)U(r)^* - U(t)H^{(k)}(0)U(t)^*\big)\psi\big\|dr.\end{aligned}$$

That the right-hand side converges to zero when $s \to t$ (from the left) now follows from the strong continuity of $U^\circ$ on $\mathcal{D}(H)$. A similar argument works for $s > t$.

(3) $\Rightarrow$ (1): Compute for $\varphi, \psi \in \mathcal{D}(H) \cap \mathcal{D}(A)$

$$\frac{d^j}{dt^j}(\varphi, \psi(t))_{|t=0} = (\varphi, H^{(j)}(0)\psi).$$

Conversely one can compute the $j$th derivative in terms of iterated commutators, and hence (1) follows. Note again, that the very first step in particular ensures that extensions are unique. □

## Examples

***1. N-body Schrödinger operators.*** Consider the operator

$$H = -\frac{1}{2}\Delta + \sum_{i<j}^{1,\dots,N} V_{ij}(x_i - x_j),$$

with *Coulomb pair potentials* $V_{ij}(x) := c_{ik}/(|x_i - x_j|)$, $c_{ik} \in \mathbb{R}$, on $L^2(X)$, where

$$X := \Big\{x = (x_1, \dots, x_N) \in \mathbb{R}^{3N} | x_j \in \mathbb{R}^3, \quad 1 \leq j \leq N, \quad \sum_{j=1}^N x_j = 0\Big\},$$

[HS00]. As a shorthand we write $x = (x_1, \dots, x_N)$. The unitary group of dilations, $U(\cdot)$ is defined by

$$(U(t)\psi)(x) := e^{t\frac{3(N-1)}{2}}\psi(e^t x),$$

and $U(t) = \exp(itA)$ for the generator of dilations $A$. From Proposition 3.11 infer for some $C > 0$

$$\|\operatorname{ad}_A^k(H)\|_{\mathfrak{B}(\mathcal{D}(p^2),\mathcal{H})} \leq C2^k.$$

It is well known, that there is a Mourre estimate for a much more general class than the Coulomb $N$-body Hamiltonian, including the following example [HS00]. This enables Theorem 3.9.

Another example for $N$-body Schrödinger operators to which Theorem 3.9 is applicable is defined with *Yukawa pair potentials*. The pair potentials $V_{ik}$ are now given by

$$V_{ij}(x) := \frac{c_{ik} e^{-\mu|x_i - x_j|}}{|x_i - x_j|}, \quad c_{ik} \in \mathbb{R}, \quad \mu > 0.$$

Observe the estimate

$$\left| \frac{d^k}{dt^k} \frac{e^{-t}}{r} e^{\mu r e^t} \right|_{|t=0} \leq k! a^k, \quad r := |x_i - x_j|,$$

for some $a > 0$. The $r$-dependent functions on the right-hand side of this inequality are infinitesimally $p^2$-bounded, which again shows the applicability of Theorem 3.9. Hence non-threshold eigenvectors are analytic vectors with respect to $A$. This reproduces known results of [BC71].

***2. The Spin-Boson Model.*** The 'matter' Hamiltonian is defined as

$$H_{\mathrm{at}} := \epsilon \sigma_3, \quad \epsilon > 0,$$

with the $2 \times 2$ Pauli-matrices $\sigma_1, \sigma_2, \sigma_3$. The corresponding Hilbert space is $\mathcal{H}_{\mathrm{at}} := \mathbb{C}^2$. We briefly list the definition of the quantised bosonic field, but for the details of *second quantisation* we refer to [DG99]. The Hilbert space of the bosonic field is the *bosonic Fock space*,

$$\mathcal{F}_+ := \bigoplus_{n=0}^{\infty} \mathcal{S}_n \mathfrak{h}^{\otimes n}, \quad \mathfrak{h} := L^2(\mathbb{R}^3, d^3k),$$

where $\mathcal{S}_n$ denotes the orthogonal projection onto the totally symmetric $n$-particle wave functions. We denote for $k \in \mathbb{R}$ with $a(k)$ and $a^\dagger(k)$ the *annihilation* and *creation* operator, respectively. The energy of the free field, $H_{\mathrm{f}}$, is defined as

$$H_{\mathrm{f}} = \int_{\mathbb{R}^3} a^\dagger(k) \omega(k) a(k) d^3k, \quad \omega(k) := \sqrt{k^2 + m^2}, \quad m > 0.$$

The Hilbert space of the compound system is

$$\mathcal{H} := \mathcal{H}_{\mathrm{at}} \otimes \mathcal{F}.$$

We define the coupling between atom and field by

$$\Phi(v) := \frac{1}{\sqrt{2}} \int_{\mathbb{R}^3} v(k) \{ G \otimes a^\dagger(k) + G^* \otimes a(k) \} d^3k,$$

with a complex $2 \times 2$ matrix $G$. The function $v$ is given by

$$v(k) := \frac{e^{-\frac{k^2}{\Lambda^2}}}{\omega(k)^{\frac{1}{2}}}, \quad \forall k \in \mathbb{R}^3.$$

The constant $\Lambda > 0$ plays the role of an ultraviolet cutoff. We define the Hamiltonian of the compound system, $H$, as

$$H := H_{\mathrm{at}} \otimes \mathbb{1} + \mathbb{1} \otimes H_{\mathrm{f}} + \Phi(v).$$

Define,

$$\alpha := \frac{i}{2} \left( \nabla_k \cdot k + k \cdot \nabla_k \right).$$

This operator is symmetric and densely defined on $L^2(\mathbb{R}^3)$ as it is the well-known generator of the strongly continuous unitary group

$$\left( u(t)\psi \right)(k) := e^{-\frac{3}{2}t} \psi \left( e^{-t} k \right).$$

We will denote the second-quantised operators of $\alpha$ and $u(t)$ by $A := d\Gamma(\alpha)$ and $U(t) := \Gamma(u(t))$, respectively. $A$ is the generator of the strongly continuous unitary group $U(t)$. Observe that

$$i^\ell \operatorname{ad}_A^\ell(H) = d\Gamma(i^\ell \operatorname{ad}_\alpha^\ell(\omega)) + (-1)^{\ell+1} \Phi \left( (i\alpha)^\ell v \right)$$

and

$$\| \Phi \left( (i\alpha)^\ell v \right) (H_{\mathrm{f}} + \mathbb{1})^{-\frac{1}{2}} \| \leq \| \omega^{-\frac{1}{2}} (i\alpha)^\ell v \|_{L^2}. \tag{3.9}$$

Since $(i\alpha)^\ell v = \frac{d^\ell}{dt^\ell} \left( e^{i\alpha t} v \right) \big|_{t=0}$, we have to estimate the multiple derivatives. Consider the map

$$\overline{B\left(0, \frac{\pi}{4}\right)} \ni z \mapsto \left( k^2 e^{-2z} + m^2 \right)^{\frac{1}{2}} = \omega\left( e^{-z} k \right), \quad k \in \mathbb{R}^3,$$

where $\overline{B\left(0, \frac{\pi}{4}\right)}$ denotes the closed ball of radius $\pi/4$, centred at 0. Observe, that

$$m \leq |\omega\left( e^{-z} k \right)| \leq e^{\frac{\pi}{4}} \omega(k) \tag{3.10}$$

where the lower bound implies that $z \mapsto \omega\left( e^{-z} k \right)^{-\frac{1}{2}}$ is holomorphic in $B\left(0, \frac{\pi}{4}\right)$, for all $k \in \mathbb{R}^3$. The upper bound ensures that $\mathcal{D}(\mathbb{1} \otimes H_{\mathrm{f}})$ is b-stable with respect to $U(\cdot)$. Below, we will also show that $\operatorname{ad}_A(H) \in \mathfrak{B}(\mathcal{D}(H), \mathcal{H})$, which implies by Proposition 3.11 that $H \in C^1(A)$. Analogously we define the holomorphic map

$$\overline{B\left(0, \frac{\pi}{4}\right)} \ni z \mapsto \frac{e^{-e^{-z} \frac{k^2}{\Lambda^2}}}{\omega(e^{-z}k)^{\frac{1}{2}}} = v\left( e^{-z} k \right), \quad k \in \mathbb{R}^3.$$

We may compute by Cauchy's formula,

$$\frac{d^\ell}{dz^\ell} \left( v(e^{-z}k) e^{-\frac{3}{2}z} \right) \Big|_{z=0} = \frac{\ell! \left( \frac{\pi}{4} \right)^{-\ell}}{2\pi} \int_0^{2\pi} e^{-\frac{3}{2}\gamma(\varphi)} v\left( e^{-\gamma(\varphi)} k \right) e^{-i\ell\varphi} d\varphi,$$

$\gamma(\varphi) := (\pi/4) e^{i\varphi}$, $\varphi \in [0, 2\pi)$. Using the estimate

$$\left| \frac{d^\ell}{dz^\ell} (v(e^{-z}k) e^{-\frac{3}{2}z}) \Big|_{z=0} \right| \leq m^{-\frac{1}{2}} e^{\frac{3\pi}{8}} e^{-e^{-\frac{\pi}{2}} \frac{k^2}{\Lambda^2}} \ell! \left( \frac{\pi}{4} \right)^{-\ell}, \quad \forall k \in \mathbb{R}^3,$$

one finds together with (3.9)

$$\|\Phi\left((i\alpha)^{\ell}v\right)(H_f+\mathbb{1})^{-\frac{1}{2}}\| \leq \ell! R^{-\ell},$$

for some $R > 0$. Analogously, we get from (3.10)

$$\left|\frac{d^{\ell}}{dz^{\ell}}(\omega(e^{-z}k))\Big|_{z=0}\right| \leq \ell!\left(\frac{\pi}{4}\right)^{-\ell} e^{\frac{\pi}{4}}\omega(k),$$

so that

$$\left\|d\Gamma(i^{\ell}\,\mathrm{ad}_{\alpha}^{\ell}(\omega))(H_{\mathrm{f}}+\mathbb{1})^{-1}\right\| \leq \|i^{\ell}\,\mathrm{ad}_{\alpha}^{\ell}(\omega)\omega^{-1}\|_{\infty} \leq \ell! c^{-\ell},$$

for some $c > 0$. From [DG99] we may infer a Mourre estimate for our model. Dereziński and Gérard use a different generator of dilations, namely

$$\alpha_{\omega} := \tfrac{i}{2}\big((\nabla_k\omega)(k)\cdot\nabla_k + \nabla_k\cdot(\nabla_k\omega)(k)\big).$$

It is also possible to prove a Mourre estimate using their techniques if $\omega(k)$ is radially increasing, $\omega(k) > 0$, $\forall k \in \mathbb{R}^3$ and 0 is the only critical point of $\omega$. Thus, we conclude by Theorem 3.9 and Proposition 3.11 that any eigenstate pertaining to an embedded non-threshold eigenvalue is an analytic vector with respect to $A$.

## 3.3 Preliminaries

In what follows, we need some regularisation techniques from operator theory. It is convenient to perform calculations involving multiple commutators by using the so-called *Helffer-Sjöstrand functional calculus*. Part and parcel of this calculus are certain extensions of a subclass of the smooth functions on $\mathbb{R}$, the *almost analytic extensions*. The following proposition allows us to define such extensions.

**Proposition 3.12.** *Consider a family of continuous functions $(f_n)_{n\in\mathbb{N}} \subset C^{\infty}(\mathbb{R})$, for which there is an $m \in \mathbb{R}$, such that $\langle x\rangle^{k-m} f_n^{(k)}$ is uniformly bounded for all $n \geq 0$. There exists a family of functions $(\tilde{f}_n)_{n\in\mathbb{N}}$, with $\tilde{f}_n \restriction_{\mathbb{R}} = f_n \restriction_{\mathbb{R}}$ for any $n \in \mathbb{N}$, such that*

1. $\mathrm{supp}(\tilde{f}_n) \subset \{z \in \mathbb{C} \,|\, \mathrm{Re}\, z \in \mathrm{supp}(f_n)$ *and* $|\mathrm{Im}\, z| \leq \langle \mathrm{Re}\, z\rangle\}$.
2. $|\bar{\partial}\tilde{f}_n(z)| \leq C_N\langle z\rangle^{m-N-1}|\mathrm{Im}\, z|^N$ *for all* $N \geq 0$.

*The constant $C_N$ does not depend on $n$.*

For a proof of this statement see [Møl00].

**Remark 3.13.** We will call these extensions for *almost analytic extensions*, because $\bar{\partial}\tilde{f}_n$ vanishes approaching the real axis.

Let $\varepsilon > 0$. For any self-adjoint operator $L$ and any $f \in C^{\infty}(\mathbb{R})$ with

$$\sup_{t\in\mathbb{R}} |f^{(k)}(t)\langle t\rangle^{k+\varepsilon}| \tag{3.11}$$

we may define a bounded operator $f(L)$, by

$$f(L) := \frac{1}{2\pi i}\int_{\mathbb{C}} \bar{\partial}\tilde{f}(z)(z-L)^{-1}dz\wedge d\bar{z}. \tag{3.12}$$

The integral on the right-hand side converges in operator norm. It is well known that this definition coincides with the operator defined by functional calculus. Concerning the class $\mathcal{B}$ however, we cannot directly apply this definition. Inspired by a construction in [MS04] we consider the following instead.

**Lemma 3.14.** *Let $r \in \mathcal{B}$. There is an almost analytic extension of $t \mapsto r(t)/t =: \rho(t)$, which satisfies due to Proposition 3.12 the bounds*

$$|\bar{\partial}\tilde{\rho}(z)| \leq C_N \langle z\rangle^{-N-2}|\operatorname{Im}(z)|^N. \tag{3.13}$$

*Proof.* Since $r$ is real analytic around 0 we observe

$$\sup_{|t|\leq 1}\left|\rho^{(k)}(t)\langle t\rangle^{k+1}\right| < \infty.$$

On the other hand, the Leibniz rule yields $r^{(k)}(t) = \rho^{(k)}(t)t + k\rho^{(k-1)}(t)$ and thus by induction

$$\sup_{|t|\geq 1}\left|\rho^{(k)}(t)\langle t\rangle^{k+1}\right| < \infty. \qquad \square$$

For any $r \in \mathcal{B}$, set $r_n(t) := nr(t/n)$, $\rho(t) := r(t)/t$, $\forall t \in \mathbb{R}$ and define $r_n(A)$ by functional calculus. If we require $\overline{\tilde{\rho}(z)} = \tilde{\rho}(\bar{z})$ the well-known formula

$$r_n(t) = \frac{1}{2\pi i}\int_{\mathbb{C}} \bar{\partial}\tilde{\rho}(z)\frac{t}{z-\frac{t}{n}}dz\wedge d\bar{z} \tag{3.14}$$

may be recovered. Observe, that

$$\frac{t}{z-\frac{t}{n}} = -n\left(1-\frac{z}{z-\frac{t}{n}}\right). \tag{3.15}$$

The first term on the right-hand side is constant and vanishes when computing commutators. Although we cannot use the formula (3.14) directly as a representation of $r_n(A)$ on $\mathcal{H}$, it is possible to use it on the domain of $A$; a fact which is useful in the next lemma.

**Lemma 3.15.** *Let $B \in C^1(A)$, where $B \in \mathfrak{B}(\mathcal{H})$. For any $r \in \mathcal{B}$ we have*

$$[B, r_n(A)] = r_n'(A)\operatorname{ad}_A(B) + R(r_n, B), \tag{3.16}$$

*with*

$$R(r_n, B) := \frac{1}{n2\pi i}\int_{\mathbb{C}} \bar{\partial}\tilde{\rho}(z)zJ_n^2(z)[\operatorname{ad}_A(B), A]J_n(z)dz\wedge d\bar{z}, \tag{3.17}$$

*where $J_n(z) := n(nz-A)^{-1}$ and the integral being norm convergent. Moreover, there is a $c > 0$*

$$\operatorname*{s-lim}_{n\to\infty} R(r_n) = 0, \text{ and } \|R(r_n, B)\| \leq c\|\operatorname{ad}_A(B)\|. \tag{3.18}$$

*If $B \in C^2(A)$, we have for any $n \in \mathbb{N}$ and some $\alpha, \beta > 0$*

$$\|AR(r_n, B)\| \le \alpha \| \operatorname{ad}_A^2(B)\|, \; \|R(r_n, B)\| \le \frac{\beta}{n} \| \operatorname{ad}_A^2(B)\|. \tag{3.19}$$

*In addition,*

$$\operatorname*{s-lim}_{n\to\infty} AR(r_n, B) = 0. \tag{3.20}$$

*Proof.* Let first $B \in C^1(A)$. If we consider $[r_n(A), B]$ as a form on $D(A) \times D(A)$, the commutator may be represented using (3.14) with $t$ replaced by $A$, more precisely for all $\psi, \phi \in D(A)$

$$(\phi, [B, r_n(A)]\psi) = \frac{1}{2\pi i} \int_{\mathbb{C}} \bar\partial\tilde\rho(z)\big\{(A\phi, J_n(z)B\psi) - (\phi, BJ_n(z)A\psi)\big\}dz \wedge d\bar z.$$

Observe, that the sum in the integrand is by definition

$$(A\phi, J_n(z)B\psi) - (\phi, BJ_n(z)A\psi) = (\phi, [AJ_n(z), B]\psi).$$

But since $B \in C^1(A)$, we obtain using (3.15)

$$\begin{aligned}(\phi, [AJ_n(z), B]\psi) &= (\phi, [nzJ_n(z), B]\psi)\\ &= (\phi, zJ_n(z)\operatorname{ad}_A(B)J_n(z)\psi)\\ &= \Big(\phi, zJ_n^2(z)\operatorname{ad}_A(B)\psi\Big) + \Big(\phi, \frac{z}{n}J_n^2(z)[\operatorname{ad}_A(B), A]J_n(z)\psi\Big).\end{aligned}$$

There is an almost analytic extension $\tilde\rho(z)$ such that

$$|\bar\partial\tilde\rho(z)|\frac{|z|}{|y|^2} \le C_N|y|^{N-2}\langle z\rangle^{-N-1}, \tag{3.21}$$

with $z = x + iy$, $x, y \in \mathbb{R}$. Choose $N = 2$ and observe that the integral

$$\frac{1}{2\pi i} \int_{\mathbb{C}} \bar\partial\tilde\rho(z)zJ_n^2(z)dz \wedge d\bar z \tag{3.22}$$

converges in norm. Moreover,

$$|\bar\partial\tilde\rho(z)|\frac{|z|^2}{|y|^3} \le C_3\langle z\rangle^{-3}.$$

Thus from $r'(t) = \rho(t) + \rho'(t)t$ we may infer that the integral in (3.22) equals $r_n'(A)$. Estimate (3.21) shows that the integral (3.17) converges in norm. Since

$$\operatorname*{s-lim}_{n\to\infty} \frac{A}{n}J_n(z) = 0, \tag{3.23}$$

the Theorem of Dominated Convergence implies (3.18).

Let now $B \in C^2(A)$. Choose in (3.13) $N = 3$, replace in (3.17) the commutator $[\operatorname{ad}_A(B), A]$ with $\operatorname{ad}_A^2(B)$ and observe that the integrand of $AR(g_n, h)(B)$ is point-wise bounded by a constant times $\langle z\rangle^{-3}$. The term $R(g_n, h)(B)$ is point-wise bounded by a constant times $\langle z\rangle^{-4}$. Both functions are in $L^1(\mathbb{R}^2)$ and hence the bounds follow. Eq. (3.20) is a consequence of (3.17), (3.23) and an application of the Theorem of Dominated Convergence. □

**Lemma 3.16.** *Let $r \in \mathcal{B}$ and $k \in \mathbb{N}$. If $B \in C^k(A)$, then*

$$\operatorname*{s-lim}_{n\to\infty} \mathrm{ad}_{r_n}^k(B) = \mathrm{ad}_A^k(B).$$

*Proof.* For $k = 1$ the statement follows from Lemma 3.15. Let $k \in \mathbb{N}$ and assume

$$\operatorname*{s-lim}_{n\to\infty} \mathrm{ad}_{r_n}^{k-1}(B) = \mathrm{ad}_A^{k-1}(B).$$

The first term on the right-hand side of

$$\mathrm{ad}_{r_n}(\mathrm{ad}_{r_n}^{k-1}(B)) = \mathrm{ad}_{r_n}^{k-1}(\mathrm{ad}_{r_n}(B)) = r_n' \,\mathrm{ad}_{r_n}^{k-1}(\mathrm{ad}_A(B)) + \mathrm{ad}_{r_n}^{k-1}(R(r_n, B))$$

converges strongly by the induction hypothesis and Lemma 3.15 since $\mathrm{ad}_A(B) \in C^{k-1}(A)$. $R(r_n, \mathrm{ad}_{r_n}^{k-1}(B))$ is a sum of two integrals:

$$\begin{aligned}\mathrm{ad}_{r_n}^{k-1}(R(r_n, B)) = &\frac{1}{2\pi i}\int_{\mathbb{C}} \bar{\partial}\tilde{\rho}(z) z \frac{A}{n} J_n^2(z)\, \mathrm{ad}_{r_n}^{k-1}(\mathrm{ad}_A(B)) J_n(z) dz \wedge d\bar{z}\\ &- \frac{1}{2\pi i}\int_{\mathbb{C}} \bar{\partial}\tilde{\rho}(z) z J_n^2(z)\, \mathrm{ad}_{r_n}^{k-1}(\mathrm{ad}_A(B)) \frac{A}{n} J_n(z) dz \wedge d\bar{z}.\end{aligned}$$

Observe, that

$$\operatorname*{s-lim}_{n\to\infty} \frac{A}{n} J_n(z) = \operatorname*{s-lim}_{n\to\infty} A(nz - A)^{-1} = 0.$$

The integrands are strongly convergent by the uniform boundedness principle and converge to the product of the strong limits. Lemma 3.15 and the Theorem of Dominated Convergence imply that we may exchange integration with the strong limit $n \to \infty$. □

We use of the following expansion formula for commutators.

**Lemma 3.17.** *Let $K, L \in \mathfrak{B}(\mathcal{H})$. Then, for any $k \in \mathbb{N}$,*

$$[K, L^k] = \sum_{j=1}^{k} \binom{k}{j} L^{k-j} \,\mathrm{ad}_L^j(K). \tag{3.24}$$

It is convenient to regularise the operator $A$ such that we may use the Helffer-Sjöstrand calculus and have sufficient flexibility in the proof. Let $g \in C_c^\infty(\mathbb{R}, \mathbb{R})$ be such that

$$g(t) = t\,\forall t \in [-1, 1],\ g(t) = 2\,\forall t \geq 3,\ g(t) = -2\,\forall t \leq -3,\ g' \geq 0, \tag{3.25}$$

and that $tg'(t)/g(t)$ has a smooth square root; clearly $g \in \mathcal{B}$. We set $g_n(t) := ng(t/n)$ and define $g_n(A)$ by functional calculus. Observe, that

$$n \mapsto g_n^2(t) \tag{3.26}$$

is monotonously increasing for all $t \in \mathbb{R}$. Set $\gamma(t) := g(t)/t$, for the function $g$ defined in (3.25). We may pick an almost analytic extension of $\gamma$, denoted by $\tilde{\gamma}$, such that $\tilde{\gamma}$ satisfies, up to a possibly different constant $C_N$, the same bounds as $\tilde{\rho}$ in (3.13).

## 3.4 Finite Regularity of Eigenstates

*Proof (Proof of Theorem 3.6).* Using the convention $A^0 = \mathbb{1}$, the statement is correct for $k = 0$. Let now be $k \in \mathbb{N}$ and assume $\psi \in \mathcal{D}(A^{k-1})$. The starting point for the proof is

$$0 = (\psi, i[h, g_n^k g_m g_n^k]\psi), \tag{3.27}$$

which may be rewritten as

$$0 = (\psi_n^{(k)}, i\,\mathrm{ad}_{g_m}(h)\psi_n^{(k)}) + 2\,\mathrm{Re}(\psi, g_m i[h, g_n^k]\psi_n^{(k)}) + 2\,\mathrm{Re}(\psi, [i[h, g_n^k], g_m]\psi_n^{(k)}), \tag{3.28}$$

where we introduced the notation $\psi_n^{(k)} := g_n^k\psi$. We abbreviate

$$I_0(n,m) := (\psi_n^{(k)}, i\,\mathrm{ad}_{g_m}(h)\psi_n^{(k)}), \tag{3.29}$$

$$I_1(n,m) := 2\,\mathrm{Re}(\psi, g_m i[h, g_n^k]\psi_n^{(k)}) \tag{3.30}$$

and

$$I_2(n,m) := 2\,\mathrm{Re}(\psi, [i[h, g_n^k], g_m]\psi_n^{(k)}) = 2\,\mathrm{Re}(\psi, i[[h, g_m], g_n^k]\psi_n^{(k)}). \tag{3.31}$$

We organise the proof in three steps. In the first step we extract from $I_1$ a term $I_0'$ which is of a similar type as $I_0$. Then, starting with (3.28) upper bounds to $I_0$, $I_0'$ are established. Finally, using Mourre's estimate we find lower bounds to $I_0$, $I_0'$, from which we conclude $\psi \in \mathcal{D}(A^k)$.

***Step 1.*** By an application of Lemma 3.17 we rewrite $I_1(n,m)$ as

$$\begin{aligned} I_1(n,m) = {} & 2\,\mathrm{Re}\left(i\sum_{j=2}^{k}\binom{k}{j}E_1(j,k,n,m)\right) + 2k\,\mathrm{Re}\left(i(\psi_n^{(k-1)}, g_m R(g_n, h)\psi_n^{(k)})\right) \\ & + 2k\,\mathrm{Re}\left(i(\psi_n^{(k-1)}, g_m g_n'\,\mathrm{ad}_A(h)\psi_n^{(k)})\right), \end{aligned} \tag{3.32}$$

where

$$E_1(j,k,n,m) := (\psi_n^{(k-j)}, g_m\,\mathrm{ad}_{g_n}^j(h)\psi_n^{(k)})$$

and

$$2k\,\mathrm{Re}(i(\psi_n^{(k-1)}, g_m R(g_n, h)\psi_n^{(k)}))$$

are present if $k \geq 2$ only, in which case $\psi \in \mathcal{D}(A)$ by induction hypothesis. We discuss the term in the last line of (3.32) first. One computes

$$\begin{aligned} 2k\,\mathrm{Re}\left(i(\psi_n^{(k-1)}, g_m g_n'\,\mathrm{ad}_A(h)\psi_n^{(k)})\right) &= 2k\,\mathrm{Re}\left(i(\psi_n^{(k)}, \gamma_m p_n^2\,\mathrm{ad}_A(h)\psi_n^{(k)})\right) \\ &= 2k\,\mathrm{Re}\left(i(\psi_n^{(k)}, \gamma_m p_n\,\mathrm{ad}_A(h)p_n\psi_n^{(k)})\right) \\ &\quad + 2k\,\mathrm{Re}\left(i(\psi_n^{(k)}, \gamma_m p_n[p_n, \mathrm{ad}_A(h)]\psi_n^{(k)})\right), \end{aligned}$$

with $\gamma_m$ being the operator $\gamma_m(A)$ and

$$p(t) := \sqrt{\frac{tg'(t)}{g(t)}},\ p_n(t) := p(t/n).$$

Hence, with

$$E_1(j,k,n) := \lim_{m\to\infty} E_1(j,k,n,m) = (A\psi_n^{(k-j)}, \mathrm{ad}_{g_n}^j(h)\psi_n^{(k)}), \quad k \ge j \ge 2,$$

we obtain

$$\begin{aligned} I_1(n) &:= \lim_{m\to\infty} I_1(n,m) \\ &= 2\,\mathrm{Re}\,\Big(i\sum_{j=2}^{k}\binom{k}{j}E_1(j,k,n)\Big) + 2k\,\mathrm{Re}\,\big(i(\psi_n^{(k-1)}, AR(g_n,h)\psi_n^{(k)})\big) \\ &\quad + 2k\,\mathrm{Re}\,\big(i(\psi_n^{(k)}, p_n[p_n, \mathrm{ad}_A(h)]\psi_n^{(k)})\big) + 2k(\psi_n^{(k)}, p_n i\,\mathrm{ad}_A(h)p_n\psi_n^{(k)}). \end{aligned} \tag{3.33}$$

Set

$$I_0'(n) := 2k(\psi_n^{(k)}, p_n i\,\mathrm{ad}_A(h)p_n\psi_n^{(k)}), \quad I_1'(n) := I_1(n) - I_0'(n). \tag{3.34}$$

***Step 2.*** First note that by an application of Lemma 3.16

$$\begin{aligned} I_2(n) &:= \lim_{m\to\infty} I_2(n,m) = 2\,\mathrm{Re}(\psi, i[\mathrm{ad}_A(h), g_n^k]\psi_n^{(k)}) \\ &= 2\,\mathrm{Re}\,\Big(i\sum_{j=1}^{k}\binom{k}{j}E_2(j,k,n)\Big), \end{aligned}$$

with

$$E_2(j,k,n) := (\psi_n^{(k-j)}, \mathrm{ad}_{g_n}^j(\mathrm{ad}_A(h))\psi_n^{(k)}), \quad k \ge j \ge 1.$$

Eq. (3.28) may be rewritten as

$$I_0(n) + I_0'(n) = -I_1'(n) - I_2(n). \tag{3.35}$$

In order to find an upper bound for the right-hand side, we first estimate $E_1(j,k,n)$, $E_2(j,k,n)$ by

$$\begin{aligned} 2|E_1(j,k,n)| &\le \epsilon_{jk}^{-1}\|\,\mathrm{ad}_{g_n}^j(h)g_n^{k-j}A\psi\|^2 + \epsilon_{jk}\|\psi_n^{(k)}\|^2, \\ 2|E_2(j,k,n)| &\le \mu_{jk}^{-1}\|\,\mathrm{ad}_{g_n}^j(\mathrm{ad}_A(h))\psi_n^{(k-j)}\|^2 + \mu_{jk}\|\psi^{(k)}\|^2, \end{aligned}$$

for all $\mu_{jk}, \epsilon_{jk} > 0$. The terms

$$\|\,\mathrm{ad}_{g_n}^j(h)g_n^{k-j}A\psi\|, \quad \|\,\mathrm{ad}_{g_n}^j(\mathrm{ad}_A(h))\psi_n^{(k-j)}\|$$

are uniformly bounded in $n$ by Lemma 3.16, $h \in C^{k+1}(A)$ and the induction hypothesis. For the remaining terms in (3.33) we have

$$\begin{aligned} 2k|(\psi_n^{(k-1)}, AR(g_n,h)\psi_n^{(k)})| &\le k\left(\delta^{-1}\|R(g_n,h)A\psi^{(k-1)}\|^2 + \delta\|\psi^{(k)}\|^2\right), \\ 2k|(\psi_n^{(k)}, p_n[p_n, \mathrm{ad}_A(h)]\psi_n^{(k)})| &\le k(\nu^{-1}\|[p_n, i\,\mathrm{ad}_A(h)]g_n\psi_n^{(k-1)}\|^2 + \nu\|\psi_n^{(k)}\|^2). \end{aligned}$$

$R(g_n, h)A$ is uniformly bounded in virtue of Lemma 3.15. The function $t \mapsto p(t)$ is by assumption smooth. Note that

$$[p_n, i\,\mathrm{ad}_A(h)]g_n = [p_n, i\,\mathrm{ad}_A(h)]A\gamma_n.$$

Further, since $p \in C_c^\infty(\mathbb{R})$, an application of Proposition 3.12 together with

$$[p_n, \mathrm{ad}_A(h)]A = \frac{-1}{2\pi i}\int_{\mathbb{C}} \bar{\partial}\tilde{p}(z)J_n(z)\,\mathrm{ad}_A^2(h)\frac{A}{n}J_n(z)dz \wedge d\bar{z}$$

shows the uniform boundedness of $[p_n, \mathrm{ad}_A(h)]g_n$. For $1 \leq j \leq k-1$ is $(\psi_n^{(j)})_{n\in\mathbb{N}}$ convergent in norm to $A^j\psi$ and hence $(\|\psi_n^j\|)_{n\in\mathbb{N}}$ is bounded. Choose now $\mu_{jk} := \binom{k}{j}^{-1}k^{-1}C_0/12$, $\epsilon_{jk} := \binom{k}{j}^{-1}(k-1)^{-1}C_0/12$, $\nu := C_0/(12k) =: \delta$ and observe

$$I_0(n) + I_0'(n) - \frac{C_0}{3} \leq I_3(n), \tag{3.36}$$

where $(I_3(n))_{n\in\mathbb{N}}$ is a bounded sequence.

***Step 3.*** Note, that we may assume $f_{\mathrm{loc}}(x) = \chi(h(x))$, $\forall x \in \mathbb{R}$, for some compactly supported smooth function $\chi$ because $h$ is chosen to be invertible on the support of $f_{\mathrm{loc}}$. This implies $f_{\mathrm{loc}}(H) \in C^{k+1}(A)$, since $h \in C^{k+1}(A)$, see [GGM04a, Prop.2.23]. Inserting the Mourre estimate from Condition 3.4 yields

$$(\psi_n^{(k)}, i[h, A]\psi_n^{(k)}) \geq C_0\|\psi_n^{(k)}\|^2 - C_1\|f_{\mathrm{loc},\perp}\psi_n^{(k)}\|^2 - (\psi_n^{(k)}, K\psi_n^{(k)}).$$

The second term is evaluated by

$$f_{\mathrm{loc},\perp}g_n^k\psi = -\sum_{l=1}^{k}\binom{k}{l}(-1)^l\,\mathrm{ad}_{g_n}^l(f_{\mathrm{loc}})g_n^{k-l}\psi,$$

where we used, that $\psi$ is an eigenstate and an adjoint version of (3.24). Thus, the contributions from this term are uniformly bounded in $n$ by Lemma 3.16 and the induction hypothesis. The spectral projection $\mathbf{1}_{|A|\leq\Lambda}(A)$ defines a partition of unity, $\mathbb{1} = \mathbf{1}_{|A|\leq\Lambda}(A) + \mathbf{1}_{|A|>\Lambda}(A)$. Hence we write

$$(\psi_n^{(k)}, K\psi_n^{(k)}) = (\psi_n^{(k)}, \mathbf{1}_{|A|\leq\Lambda}(A)K\psi_n^{(k)}) + (\psi_n^{(k)}, \mathbf{1}_{|A|>\Lambda}(A)K\psi_n^{(k)}).$$

Furthermore, we may estimate

$$|(\psi_n^{(k)}, \mathbf{1}_{|A|\leq\Lambda}(A)K\psi_n^{(k)})| \leq \frac{1}{2}\left(\frac{\|K\mathbf{1}_{|A|\leq\Lambda}(A)\psi_n^{(k)}\|^2}{\nu} + \nu\|\psi_n^{(k)}\|^2\right)$$

and

$$|(\psi_n^{(k)}, \mathbf{1}_{|A|>\Lambda}(A)K\psi_n^{(k)})| \leq \frac{1}{2}\left(\frac{\|\mathbf{1}_{|A|>\Lambda}(A)K\|^2}{\delta} + \delta\right)\|\psi_n^{(k)}\|^2.$$

Observe that since $K$ is compact and $\text{s-lim}_{\Lambda\to\infty} \chi_{|A|>\Lambda} = 0$ we have

$$\forall \epsilon > 0\, \exists \Lambda_\epsilon > 0 : \ \|\chi_{|A|>\Lambda_\epsilon} K\| < \epsilon,$$

but this implies $\forall \Lambda \geq \Lambda_\epsilon$

$$\|\mathbf{1}_{|A|>\Lambda}(A)K\| = \|\mathbf{1}_{|A|>\Lambda}(A)\mathbf{1}_{|A|>\Lambda_\epsilon}(A)K\| \leq \epsilon.$$

Thus, we may choose $\nu = C_0/9$, $\delta = C_0/9$ and pick then a $\Lambda > 0$ big enough, such that

$$2\|\mathbf{1}_{|A|>\Lambda}(A)K\|^2 \leq C_0^2/(9)^2, \tag{3.37}$$

i.e. $C_0 - \nu - \delta - \epsilon = C_0/3$. Thus we arrive at

$$I_0(n) + \frac{9\|K\mathbf{1}_{|A|\leq\Lambda}(A)\psi_n^{(k)}\|^2}{2C_0} + C_1 \left\| \sum_{l=1}^{k} \binom{k}{l} \operatorname{ad}_{g_n}^l(f_{\mathrm{loc}}) g_n^{k-l}\psi \right\|^2 \geq \frac{2C_0}{3}\|\psi_n^k\|^2.$$

The left-hand side is bounded in $n$ by *Step 2* and the induction hypothesis. Analogously, one finds for $I_0'(n)$

$$I_0'(n) + b_n \geq \frac{C_0}{3}\|p_n\psi_n^{(k)}\|^2,$$

for some $b_n \geq 0$, $n \in \mathbb{N}$ and $\sup_{n\in\mathbb{N}} b_n < \infty$. Let

$$I_4(n) := b_n + \frac{9\|K\mathbf{1}_{|A|\leq\Lambda}(A)\psi_n^{(k)}\|^2}{2C_0} + C_1 \left\| \sum_{l=1}^{k} \binom{k}{l} \operatorname{ad}_{g_n}^l(f_{\mathrm{loc}}) g_n^{k-l}\psi \right\|^2.$$

Finally, this gives with (3.36)

$$\tfrac{C_0}{3}\left(\|p_n\psi_n^{(k)}\|^2 + \|\psi_n^{(k)}\|^2\right) \leq I_3(n) + I_4(n),$$

where the right-hand side is bounded in $n$. By definition of $g$ the result is now a consequence of the Theorem of Monotone Convergence applied to the left-hand side. □

## 3.5 Eigenstates as analytic vectors

To obtain explicit bounds, independent of the regularisations of $A$, we apply Lemma 3.16 and use (3.35) as a starting point.

**Proposition 3.18.** *Let $k \in \mathbb{N}$, $h_\lambda(H) \in C^{k+1}(A)$ and Condition 3.4 be satisfied. Then, for any eigenstate $\psi$ of $H$ with eigenvalue $\lambda \in \operatorname{supp}(f_{\mathrm{loc}})$ and $\Lambda \geq 0$ being* *chosen as in (3.37) we have*

$$
\begin{aligned}
\|A^k\psi\|^2 \le{}& \frac{27\|K\mathbf{1}_{|A|\le\Lambda}(A)A^k\psi\|^2}{C_0^2} + \frac{6C_1}{C_0}\Big\|\sum_{l=1}^{k}\binom{k}{l}\operatorname{ad}_A^l(f_{\mathrm{loc}})A^{k-l}\psi\Big\|^2 \\
&+ \frac{96}{((1+2k)C_0)^2}\Big(\|\operatorname{ad}_A^{k+1}(h)\psi\|^2 + k^2\|\operatorname{ad}_A^2(h)A^{k-1}\psi\|^2\Big) \\
&+ \frac{12}{(1+2k)C_0}\sum_{j=2}^{k-1}\binom{k+1}{j+1}\Big(|(A^{k+1-j}\psi, \operatorname{ad}_A^{j+1}(h)A^{k-1}\psi)| \\
&\qquad + |(A^{k-j}\psi, \operatorname{ad}_A^{j+2}(h)A^{k-1}\psi)|\Big). \qquad (3.38)
\end{aligned}
$$

**Remark 3.19.** The bounds derived in this proposition make the locally uniform boundedness of $A^k\psi$ in the sense of Condition 1.10 of [FlS10b] apparent.

*Proof.* Note that $\psi \in \mathcal{D}(A^k)$ by Theorem 3.6. We observe

$$
\lim_{n\to\infty}[p_n, \operatorname{ad}_A(h)] = \lim_{n\to\infty}\frac{-1}{n2\pi i}\int_{\mathbb{C}}\bar\partial\tilde p(z)J_n(z)\operatorname{ad}_A^2(h)J_n(z)dz\wedge d\bar z = 0,
$$

since $\bar\partial\tilde p$ has compact support and $h \in C^{k+1}(A)$. Further with $\psi^{(l)} := A^l\psi$, for $0 \le l \le k$,

$$
\begin{aligned}
\lim_{n\to\infty} E_1(j,k,n) &= (\psi^{(k+1-j)}, \operatorname{ad}_A^j(h)\psi^{(k)}) =: E_1(j,k), \quad k \ge j \ge 2, \\
\lim_{n\to\infty} E_2(j,k,n) &= (\psi^{(k-j)}, \operatorname{ad}_A^{j+1}(h)\psi^{(k)}) =: E_2(j,k), \quad k \ge j \ge 1.
\end{aligned}
$$

Note that $E_1(j+1,k) = E_2(j,k)$ for $k-1 \ge j \ge 1$. Thus, Eq. (3.35) reads after taking the limit $n \to \infty$

$$
(1+2k)(\psi^{(k)}, i\operatorname{ad}_A(h)\psi^{(k)}) = 2\operatorname{Re}\Big(i\sum_{j=1}^{k-1}\binom{k+1}{j+1}E_2(j,k)\Big) + 2\operatorname{Re} iE_2(k,k).
$$

The term $E_2(k,k)$ is singular in the sense that one cannot commute one power of $A$ to the left-hand side and the estimate for $E_2(1,k)$ does not improve under such a manipulation. To estimate $E_2(1,k)$ we note

$$
-2\operatorname{Re}(\psi^{(k-1)}, i\operatorname{ad}_A^2(h)\psi^{(k)}) \le \tfrac{1}{\epsilon}\|\operatorname{ad}_A^2(h)\psi^{(k-1)}\|^2 + \epsilon\|\psi^{(k)}\|^2.
$$

We pick up a combinatorial factor $(k+1)k/2$ and thus choose

$$
\epsilon = \frac{(1+2k)C_0}{(k+1)k}2^{-3}.
$$

For $E_2(k,k)$, the combinatorial factor is 1 and we estimate

$$
-2\operatorname{Re}(\psi, i\operatorname{ad}_A^{k+1}(h)\psi^{(k)}) \le \tfrac{1}{\mu}\|\operatorname{ad}_A^{k+1}(h)\psi\|^2 + \mu\|\psi^{(k)}\|^2.
$$

Choose now

$$
\mu = (1+2k)C_0 2^{-4}.
$$

This gives with $(k+1)k/2 \leq k^2$ the inequality

$$(\psi^{(k)}, i\,\mathrm{ad}_A(h)\psi^{(k)}) - C_0 2^{-3}\|\psi^{(k)}\|^2 \leq \frac{2}{1+2k}\sum_{j=2}^{k-1}\binom{k+1}{j+1}|E_2(j,k)| + \frac{16}{(1+2k)^2 C_0}\left(\|\,\mathrm{ad}_A^{k+1}(h)\psi\|^2 + k^2\|\,\mathrm{ad}_A^2(h)\psi^{(k-1)}\|^2\right).$$

Note, that the upper bounds are modified as compared to the bounds in *Step 2* of the proof of Theorem 3.6. Namely we use for $2 \leq j \leq k-1$,

$$E_2(j,k) = (\psi^{(k+1-j)}, \mathrm{ad}_A^{j+1}(h)\psi^{(k-1)}) + (\psi^{(k-j)}, \mathrm{ad}_A^{j+2}(h)\psi^{(k-1)}).$$

Next, lower bounds are established using an analogous argument as in *Step 3* of the proof of Theorem 3.6. Observe that

$$(\psi^{(k)}, i\,\mathrm{ad}_A(h)\psi^{(k)}) + \frac{9\|K\mathbf{1}_{|A|\leq\Lambda}(A)\psi^{(k)}\|^2}{2C_0} + C_1\left\|\sum_{l=1}^{k}\binom{k}{l}\mathrm{ad}_A^l(f_{\mathrm{loc}})\psi^{(k-l)}\right\|^2 - C_0 2^{-3}\|\psi^{(k)}\|^2 \geq \frac{C_0}{6}\|\psi^{(k)}\|^2.$$

Finally, we arrive at

$$\frac{C_0}{6}\|\psi^{(k)}\|^2 \leq \frac{9\|K\mathbf{1}_{|A|\leq\Lambda}(A)A^k\psi\|^2}{2C_0} + C_1\left\|\sum_{l=1}^{k}\binom{k}{l}\mathrm{ad}_A^l(f_{\mathrm{loc}})A^{k-l}\psi\right\|^2 + \frac{16}{(1+2k)^2 C_0}\left(\|\,\mathrm{ad}_A^{k+1}(h)\psi\|^2 + k^2\|\,\mathrm{ad}_A^2(h)A^{k-1}\psi\|^2\right) + \frac{2}{1+2k}\sum_{j=2}^{k-1}\binom{k+1}{j+1}|E_2(j,k)|,$$

which implies (3.38). □

**Lemma 3.20.** *Let $K, L \in \mathfrak{B}(\mathcal{H})$ and $J(z) := (z-K)^{-1}$ for $z \in \rho(K)$. Then,*

$$\mathrm{ad}_L^k(J(z)) = \sum_{a\in C(k)}\frac{k!}{a_1!\cdot\dots\cdot a_{n_a}!}J(z)\prod_{i=1}^{n_a}\mathrm{ad}_L^{a_i}(K)J(z), \tag{3.39}$$

*where $C(k)$ denotes the set of all possible decompositions of $k = a_1 + \dots + a_{n_a}$ in sums of natural numbers and further $a := (a_1, \dots, a_{n_a})$.*

The formula may easily be observed to be correct. For a proof of similar statement see [Ras10].

*Proof (Proof of Lemma 3.2).* We proof the statement by establishing the formula (3.39) inductively for $K$ replaced by $H$ and $L$ replaced by $A$. For $k=1$ we observe $\mathrm{ad}_A(J(z)) = J(z)\,\mathrm{ad}_A(H)J(z)$, since $H \in C^1(A)$. Assume now for $k-1 \in \mathbb{N}$, $\rho(H)$,

$$\mathrm{ad}_A^{k-1}(J(z)) = \sum_{a\in C(k-1)}\frac{(k-1)!}{a_1!\cdot\dots\cdot a_{n_a}!}J(z)\prod_{j=1}^{n_a}\mathrm{ad}_A^{a_j}(H)J(z). \tag{3.40}$$

Observe, that $\mathrm{ad}_A^{a_j}(H)J(z) \in \mathfrak{B}(\mathcal{H})$, for all $1 \le j \le n_a$. It is well known that the bounded elements in $C^1(A)$ form an algebra. This means that it suffices to check that each of the operators $\mathrm{ad}_A^{a_j}(H)J(z)$ is in $C^1(A)$. For $0 \le m \le k-1$ we consider $[\mathrm{ad}_A^m(H)J(z), A]$. Let $\psi, \phi \in \mathcal{D}(A) \cap \mathcal{D}(H)$, then

$$\begin{aligned}(\psi, [\mathrm{ad}_A^m(H)J(z), A]\phi) &= ((-1)^m J(\bar{z})\,\mathrm{ad}_A^m(H)\psi, A\phi) \\ &\quad + (A\psi, \mathrm{ad}_A^m(H)J(z)\phi) \\ &= (\psi, [\mathrm{ad}_A^m(H), A]J(z)\phi) \\ &\quad + ((-1)^m\,\mathrm{ad}_A^m(A)\psi, J(z)\,\mathrm{ad}_A(H)J(z)\phi),\end{aligned}$$

where in the last line we used

$$AJ(z)\psi = J(z)A\psi + J(z)\,\mathrm{ad}_A(H)J(z)\psi, \quad \forall \psi \in \mathcal{D}(H).$$

By assumption, $[\mathrm{ad}_A^m(H), A]$ extends to a an element

$$\mathrm{ad}_A^{m+1}(H) \in \mathfrak{B}(\mathcal{D}(H), \mathcal{H}),$$

which implies that $[\mathrm{ad}_A^m(H)J(z), A]$ extends to a bounded operator for $0 \le m \le k-1$, i.e. $\mathrm{ad}_A^m(H)J(z) \in C^1(A)$. Hence $H \in C^k(A)$. □

We devote the rest of this section to prove Theorem 3.9.

*Proof (of Theorem 3.9).* We organise the proof for analyticity in two steps and, for simplicity, we suppose the eigenvalue $\lambda$ with respect to $H, \psi$ is 0. We consider $h(x) := x(1+\nu x^2)^{-1}$, for sufficiently small $\nu > 0$, see Section 3.6 and replace $f_{\mathrm{loc}}$ by $f_{\mathrm{ana}}$, defined in (3.48). By assumption and Section 3.6, this $h$ satisfies Condition 3.4. The first step consists of proving that $\psi$ is an analytic vector for $A$ under the condition

$$\|\,\mathrm{ad}_A^k(h)\|, \|\,\mathrm{ad}_A^k(f_{\mathrm{ana}})\| \le k! w^{-k}, \quad \forall k \in \mathbb{N}, \tag{3.41}$$

for some $w \in \mathbb{R}_+$ to be fixed later in the proof. In the second step we prove (3.41) using Condition 3.8. Note, that it is sufficient to prove analyticity of the map $\theta \mapsto \exp(i\theta A)\psi =: \psi(\theta)$ in some ball around 0. Namely, if $\psi(\cdot)$ is analytic in a ball then $\tilde{\psi}(t+\theta) := \exp(itA)\psi(\theta)$, $t \in \mathbb{R}$ defines an analytic extension of this map to a strip. Alternatively, one observes the bounds in (3.38) to be invariant under conjugation of $H$ with $\exp(itA)$, $t \in \mathbb{R}$ and hence $\psi(\cdot)$ extends to an analytic function in a strip around the real axis.

***Step 1.*** Assume Condition (3.41) to be satisfied and abbreviate

$$\begin{aligned}\alpha(j,k) &:= \frac{12}{(1+2k)C_0}\binom{k+1}{j+1}|(\psi^{(k+1-j)}, \mathrm{ad}_A^{j+1}(h)\psi^{(k-1)})|, \\ \beta(j,k) &:= \frac{12}{(1+2k)C_0}\binom{k+1}{j+1}|(\psi^{(k-j)}, \mathrm{ad}_A^{j+2}(h)\psi^{(k-1)})|.\end{aligned}$$

Motivated by Condition (3.41), we use the ansatz

$$\|\psi^{(l)}\| \le l! q^{-l}, \quad \text{for } 1 \le l \le k-1,$$

for some $q \in \mathbb{R}_+$, $q < w$, independent of $l$. Employing the assumptions gives

$$\alpha(j,k) \leq k!^2 q^{-2k} \frac{12}{C_0 w k}(k+1-j)\left(\frac{q}{w}\right)^j,$$

thus

$$(k!^2 q^{-2k})^{-1} \sum_{j=2}^{k-1} \alpha(j,k) \leq \frac{12}{C_0 w}\left(\frac{q}{w}\right)^2 \sum_{j=0}^{k-3}\left(\frac{q}{w}\right)^j \leq \frac{12}{C_0 w}\left(\frac{q}{w}\right)^2 \frac{1}{1-\left(\frac{q}{w}\right)}.$$

Analogously,

$$\beta(j,k) \leq k!^2 q^{-2k} \frac{12}{C_0 w k}(j+2)\left(\frac{q}{w}\right)^{j+1}$$

and consequently

$$(k!^2 q^{-2k})^{-1} \sum_{j=2}^{k-1} \beta(j,k) \leq \frac{24}{C_0 w}\left(\frac{q}{w}\right)^3 \sum_{j=0}^{k-3}\left(\frac{q}{w}\right)^j \leq \frac{24}{C_0 w}\left(\frac{q}{w}\right)^3 \frac{1}{1-\left(\frac{q}{w}\right)}.$$

We continue by estimating (3.24),

$$\begin{aligned}\left(\frac{6C_1}{C_0}\right)^{\frac{1}{2}} \|f_{\mathrm{ana},\perp}\psi^{(k)}\| &\leq \left(\frac{6C_1}{C_0}\right)^{\frac{1}{2}} \sum_{j=1}^{k}\binom{k}{j} j!(k-j)!\left(\frac{q}{w}\right)^j q^{-k} \\ &\leq k! q^{-k}\left(\frac{6C_1}{C_0}\right)^{\frac{1}{2}}\left(\frac{q}{w}\right)\frac{1}{1-\left(\frac{q}{w}\right)}.\end{aligned}$$

Further,

$$\begin{aligned}\frac{96k^2\|\operatorname{ad}_A^2(h)\psi^{(k-1)}\|^2}{C_0^2(1+2k)^2} &\leq \frac{24}{C_0^2 k^2 w^2}\left(\frac{q}{w}\right)^2 k!^2 q^{-2k}, \\ \frac{96\|\operatorname{ad}_A^{k+1}(h)\psi\|^2}{C_0^2(1+2k)^2} &\leq \frac{96}{C_0^2 w^2}\left(\frac{q}{w}\right)^{2k} k!^2 q^{-2k}\end{aligned}$$

and finally

$$\frac{27}{C_0^2}\|K\mathbf{1}_{|A|\leq\Lambda}(A)\psi^{(k)}\|^2 \leq \frac{27\|K\|^2(\Lambda q)^{2k}}{C_0^2 k!^2} k!^2 q^{-2k}.$$

Pick now $q$ sufficiently small, such that all pre-factors of $k!^2 q^{-2k}$ are less than $1/6$ and observe that this can be done uniformly in $k$. Then, we obtain for our specified $q$

$$\|\psi^{(k-1)}\| \leq (k-1)! q^{-(k-1)} \Longrightarrow \|\psi^{(k)}\| \leq k! q^{-k}.$$

This proves that $\psi$ is an analytic vector for $A$, given condition (3.41).

***Step 2.*** We first compute the multiple commutators of $h$. For some $n_0 \in \mathbb{N}$, see Section 3.6, the function

$$h(x) = -\tfrac{1}{2}((i - x/n_0)^{-1} + (-i - x/n_0)^{-1})$$

and (3.48) satisfy Condition 3.4. It follows from Condition 3.8 and (3.40) in the proof of Lemma 3.2 that the multiple commutators of $h$ may be expressed in terms of the multiple commutators of $J(z) := (z - H/n_0)^{-1}$,

$$\mathrm{ad}_A^k(J(\pm i)) = n_0^{-k} \sum_{a \in C(k)} \frac{k!}{a_1! \cdot \dots \cdot a_{n_a}!} J(\pm i) \prod_{i=1}^{n_a} \mathrm{ad}_A^{a_i}(H) J(\pm i), \tag{3.42}$$

for any $z$ in the resolvent set of $H$. The number of elements in $C(k)$ is given by $2^k - 1$, which may be verified by induction. Thus, we may estimate (3.42) further in virtue of (3.6).

$$\| \mathrm{ad}_A^k(J(\pm i)) \| \le k! v^{-k} (2^k - 1) \le k! w^{-k} \left( \frac{2w}{v} \right)^k .$$

Choose now $\mathbb{R} \ni w > 0$ such that $4w \le v$ and conclude as in *Step 1* by induction that for $h$, Condition 3.8 implies (3.41) and in particular, $h \in C^\infty(A)$. It is obvious that $f_{\mathrm{ana}}$ gives the same bounds, which completes the proof. □

**Remark 3.21.**
1. If we had used $\arctan(x)$ instead of $h(x) = x(1 + x^2)^{-1}$, we would have encountered the problem that the bounds (3.41) are easily obtained from (3.6) in graph norm w.r.t. $H$, only. In contrast, the decay at infinity of our choice of $h$ allows naturally for bounds in operator norm.

2. Note, that the first step in the proof uses the relations (3.41) only and is, abstractly, independent of the stronger assumption (3.6).

## 3.6 The Mourre estimate in localised form

The Mourre estimate is usually cast in a different form than it is used here. Let $H, A$ be self-adjoint operators, $H \in C^1(A)$. Let now $\tilde{C}_0 > 0$ and $\tilde{K}$ be a compact operator. We denote by $\mathbf{1}_I(H)$ spectral projections of $H$ for an interval $I \subset \mathbb{R}$. Suppose, that in the sense of quadratic forms on $\mathcal{H} \times \mathcal{H}$

$$\mathbf{1}_I(H) i[H, A] \mathbf{1}_I(H) \ge \tilde{C}_0 \mathbf{1}_I(H) - \tilde{K}. \tag{3.43}$$

This inequality is usually referred to as a *Mourre estimate*. Choose $f_{\mathrm{loc}} \in C_c^\infty(\mathbb{R})$ such that $\mathrm{supp}(f_{\mathrm{loc}}(H)) \subseteq I$ and $f_{\mathrm{loc}}(\lambda) = 1$. Set $f_{\mathrm{loc},\perp} := 1 - f_{\mathrm{loc}}$. Then, multiplying (3.43) from the left and the right with $f_{\mathrm{loc}}(H)$ yields

$$f_{\mathrm{loc}} i[H, A] f_{\mathrm{loc}} \ge \tilde{C}_0 + \tilde{C}_0 f_{\mathrm{loc},\perp}^2 - 2\tilde{C}_0 f_{\mathrm{loc},\perp} - K,$$

where $K := f_{\mathrm{loc}} \tilde{K} f_{\mathrm{loc}}$ is compact. As forms we observe $\forall \epsilon > 0$

$$2 f_{\mathrm{loc},\perp} \le \epsilon + \tfrac{1}{\epsilon} f_{\mathrm{loc},\perp}^2 .$$

Pick $\epsilon = 1/4$. Therefore, we may rewrite (3.45) as

$$f_{\mathrm{loc}} i[H, A] f_{\mathrm{loc}} \ge \tilde{C}_0 \tfrac{3}{4} - 3\tilde{C}_0 f_{\mathrm{loc},\perp}^2 - K. \tag{3.44}$$

Let $h \in \mathcal{B}$. Set $h(t) := h(t-\lambda)$. By possibly shrinking the support of $f_{\mathrm{loc}}$ we may assume $\mathrm{supp}(f_{\mathrm{loc}}) \subseteq \mathrm{supp}(h_\lambda)$. To avoid obscuring the computations notationally, we refrain from writing $h_\lambda$ and use $h$ instead. Set $h_n(t) := nh(t/n)$, $\forall t \in \mathbb{R}$ and abbreviate $K_n(z) := (z - H/n)^{-1}$. Then, by similar arguments as in Lemma 3.15,

$$f_{\mathrm{loc}} i\,\mathrm{ad}_A(h_n) f_{\mathrm{loc}} = f_{\mathrm{loc}} h_n' i\,\mathrm{ad}_A(H) f_{\mathrm{loc}} + R,$$

where

$$R := \frac{1}{2\pi n}\int_{\mathbb{C}} \bar{\partial}\widetilde{\left(\frac{h}{t}\right)}(z) z K_n(z)^2 f_{\mathrm{loc}}[\mathrm{ad}_A(H), H] f_{\mathrm{loc}} K_n(z)\, dz \wedge d\bar{z}.$$

Note that

$$f_{\mathrm{loc}} i\,\mathrm{ad}_A(H) f_{\mathrm{loc}} = f_{\mathrm{loc}} \mathbf{1}_I(H) i\,\mathrm{ad}_A(H) \mathbf{1}_I(H) f_{\mathrm{loc}}$$

is a bounded operator on $\mathcal{H}$. Analogue estimates as in the proof of Lemma 3.15 yield

$$\|R\| \le \frac{C}{n},$$

for a $C \ge 0$. This gives

$$\begin{aligned}\|f_{\mathrm{loc}} i\,\mathrm{ad}_A(H-h_n) f_{\mathrm{loc}}\| &\le \|(\mathbb{1}-h_n') f_{\mathrm{loc}} i\,\mathrm{ad}_A(H) f_{\mathrm{loc}}\| + \frac{C}{n} \\ &\le C'\Big(\|(\mathbb{1}-h_n')\mathbf{1}_{\mathrm{supp}(f_{\mathrm{loc}})}(H)\| + \tfrac{1}{n}\Big),\end{aligned}$$

for some $C' > 0$. Taylor's theorem implies for positive $t \in \mathrm{supp}(f_{\mathrm{loc}})$

$$|1 - h_n'(t)| \le \int_0^{\frac{t}{n}} |h''(s)| ds \le \frac{\sup_{t\in\mathrm{supp}(f_{\mathrm{loc}})}|t|}{n} \sup_{s\in\mathrm{supp}(f_{\mathrm{loc}})} |h''(s)|$$

and analogously for negative $t \in \mathrm{supp}(f_{\mathrm{loc}})$. Thus, there is a $C'' > 0$ such that

$$f_{\mathrm{loc}} i\,\mathrm{ad}_A(H-h_n) f_{\mathrm{loc}} \le \frac{C''}{n}.$$

Choose $n_0 \in \mathbb{N}$ large enough such that

$$f_{\mathrm{loc}} i\,\mathrm{ad}_A(H-h_{n_0}) f_{\mathrm{loc}} \le \frac{\tilde{C}_0}{4}. \tag{3.45}$$

Using $f_{\mathrm{loc},\perp} = 1 - f_{\mathrm{loc}}$ we obtain from (3.45), (3.44)

$$i[h_{n_0}, A] \ge \tfrac{\tilde{C}_0}{2} - 3\tilde{C}_0 f_{\mathrm{loc},\perp}^2 - K - f_{\mathrm{loc},\perp} i[h_{n_0}, A] f_{\mathrm{loc},\perp} - 2\,\mathrm{Re}(f_{\mathrm{loc},\perp} i[h_{n_0}, A]), \tag{3.46}$$

Note, that all operators appearing in (3.46) are self-adjoint. With

$$\begin{aligned} & f_{\mathrm{loc},\perp} i\,\mathrm{ad}_A(h_{n_0}) f_{\mathrm{loc},\perp} \le \|\,\mathrm{ad}_A(h_{n_0})\| f_{\mathrm{loc},\perp}^2, \\ \forall \delta > 0: \qquad & \pm 2\,\mathrm{Re}(f_{\mathrm{loc},\perp} i\,\mathrm{ad}_A(h_{n_0})) \le \delta \|\,\mathrm{ad}_A(h_{n_0})\|^2 + \tfrac{1}{\delta} f_{\mathrm{loc},\perp}^2,\end{aligned}$$

and a choice of $\delta$ such that $\delta\|\,\mathrm{ad}_A(h_{n_0})\|^2 \leq \tilde{C}_0/4$ we find

$$i[h_{n_0}, A] \geq C_0 - C_1 f_{\mathrm{loc},\perp}^2 - K, \tag{3.47}$$

where $0 < C_0 := \tilde{C}_0/4$. The other constant is $C_1 := 3\tilde{C}_0 + \delta^{-1} + \|\,\mathrm{ad}_A(h_{n_0})\|$.

We may choose an $h$ which is real analytic and extends to an analytic function in a strip around the real axis. Thus it is possible to reformulate inequality (3.47) using analytic functions only; a fact we rely on in the proof of our analyticity result.

Consider the real analytic function

$$f_{\mathrm{ana}}(x) := \frac{1}{1+(x-\lambda)^2} = \frac{1}{2}\left(\frac{1}{1+i(x-\lambda)} + \frac{1}{1-i(x-\lambda)}\right), \forall x \in \mathbb{R}. \tag{3.48}$$

Replacing the constant $C_1$ with

$$C_1 \sup_{x\in\mathbb{R}} \left(\frac{f_{\mathrm{loc},\perp,}(x)}{f_{\mathrm{ana},\perp}(x)}\right),$$

where $f_{\mathrm{ana},\perp} := 1 - f_{\mathrm{ana}}$, we may rewrite the Mourre estimate (3.47) as

$$i[h, A] \geq C_0 - C_1 f_{\mathrm{ana},\perp}^2 - K. \tag{3.49}$$

We denote the constant in front of $f_{\mathrm{ana},\perp}^2$ in a slight abuse of notation again with $C_1$.

### Acknowledgements

M. Westrich thanks Johannes-Gutenberg Universität Mainz, and V. Bach in particular, for support. Moreover, both authors thank the Erwin Schrödinger Institut (ESI) for hospitality, and in the case of M. Westrich for financial support in the form of a 'Junior Research Fellowship'.

## 3.7 Bibliography

[AdMG96] W. Amrein, A. Boutet de Monvel, and V. Georgescu, *$C_0$-groups, commutator methods, and spectral theory of N-body Hamiltonians*, Birkhäuser, 1996.

[Amm00] Z. Ammari, *Asymptotic completeness for a renormalized nonrelativistic Hamiltonian in quantum field theory: The Nelson model*, Math. Phys. Anal. Geom. **3** (2000), 217–285.

[BC71] E. Balslev and J. M. Combes, *Spectral Properties of Many-body Schrödinger Operators with Dilatation-analytic interactions*, Commun. Math. Phys. **22** (1971), 280–294.

[CGH06] L. Cattaneo, G. M. Graf, and W. Hunziker, *A general resonance theory based on Mourre's inequality*, Ann. Henri Poincaré **7** (2006), 583–601.

[DG99] J. Dereziński and C. Gérard, *Asymptotic completeness in quantum field theory. Massive Pauli-Fierz Hamiltonians*, Rev. Math. Phys. **11** (1999), 383–450.

[DG00] ______, *Spectral and scattering theory of spatially cut-off $P(\phi)_2$ Hamiltonians*, Comm. Math. Phys. **213** (2000), 39–125.

[DJ01] J. Dereziński and V. Jaksic, *Spectral theory of Pauli-Fierz operators*, J. Funct. Anal. **180** (2001), 243–327.

[FGS01] J. Fröhlich, M. Griesemer, and B. Schlein, *Asymptotic electromagnetic fields in models of quantum-mechanical matter interacting with the quantized radiation field*, Adv. Math. **164** (2001), 349–398.

[FGS08] J. Fröhlich, M. Griesemer, and I. M. Sigal, *Spectral theory for the standard model of non-relativistic QED*, Comm. Math. Phys. **283** (2008), 613–646.

[FH82] R. Froese and I. Herbst, *A new proof of the Mourre estimate*, Duke Math. J. **49** (1982), 1075–1085.

[FlS10a] J. Faupin, J.S. Møller, and E. Skibsted, *Regularity of Bound States*, arXiv:1006.5871 (2010).

[FlS10b] ______, *Second order perturbation theory for embedded eigenvalues*, arXiv:1006.5869 (2010).

[GGM04a] V. Georgescu, C. Gérard, and J. S. Møller, *Commutators, $C_0$-semigroups and resolvent estimates*, J. Funct. Anal. **216** (2004), 303–361.

[GGM04b] ______, *Spectral theory of massless Pauli-Fierz models*, Comm. Math. Phys. **249** (2004), 29–78.

[Gol09] S. Golénia, *Positive commutators, Fermi golden rule and the spectrum of zero temperature Pauli-Fierz Hamiltonians*, J. Funct. Anal. **256** (2009), 2587–2620.

[HS00] W. Hunziker and I. M. Sigal, *The quantum N-body problem*, J. Math. Phys. **41** (2000), 3448–3510.

[Møl00] J. S. Møller, *An abstract radiation condition and applications to N-body systems*, Rev. Math. Phys. **12** (2000), 767–803.

[Mou81] E. Mourre, *Absence of singular continuous spectrum for certain self-adjoint operators*, Comm. Math. Phys. **78** (1981), 391–408.

[MR10] J. S. Møller and M. G. Rasmussen, *The massive translation invariant Nelson model II.*, in preparation (2010).

[MS04] J. S. Møller and E. Skibsted, *Spectral theory for time-periodic many-body systems*, Adv. Math. **188** (2004), 137–221.

[Ras10] M.G. Rasmussen, *PhD Thesis, Aarhus University*, 2010.

[RS75] M. Reed and B. Simon, *Methods of modern mathematical physics: II. Fourier analysis and self-adjointness*, 1 ed., Academic Press, San Diego, 1975.

[Sah97] J. Sahbani, *The conjugate operator method for locally regular Hamiltonians*, J. Operator Theory **38** (1997), 297–322.

[SAS89] I. Herbst S. Agmon and E. Skibsted, *Perturbation of embedded eigenvalues in the generalized N-body problem*, Commun. Math. Phys. **122** (1989), 411–438.

[Ski98] E. Skibsted, *Spectral analysis of N-body systems coupled to a bosonic field*, Rev. Math. Phys. **10** (1998), 989–1026.

# Part III

# A Pumping Scheme for Solid State Lasers

CHAPTER 4

# Characterisation of the Quasi-Stationary State of an Impurity Driven by Monochromatic Light I - The Effective Theory

J.-B. BRU, W. A. DE SIQUEIRA PEDRA, M. WESTRICH

**Abstract**

We study rigorously a pumping scheme of a solid state laser model deriving from a microscopical model, which is composed of an impurity in a crystal interacting with a monochromatic external light source. The main purpose of the present work is the analysis of its effective dynamics and in a companion paper the link to the microscopical model is established. We prove for the effective dynamics the existence of and relaxation to a quasi-stationary state, which is a stationary state up to Rabi-Oscillations due to the external light source. Moreover, we characterise the state in terms of "generalised Einstein relations" of spontaneous/stimulated emission/absorption, which are conceptually related to the phenomenological relations derived by Einstein in 1916. Our approach is based on a spectral analysis of the evolution semigroup pertaining to the non-autonomous Cauchy problem.

## 4.1 Introduction

In the present paper and in a companion one [BPW11b], we study the dynamics of an impurity in a crystal, which serves as a thermal reservoir, interacting with an external monochromatic light source. In the corresponding microscopical model, impurity, crystal and external light source are described by selfadjoint Hamilton operators. The crystal is modelled by electrons in thermal equilibrium. By unitarity of the evolution, the compound system does not exhibit dissipation. However, our main interest is to obtain an effective description of the time-evolution of the population of the energy levels of the impurity and especially its long-time behaviour. We derive an effective evolution for the population of the energy levels of the impurity, which differs from the phenomenological dynamics usually used in the physical literature, [AL07], in the sense, that the corresponding equation of motion is a integro-differential equation, whereas the phenomenological equation, called Pauli equation, is an autonomous linear differential equation. The long time behaviour of our equation is in generic situations however the same as the one predicted by the Pauli equation. It turns out, that for large time the dynamics attains a quasi-stationary state, i.e. it is stationary up to an oscillation of a certain frequency. Moreover, we find conditions on the structure of the quasi-stationary state in terms of the generator of the large time dynamics. These conditions are are expressed in terms of certain relations, which are conceptually related to the famous Einstein relations for spontaneous and stimulated transition rates of an atom interacting with the radiation field, [Ein16].

Models related to our setup without external light source have been studied extensively, see for instance [AL07, AJP06a, AJP06b, AJP06c] and references therein. The most important questions which have been considered in this context are existence and asymptotic stability of stationary states, especially asymptotic stability of thermal equilibrium states, the so-called "return to equilibrium" (RTE), [AJP06a, AJP06b, AJP06c, BFS00, JP96]. The thermal equilibrium satisfies a balance relation, which is called *detailed balance condition*. It states, that the transition rate from level $E_j$ to level $E_\ell$, equals the transition rate from $E_\ell$ to $E_j$ times a Boltzmann factor, $\exp\left(-\beta\left(E_\ell - E_j\right)\right)$.

RTE typically occurs in models involving one thermal reservoir at a given temperature $T$ weakly coupled to a confined atom. As soon as there are several thermal reservoirs at distinct temperature, the system does not possess a thermal equilibrium state but rather a "non-equilibrium stationary state", (NESS), [JP02, MMS07]. In our setting we certainly do not expect a thermal equilibrium state to exist. On the other hand it is a basic model for pumping schemes of doped crystals, [SY68]. For a not too strong external light source, henceforth called (optical) pump, one expects for large time a steady emission of photons with frequency corresponding to a specific energy difference of eigenvalues of the Hamiltonian describing the impurity. The steady emission is due to a stronger occupation of a energy level of the impurity with energy $E_2$ as compared to an energy level $E_1 < E_2$. This effect is called "inversion of population" and it is a central mechanism in lasers. Therefore, we expect a stationary state up to small oscillations of the density of population of the impurity energy levels, with a specific frequency, to exist. These oscillations are the "Rabi–Oscillations", [AL07, AGF10], which are imposed by the optical pump.

The general strategy of this project this is as follows: In [BPW11b] we use a reformulation of the two-parameter family of automorphisms describing the evolution of the compound system using a non-autonomous analogue of $C$-Liouvilleans, introduced by Jaksic and Pillet in [JP02]. The $C$-Liouvillean is the generator of a strongly continuous one–parameter semigroup and in general not selfadjoint, but well suited for the analysis of systems which do not possess a thermal equilibrium state. We then prove that the non-autonomous $C$-Liouvillean dynamics is uniformly in time, on the impurity's degrees of freedom, perturbatively close to a dynamics which is generated by a non-autonomous Markovian approximation of the original dynamics. In the present paper, we start with the Markovian approximation and employ a Floquet analysis of the corresponding evolution semigroup. This allows us to derive general properties of the quasi-stationary state without any phenomenological approximations, as the rotating wave approximation, [AL07]. In this vein, we find a balance condition of the quasi-stationary state, which represents a natural replacement of the detailed balance condition.

A motivation for this work comes from the following consideration. The laser effect is based on a phase transition of incoherent light to a directed coherent light beam. To our knowledge there is only one setup for which this phase transition has been successfully proven, namely for the Dicke maser/laser model by Hepp and Lieb, . The model consists in a Hamiltonian approach of a radiation field serving as a reservoir, a finite number, $N$, of two-level atoms, finitely many quantised "radiation-modes" and linear couplings of atoms and reservoir with atoms and atoms with the radiation modes, [HL73]. The system undergoes a phase transition in the limit $N \to \infty$ in the sense, that the radiation becomes coherent. More than 20 years later, Alli and Sewell, [AS95], and related to this Bagarello, [Bag02], proved some generalisations of these results, but in a weak coupling limit regime. On the other hand, solid state lasers are usually constructed with weakly doped crystals, [SY68]. Thus a limit of many particles is not suitable. The present work is in this sense a first step to a laser model with fixed $N$, namely to understand its pumping scheme. An important open problem remains however to find a realistic description of a cavity. Recent work in this direction is due to Bruneau and Pillet, [BD09].

Another motivation is drawn from the structure of transition rates between different energy levels of the impurity. These rates derive from relations which are of a similar form as the famous Einstein relations, [Ein16], which Einstein derived phenomenologically, assuming essentially only

- Wien's displacement law,
- that the thermal equilibrium state of the atom, the Gibbs state, is stationary w.r.t. the interaction with the radiation,
- that the radiation density diverges if the temperature tends to infinity.

The situation he discussed is the interaction of an atom interacting with the radiation field. The corresponding initial state was assumed to yield a non-zero radiation density. He found in particular, that the rates for the stimulated processes are proportional to the radiation density and the rates of the spontaneous processes. In contrast, we consider a situation where the initial radiation density is zero, but instead there is an optical pump. Therefore one can not expect the same relation between the stimulated and the spontaneous processes as in Einstein's work. In our model we find that the stimulated processes are proportional to the intensity of the radiation as in Einstein's work and that the matrix for rates of the stimulated processes are determined by the "off-diagonal part" of the inverse matrix for the rates of the spontaneous processes, $A_{OD}^{-1}$. A recent work of Berman, Merkli and Sigal, [BMS08], relates the time of decoherence, $\tau_{dec}$, which typically measures the time until a quantum statistical system becomes a classical statistical system, to $A_{OD}^{-1}$, i.e. $\tau_{dec} \sim A_{OD}^{-1}$. In another recent work of Bach, Merkli, Pedra and Sigal, [BMPS11], the possibility to control $\tau_{dec}$ using a special external light source, very much different form ours, is investigated. In certain situations control of decoherence could thus enhance the inversion of the population. On the other hand, by measuring the threshold of the pump intensity needed for inversion of populations could yield a simple experimental test for control of decoherence.

In the present paper we focus on the derivation and analysis of the structure of the quasi-stationary state of the corresponding time-dependent optical equation for the impurity. To this end, we replace the electron field–impurity coupling by its Markov–approximation, point-wise in time. In a companion paper, [BPW11b], we complete the analysis of full microscopic dynamics for translation analytic electron field-impurity couplings. In particular, the approximation of the dynamics by a time-dependent optical equation is justified for this class of couplings.

We organise the paper as follows. In Section 4.2 we define the microscopic model and specify the initial state of the system. Then, in Section 4.3 we first define the effective master equation and specify its relation to the microscopic model, see Section 4.3.1. In Section 4.3.2, we reformulate the non-autonomous effective master equation as a so-called evolution semigroup in a enlarged Hilbert space, in which the physical time is regarded as a new degree of freedom. Moreover, a spectral analysis of its generator yields an optical equation, which in Section 4.4 leads to a characterisation of the quasi-stationary state in terms of generalised Einstein relations. In the appendix we gathered some results used in the text for the reader's convenience.

## 4.2 Mathematical description of particle systems in interaction with a reservoir

### 4.2.1 The reservoir

We introduce now well know objects and one may for instance consult [BR87, BR96]. Let $\mathfrak{h}_1 := L^2(\mathbb{R}^3, \mathbb{C})$ be the separable Hilbert space representing the one–particle space of the reservoir. The one–particle Hamiltonian $h_1$ is then defined by using a dispersion relation. Consider some measurable, rotationally invariant function $\mathbf{E} : \mathbb{R}^3, \rightarrow \mathbb{R}$, i.e. $\mathbf{E}(p) = E(|p|)$ and define the multiplication operator $h_1 = h_1(E)$, $f(p) \mapsto E(p)f(p)$ on $\mathfrak{h}_1$. Physically, $E$ represents the energy of one particle at momentum $p$.

In the context of the Markov–approximations, also $L^2$ spaces on Brillouin zones, which model crystals in a more realistic way, could also be used as one–particle spaces. The results obtained are qualitatively the same. In particular the rotation symmetry in not essential to the analysis performed below. As we seek to keep technical aspects as simple as possible in the sequel, yet maintaining mathematical rigour, we even demand:

**Assumption 4.1 (E).** $\mathbf{E}(p) \equiv |p|$.

We consider a fermion reservoir which models electrons in thermal equilibrium interacting with an impurity in a crystal. In the following, we occasionally say "atom", instead of "impurity", especially as indices in formulas. From physical point of view, this is not an unnatural name. An interaction of the impurity with bosonic particles like phonons can also be implemented, but for simplicity we refrain from considering it as it qualitatively leads to similar results w.r.t. the dynamics of the atomic state.

Thus, observables of the reservoir are selfadjoint elements of the fermion $C^*$–algebra $\mathcal{V}_{\mathcal{R}}$, which is defined as follows. For any $f \in \mathfrak{h}_1$, let $a(f)$ and $a^+(f) := a(f)^*$ be the fermionic annihilation and creation operators on the antisymmetric Fock space $\mathcal{F}_-(\mathfrak{h}_1)$. These operators implement the canonical anti-commutation relations (CAR):

$$a(f_1)a^+(f_2) + a^+(f_2)a(f_1) = \langle f_1, f_2 \rangle, \tag{4.1}$$

which yield the boundedness of $a(f)$ and $a^+(f)$:

$$\|a^+(f)\|_{\mathcal{F}_-(\mathfrak{h}_1)} = \|a(f)\|_{\mathcal{F}_-(\mathfrak{h}_1)} = \|f\|_{\mathfrak{h}_1}, \quad f_1, f_2 \in \mathfrak{h}_1. \tag{4.2}$$

The fermion algebra

$$\begin{aligned} \mathcal{V}_{\mathcal{R}} \quad := \quad & \overline{\mathrm{lin}\Big\{ \mathbf{1}_{\mathcal{R}} \Big\} \cup \Big\{ a^+(f_1) \ldots a^+(f_m) a(f_{m+1}) \ldots} \\ & \overline{\ldots a^+(f_{m+n}) \mid f_1, \ldots, f_{m+n} \in \mathfrak{h}_1 \Big\} \Big\}}^{\|\cdot\|_{\mathcal{B}(\mathcal{F}_-(\mathfrak{h}_1))}} \end{aligned} \tag{4.3}$$

is defined as being the $C^*$–algebra generated by annihilation operators $\{a(f)\}_{f \in \mathfrak{h}_1}$. Note that $\mathcal{V}_{\mathcal{R}} \subsetneq \mathcal{B}(\mathcal{F}_-(\mathfrak{h}_1))$ is strictly smaller than the $C^*$–algebra of all bounded operators $\mathcal{B}(\mathcal{F}_-(\mathfrak{h}_1))$.

The unperturbed dynamics of the reservoir is defined by a Bogoliubov automorphism on the algebra $\mathcal{V}_{\mathcal{R}}$:

$$\tau_t^{\mathcal{R}}(a(f)) = a(e^{ith_1} f), \quad f \in \mathfrak{h}_1, \ t \in \mathbb{R}. \tag{4.4}$$

This condition physically means that the fermionic particles of the reservoir do not interact with each other, i.e., they form an ideal Fermi gas. The latter equality uniquely defines an one–parameter group $\{\tau_t^{\mathcal{R}}\}_{t \in \mathbb{R}}$ on $\mathcal{V}_{\mathcal{R}}$. By (4.2), this group is strongly continuous and hence, $(\mathcal{V}_{\mathcal{R}}, \tau_t^{\mathcal{R}})$ is a $C^*$–dynamical system.

We denote its generator by $\delta_{\mathcal{R}}$. Generators of $C^*$–dynamical systems are symmetric derivations. This means that the domain $\mathrm{Dom}(\delta_{\mathcal{R}})$ of the generator $\delta_{\mathcal{R}}$ is a dense sub–$*$–algebra of $\mathcal{V}_{\mathcal{R}}$ and, for all $A, B \in \mathrm{Dom}(\delta_{\mathcal{R}})$,

$$\delta_{\mathcal{R}}(A)^* = \delta_{\mathcal{R}}(A^*), \quad \delta_{\mathcal{R}}(AB) = \delta_{\mathcal{R}}(A)B + A\delta_{\mathcal{R}}(B). \tag{4.5}$$

Thermal states of the reservoir are defined through the bounded positive operators

$$d_{\mathcal{R}} := \frac{1}{1+e^{\beta h_1}} \tag{4.6}$$

acting on $\mathfrak{h}_1$ for all (inverse temperature) $\beta \in (0,\infty)$. Indeed, the so–called *symbol* $d_{\mathcal{R}}$ uniquely defines a (faithful) quasi–free state

$$\omega_{\mathcal{R}} := \omega_{d_{\mathcal{R}}} \tag{4.7}$$

on the fermion algebra $\mathcal{V}_{\mathcal{R}}$, by the following theorem:

**Theorem 4.2 (Two-point correlation functions and quasi–free states).** *Let $d$ be any bounded operator on $\mathfrak{h}_1$ satisfying $0 \leq d \leq 1$. Then the correlation functions*

$$\omega_d(\mathbf{1}_{\mathcal{R}}) := 1 \tag{4.8}$$

$$\omega_d\left(a^+(f_1)\dots a^+(f_m)a(g_1)\dots a(g_n)\right) := \delta_{mn}\det\left([\langle f_j, dg_k\rangle]_{j,k}\right) \tag{4.9}$$

*for all $\{f_j\}_{j=1}^n, \{g_j\}_{j=1}^n \subset \mathfrak{h}_1$ define a functional which is the unique bounded linear extension to the algebra $\mathcal{V}_{\mathcal{R}}$ is a state $\omega_d$. The operator $d$ is called the symbol of $\omega_d$.*

We call $\omega_{\mathcal{R}}$ the thermal state of the reservoir at inverse temperature $\beta$. This definition of thermal states is rather abstract but can physically be motivated as follows: Confining the particles in a box of side length $L$ corresponds to the replacement of the momentum space $\mathbb{R}^3$ by $\frac{2\pi}{L}\mathbb{Z}^3$, i.e., $L^2(\mathbb{R}^3)$ by $\ell^2(\frac{2\pi}{L}\mathbb{Z}^3)$. In particular, the spectrum of $H_{\mathcal{R}}$ (and hence of its fermionic second quantisation $\mathrm{d}\Gamma_-(H_{\mathcal{R}})$) is purely discrete. Moreover, the operators $e^{-\beta \mathrm{d}\Gamma_-(H_{\mathcal{R}})}$ are trace–class for all side lengths $L$. Thus we can define Gibbs states

$$\mathfrak{g}_{\mathcal{R}}^{(L)}(\cdot) := \frac{\mathrm{Tr}(\,\cdot\, e^{-\beta \mathrm{d}\Gamma_-(H_{\mathcal{R}})})}{\mathrm{Tr}(e^{-\beta \mathrm{d}\Gamma_-(H_{\mathcal{R}})})}, \tag{4.10}$$

which has the thermal state $\omega_{\mathcal{R}}$ as unique weak–$*$ limit when $L \to \infty$. In particular, it follows that thermal states inherit the KMS property of Gibbs states, [BR96, Sim93]:

**Theorem 4.3 (Thermal states and KMS property).** *For any $\beta \in (0,\infty)$ and $A, B \in \mathcal{V}_{\mathcal{R}}$, there is a continuous function $F_{A,B} : \mathbb{R} + i[0,\beta] \to \mathbb{C}$, holomorphic on $\mathbb{R} + i(0,\beta)$, such that, for all $t \in \mathbb{R}$,*

$$F_{A,B}(t) = \omega_{\mathcal{R}}(A\tau_t^{\mathcal{R}}(B)), \quad F_{A,B}(t+i\beta) = \omega_{\mathcal{R}}(\tau_t^{\mathcal{R}}(B)A). \tag{4.11}$$

*In particular, the thermal state $\omega_{\mathcal{R}}$ is stationary.*

### 4.2.2 The atom

The atom is modelled by a finite quantum system, i.e., its observables are self–adjoint elements of the finite–dimensional $C^*$–algebra $\mathcal{B}(\mathbb{C}^d)$ of all linear (bounded) operators on $\mathbb{C}^d$ for $d \in \mathbb{N}$.

In the sequel it is convenient to define left and right multiplication on $\mathcal{B}(\mathbb{C}^d)$: For all $A \in \mathcal{B}(\mathbb{C}^d)$ we define linear operators, $\underset{\rightarrow}{A}$ and $\underset{\leftarrow}{A}$, by

$$B \mapsto \underset{\rightarrow}{A} B := AB \quad \text{and} \quad B \mapsto \underset{\leftarrow}{A} B := BA. \tag{4.12}$$

The Hamiltonian of the atom is an arbitrary observable $H_{\mathrm{at}} = H_{\mathrm{at}}^* \in \mathcal{B}(\mathbb{C}^d)$ representing its total energy. We denote its eigenvalues and corresponding eigenspaces respectively by $E_k \in \mathbb{R}$ and $\mathcal{H}_k \subset \mathbb{C}^d$ for $k \in \{1, \ldots, N\}$. $E_k$ is chosen such that $E_j < E_k$ whenever $j < k$. In other words, $E_k$ is the energy of the $k$th atomic level and vectors of $\mathcal{H}_k$ described the sub–band structure of the corresponding level. The dimension $n_k$ of $\mathcal{H}_k$ is the degeneracy of the $k$th atomic level.

The Hamiltonian $H_{\mathrm{at}}$ defines the free atomic dynamics, i.e., a continuous one–parameter group of $*$–automorphisms $\{\tau_t^{\mathrm{at}}\}_{t \in \mathbb{R}}$ of the $C^*$–algebra $\mathcal{B}(\mathbb{C}^d)$, by

$$\tau_t^{\mathrm{at}}(A) := e^{itH_{\mathrm{at}}} A e^{-itH_{\mathrm{at}}}, \quad A \in \mathcal{B}(\mathbb{C}^d). \tag{4.13}$$

The thermal states of the free atom are Gibbs states $\mathfrak{g}_{\mathrm{at}}$ for any inverse temperature $\beta \in (0, \infty)$, given by the density matrix

$$\rho_{\mathfrak{g}} := \frac{e^{-\beta H_{\mathrm{at}}}}{\mathrm{Tr}_{\mathbb{C}^d}\left(e^{-\beta H_{\mathrm{at}}}\right)}. \tag{4.14}$$

However, in presence of interactions with the pump or the reservoir, the state $\omega$ of the atom is generally far from any Gibbs state $\mathfrak{g}_{\mathrm{at}}$.

We thus proceed to consider arbitrary atomic states $\omega_{\mathrm{at}}$. For any state $\omega_{\mathrm{at}}$ on $\mathcal{B}(\mathbb{C}^d)$, there is a unique trace–one positive operator $\rho_{\mathrm{at}}$ on $\mathbb{C}^d$, the so–called density matrix of $\omega_{\mathrm{at}}$, such that

$$\omega_{\mathrm{at}}(A) = \mathrm{Tr}_{\mathbb{C}^d}\left(\rho_{\mathrm{at}}\, A\right), \qquad A \in \mathcal{B}(\mathbb{C}^d).$$

Any state $\omega_{\mathrm{at}}$ on $\mathcal{B}(\mathbb{C}^d)$ can be represented as a vector state via its GNS representation $(\mathfrak{H}_{\mathrm{at}}, \pi_{\mathrm{at}}, \Omega_{\mathrm{at}})$, see for instance [BR87]. If $\omega_{\mathrm{at}}$ is faithful, then there is a direct way to construct the representation $(\mathfrak{H}_{\mathrm{at}}, \pi_{\mathrm{at}}, \Omega_{\mathrm{at}})$. The Hilbert space $\mathfrak{H}_{\mathrm{at}}$ corresponds to the linear space $\mathcal{B}(\mathbb{C}^d)$ endowed with the Hilbert–Schmidt scalar product

$$\langle A, B \rangle_{\mathrm{at}} := \mathrm{Tr}(A^* B), \qquad A, B \in \mathcal{B}(\mathbb{C}^d).$$

The representation $\pi_{\mathrm{at}}$ is the left multiplication, i.e.,

$$\pi_{\mathrm{at}}(A) = \underset{\rightarrow}{A}, \qquad A \in \mathcal{B}(\mathbb{C}^d),$$

see (4.12) and the cyclic vector of the GNS representation of $\omega_{\mathrm{at}}$ is given by

$$\Omega_{\mathrm{at}} := \rho_{\mathrm{at}}^{1/2} \in \mathfrak{H}_{\mathrm{at}}, \tag{4.15}$$

with $\rho_{\mathrm{at}} \in \mathcal{B}(\mathbb{C}^d)$ denotes the density matrix of $\omega_{\mathrm{at}}$. In particular,

$$\omega_{\mathrm{at}}(A) = \left\langle \Omega_{\mathrm{at}}, \underset{\rightarrow}{A}\, \Omega_{\mathrm{at}} \right\rangle_{\mathrm{at}}, \qquad A \in \mathcal{B}(\mathbb{C}^d).$$

The dynamics of the continuous one–parameter group of $*$–automorphisms $\{\tau_t^{\mathrm{at}}\}_{t\in\mathbb{R}}$ of the $C^*$–algebra $\mathcal{B}(\mathbb{C}^d)$ defined by (4.13) can be represented in the Schrödinger picture of Quantum Mechanics through the so–called (standard) *Liouvillean* operator

$$L_{\mathrm{at}} := \left( \underrightarrow{H_{\mathrm{at}}} - \underleftarrow{H_{\mathrm{at}}} \right) = [H_{\mathrm{at}}, \cdot] = L_{\mathrm{at}}^* \tag{4.16}$$

acting on $\mathfrak{H}_{\mathrm{at}}$. Indeed, it is easy to check that:

**Lemma 4.4 (Schrödinger picture of $\{\tau_t^{\mathrm{at}}\}_{t\in\mathbb{R}}$).**
*For all $t \in \mathbb{R}$ and all $A \in \mathcal{B}(\mathbb{C}^d)$,*

$$\omega_{\mathrm{at}}\left(\tau_t^{\mathrm{at}}(A)\right) = \langle \Omega_{\mathrm{at}}(t), \pi_{\mathrm{at}}(A)\, \Omega_{\mathrm{at}}(t)\rangle_{\mathrm{at}}, \qquad \Omega_{\mathrm{at}}(t) := e^{-itL_{\mathrm{at}}}\Omega_{\mathrm{at}}.$$

### 4.2.3 The pump

The pump, i.e. monochromatic field interacting with the atom, is described by the following time–periodic term in the atomic Hamiltonian:

$$\eta \cos(\varpi t) H_{\mathrm{p}}, \qquad \varpi := E_N - E_1 > 0. \tag{4.17}$$

$H_{\mathrm{p}} = H_{\mathrm{p}}^* \in \mathcal{B}(\mathbb{C}^d)$ is a selfadjoint matrix satisfying the following condition:

**Assumption 4.5 (P).** $H_{\mathrm{p}} = h_{\mathrm{p}} + h_{\mathrm{p}}^*$, $h_{\mathrm{p}} \in \mathcal{B}(\mathbb{C}^d)$, with

$$\ker\left(h_{\mathrm{p}}\right)^{\perp} \subseteq \operatorname{ran}\left(\mathbf{1}\left[H_{\mathrm{at}} = E_1\right]\right), \ \operatorname{ran}\left(h_{\mathrm{p}}\right) \subseteq \operatorname{ran}\left(\mathbf{1}\left[H_{\mathrm{at}} = E_N\right]\right).$$

In other words, by (4.17), the pump produces only transitions between the lowest and the highest atomic levels 1 and $N$.

From the physical point of view, the time–dependent pump may be regarded as a partial classical limit of a closed physical system involving a "quantised pump energy". The corresponding initial state for this "quantised pump energy" is given by a coherent state and hence, it is not a KMS state, [Hep74, Wes08].

### 4.2.4 The reservoir–atom–pump system

Define the $C^*$–algebra $\mathcal{V} := \mathcal{B}(\mathbb{C}^d) \otimes \mathcal{V}_{\mathcal{R}}$. As both $C^*$–algebras $\mathcal{B}(\mathbb{C}^d)$ and $\mathcal{V}_{\mathcal{R}}$ are already realised as algebras of bounded operators on Hilbert spaces and since $\mathcal{B}(\mathbb{C}^d)$ is finite dimensional, we do not have to specify the meaning of the tensor product. Observables of the reservoir–atom system are selfadjoint elements of $\mathcal{V}$. Its free dynamics is induced by the one–parameter group $\{\tau_t\}_{t\in\mathbb{R}}$ of $*$–automorphisms of $\mathcal{V}$ defined by

$$\tau_t := \tau_t^{\mathrm{at}} \otimes \tau_t^{\mathcal{R}}, \quad t \in \mathbb{R}. \tag{4.18}$$

This tensor product is well–defined and unique because the atomic algebra $\mathcal{B}(\mathbb{C}^d)$ is finite dimensional. The generator of the free dynamics $\tau_t$ is the symmetric derivation $\delta$.

Let $\omega_{\mathrm{at}}$ be any initial state of the atom and define the initial state of the atom–reservoir system by

$$\omega_0 := \omega_{\mathrm{at}} \otimes \omega_{\mathcal{R}}. \tag{4.19}$$

Again, the latter is well–defined and unique, by finite dimensionality of $\mathcal{B}(\mathbb{C}^d)$. If $\omega^{\mathrm{at}} = \mathfrak{g}_{\mathrm{at}}$ is the Gibbs state then $\omega_0$ is clearly a $(\beta, \tau)$–KMS state. Observe also that $\mathfrak{g}_{\mathrm{at}}$ is a faithful state and we assume without loss of generality that $\omega^{\mathrm{at}}$ is a faithful state. The set of faithful states is dense in the set of all states of the atom. Since the quasi–free state $\omega_{\mathcal{R}}$ of the reservoir is also faithful, this property carries over to the initial state $\omega_0$ of the composite system.

**The atom–reservoir interaction**

The interaction between the atom and the reservoir involves *fermion field operators,*

$$\Phi(f) := \frac{1}{\sqrt{2}}(a^+(f) + a(f)) = \Phi(f)^* \in \mathcal{B}(\mathcal{F}_-(\mathfrak{h}_1))$$

defined for all $f \in \mathfrak{h}_1$.

Choose a collection $\{Q_\ell\}_{\ell=1}^m \subset \mathcal{B}(\mathbb{C}^d)$ of self–adjoint matrices and an orthonormal system $\{f_\ell\}_{\ell=1}^m \subset \mathfrak{h}_1$, $f_\ell(p) = g_\ell(|p|)$. Here, we assume again rotation invariance of the functions $f_\ell$, for technical simplicity. More general choices lead to results which are qualitatively of the same type as ours. The atom–reservoir interaction is implemented by the symmetric derivation

$$\delta_{\mathrm{at},\mathcal{R}} := i \left[ \sum_{\ell=1}^m Q_\ell \otimes \Phi(f_\ell), \ \cdot \right]. \tag{4.20}$$

Note that the orthonormality of the family $\{f_\ell\}_{\ell=1}^m$ does not inflict loss of generality as for an arbitrary set $\{\tilde{Q}_\ell\}_{\ell=1}^{\tilde{m}} \subset \mathcal{B}(\mathbb{C}^d)$ of selfadjoint matrices and (possibly not orthonormal) family $\{\tilde{f}_\ell\}_{\ell=1}^{\tilde{m}} \subset \mathfrak{h}_1$, there are $m \in \mathbb{N}$, $\{Q_\ell\}_{\ell=1}^m \subset \mathcal{B}(\mathbb{C}^d)$ and an orthonormal system $\{f_\ell\}_{\ell=1}^m \subset \mathfrak{h}_1$ such that

$$\sum_{\ell=1}^m Q_\ell \otimes \Phi(f_\ell) = \sum_{\ell=1}^{\tilde{m}} \tilde{Q}_\ell \otimes \Phi(\tilde{f}_\ell).$$

**The atom–reservoir-pump dynamics**

The full dynamics of the system involves the classical pump described in Section 4.2.3, which is a perturbation of the free dynamics. It modifies the symmetric derivation $\delta$ by adding the time–depending generator $\eta \cos(\varpi t)\delta_{\mathrm{at,p}}$ with

$$\delta_{\mathrm{at,p}} := i[H_{\mathrm{p}} \otimes \mathbf{1}_{\mathcal{R}}, \ \cdot \ ]$$

and $\eta \in \mathbb{R}$. In other words, the atom–reservoir–pump dynamics is generated by

$$\delta_t^{(\lambda,\eta)} := \delta + \eta \cos(\varpi t)\delta_{\mathrm{at,p}} + \lambda \delta_{\mathrm{at},\mathcal{R}}, \quad t \in \mathbb{R}. \tag{4.21}$$

Here, $\lambda, \eta \in \mathbb{R}$ represent the strength of the atom–reservoir coupling and the atom–pump coupling, respectively.

As $\delta_{\mathrm{at},\mathcal{R}}$ and $\delta_{\mathrm{at,p}}$ are bounded symmetric derivations, $\delta_t^{(\lambda,\eta)}$ is the generator of a strongly continuous one–parameter group of $*$–automorphisms of $\mathcal{V}$. As the map

$$t \mapsto \delta_t^{(\lambda,\eta)} - \delta_0^{(\lambda,\eta)}$$

is norm–continuous, $\delta_t^{(\lambda,\eta)}$ generates a strongly continuous two–parameter family of automorphisms $\tau_{t,s}^{(\lambda,\eta)}$ of $\mathcal{V}$ corresponding to the non–autonomous dynamics of the atom–reservoir–pump system. As $\eta \cos(\varpi t)\delta_{\mathrm{at,p}}$ is bounded and cos is a smooth function, the two–parameter family $\tau_{t,s}^{(\lambda,\eta)}$ may be constructed by the Dyson series.

Consequently, the time–dependent state of the full system is given by

$$\omega_t := \omega_0 \circ \tau_{t,0}^{(\lambda,\eta)} = (\omega_{\mathrm{at}} \otimes \omega_{\mathcal{R}}) \circ \tau_{t,0}^{(\lambda,\eta)}, \quad t \in \mathbb{R}_0^+.$$

This state reduced to the atomic part only yields a state

$$\omega_{\mathrm{at}}(t)(A) := \omega_t(A \otimes \mathbf{1}_{\mathcal{R}}), \qquad A \in \mathcal{B}(\mathbb{C}^d), \tag{4.22}$$

for any $t \in \mathbb{R}_0^+$.

We will take later $|\lambda|, |\eta| \ll 1$. In other words, we will take the atom–reservoir and atom–pump interactions as a small, but non–vanishing, perturbation of the free dynamics. Moreover, we assume that the pump is moderate w.r.t. the atom–reservoir interaction in the following sense:

**Assumption 4.6 (MP).** For any $\lambda \in \mathbb{R}$, $|\eta| \leq c\lambda^2$ for some fixed $c \in (0, \infty)$.

Actually, it would suffice to impose $|\eta| \leq c|\lambda|$ for some sufficiently small constant $c > 0$, but the above condition is technically convenient. In the opposite situation when $|\eta| >> |\lambda|$ and at small $(\eta, \lambda) \in \mathbb{R}^2$, the atomic populations undergo Rabi oscillations, typically. We are rather interested in the regime where the evolution of the full system is described (up to negligibly small oscillations) by some relaxing dynamics in order to see, for instance, a persisting inversion of population.

As it will be shown below, the contribution of the pump to the final state of the atom is of order $\eta^2/\lambda^4$ whereas the contribution of the interaction with the reservoir is of order one. Thus imposing $|\eta| \simeq \lambda^2$ means physically that both the pump and the reservoir contribute in an essential way to the final state of the atom. Hence, we say in this context that the pump is weak whenever $|\eta| \ll \lambda^2$.

## 4.3 The effective atomic master equation

### 4.3.1 Definitions

The aim of this section is to analyse the atomic dynamics resulting from the restriction on $\mathcal{B}(\mathbb{C}^d)$ of the full dynamics generated by the symmetric derivation $\delta_t^{(\lambda,\eta)}$, see (4.21). This corresponds to study the family of states

$\{\omega_{\mathrm{at}}(t)\}_{t\in\mathbb{R}_0^+}$ defined by (4.22) or, equivalently, to study the corresponding family $\{\rho_{\mathrm{at}}(t)\}_{t\in\mathbb{R}_0^+}$ of density matrices. We are more precisely interested in the time behaviour of observables related to atomic levels only, and not to correlations between different levels. Mathematically, this amounts to study the orthogonal projection $P_{\mathfrak{D}}(\rho_{\mathrm{at}}(t))$ of the density matrix $\rho_{\mathrm{at}}(t)$ on the subspace

$$\mathfrak{D} = \mathfrak{D}(H_{\mathrm{at}}) := \mathcal{B}(\mathcal{H}_1) \oplus \cdots \oplus \mathcal{B}(\mathcal{H}_{\mathrm{N}}) \subset \mathfrak{H}_{\mathrm{at}}. \tag{4.23}$$

In other words, we analyse the density matrix

$$P_{\mathfrak{D}}(\rho_{\mathrm{at}}(t)) = \sum_{k=1}^{N} \mathbf{1}[H_{\mathrm{at}} = E_k]\ \rho_{\mathrm{at}}(t)\ \mathbf{1}[H_{\mathrm{at}} = E_k]$$

for any $t \in \mathbb{R}_0^+$. The density matrix $\rho_{\mathrm{at}}(t)$ is approximated by the solution of an effective non-autonomous initial value problem in $\mathcal{B}(\mathbb{C}^d)$ called the effective atomic master equation. Its generator is a time–dependent Lindbladian $\mathfrak{L}_t^{(\lambda,\eta)}$, i.e. it generates for any $t \in \mathbb{R}$ a completely positive group, see Section 4.5.1.

Similar to (4.21) this Lindbladian $\mathfrak{L}_t^{(\lambda,\eta)} \in \mathcal{B}(\mathfrak{H}_{\mathrm{at}})$ is defined by the following sum:

$$\mathfrak{L}_t^{(\lambda,\eta)}(\rho) := \mathfrak{L}_{\mathrm{at}}(\rho) + \eta\cos(\varpi t)\mathfrak{L}_{\mathrm{p}}(\rho) + \lambda^2\mathfrak{L}_{\mathcal{R}}(\rho), \qquad \rho \in \mathfrak{H}_{\mathrm{at}}. \tag{4.24}$$

The first term is the Lindbladian of the free atomic dynamics which is the anti–selfadjoint operator defined by

$$\mathfrak{L}_{\mathrm{at}}(\rho) := -i[H_{\mathrm{at}}, \rho] = -\mathfrak{L}_{\mathrm{at}}^*(\rho), \qquad \rho \in \mathfrak{H}_{\mathrm{at}}. \tag{4.25}$$

Similarly, the second term of (4.24) corresponds to the Lindbladian

$$\mathfrak{L}_{\mathrm{p}}(\rho) := -i[H_{\mathrm{p}}, \rho] = -\mathfrak{L}_{\mathrm{p}}^*(\rho), \qquad \rho \in \mathfrak{H}_{\mathrm{at}}. \tag{4.26}$$

The third term includes a dissipative part $\mathfrak{L}_d \in \mathcal{B}(\mathfrak{H}_{\mathrm{at}})$, i.e., $\mathfrak{L}_{\mathcal{R}} \in \mathcal{B}(\mathfrak{H}_{\mathrm{at}})$ is not anti–selfadjoint, which results from the Markov–approximation of atom–reservoir interaction. More precisely, the Lindbladian $\mathfrak{L}_{\mathcal{R}}$ equals

$$\mathfrak{L}_{\mathcal{R}}(\rho) := -i[H_{\mathrm{Lamb}}, \rho] + \mathfrak{L}_d(\rho), \qquad \rho \in \mathfrak{H}_{\mathrm{at}}. \tag{4.27}$$

The so–called *atomic Lamb shift* $H_{\mathrm{Lamb}}$ and *effective atomic dissipation* $\mathfrak{L}_d$ encode, in the weak coupling limit, the influence of the electron field-impurity interaction on the dynamics of the impurity and are defined as follows. Denoting the spectrum of any operator $A$ by $\sigma(A)$, for each

$$\epsilon \in \sigma(i[H_{\mathrm{at}}, \cdot]) = \left\{E_j - E_k : j,k \in \{1,2,\ldots N\}\right\}, \tag{4.28}$$

we define the sets

$$\mathfrak{t}_\epsilon := \{(j,k) : E_j - E_k = \epsilon\} \subset \{1,2,\ldots N\} \times \{1,2,\ldots N\}.$$

Then, for every $j,k \in \{1,2,\ldots N\}$ and any $\ell \in \{1,2,\ldots m\}$, let $V_{j,k}^{(\ell)} \in \mathcal{B}(\mathbb{C}^d)$ be defined by

$$V_{j,k}^{(\ell)} := \mathbf{1}\left[H_{\mathrm{at}} = E_j\right]\ Q_\ell\, \mathbf{1}\left[H_{\mathrm{at}} = E_k\right]. \tag{4.29}$$

Using the family $\{V_{j,k}^{(\ell)}\}_{j,k,\ell}$ of linear operators, the atomic Lamb shift $H_{\mathrm{Lamb}} \in \mathcal{B}(\mathbb{C}^d)$ is the selfadjoint element

$$H_{\mathrm{Lamb}} = \sum_{\epsilon \in \sigma(i[H_{\mathrm{at}},\cdot])\backslash\{0\}} \sum_{(j,k)\in \mathfrak{t}_\epsilon} \sum_{\ell=1}^{m} d_{j,k}^{(\ell)} V_{j,k}^{(\ell)} V_{j,k}^{(\ell)*}, \tag{4.30}$$

where

$$d_{j,k}^{(\ell)} := \mathcal{PP}\left[ f_\ell^{(\beta)}\left(\cdot - (E_j - E_k)\right)\right], \tag{4.31}$$

where

$$f_\ell^{(\beta)}(x) := \frac{|g_\ell(|x|)|^2}{1+\mathrm{e}^{-\beta x}}$$

and $\mathcal{PP}[f]$ denotes the principal part of the function $f$. Meanwhile, the effective atomic dissipation $\mathfrak{L}_d \in \mathcal{B}(\mathfrak{H}_{\mathrm{at}})$ is defined by

$$\begin{aligned} \mathfrak{L}_d(\rho) \quad &:= \quad \frac{1}{2} \sum_{\epsilon\in\sigma(\mathfrak{L}_{\mathrm{at}})\backslash\{0\}} \sum_{(j,k)\in\mathfrak{t}_\epsilon} \sum_{\ell=1}^{m} c_{j,k}^{(\ell)} \mathfrak{L}_{j,k}^{(\ell)}(\rho) \\ &= \quad \frac{1}{2} \sum_{\epsilon\in\sigma^+(\mathfrak{L}_{\mathrm{at}})} \sum_{(j,k)\in\mathfrak{t}_\epsilon} \sum_{\ell=1}^{m} c_{j,k}^{(\ell)} \mathfrak{L}_{j,k}^{(\ell)}(\rho) \\ &\quad + \frac{e^{-\beta\epsilon}}{2} \sum_{\epsilon\in\sigma^+(\mathfrak{L}_{\mathrm{at}})} \sum_{(j,k)\in\mathfrak{t}_\epsilon} \sum_{\ell=1}^{m} c_{j,k}^{(\ell)} \left(\mathfrak{L}_{j,k}^{(\ell)}\right)^*(\rho), \end{aligned} \tag{4.32}$$

with $\sigma^+(\mathfrak{L}_{\mathrm{at}}) := \sigma(\mathfrak{L}_{\mathrm{at}}) \cap \mathbb{R}_+$, for all $\rho \in \mathfrak{H}_{\mathrm{at}}$, where

$$\mathfrak{L}_{j,k}^{(\ell)}(\rho) \quad := \quad 2V_{j,k}^{(\ell)}\rho V_{j,k}^{(\ell)*} - V_{j,k}^{(\ell)*}V_{j,k}^{(\ell)}\rho - \rho V_{j,k}^{(\ell)*}V_{j,k}^{(\ell)}, \tag{4.33}$$

$$\left(\mathfrak{L}_{j,k}^{(\ell)}\right)^*(\rho) \quad := \quad 2V_{j,k}^{(\ell)*}\rho V_{j,k}^{(\ell)} - V_{j,k}^{(\ell)}V_{j,k}^{(\ell)*}\rho - \rho V_{j,k}^{(\ell)}V_{j,k}^{(\ell)*}, \tag{4.34}$$

and

$$c_{j,k}^{(\ell)} := f_\ell^{(\beta)}(E_j - E_k). \tag{4.35}$$

Note that the second equality in (4.32) follows from

$$f_\ell^{(\beta)}(x) = \mathrm{e}^{-\beta x} f_\ell^{(\beta)}(x), \quad \left(\mathfrak{L}_{j,k}^{(\ell)}\right)^*(\rho) = \mathfrak{L}_{k,j}^{(\ell)}(\rho). \tag{4.36}$$

The terms $V_{j,k}^{(\ell)}\rho V_{j,k}^{(\ell)*}$ and $V_{j,k}^{(\ell)*}\rho V_{j,k}^{(\ell)}$ correspond to transitions between the $j$th and $k$th atomic levels, whereas the other terms guarantee the Markov properties of the evolution, i.e., the preservation of the trace of the density matrix.

A priori, the family $\{P_{\mathfrak{D}}(\rho_{\mathrm{at}}(t))\}_{t\in\mathbb{R}_0^+}$ of density matrices can have several limits (depending on initial conditions) or even be oscillating, as $t \to \infty$. We would like to avoid this situation and we thus assume the following sufficient condition to obtain the uniqueness of the final density matrix in the limit $t \to \infty$.

**Assumption 4.7 (B).** Denote with $M''$ the bi–commutant, of $M \subset \mathcal{B}(\mathbb{C}^d)$. Then,

$$\left( \bigcup_{(j,k,\ell),\, c_{j,k}^{(\ell)} \neq 0} \left\{ V_{j,k}^{(\ell)} \right\} \right)'' = \mathcal{B}(\mathbb{C}^d).$$

Indeed, this assumption implies that the semigroup generated by $\mathfrak{L}_{\mathcal{R}}$ (or $\mathfrak{L}_d$) is relaxing and 0 is a non–degenerated eigenvalue of $\mathfrak{L}_{\mathcal{R}}$ and $\mathfrak{L}_d$, see Theorem 4.35. The uniqueness of the final density matrix then follows from Corollary 4.19.

In order to illustrate this condition, consider the following example: Assume that $m = 1$ and the degeneracy $n_k$ of the $k$th atomic level equal $n_k = 1$ for any $k \in \{1, \ldots, N = d\}$. Let $\{\varphi_k\}_{k=1}^d \subset \mathbb{C}^d$ be an orthonormal basis of eigenvectors of $H_{\mathrm{at}}$ with $H_{\mathrm{at}}\varphi_k = E_k \varphi_k$. If

$$Q_1 \varphi_k = \sum_{j=1}^{d} \varphi_j, \qquad k \in \{1, \ldots, d\},$$

then the family $\{V_{j,k}^{(1)}\}_{j,k=1}^d$ satisfies $V_{j,n}^{(1)} V_{n,k}^{(1)} = V_{j,k}^{(1)}$ for all $j, k, n$ and forms an orthonormal basis of $\mathfrak{H}_{\mathrm{at}}$. We assume the family of non–negative numbers $\{c_{j,k}^{(1)}\}_{j,k=1}^d$ is irreducible in the sense that, for all $j \neq k$, there is a sequence $(j_1, k_1), \ldots, (j_n, k_n)$ such that $c_{j_1,k_1}^{(1)}, \ldots, c_{j_n,k_n}^{(1)} \neq 0$, $j_1 = j$, $k_n = k$, and $k_l = j_{l+1}$ for $l \in \{1, 2, \ldots k-1\}$. Physically speaking it means that any arbitrary pair of atomic levels is connected by non–vanishing transitions. By using the commutator identity

$$\left[ A, V_{j,k}^{(1)} \right] = \left[ A, V_{j,n}^{(1)} V_{n,k}^{(1)} \right] = V_{j,n}^{(1)} \left[ A, V_{n,k}^{(1)} \right] + \left[ A, V_{j,n}^{(1)} \right] V_{n,k}^{(1)}$$

for all $j, n, k$ and the irreducibility of the family $\{c_{j,k}^{(1)}\}_{j,k=1}^d$ one can check that the commutant

$$\left( \bigcup_{(j,k),\, c_{j,k}^{(1)} \neq 0} \left\{ V_{j,k}^{(1)} \right\} \right)' = \mathbb{C}.\mathbf{1}_{\mathbb{C}^d} \ ,$$

from which Assumption (B) follows. This is in perfect analogy to well–known results about unicity of invariant states of discrete Markov chains.

Assumption (B) concludes the list of required conditions and from now on, we assume *all of them* to be satisfied.

We define now the effective atomic master equation as the initial value problem

$$\forall t \geq 0 : \qquad \frac{d}{dt}\rho(t) = \mathfrak{L}_t^{(\lambda,\eta)}(\rho(t)), \qquad \rho(0) = \rho_{\mathrm{at}}(0) \equiv \rho_{\mathrm{at}}. \qquad (4.37)$$

This evolution equation clearly has a unique solution, by finite dimensionality. Recall that $\rho_{\mathrm{at}}$ is the density matrix of the initial state $\omega_{\mathrm{at}}$ of the atom and $\rho_{\mathrm{at}}(t)$ is the density matrix of the time–dependent state $\omega_{\mathrm{at}}(t)$ defined by (4.22) for any $t \geq 0$. Observe that the initial value problem (4.37) defines a continuous two–parameter family denoted by $\{\hat{\tau}_{t,s}^{(\lambda,\eta)}\}_{t \geq s}$. Since $\hat{\tau}_{t,s}^{(\lambda,\eta)}$ preserves positivity and the trace, this family is norm bounded. Indeed for some finite constant $C$ not depending on $\lambda$, $\eta$, $s$, and $t$,

$$\forall \lambda, \eta, s, t \in \mathbb{R}, \, t \geq s : \qquad \| \, \hat{\tau}_{t,s}^{(\lambda,\eta)} \, \| \leq C. \tag{4.38}$$

When the atom–pump interaction is absent, the dynamics become autonomous and thus, the family $\{\hat{\tau}_{t,s}^{(\lambda,0)}\}_{t \geq s}$ corresponds to a one–parameter semigroup denoted for simplicity by

$$\forall t \geq 0 : \qquad \hat{\tau}_{t}^{(\lambda,0)} := \hat{\tau}_{t,0}^{(\lambda,0)}. \tag{4.39}$$

Under certain technical assumptions of the electron field–impurity coupling the following theorem about the dynamics of the orthogonal projection $P_{\mathfrak{D}}(\rho_{\mathrm{at}}(t))$ of the density matrix $\rho_{\mathrm{at}}(t)$ on the subspace $\mathfrak{D}$ of block–diagonal density matrix can be proven, see [BPW11b].

**Theorem 4.8 (Validity of the Non–Autonomous Master Equation).**
*The unique solution $\{\rho(t)\}_{t \geq 0}$ of the effective atomic master equation (4.37) and the atomic density matrix $\{\rho_{\mathrm{at}}(t)\}_{t \geq 0}$ obey the uniform bound*

$$\left\| P_{\mathfrak{D}} \left( \rho_{\mathrm{at}}(t) - \rho(t) \right) \right\| \leq C(\lambda^2 + |\lambda| |\varpi|^{-1}),$$

*for some constant $C < \infty$ which neither depends on the initial state $\omega_{\mathrm{at}}$ of the atom nor on the parameters $t$, $\varpi$, $\lambda$, and $\eta$.*

**Remark 4.9.** The effective atomic master equation, (4.37), may be obtained as a weak coupling limit, or Markov approximation, of the dynamics $\{\tau_{t,s}^{(\lambda,\mu)}\}_{t \geq s}$ w.r.t. the fermion degrees of freedom, similar to the results of Davies, [Dav74, Dav76, Dav75]; see also [DF06] and references therein. These results cover the autonomous case and one has to control the influence of the pump while taking the weak coupling limit. As Theorem 4.8 provides a uniform bound in $t$, i.e. it is not restricted to the van Hove timescale, $t\lambda^2 = \text{const.}$, it contains any weak coupling limit results, which prove convergence uniformly on compact intervals for $t\lambda^2$, typically. We stress, that the weak coupling limit is taken in the GNS representation of the initial state $\omega_0$, taking thermal effects into account.

### 4.3.2 Evolution Semigroup of the Non–Autonomous Master Equation

In this subsection we perform a spectral analysis of the evolution semigroup of the non–autonomous master equation, that is, the initial value problem (4.37). To this end, we represent this non–autonomous evolution as an *autonomous* dynamics on an enlarged Hilbert space emerging through an additional degree of freedom, which is a new time variable denoted by $\alpha$. This method enables a long–time analysis of the non-autonomous dynamics via a spectral analysis of the generator of the associated evolution semigroup.

We thus proceed by first defining this enlarged space, which is the Hilbert space

$$\mathfrak{H}_{\mathrm{evo}} := L^2(\mathbb{T}_{\varpi}, \mathfrak{H}_{\mathrm{at}}), \quad \mathbb{T}_{\varpi} := \mathbb{R}/_{\frac{2\pi}{\varpi}\mathbb{Z}}, \tag{4.40}$$

of time–dependent $2\pi\varpi^{-1}$–*periodic* density matrices. The scalar product on $\mathfrak{H}_{\mathrm{evo}}$ is naturally defined, for all $f, g \in \mathfrak{H}_{\mathrm{evo}}$, by

$$\langle f, g \rangle_{\mathrm{evo}} := \frac{\varpi}{2\pi} \int_0^{\frac{2\pi}{\varpi}} \langle f(t), g(t) \rangle_{\mathrm{at}} \,\mathrm{d}t = \frac{\varpi}{2\pi} \int_0^{\frac{2\pi}{\varpi}} \mathrm{Tr}\left( f(t)^* g(t) \right) \mathrm{d}t.$$

Then, there is a strongly continuous one–parameter semigroup $\{\mathcal{T}_\alpha\}_{\alpha \geq 0}$ such that, for all $\alpha \geq 0$ and $f \in \mathfrak{H}_{\mathrm{evo}}$,

$$\forall t \in \mathbb{T}_{\varpi} \text{ a.e.} : \qquad \mathcal{T}_\alpha(f)(t) = \hat{\tau}_{t,t-\alpha}^{(\lambda,\eta)} f(t-\alpha),$$

where we recall that $\{\hat{\tau}_{t,s}^{(\lambda,\eta)}\}_{t \geq s}$ is the continuous two–parameter family defined from the non–autonomous master equation (4.37). Observe that $\{\hat{\tau}_{t,s}^{(\lambda,\eta)}\}_{t \geq s}$ is periodic in the sense that

$$\hat{\tau}_{t,s}^{(\lambda,\eta)} = \hat{\tau}_{t+2\pi\varpi^{-1}k, s+2\pi\varpi^{-1}k}^{(\lambda,\eta)} \tag{4.41}$$

for all $k \in \mathbb{Z}$ and $t \geq s$. Therefore, $\mathcal{T}_\alpha(f) \in \mathfrak{H}_{\mathrm{evo}}$. Moreover, the semigroup $\{\mathcal{T}_\alpha\}_{\alpha \geq 0}$ is norm bounded, by the norm boundedness of the operator family $\{\hat{\tau}_{t,s}^{(\lambda,\eta)}\}_{t \geq s}$. Indeed, for some finite constant $C$ not depending on $\lambda$, $\eta$, and $\alpha$,

$$\forall \lambda, \eta \in \mathbb{R}, \alpha \geq 0 : \qquad \| \mathcal{T}_\alpha \| \leq C. \tag{4.42}$$

The generator of the strongly continuous semigroup $\{\mathcal{T}_\alpha\}_{\alpha \geq 0}$ is the closed operator

$$G^{(\lambda,\eta)} := -\frac{d}{dt} + \mathfrak{L}_{\mathrm{evo}}^{(\lambda,\eta)}, \ \mathcal{D}\left(G^{(\lambda,\mu)}\right) = \mathcal{D}\left(\frac{d}{dt}\right), \tag{4.43}$$

where $\mathfrak{L}_{\mathrm{evo}}^{(\lambda,\eta)}$ is the bounded operator defined, for all $f \in \mathfrak{H}_{\mathrm{evo}}$, by

$$\forall t \in \mathbb{T}_{\varpi} \text{ a.e.} : \qquad \mathfrak{L}_{\mathrm{evo}}^{(\lambda,\eta)}(f)(t) := \mathfrak{L}_t^{(\lambda,\eta)}(f(t))$$

The derivative operator is the closed, unbounded operator with domain

$$\mathcal{D}\left(\frac{d}{dt}\right) = \left\{ \sum_{k=-\infty}^{\infty} a_k e^{ik\varpi t} \ : \ a_k \in \mathfrak{H}_{\mathrm{at}}, \ \sum_{k=-\infty}^{\infty} \|k\, a_k\|_{\mathrm{at}}^2 < \infty \right\}.$$

Observe that the spectrum of the generator $G^{(0,0)}$ is purely discrete. In the following we identify all vectors $\rho \in \mathfrak{H}_{\mathrm{at}}$ with constant functions $\rho(t) = \rho$ of $\mathfrak{H}_{\mathrm{evo}}$.

In the next Lemma we show that the scalar products of the form

$$\langle \mathcal{T}_\alpha(\rho), A \rangle_{\mathrm{evo}}$$

properly describe the time evolution of

$$\langle \rho(\alpha), A \rangle_{\mathrm{at}} := \mathrm{Tr}\left(\rho(\alpha) A\right)$$

whenever the pump frequency, $\varpi$, is sufficiently large.

**Lemma 4.10 (Effective behaviour of $\rho\,(t)$–I).**
*For any state $\rho \in \mathfrak{D} \subset \mathfrak{H}_{\mathrm{at}}$, with $\rho = \rho(0)$, and any observable $A \in \mathfrak{D} \subset \mathcal{B}(\mathbb{C}^d) \equiv \mathfrak{H}_{\mathrm{at}}$, the unique solution $\{\rho(t)\}_{t\geq 0}$ of the effective atomic master equation (4.37) satisfies the bound*

$$\left|\langle \rho(\alpha), A\rangle_{\mathrm{at}} - \langle \mathcal{T}_\alpha\,(\rho)\,, A\rangle_{\mathrm{evo}}\right| \leq C\,\|A\|\,\frac{|\lambda|(1+|\lambda|)}{\varpi}, \tag{4.44}$$

*where $C$ is a finite constant not depending on $\rho$, $A$, $\lambda$, $\eta$, $\varpi$, and $\alpha$.*

*Proof.* By Assumption (MP) $|\eta| \leq c\lambda^2$, for some fixed $c \in (0,\infty)$. The "variation of constants formula" provides a relation between the continuous two–parameter family $\{\hat{\tau}_{t,s}^{(\lambda,\eta)}\}_{t\geq s}$ and the semigroup $\{\hat{\tau}_t^{(0,0)}\}_{t\geq 0}$, defined by (4.39), is given by the integral equation

$$\forall s,t{\in}\mathbb{R},\ t\geq s: \qquad \hat{\tau}_{t,s}^{(\lambda,\eta)} = \hat{\tau}_{t-s}^{(0,0)} + \int_s^t \hat{\tau}_{t-v}^{(0,0)}\mathfrak{W}_v^{(\lambda,\eta)}\hat{\tau}_{v,s}^{(\lambda,\eta)}\mathrm{d}v\,. \tag{4.45}$$

Here, for any $t\geq 0$, the operator

$$\mathfrak{W}_t^{(\lambda,\eta)} := \mathfrak{L}_t^{(\lambda,\eta)} - \mathfrak{L}_t^{(0,0)} = \eta\cos(\varpi t)\mathfrak{L}_{\mathrm{p}} + \lambda^2\mathfrak{L}_{\mathcal{R}}$$

is the difference between the full Lindbladian $\mathfrak{L}_t^{(\lambda,\eta)}$, (4.24), and the free one $\mathfrak{L}_t^{(0,0)} \equiv \mathfrak{L}_{\mathrm{at}}$, (4.25). Since

$$\langle \rho(\alpha), A\rangle_{\mathrm{at}} - \langle \mathcal{T}_\alpha\,(\rho)\,, A\rangle_{\mathrm{evo}} = \frac{\varpi}{2\pi}\int_0^{\frac{2\pi}{\varpi}} \left\langle \left(\hat{\tau}_{\alpha,0}^{(\lambda,\eta)} - \hat{\tau}_{t,t-\alpha}^{(\lambda,\eta)}\right)(\rho)\,, A\right\rangle_{\mathrm{at}}\mathrm{d}t, \tag{4.46}$$

we proceed by estimating the difference

$$\|\ \hat{\tau}_{\alpha,0}^{(\lambda,\eta)} - \hat{\tau}_{t,t-\alpha}^{(\lambda,\eta)}\ \|$$

for any $\alpha\geq 0$ and $t\in\left[0,2\pi\varpi^{-1}\right)$. To this end, we choose, for any $\alpha \geq 0$, the parameter $r\,(\alpha) \in 2\pi\varpi^{-1}\mathbb{N}_0$ such that

$$0 \leq r\,(\alpha) - \alpha \leq 2\pi\varpi^{-1}.$$

Since $\mathfrak{W}_t^{(\lambda,\eta)}$ is periodic with period $2\pi\varpi^{-1}$,

$$\hat{\tau}_{t,s}^{(\lambda,\eta)} = \hat{\tau}_{t+r(\alpha),s+r(\alpha)}^{(\lambda,\eta)}$$

(cf. (4.41)) and thus, for any $t\in\left[0,2\pi\varpi^{-1}\right]$,

$$\hat{\tau}_{\alpha,0}^{(\lambda,\eta)} - \hat{\tau}_{t,t-\alpha}^{(\lambda,\eta)} = \hat{\tau}_{\alpha,0}^{(\lambda,\eta)} - \hat{\tau}_{\delta+\alpha,\delta}^{(\lambda,\eta)} \tag{4.47}$$

with

$$\delta := t + r\,(\alpha) - \alpha \in \left[0,4\pi\varpi^{-1}\right].$$

Using the cocycle property satisfied by the two–parameter family $\{\hat{\tau}_{t,s}^{(\lambda,\eta)}\}_{t\geq s}$ together with (4.47),

$$\hat{\tau}_{\alpha,0}^{(\lambda,\eta)} - \hat{\tau}_{t,t-\alpha}^{(\lambda,\eta)} = \hat{\tau}_{\alpha+\delta,\delta}^{(\lambda,\eta)}(\hat{\tau}_{\delta,0}^{(\lambda,\eta)} - \mathbf{1}) + (\mathbf{1}{-}\hat{\tau}_{\alpha+\delta,\alpha}^{(\lambda,\eta)})\hat{\tau}_{\alpha,0}^{(\lambda,\eta)} \tag{4.48}$$

with $\delta \in [0, 4\pi\varpi^{-1}]$. Note that $\|[H_{at}, \cdot]\| = \mathcal{O}(\varpi)$ and thus we cannot expect $\left\|(\mathbf{1} - \hat{\tau}_{\delta,0}^{(\lambda,\eta)})\right\|$ and $\left\|(\hat{\tau}_{\alpha+\delta,\alpha}^{(\lambda,\eta)} - \mathbf{1})\right\|$ to be small at $\delta = \mathcal{O}(\varpi^{-1})$. However, for $\rho, A \in \mathfrak{D} \subset B(\mathbb{C}^d)$, $\left\|(\mathbf{1} - \hat{\tau}_{\delta,0}^{(\lambda,\eta)})(\rho)\right\|$ and $\left\|(\hat{\tau}_{\alpha+\delta,\alpha}^{(\lambda,\eta)} - \mathbf{1})^*(A)\right\|$ are indeed small at $\delta = \mathcal{O}(\varpi^{-1})$: We infer from the integral equation (4.45) that, for all $s \in \mathbb{R}$ and $\delta \in [0, 4\pi\varpi^{-1}]$,

$$\mathbf{1} - \hat{\tau}_{s+\delta,s}^{(\lambda,\eta)} = (\mathbf{1} - \hat{\tau}_{\delta}^{(0,0)}) + \int_s^{s+\delta} \hat{\tau}_{s+\delta-v}^{(0,0)} \mathfrak{W}_v^{(\lambda,\eta)} \hat{\tau}_{v,s}^{(\lambda,\eta)} \mathrm{d}v.$$

As

$$(\mathbf{1} - \hat{\tau}_{\delta,0}^{(0,0)})(\rho) = (\hat{\tau}_{\alpha+\delta,\alpha}^{(0,0)} - \mathbf{1})^*(A) = 0,$$

for all $\rho, A \in \mathfrak{D} \subset B(\mathbb{C}^d)$, it follows that

$$\begin{aligned} \left\|(\mathbf{1} - \hat{\tau}_{\delta,0}^{(\lambda,\eta)})(\rho)\right\| &\leq C_1 \frac{|\lambda|(1+|\lambda|)}{\varpi} \|\rho\|, \\ \left\|(\hat{\tau}_{\alpha+\delta,\alpha}^{(\lambda,\eta)} - \mathbf{1})^*(A)\right\| &\leq C_1 \frac{|\lambda|(1+|\lambda|)}{\varpi} \|A\|, \end{aligned}$$

for all $\rho, A \in \mathfrak{D}$ and some $C_1 < \infty$ not depending on $\rho$, $A$, $\lambda$ and $\eta$. On the other hand, the family $\{\hat{\tau}_{t,s}^{(\lambda,\eta)}\}_{t \geq s}$ is uniformly bounded by (4.38). Hence, it follows that

$$\forall t \in \left[0, 2\pi\varpi^{-1}\right] : \qquad \| \hat{\tau}_{\alpha,0}^{(\lambda,\eta)} - \hat{\tau}_{t,t-\alpha}^{(\lambda,\eta)} \| \leq C_2 \frac{|\lambda|(1+|\lambda|)}{\varpi}$$

with $C_2 < \infty$ not depending on $\rho$, $A$, $\lambda$, $\eta$, $\varpi$, $t$ and $\alpha$. Combining this with (4.46), we arrive at the estimate (4.44). □

This lemma allows us to analyse the long–time behaviour of the solution $\{\rho(t)\}_{t \geq 0}$ of the non–autonomous master equation (4.37) via the autonomous dynamics described by the evolution semigroup $\{\mathcal{T}_\alpha\}_{\alpha \geq 0}$.

The semigroup $\{\mathcal{T}_\alpha\}_{\alpha \geq 0}$ acts on an infinite dimensional Hilbert space $\mathfrak{H}_{\mathrm{evo}}$, but the initial conditions we are interested in are constant functions, i.e., elements of $\mathfrak{H}_{\mathrm{at}} \subset \mathfrak{H}_{\mathrm{evo}}$. It turns out that $\mathfrak{H}_{\mathrm{at}}$ is almost parallel to some invariant finite dimensional subspace of $\{\mathcal{T}_\alpha\}_{\alpha \geq 0}$, see (4.51) below. As this semigroup is bounded (see (4.42)), the restriction of the dynamics onto this invariant subspace describes – up to small errors – the evolution of $\{\rho(t)\}_{t \geq 0}$.

More precisely, the invariant, finite dimensional subspace is defined by

$$\mathfrak{H}_{\mathrm{inv}}^{(\lambda,\eta)} := \mathrm{span} \left\{ \bigcup_{\epsilon \in \sigma(i[H_{\mathrm{at}},\cdot])} \mathfrak{H}_\epsilon^{(\lambda,\eta)} \right\}.$$

Here, for each $\epsilon \in \sigma(i[H_{\mathrm{at}}, \cdot])$,

$$\mathfrak{H}_\epsilon^{(\lambda,\eta)} := P_\epsilon^{(\lambda,\eta)} \mathfrak{H}_{\mathrm{evo}}$$

is an invariant, finite dimensional subspace (see [Kat76, Chapter II]) of the evolution semigroup $\{\mathcal{T}_\alpha\}_{\alpha \geq 0}$ and

$$P_\epsilon^{(\lambda,\eta)} := \frac{1}{2\pi i} \oint_{|z-\epsilon| = \frac{R}{4}} \left(z - G^{(\lambda,\eta)}\right)^{-1} \mathrm{d}z \tag{4.49}$$

is the Kato projection. Here,

$$R := \min\left\{\left|\epsilon - \epsilon'\right| : \epsilon, \epsilon' \in \sigma(i[H_{\mathrm{at}}, \cdot]), \epsilon \neq \epsilon'\right\} > 0 \tag{4.50}$$

and we assume in the following that $\lambda^2$ (and thus $|\eta|$, by Assumption (MP)) is small enough such that, for any $\epsilon \in \sigma(i[H_{\mathrm{at}}, \cdot])$ and $z \in \mathbb{C}$ with $|z| = \frac{R}{4}$, we have $\epsilon + z \notin \sigma\left(G^{(\lambda,\eta)}\right)$. In other words, we choose $R$ and $\lambda$ small enough to ensure that the Kato projection, $P_{\epsilon}^{(\lambda,\eta)}$, is well–defined.

Next, we study the restriction of the dynamics described by the semigroup $\{\mathcal{T}_\alpha\}_{\alpha\geq 0}$ onto the invariant subspace $\mathfrak{H}_{\mathrm{inv}}^{(\lambda,\eta)}$. In particular, if $\lambda$, $\eta$ are sufficiently small and $\varpi$ is large enough, then we show below that this restriction describes the time behaviour of $\{\mathcal{T}_\alpha\left(\rho\right)\}_{\alpha\geq 0}$ provided that the initial value is a constant function, i.e., an element $\rho \in \mathfrak{H}_{\mathrm{at}}$. Using Lemma 4.10, it yields

**Corollary 4.11 (Effective behavior of $\rho\left(t\right)$–II).**
*For any $\rho \in \mathfrak{D} \subset \mathfrak{H}_{\mathrm{at}}$, with $\rho = \rho(0)$, and any observable $A \in \mathcal{B}(\mathbb{C}^d) \cap \mathfrak{D}$, the unique solution $\{\rho(t)\}_{t\geq 0}$ of the effective atomic master equation (4.37) satisfies the bound*

$$\begin{aligned}&\left|\langle \rho(\alpha), A\rangle_{\mathrm{at}} - \sum_{\epsilon\in\sigma(i[H_{\mathrm{at}},\cdot])}\left\langle \exp\left(\alpha\, P_{\epsilon}^{(\lambda,\eta)} G^{(\lambda,\eta)} P_{\epsilon}^{(\lambda,\eta)}\right)\rho, A\right\rangle_{\mathrm{evo}}\right| \\ \leq\ & C\,\|A\|\left(\lambda^2 + \frac{|\lambda|(1+|\lambda|)}{\varpi}\right),\end{aligned}$$

*where $C$ is a finite constant independent of $\rho$, $A$, $\lambda$, $\eta$, $\varpi$, and $\alpha$.*

*Proof.* Define the projection

$$P_{\mathrm{inv}}^{(\lambda,\eta)} := \sum_{\epsilon\in\sigma(i[H_{\mathrm{at}},\cdot])} P_{\epsilon}^{(\lambda,\eta)}$$

onto the invariant subspace $\mathfrak{H}_{\mathrm{inv}}^{(\lambda,\eta)}$. Note that

$$\forall \rho \in \mathfrak{H}_{\mathrm{at}} \subset \mathfrak{H}_{\mathrm{evo}} : \qquad P_{\mathrm{inv}}^{(0,0)}\rho = \rho,$$

whereas, by Kato's perturbation theory of discrete eigenvalues, there is a constant $C_3 < \infty$ such that

$$\left\|P_{\mathrm{inv}}^{(\lambda,\eta)} - P_{\mathrm{inv}}^{(0,0)}\right\| \leq C_3\lambda^2. \tag{4.51}$$

Meanwhile, we also observe that the operator families

$$\left\{\exp\left(\alpha\, P_{\epsilon}^{(\lambda,\eta)} G^{(\lambda,\eta)} P_{\epsilon}^{(\lambda,\eta)}\right)\right\}_{\alpha\geq 0},$$

for all $\epsilon \in \sigma(i[H_{\mathrm{at}}, \cdot])$, are bounded semigroups because there are restrictions of the bounded semigroup $\{\mathcal{T}_\alpha\}_{\alpha\geq 0}$ onto invariant subspaces:

$$\forall \alpha \geq 0,\ \epsilon \in \sigma(i[H_{\mathrm{at}}, \cdot]) : \qquad \mathcal{T}_\alpha P_{\epsilon}^{(\lambda,\eta)} = \exp\left(\alpha\, P_{\epsilon}^{(\lambda,\eta)} G^{(\lambda,\eta)} P_{\epsilon}^{(\lambda,\eta)}\right).$$

Hence, using the equality

$$\begin{aligned}\mathcal{T}_\alpha(\rho) &= \mathcal{T}_\alpha\left(\left(\mathbf{1} - P_{\mathrm{inv}}^{(\lambda,\eta)}\right)\rho\right) + \mathcal{T}_\alpha\left(P_{\mathrm{inv}}^{(\lambda,\eta)}\rho\right)\\ &= \mathcal{T}_\alpha\left(\left(P_{\mathrm{inv}}^{(0,0)} - P_{\mathrm{inv}}^{(\lambda,\eta)}\right)\rho\right) + \sum_{\epsilon\in\sigma(i[H_{\mathrm{at}},\cdot])} \exp\left(\alpha\, P_\epsilon^{(\lambda,\eta)} G^{(\lambda,\eta)} P_\epsilon^{(\lambda,\eta)}\right)\rho\end{aligned}$$

we obtain the upper bound

$$\left|\langle \mathcal{T}_\alpha(\rho), A\rangle_{\mathrm{evo}} - \sum_{\epsilon\in\sigma(i[H_{\mathrm{at}},\cdot])}\left\langle \exp\left(\alpha\, P_\epsilon^{(\lambda,\eta)} G^{(\lambda,\eta)} P_\epsilon^{(\lambda,\eta)}\right)\rho, A\right\rangle_{\mathrm{evo}}\right| \le C_4\,\|A\|\,\lambda^2,$$

where $C_4 < \infty$ is a constant not depending on $\rho$, $A$, $\lambda$, $\eta$, $\varpi$, and $\alpha$. The assertion follows now from Lemma 4.10. □

As a consequence, we may reduce the dimension of the problem to the finite–dimensional subspace $\mathfrak{H}_{\mathrm{inv}}^{(\lambda,\eta)}$.

Theorem 4.8 only compares the orthogonal projections $P_{\mathfrak{D}}(\rho(t))$ and $P_{\mathfrak{D}}(\rho_{\mathrm{at}}(t))$ of $\{\rho(t)\}_{t\ge 0}$ and the atomic density matrix $\{\rho_{\mathrm{at}}(t)\}_{t\ge 0}$, respectively (see (4.23)). Therefore, our analysis is restricted to the evolution of $\{P_{\mathfrak{D}}(\rho(t))\}_{t\ge 0}$. This quantity is related to the subspace $\mathfrak{H}_0^{(\lambda,\eta)}$ as shown in the following lemma.

**Lemma 4.12 (Effective behaviour of $P_{\mathfrak{D}}(\rho(t))$–I).**
*For any $\rho \in \mathfrak{D} \subset \mathfrak{H}_{\mathrm{at}}$, with $\rho = \rho(0)$, and any observable $A \in \mathcal{B}(\mathbb{C}^d) \equiv \mathfrak{H}_{\mathrm{at}}$, the unique solution $\{\rho(t)\}_{t\ge 0}$ of the effective atomic master equation (4.37) satisfies the bound*

$$\begin{aligned}&\left|\langle P_{\mathfrak{D}}(\rho(\alpha)), A\rangle_{\mathrm{at}} - \left\langle \exp\left(\alpha\, P_0^{(\lambda,\eta)} G^{(\lambda,\eta)} P_0^{(\lambda,\eta)}\right)\rho, A\right\rangle_{\mathrm{evo}}\right|\\ \le\ & C\,\|A\|\left(\lambda^2 + \frac{|\lambda|(1+|\lambda|)}{\varpi}\right),\end{aligned}$$

*where C is a finite constant not depending on $\rho$, $A$, $\lambda$, $\eta$, $\varpi$, and $\alpha$.*

*Proof.* The orthogonal projection $P_{\mathfrak{D}}$ on $\mathfrak{H}_{\mathrm{at}}$ naturally induces an orthogonal projection, again denoted by $P_{\mathfrak{D}}$, on the Hilbert space $\mathfrak{H}_{\mathrm{evo}}$ of time–dependent density matrices by the equalities

$$\forall t \in \mathbb{T}_\varpi,\ f \in \mathfrak{H}_{\mathrm{evo}}: \qquad P_{\mathfrak{D}}(f)(t) := P_{\mathfrak{D}}(f(t)).$$

Using this definition we get

$$\begin{aligned}&\sum_{\epsilon\in\sigma(i[H_{\mathrm{at}},\cdot])}\left\langle \exp\left(\alpha\, P_\epsilon^{(\lambda,\eta)} G^{(\lambda,\eta)} P_\epsilon^{(\lambda,\eta)}\right)\rho, P_{\mathfrak{D}}(A)\right\rangle_{\mathrm{evo}}\\ =\ &\sum_{\epsilon\in\sigma(i[H_{\mathrm{at}},\cdot])}\left\langle P_{\mathfrak{D}}\left(\exp\left(\alpha\, P_\epsilon^{(\lambda,\eta)} G^{(\lambda,\eta)} P_\epsilon^{(\lambda,\eta)}\right)\rho\right), A\right\rangle_{\mathrm{evo}},\end{aligned}$$

since

$$\langle P_{\mathfrak{D}}(\rho(\alpha)), A\rangle_{\mathrm{at}} = \langle \rho(\alpha), P_{\mathfrak{D}}(A)\rangle_{\mathrm{at}}.$$

We use now Corollary 4.11 to obtain the bound

$$\begin{aligned}&\left|\langle P_{\mathfrak{D}}\left(\rho(\alpha)\right), A\rangle_{\mathrm{at}} - \sum_{\epsilon\in\sigma(i[H_{\mathrm{at}},\cdot])} \left\langle P_{\mathfrak{D}}\left(P_\epsilon^{(\lambda,\eta)} e^{\alpha G^{(\lambda,\eta)} P_\epsilon^{(\lambda,\eta)}} \rho\right), A\right\rangle_{\mathrm{evo}}\right| \\ \leq\ & C_5 \|A\| \left(\lambda^2 + \frac{|\lambda|(1+|\lambda|)}{\varpi}\right) \end{aligned} \tag{4.52}$$

with $C_5 < \infty$. For any $\epsilon \in \sigma(i[H_{\mathrm{at}}, \cdot])$, note that

$$P_{\mathfrak{D}} P_\epsilon^{(\lambda,\eta)} = P_{\mathfrak{D}} P_\epsilon^{(0,0)} + P_{\mathfrak{D}}(P_\epsilon^{(\lambda,\eta)} - P_\epsilon^{(0,0)}) = \delta_{\epsilon,0} P_{\mathfrak{D}} + P_{\mathfrak{D}}(P_\epsilon^{(\lambda,\eta)} - P_\epsilon^{(0,0)}), \tag{4.53}$$

with the Kronecker symbol, $\delta_{\epsilon,\epsilon'}$. Similar to (4.51), there is a constant $C_6 < \infty$ such that

$$\max_{\epsilon\in\sigma(i[H_{\mathrm{at}},\cdot])} \left\| P_\epsilon^{(\lambda,\eta)} - P_\epsilon^{(0,0)} \right\| \leq C_6 \lambda^2. \tag{4.54}$$

Therefore, we infer from (4.52)–(4.54) that

$$\begin{aligned}&\left|\langle P_{\mathfrak{D}}\left(\rho(\alpha)\right), A\rangle_{\mathrm{at}} - \left\langle P_{\mathfrak{D}}\left(\exp\left(\alpha\, G^{(\lambda,\eta)} P_0^{(\lambda,\eta)}\right)\rho\right), A\right\rangle_{\mathrm{evo}}\right| \\ \leq\ & C_7 \|A\| \left(\lambda^2 + \frac{|\lambda|(1+|\lambda|)}{\varpi}\right) \end{aligned} \tag{4.55}$$

with $C_7 < \infty$. Finally, observe that

$$\begin{aligned} \left\langle P_{\mathfrak{D}}\left(e^{\alpha G^{(\lambda,\eta)} P_0^{(\lambda,\eta)}} \rho\right), A\right\rangle_{\mathrm{evo}} &= \left\langle e^{\alpha G^{(\lambda,\eta)} P_0^{(\lambda,\eta)}} \rho, P_{\mathfrak{D}}(A)\right\rangle_{\mathrm{evo}} \\ &= \left\langle e^{\alpha G^{(\lambda,\eta)} P_0^{(\lambda,\eta)}} \rho, P_0^{(0,0)}(A)\right\rangle_{\mathrm{evo}} \\ &= \left\langle P_0^{(0,0)}\left(e^{\alpha G^{(\lambda,\eta)} P_0^{(\lambda,\eta)}} \rho\right), A\right\rangle_{\mathrm{evo}}. \end{aligned}$$

Thus, using (4.54) and (4.55) we arrive at the assertion. □

The invariant spaces $\mathfrak{H}_0^{(\lambda,\eta)}$, related to the projectors $P_0^{(\lambda,\eta)}$, are not explicit enough for practical purposes. Therefore, the next step is to reduce the dynamics onto the spaces $\mathfrak{H}_0^{(0,0)}$, which are explicitly known. To this end, we denote the restriction of $G^{(\lambda,\eta)}$ onto the space $\mathfrak{H}_0^{(0,0)}$ by

$$\Lambda^{(\lambda,\eta)} := P_0^{(0,0)} G^{(\lambda,\eta)} P_0^{(0,0)}. \tag{4.56}$$

It turns out that the dynamics of $P_{\mathfrak{D}}(\rho(t))$ is properly described by the semigroup generated by $\Lambda^{(\lambda,\eta)}$:

**Theorem 4.13.**
*For any $\varepsilon \in (0,1)$, there is a constant $C_\varepsilon \in (0,\infty)$ such that,*

$$\left\| \exp\left(\alpha \Lambda^{(\lambda,\eta)}\right) - \exp\left(\alpha P_0^{(\lambda,\eta)} G^{(\lambda,\eta)} P_0^{(\lambda,\eta)}\right) \right\| \leq C_\varepsilon |\lambda|^{2(1-\varepsilon)}.$$

In particular, Lemma 4.12 and Theorem 4.13 directly yield the following corollary:

**Corollary 4.14 (Effective behaviour of $P_{\mathfrak{D}}(\rho(t))$–II).**
*For any $\varepsilon \in (0,1)$, any state $\rho \in \mathfrak{D} \subset \mathfrak{H}_{\mathrm{at}}$, with $\rho = \rho(0)$, and any observable $A \in \mathcal{B}(\mathbb{C}^d) \equiv \mathfrak{H}_{\mathrm{at}}$, the unique solution $\{\rho(t)\}_{t\geq 0}$ of the effective atomic master equation (4.37) satisfies the bound*

$$\begin{aligned} &\left|\langle P_{\mathfrak{D}}(\rho(\alpha)), A\rangle_{\mathrm{at}} - \left\langle \exp\left(\alpha\Lambda^{(\lambda,\eta)}\right)\rho, A\right\rangle_{\mathrm{evo}}\right| \\ \leq\ & C\,\|A\|\left(|\lambda|^{2(1-\varepsilon)} + \frac{|\lambda|(1+|\lambda|)}{\varpi}\right), \end{aligned}$$

*where $C$ is a finite constant independent of $\rho$, $A$, $\lambda$, $\eta$, $\varpi$, and $\alpha$.*

The proof of Theorem 4.13 needs some technical preparations. For the sake of clarity we defer it to Section 4.3.3 and continue our discussion on the large time behaviour of $P_{\mathfrak{D}}(\rho(t))$.

Observe that the Hilbert space $\mathfrak{H}_0^{(0,0)}$ is not a subspace of $\mathfrak{H}_{\mathrm{at}} \subset \mathfrak{H}_{\mathrm{evo}}$, because of oscillating terms present in it. Indeed, by taking any ONB $\{e_n^{(k)}\}_{n\in K_k}$, $K_k := \{1,\ldots,\dim(\mathcal{H}_k)\} \subset \mathbb{N}$, of the eigenspace $\mathcal{H}_k \subset \mathbb{C}^d$, $k \in \{1,\ldots,N\}$, of the atomic Hamiltonian $H_{\mathrm{at}}$ (see Section 4.2.2), we define the family

$$\{W_{(k,n)}^{(k',n')}\}_{k,k'\in\{1,\ldots,N\},\ n\in K_k,\ n'\in K_{k'}} \subset \mathfrak{H}_{\mathrm{at}} \equiv \mathcal{B}(\mathbb{C}^d)$$

of vectors by

$$W_{(k,n)}^{(k',n')} e_{n''}^{(k'')} := \delta_{n,n''}\delta_{k,k''} e_{n'}^{(k')}. \tag{4.57}$$

Then, the Hilbert space $\mathfrak{H}_0^{(0,0)}$ is equal to

$$\mathfrak{H}_0^{(0,0)} = \mathrm{span}\left\{ e^{-itE_{kk'}} W_{(k,n)}^{(k',n')} \mid (k,k') \in \bigcup_{m\in\{-1,0,1\}} \mathfrak{t}_{m\varpi},\ n \in K_k,\ n' \in K_{k'} \right\},$$

where $E_{kk'} := E_k - E_{k'}$. We next remove the oscillating terms by defining a unitary map $U$ from $\mathfrak{H}_0^{(0,0)}$ to the subspace

$$\tilde{\mathfrak{H}}_0^{(0,0)} := \mathrm{span}\left\{ W_{(k,n)}^{(k',n')} \mid (k,k') \in \bigcup_{m\in\{-1,0,1\}} \mathfrak{t}_{m\varpi},\ n \in K_k,\ n' \in K_{k'} \right\} \subset \mathfrak{H}_{\mathrm{at}} \tag{4.58}$$

as follows:

$$U\left(e^{-it(E_k - E_{k'})} W_{(k,n)}^{(k',n')}\right) := W_{(k,n)}^{(k',n')}. \tag{4.59}$$

The behaviour of $P_{\mathfrak{D}}(\rho(\alpha))$ can be studied through the generator $\Lambda^{(\lambda,\eta)}$, which acts (non–trivially) on $\mathfrak{H}_0^{(0,0)} \not\subseteq \mathfrak{H}_{\mathrm{at}}$, see (4.56) and Corollary 4.14. As far as the large time behaviour of $P_{\mathfrak{D}}(\rho(\alpha))$ is concerned, we can analyse instead the evolution semigroup given by the generator

$$\tilde{\Lambda}^{(\lambda,\eta)} := U\Lambda^{(\lambda,\eta)}U^* \tag{4.60}$$

acting now on the subspace $\tilde{\mathfrak{H}}_0^{(0,0)} \subset \mathfrak{H}_{\text{at}}$. This follows, for any initial density matrix $\rho \in \mathfrak{H}_{\text{at}}$, from the equality

$$\begin{aligned} P_{\mathfrak{D}}\left(\exp\left(\alpha\Lambda^{(\lambda,\eta)}\right)\rho\right) &= P_{\mathfrak{D}}\left(\exp\left(\alpha\Lambda^{(\lambda,\eta)}\right)P_0^{(0,0)}(\rho)\right) \\ &= P_{\mathfrak{D}}\left(U^*\exp\left(\alpha\tilde{\Lambda}^{(\lambda,\eta)}\right)UP_{\mathfrak{D}}(\rho)\right) \\ &= P_{\mathfrak{D}}\left(\exp\left(\alpha\tilde{\Lambda}^{(\lambda,\eta)}\right)P_{\mathfrak{D}}(\rho)\right) \\ &=: \rho_{\mathfrak{D}}(\alpha) \end{aligned} \tag{4.61}$$

and Theorem 4.35. We describe this more precisely in the following theorem:

**Theorem 4.15 (Long–time behaviour of $P_{\mathfrak{D}}(\rho(t))$).**
(i) *For all $\rho \in \tilde{\mathfrak{H}}_0^{(0,0)}$,*

$$\tilde{\Lambda}^{(\lambda,\eta)}(\rho) = \frac{\eta}{2}\mathfrak{L}_{\text{p}}(\rho) + \lambda^2\mathfrak{L}_{\mathcal{R}}(\rho)$$

*with $\mathfrak{L}_{\text{p}}(\rho)$ and $\mathfrak{L}_{\mathcal{R}}(\rho)$ defined by (4.26) and (4.27) respectively.*
(ii) *There is a unique density matrix $\tilde{\rho}_\infty \in \tilde{\mathfrak{H}}_0^{(0,0)}$ such that $\tilde{\Lambda}^{(\lambda,\eta)}(\tilde{\rho}_\infty) = 0$. Moreover, for all $\rho \in \mathfrak{H}_{\text{at}}$ and any $\varepsilon \in (0,1)$,*

$$\limsup_{\alpha\to\infty}\|P_{\mathfrak{D}}(\rho(\alpha)) - P_{\mathfrak{D}}(\tilde{\rho}_\infty)\| \le C\left(|\lambda|^{2(1-\varepsilon)} + \frac{|\lambda|(1+|\lambda|)}{\varpi}\right), \tag{4.62}$$

*where $C$ is a finite constant independent of $\rho$, $A$, $\lambda$, $\eta$, $\varpi$, and $\alpha$.*

*Proof.* (i) This assertion readily follows from explicit computations.
(ii) Note that $\tilde{\Lambda}^{(\lambda,\eta)}$, given by the equality in (i) makes sense for all $\rho \in \mathfrak{H}_{\text{at}}$ whereas $\tilde{\mathfrak{H}}_0^{(0,0)} \subset \mathfrak{H}_{\text{at}}$ is an invariant space of $\tilde{\Lambda}^{(\lambda,\eta)} \in \mathcal{B}(\mathfrak{H}_{\text{at}})$. By Theorem 4.35 and Assumption (B), $\tilde{\Lambda}^{(\lambda,\eta)} \in \mathcal{B}(\mathfrak{H}_{\text{at}})$ is the generator of a relaxing Markov CP and $C_0$ semigroup, see Definition 4.34. In particular, there is a unique density matrix $\tilde{\rho}_\infty \in \mathfrak{H}_{\text{at}}$ such that, for any density matrix $\rho \in \mathfrak{H}_{\text{at}}$,

$$\lim_{\alpha\to\infty}\left(\exp\left(\alpha\tilde{\Lambda}^{(\lambda,\eta)}\right)\rho\right) = \tilde{\rho}_\infty. \tag{4.63}$$

It follows that $\tilde{\rho}_\infty \in \mathfrak{H}_{\text{at}}$ is the unique density matrix satisfying $\tilde{\Lambda}^{(\lambda,\eta)}(\tilde{\rho}_\infty) = 0$. As $\tilde{\mathfrak{H}}_0^{(0,0)}$ is an invariant space of $\tilde{\Lambda}^{(\lambda,\eta)} \in \mathcal{B}(\mathfrak{H}_{\text{at}})$ containing density matrices, one then has $\tilde{\rho}_\infty \in \tilde{\mathfrak{H}}_0^{(0,0)}$. Using (4.61)

$$\lim_{\alpha\to\infty}P_{\mathfrak{D}}\left(\exp\left(\alpha\Lambda^{(\lambda,\eta)}\right)\rho\right) = P_{\mathfrak{D}}(\tilde{\rho}_\infty)$$

as $P_{\mathfrak{D}}(\rho) \in \mathfrak{H}_{\text{at}}$ is also a density matrix. The inequality (4.62) then results from Corollary 4.14 and the finite dimensionality of $\mathfrak{H}_{\text{at}}$. □

It now remains to characterise more precisely the density matrix $\tilde{\rho}_\infty \in \tilde{\mathfrak{H}}_0^{(0,0)}$ of Theorem 4.15 (ii).

Denote

$$P_{\mathfrak{D}}^{\perp} := \mathbf{1} - P_{\mathfrak{D}}$$

and observe that $P_{\mathfrak{D}}(\tilde{\mathfrak{H}}_0^{(0,0)})$ and $P_{\mathfrak{D}}^{\perp}(\tilde{\mathfrak{H}}_0^{(0,0)})$ are invariant subspaces of the Lindbladian $\mathfrak{L}_{\mathcal{R}}$ (4.27), whereas $\mathfrak{L}_{\mathrm{p}}$ (4.26) maps $P_{\mathfrak{D}}(\tilde{\mathfrak{H}}_0^{(0,0)})$ to $P_{\mathfrak{D}}^{\perp}(\tilde{\mathfrak{H}}_0^{(0,0)})$, and vice versa. These properties allow a characterisation of the density matrix $P_{\mathfrak{D}}(\tilde{\rho}_{\infty})$ by means of a "*pre–master equation*" on the (smaller) subspace $P_{\mathfrak{D}}(\tilde{\mathfrak{H}}_0^{(0,0)})$ for the semigroups $\{\exp(\alpha\tilde{\Lambda}^{(\lambda,\eta)})\}_{\alpha\geq 0}$.

**Theorem 4.16 (The pre–master equation).**
*The family $\{\rho_{\mathfrak{D}}(\alpha)\}_{\alpha\geq 0}$ of density matrices defined by (4.61) for any initial density matrix $\rho\in\mathfrak{H}_{\mathrm{at}}$ obeys the integro–differential equation*

$$\begin{aligned}\frac{d}{d\alpha}\rho_{\mathfrak{D}}(\alpha) &= \lambda^2\mathfrak{L}_{\mathcal{R}}(\rho_{\mathfrak{D}}(\alpha)) \\ &\quad +\frac{\eta^2}{4\lambda^2}\int_0^{\alpha\lambda^{-2}} P_{\mathfrak{D}}\mathfrak{L}_{\mathrm{p}}P_{\mathfrak{D}}^{\perp}e^{s\mathfrak{L}_{\mathcal{R}}}P_{\mathfrak{D}}^{\perp}\mathfrak{L}_{\mathrm{p}}P_{\mathfrak{D}}\left(\rho_{\mathfrak{D}}\left(\alpha-s\lambda^{-2}\right)\right)\mathrm{d}s,\end{aligned}$$

*called here the* pre–master equation*.*

*Proof.* The result follows from standard considerations and may for instance be taken from [JZK⁺03, Chapter 7]. □

By combining (4.63) with the equality $\tilde{\Lambda}^{(\lambda,\eta)}(\tilde{\rho}_{\infty})=0$ (Theorem 4.15 (ii)), the density matrix $\rho_{\mathfrak{D}}(\alpha)$ must converge to $P_{\mathfrak{D}}(\tilde{\rho}_{\infty})$ as $\alpha\to\infty$ and its derivative must vanish in the limit $\alpha\to\infty$. Using Theorem 4.20 proven below, we get that

$$\left\|P_{\mathfrak{D}}\mathfrak{L}_{\mathrm{p}}P_{\mathfrak{D}}^{\perp}e^{s\mathfrak{L}_{\mathcal{R}}}P_{\mathfrak{D}}^{\perp}\mathfrak{L}_{\mathrm{p}}P_{\mathfrak{D}}\right\|\leq C_7e^{-sC_8}, \tag{4.64}$$

for some constants $C_7<\infty$ and $C_8>0$. The latter ensures the integrability of the integrand in the pre–master equation on the whole positive real line $[0,\infty)$. As a consequence, by Lebesgue's dominated convergence theorem, the limit $P_{\mathfrak{D}}(\tilde{\rho}_{\infty})$ satisfies the following *balance condition*, which is defined by the equation:

$$\mathfrak{L}_{\mathcal{R}}(\rho)+\frac{\eta^2}{4\lambda^4}\mathfrak{B}(\rho)=0 \tag{4.65}$$

for $\rho\in\mathfrak{H}_{\mathrm{at}}$ and where

$$\mathfrak{B}:=\int_0^{\infty}P_{\mathfrak{D}}\mathfrak{L}_{\mathrm{p}}P_{\mathfrak{D}}^{\perp}e^{s\mathfrak{L}_{\mathcal{R}}}P_{\mathfrak{D}}^{\perp}\mathfrak{L}_{\mathrm{p}}P_{\mathfrak{D}}\mathrm{d}s\in\mathcal{B}(\mathfrak{H}_{\mathrm{at}}).$$

We note, however, that the balance condition (4.65) might, a priori, have more than one density matrix as a solution. Next we give a criterion for $\mathfrak{B}$ to be associated with a generator of a CP Markov semigroup, which we use to employ Theorem 4.35 for $\mathfrak{L}_{\mathcal{R}}+\mathfrak{B}$ in order to obtain a unique solution. It is useful to introduce the projections

$$P_{jk}:=\underrightarrow{\mathbf{1}\left[H_{\mathrm{at}}=E_j\right]}\,\underleftarrow{\mathbf{1}\left[H_{\mathrm{at}}=E_k\right]}, \tag{4.66}$$

for $j,k=1,\ldots,N$. Note that

$$1_{\mathfrak{H}_{\mathrm{at}}}=\sum_{j,k=1}^{N}P_{jk}.$$

**Proposition 4.17 (CP criterion for $\mathfrak{B}$).**

If
$$P_{N1}\mathfrak{L}_{\mathcal{R}}P_{N1} = \alpha_{N1}P_{N1},$$
for some $\alpha_{N1} \in \mathbb{C}$, then $\mathfrak{B}$ is the restriction of a generator $\tilde{\mathfrak{B}} \in \mathcal{B}\left(\mathfrak{H}_{\mathrm{at}}\right)$ of a CP Markov semigroup, i.e.
$$\mathfrak{B} = \tilde{\mathfrak{B}} \restriction_{\mathrm{ran}(P_{\mathfrak{D}})} .$$

*Proof.* Note, that since $\mathfrak{L}_{\mathcal{R}}$ is the generator of a completely positive Markov semigroup, $\mathrm{Re}\left(\alpha_{jk}\right) \geq 0$. By (4.64) follows that
$$\left(\mathfrak{L}_{\mathrm{P}}\right)^{-1} := \left(P_{\mathfrak{D}}^{\perp}\mathfrak{L}_{\mathrm{P}}P_{\mathfrak{D}}^{\perp}\right)^{-1} = \int_0^{\infty} ds\, P_{\mathfrak{D}}^{\perp}e^{s\mathfrak{L}_{\mathcal{R}}}P_{\mathfrak{D}}^{\perp}$$
exists, using Theorem 4.20 and that $P_{\mathfrak{D}}^{\perp}$ is a projection onto an invariant space of $\mathfrak{L}_{\mathcal{R}}$. From Assumption (P) follows then for any $s \in \mathbb{R}_0^+$,
$$P_{\mathfrak{D}}\mathfrak{L}_{\mathrm{p}}P_{\mathfrak{D}}^{\perp}\left(\mathfrak{L}_{\mathrm{P}}\right)^{-1}P_{\mathfrak{D}}^{\perp}\mathfrak{L}_{\mathrm{p}}P_{\mathfrak{D}} = \sum_{j,k=1}^{N}\mathfrak{B}_{jk},$$
where the $\mathfrak{B}_{jk}$ are given by
$$\begin{aligned}
\mathfrak{B}_{N1} \;:=\;& P_{NN}\underrightarrow{h_{\mathrm{P}}}P_{1N}\left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}P_{N1}\underrightarrow{h_{\mathrm{P}}}P_{11} - P_{NN}\underrightarrow{h_{\mathrm{P}}}P_{1N}\left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}P_{1N}\underleftarrow{h_{\mathrm{P}}^*}P_{11}\\
&-P_{NN}\underleftarrow{h_{\mathrm{P}}^*}P_{N1}\left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}P_{N1}\underrightarrow{h_{\mathrm{P}}}P_{11} + P_{NN}\underleftarrow{h_{\mathrm{P}}^*}P_{N1}\left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}P_{1N}\underleftarrow{h_{\mathrm{P}}^*}P_{11}\\
\mathfrak{B}_{1N} \;:=\;& P_{11}\underrightarrow{h_{\mathrm{P}}^*}P_{N1}\left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}P_{1N}\underrightarrow{h_{\mathrm{P}}^*}P_{NN} - P_{11}\underrightarrow{h_{\mathrm{P}}^*}P_{N1}\left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}P_{N1}\underleftarrow{h_{\mathrm{P}}}P_{NN}\\
&-P_{11}\underleftarrow{h_{\mathrm{P}}}P_{1N}\left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}P_{1N}\underrightarrow{h_{\mathrm{P}}^*}P_{NN} + P_{11}\underleftarrow{h_{\mathrm{P}}}P_{1N}\left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}P_{N1}\underleftarrow{h_{\mathrm{P}}}P_{NN}\\
\mathfrak{B}_{NN} \;:=\;& P_{NN}\underrightarrow{h_{\mathrm{P}}}P_{1N}\left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}P_{1N}\underrightarrow{h_{\mathrm{P}}^*}P_{NN} - P_{NN}\underrightarrow{h_{\mathrm{P}}}P_{1N}\left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}P_{N1}\underleftarrow{h_{\mathrm{P}}}P_{NN}\\
&-P_{NN}\underleftarrow{h_{\mathrm{P}}^*}P_{N1}\left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}P_{1N}\underrightarrow{h_{\mathrm{P}}^*}P_{NN} + P_{NN}\underleftarrow{h_{\mathrm{P}}^*}P_{N1}\left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}P_{N1}\underleftarrow{h_{\mathrm{P}}}P_{NN}\\
\mathfrak{B}_{11} \;:=\;& P_{11}\underrightarrow{h_{\mathrm{P}}^*}P_{N1}\left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}P_{N1}\underrightarrow{h_{\mathrm{P}}}P_{11} - P_{11}\underrightarrow{h_{\mathrm{P}}^*}P_{N1}\left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}P_{1N}\underleftarrow{h_{\mathrm{P}}^*}P_{11}\\
&-P_{11}\underleftarrow{h_{\mathrm{P}}}P_{1N}\left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}P_{N1}\underrightarrow{h_{\mathrm{P}}}P_{11} + P_{11}\underleftarrow{h_{\mathrm{P}}}P_{1N}\left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}P_{1N}\underleftarrow{h_{\mathrm{P}}^*}P_{11},
\end{aligned}$$
and $\mathfrak{B}_{jk} = 0$ if $j$ or $k$ is in $\{2, \dots, N-1\}$. Recall that $\mathrm{ran}\left(P_{jk}\right)$ are invariant spaces of $\mathfrak{L}_{\mathcal{R}}$ and hence
$$P_{1N}\left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}P_{N1} = 0 = P_{N1}\left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}P_{1N}.$$
Theorem 4.20 implies $\mathrm{Re}\left(\alpha_{N1}\right) < 0$. Observe, that
$$\bar{\alpha}_{N1}P_{1N} = \left(P_{N1}\mathfrak{L}_{\mathcal{R}}P_{N1}\right)^{*\rho_{\mathfrak{g}}} = P_{1N}\mathfrak{L}_{\mathcal{R}}P_{1N} =: \alpha_{1N}P_{1N},$$
where $(\cdot)^{*\rho_{\mathfrak{g}}}$ denotes the adjoint with respect to the scalar product induced by the Gibbs state $\rho_{\mathfrak{g}}$,
$$\langle A, B\rangle_{\rho_{\mathfrak{g}}} := \mathrm{Tr}\left(\rho_{\mathfrak{g}}A^*B\right),$$

with the inverse temperature $\beta$ of the reservoir, determined by the choice of the KMS state $\omega_{\mathcal{R}}$. Hence, $\alpha := \alpha_{N1} = \bar{\alpha}_{1N}$. Thus,

$$\begin{aligned}\mathfrak{B}_{N1} &= -\bar{\alpha}^{-1} P_{NN} \underrightarrow{h_{\mathrm{P}}} P_{1N} \underleftarrow{h_{\mathrm{P}}^*} P_{11} - \alpha^{-1} P_{NN} \underleftarrow{h_{\mathrm{P}}^*} P_{N1} \underrightarrow{h_{\mathrm{P}}} P_{11} \\ &= -\frac{2\mathrm{Re}\,(\alpha)}{|\alpha|^2} \underrightarrow{h_{\mathrm{P}}} \underleftarrow{h_{\mathrm{P}}^*},\end{aligned}$$

as one easily checks, using Assumption (P). Similarly one observes

$$\mathfrak{B}_{1N} = -\frac{2\mathrm{Re}\,(\alpha)}{|\alpha|^2} \underrightarrow{h_{\mathrm{P}}^*} \underleftarrow{h_{\mathrm{P}}}.$$

For any $\rho \in \mathcal{B}\,(\mathfrak{H}_{\mathrm{at}})$ we have

$$\begin{aligned}\mathfrak{B}_{NN}\,(\rho) &= \bar{\alpha}^{-1} h_{\mathrm{P}} h_{\mathrm{P}}^* \rho \mathbf{1}\,[H_{\mathrm{at}} = E_N] + \alpha^{-1} \mathbf{1}\,[H_{\mathrm{at}} = E_N]\,\rho h_{\mathrm{P}} h_{\mathrm{P}}^* \\ \mathfrak{B}_{11}\,(\rho) &= \alpha^{-1} h_{\mathrm{P}}^* h_{\mathrm{P}} \rho \mathbf{1}\,[H_{\mathrm{at}} = E_1] + \bar{\alpha}^{-1} \mathbf{1}\,[H_{\mathrm{at}} = E_1]\,\rho h_{\mathrm{P}}^* h_{\mathrm{P}}.\end{aligned}$$

Define now the completely positive map

$$\Xi := \mathfrak{B}_{1N} + \mathfrak{B}_{N1} + \tilde{\mathfrak{B}}_{NN} + \tilde{\mathfrak{B}}_{11},$$

with

$$\begin{aligned}\tilde{\mathfrak{B}}_{NN} &:= \frac{\mathrm{Re}\,(\alpha)}{|\alpha|^2} \left( \underrightarrow{h_{\mathrm{P}}} \underrightarrow{h_{\mathrm{P}}^*} + \underleftarrow{h_{\mathrm{P}}} \underleftarrow{h_{\mathrm{P}}^*} \right) \\ \tilde{\mathfrak{B}}_{11} &:= \frac{\mathrm{Re}\,(\alpha)}{|\alpha|^2} \left( \underrightarrow{h_{\mathrm{P}}^*} \underrightarrow{h_{\mathrm{P}}} + \underleftarrow{h_{\mathrm{P}}^*} \underleftarrow{h_{\mathrm{P}}} \right).\end{aligned}$$

Moreover, setting

$$\Delta := \frac{i\mathrm{Im}\,(\alpha)}{|\alpha|^2} \left( h_{\mathrm{P}} h_{\mathrm{P}}^* - h_{\mathrm{P}}^* h_{\mathrm{P}} \right),$$

and observing that $\Delta \in \mathcal{B}\,(\mathcal{H}_{\mathrm{at}})$ is anti–selfadjoint we arrive at

$$\tilde{\mathfrak{B}} := \underrightarrow{\Delta} + \underleftarrow{\Delta^*} + \Xi.$$

Since

$$\Xi^{*1} \equiv \Xi, \qquad \square$$

where $(\cdot)^{*1}$ is the adjoint with respect to the scalar product $\langle \cdot, \cdot \rangle_{\mathrm{at}}$, we conclude $\Xi\,(1) = 0$, and $\tilde{B}$ is thus by Theorem 4.32 a generator of a CP Markov (semi)group.

**Remark 4.18.**

1. The assumption in Proposition 4.17 corresponds physically to a *fully resonant* pump, i.e. where the reservoir–impurity interaction does not split the spectral line of the $N1$–transition. In this case, the $N1$ decoherence time is a number, not a general operator.

2. As another criterion to obtain $\mathfrak{B}$ being associated with the generator of a CP Markov semigroup we do expect that for a strong decoherence, i.e. the order of magnitude of the real part of $\mathfrak{L}_{\mathcal{R}} P_{\mathfrak{D}}^{\perp}$ compared to the real part of $\mathfrak{L}_{\mathcal{R}} P_{\mathfrak{D}}$ being big, $\mathfrak{B}$ may be obtained as a weak coupling limit, where the coupling parameter is given by the ratio $\eta/\lambda^2$. This would then imply that $\mathfrak{B}$ is a (restriction of) generator of a CP Markov semigroup, even if the reservoir–impurity interaction creates a fine–structure splitting of the $N1$–transition.

3. We only need that the ground state of $\mathfrak{L}_{\mathcal{R}} + \eta^2/\lambda^4 \mathfrak{B}$ is unique for the characterisation of the quasi–stationary state. By Kato's perturbation theory of discrete eigenvalues this is always true for the *weak pump*, i.e. sufficiently small ratio $\eta/\lambda^2$.

Using Proposition 4.17 and Theorem 4.35 in combination with Remark 4.31, the solution of (4.65) is uniquely determined in the set of density matrices of $\mathfrak{H}_{\mathrm{at}}$ and hence characterises $P_{\mathfrak{D}}(\tilde{\rho}_\infty)$ completely.

**Corollary 4.19 (Characterisation of $P_{\mathfrak{D}}(\tilde{\rho}_\infty)$ via the balance condition).**

*Let*

$$P_{N1} \mathfrak{L}_{\mathcal{R}} P_{N1} = \alpha_{N1} P_{N1},$$

*for some $\alpha_{N1} \in \mathbb{C}$. Then, $P_{\mathfrak{D}}(\tilde{\rho}_\infty)$ is the unique density matrix satisfying the balance condition*

$$\mathfrak{L}_{\mathcal{R}}\left(P_{\mathfrak{D}}(\tilde{\rho}_\infty)\right) + \frac{\eta^2}{4\lambda^4} \mathfrak{B}\left(P_{\mathfrak{D}}(\tilde{\rho}_\infty)\right) = 0.$$

### 4.3.3 Proof of Theorem 4.13

In this subsection, it is useful to extend the definition of $\Lambda^{(\lambda,\eta)}$ (4.56), $\tilde{\mathfrak{H}}_0^{(0,0)}$ (4.58), $U$ (4.59), and $\tilde{\Lambda}^{(\lambda,\eta)}$ (4.60) to all $\epsilon \in \sigma(i[H_{\mathrm{at}}, \cdot])$ as follows:

$$\begin{aligned}
&\Lambda_\epsilon^{(\lambda,\eta)} := P_\epsilon^{(0,0)} G^{(\lambda,\eta)} P_\epsilon^{(0,0)}. \\
&\tilde{\mathfrak{H}}_\epsilon^{(0,0)} := \operatorname{span}\left\{ W_{(k,n)}^{(k',n')} \mid (k,k') \in \bigcup_{m \in \{-2,-1,0,1,2\}} \mathfrak{t}_{\epsilon+m\varpi},\ n \in K_k,\ n' \in K_{k'} \right\} \\
&U_\epsilon\left(e^{it\left(\epsilon - E_k + E_{k'}\right)} W_{(k,n)}^{(k',n')}\right) := W_{(k,n)}^{(k',n')}. \\
&\tilde{\Lambda}_\epsilon^{(\lambda,\eta)} := U_\epsilon \Lambda_\epsilon^{(\lambda,\eta)} U_\epsilon^* .
\end{aligned} \tag{4.67}$$

Observe that

$$\tilde{\mathfrak{H}}_\epsilon^{(0,0)} \subset \mathfrak{H}_{\mathrm{at}}, \quad \tilde{\mathfrak{H}}_{-\varpi}^{(0,0)} = \tilde{\mathfrak{H}}_0^{(0,0)} = \tilde{\mathfrak{H}}_\varpi^{(0,0)},$$

whereas

$$\forall \epsilon \in \sigma(i[H_{\mathrm{at}}, \cdot]) \backslash \{-\varpi, 0, \varpi\} : \qquad \tilde{\mathfrak{H}}_0^{(0,0)} \perp \tilde{\mathfrak{H}}_\epsilon^{(0,0)}.$$

Using these observations we can deduce the structure of the spectrum of the generators $\Lambda_\epsilon^{(\lambda,\eta)}$:

**Theorem 4.20 (Spectrum of $\Lambda_\epsilon^{(\lambda,\eta)}$).**
*For all $\epsilon \in \sigma(i[H_{\mathrm{at}},\cdot])\backslash\{-\varpi,0,\varpi\}$,*

$$\sigma(\Lambda_\epsilon^{(\lambda,\eta)}) \subset i\mathbb{R}-\mathbb{R}_+,$$

*i.e., any eigenvalue of $\Lambda_\epsilon^{(\lambda,\eta)}$, $\epsilon \in \mathfrak{t}\backslash\{-\varpi,0,\varpi\}$, has a strictly negative real part. Moreover, $-\varpi$, $0$, $\varpi$ are non–degenerated eigenvalues of $\Lambda_{-\varpi}^{(\lambda,\eta)}$, $\Lambda_0^{(\lambda,\eta)}$, and $\Lambda_\varpi^{(\lambda,\eta)}$, respectively.*

*Proof.* Direct computations shows that

$$\tilde{\Lambda}_\epsilon^{(\lambda,\eta)} = \left(-i\epsilon + \frac{\eta}{2}\mathfrak{L}_{\mathrm{p}} + \lambda^2\mathfrak{L}_{\mathcal{R}}\right)\Big|_{\tilde{\mathfrak{H}}_\epsilon^{(0,0)}}$$

from which we infer

$$\sigma(\Lambda_\epsilon^{(\lambda,\eta)}) = \sigma(\tilde{\Lambda}_\epsilon^{(\lambda,\eta)}) = -i\epsilon + \sigma\left(\ \tilde{\Lambda}^{(\lambda,\eta)}\Big|_{\tilde{\mathfrak{H}}_\epsilon^{(0,0)}}\ \right),$$

where $\tilde{\Lambda}^{(\lambda,\eta)} \in \mathcal{B}(\mathfrak{H}_{\mathrm{at}})$ is seen as an operator acting on $\mathfrak{H}_{\mathrm{at}}$, see proof of Theorem 4.15. $\tilde{\mathfrak{H}}_\epsilon^{(0,0)}$ is an invariant space of $\tilde{\Lambda}^{(\lambda,\eta)} \in \mathcal{B}(\mathfrak{H}_{\mathrm{at}})$. By Theorem 4.35 and Assumption (B), 0 is a non–degenerate eigenvalue of $\tilde{\Lambda}^{(\lambda,\eta)}$. The corresponding eigenvector is an element of $\tilde{\mathfrak{H}}_\epsilon^{(0,0)} = \tilde{\mathfrak{H}}_{\pm\varpi}^{(0,0)}$. Since $\tilde{\Lambda}^{(\lambda,\eta)}$ generates a relaxing Markov CP and $C_0$ semigroup, all non–zero elements $p \in \sigma(\ \tilde{\Lambda}^{(\lambda,\eta)}\Big|_{\tilde{\mathfrak{H}}_\epsilon^{(0,0)}})\backslash\ \{0\}$ have a strictly negative real part $\mathrm{Re}\,(p) < 0$. □

**Lemma 4.21 (Stability of Assumption B under block localisation).**
*Let $H \in \mathcal{B}(\mathbb{C}^d)$ be selfadjoint and denote by $\mathbf{1}_\varepsilon$ the spectral projection of $[H,\cdot]$ onto the eigenspace corresponding to an eigenvalue $\varepsilon \in \sigma([H,\cdot])$. Then, there are $\tilde{m} \in \mathbb{N}$, positive real number $\tilde{c}_{j,k}^{(\tilde{\ell})} \in \mathbb{R}_+$, and $\tilde{V}_{j,k}^{(\tilde{\ell})} \in \mathcal{B}(\mathbb{C}^d)$ such that*

$$\begin{aligned}\sum_{\varepsilon\in\sigma([H,\cdot])} \mathbf{1}_\varepsilon \mathfrak{L}_d \mathbf{1}_\varepsilon(\rho) \quad &= \quad \frac{1}{2}\sum_{\varepsilon\in\sigma^+(\mathfrak{L}_{\mathrm{at}})}\ \sum_{(j,k)\in\mathfrak{t}_\epsilon}\ \sum_{\tilde{\ell}=1}^{\tilde{m}} \tilde{c}_{j,k}^{(\tilde{\ell})}\tilde{\mathfrak{L}}_{j,k}^{(\tilde{\ell})}(\rho) \\ &\quad + \frac{e^{-\beta\epsilon}}{2}\sum_{\varepsilon\in\sigma^+(\mathfrak{L}_{\mathrm{at}})}\ \sum_{(j,k)\in\mathfrak{t}_\epsilon}\ \sum_{\tilde{\ell}=1}^{\tilde{m}} \tilde{c}_{j,k}^{(\tilde{\ell})}\left(\tilde{\mathfrak{L}}_{j,k}^{(\tilde{\ell})}\right)^*(\rho),\end{aligned}$$

*with*

$$\begin{aligned}\tilde{\mathfrak{L}}_{j,k}^{(\tilde{\ell})}(\rho) \quad &:= \quad 2\tilde{V}_{j,k}^{(\tilde{\ell})}\rho\tilde{V}_{j,k}^{(\tilde{\ell})*} - \tilde{V}_{j,k}^{(\tilde{\ell})*}\tilde{V}_{j,k}^{(\tilde{\ell})}\rho - \rho\tilde{V}_{j,k}^{(\tilde{\ell})*}\tilde{V}_{j,k}^{(\tilde{\ell})}, \\ \left(\tilde{\mathfrak{L}}_{j,k}^{(\tilde{\ell})}\right)^*(\rho) \quad &:= \quad 2\tilde{V}_{j,k}^{(\tilde{\ell})*}\rho\tilde{V}_{j,k}^{(\tilde{\ell})} - \tilde{V}_{j,k}^{(\tilde{\ell})}\tilde{V}_{j,k}^{(\tilde{\ell})*}\rho - \rho\tilde{V}_{j,k}^{(\tilde{\ell})}\tilde{V}_{j,k}^{(\tilde{\ell})*}.\end{aligned}$$

*Moreover,*

$$\left[\bigcup_{(j,k,\tilde{\ell}),\tilde{c}_{j,k}^{(\tilde{\ell})}\neq 0}\left\{\tilde{V}_{j,k}^{(\tilde{\ell})}\right\}\right]'' = \mathcal{B}(\mathbb{C}^d), \tag{4.68}$$

*whenever Assumption (B) is satisfied. In particular,*

$$\sum_{\varepsilon\in\sigma([H,\cdot])} \mathbf{1}_\varepsilon \mathfrak{L}_d \mathbf{1}_\varepsilon(\rho)$$

*is the generator of a Markov CP and $C_0$ semigroup satisfying Assumption (B).*

*Proof.* For any $V \in \mathcal{B}(\mathbb{C}^d)$ and all

$$\varepsilon \in \sigma([H,\cdot]) = \left\{\tilde{E}_j - \tilde{E}_k : j,k \in \{1,2,\dots M\}\right\},$$

we define the matrix $V_\varepsilon \in \mathcal{B}(\mathbb{C}^d)$ by

$$V_\varepsilon := \mathbf{1}_\varepsilon(V) = \sum_{(j,k)\in\mathfrak{t}_\varepsilon} \mathbf{1}\left[H = \tilde{E}_k\right] \; V \, \mathbf{1}\left[H = \tilde{E}_j\right],$$

where $\{\tilde{E}_j\}_{j=1}^M$ are the eigenvalues of $H$ and

$$\mathfrak{t}_\varepsilon := \{(j,k) : \tilde{E}_j - \tilde{E}_k = \varepsilon\} \subset \{1,2,\dots M\} \times \{1,2,\dots M\}.$$

By construction, note that

$$\sum_{\varepsilon\in\sigma([H,\cdot])} V_\varepsilon = V.$$

In particular, one has

$$V \in \operatorname{span}\left\{\bigcup_{\varepsilon\in\sigma([H,\cdot])} V_\varepsilon\right\}.$$

Therefore, by defining

$$\tilde{V}_{j,k}^{(\ell,\varepsilon)} := \mathbf{1}_\varepsilon(V_{j,k}^{(\ell)})$$

and identifying the finite sets $\{1,2,\dots m\} \times \sigma([H,\cdot])$ and $\{1,2,\dots \tilde{m}\}$, we deduce (4.68), by Assumption (B). Furthermore, since, for all eigenvectors $A_\varepsilon, B_{\tilde{\varepsilon}} \in \mathcal{B}(\mathbb{C}^d)$ of $[H,\cdot]$ with eigenvalues $\varepsilon, \tilde{\varepsilon} \in \sigma([H,\cdot])$ respectively, i.e., $\mathbf{1}_\varepsilon(A_\varepsilon) = A_\varepsilon$ and $\mathbf{1}_{\tilde{\varepsilon}}(B_{\tilde{\varepsilon}}) = B_{\tilde{\varepsilon}}$,

$$A_\varepsilon B_{\tilde{\varepsilon}} = C_{\varepsilon+\tilde{\varepsilon}}, \qquad \text{with} \qquad \mathbf{1}_{\varepsilon+\tilde{\varepsilon}}(C_{\varepsilon+\tilde{\varepsilon}}) = C_{\varepsilon+\tilde{\varepsilon}}, \qquad \square$$

we obtain the equalities

$$\begin{aligned} \sum_{\varepsilon\in\sigma([H,\cdot])} \mathbf{1}_\varepsilon(V\mathbf{1}_\varepsilon(\rho)V^*) &= \sum_{\varepsilon\in\sigma([H,\cdot])} \mathbf{1}_\varepsilon\left(\sum_{\tilde{\varepsilon}\in\sigma([H,\cdot])} V_{\tilde{\varepsilon}}\mathbf{1}_\varepsilon(\rho) \sum_{\hat{\varepsilon}\in\sigma([H,\cdot])} V_{\hat{\varepsilon}}^*\right) \\ &= \sum_{\varepsilon\in\sigma([H,\cdot])}\sum_{\tilde{\varepsilon}\in\sigma([H,\cdot])} V_{\tilde{\varepsilon}}\mathbf{1}_\varepsilon(\rho)(V_{-\tilde{\varepsilon}})^* \\ &= \sum_{\tilde{\varepsilon}\in\sigma([H,\cdot])} V_{\tilde{\varepsilon}}\rho V_{\tilde{\varepsilon}}^*. \end{aligned}$$

Similarly,

$$\begin{aligned} &\sum_{\varepsilon\in\sigma([H,\cdot])} 2\,\mathbf{1}_\varepsilon(V\mathbf{1}_\varepsilon(\rho)V^*) - \mathbf{1}_\varepsilon(V^*V\mathbf{1}_\varepsilon(\rho)) - \mathbf{1}_\varepsilon(\mathbf{1}_\varepsilon(\rho)VV^*) \\ = &\sum_{\varepsilon\in\sigma([H,\cdot])} 2V_\varepsilon\rho V_\varepsilon^* - V_\varepsilon^*V_\varepsilon\rho - \rho V_\varepsilon^*V_\varepsilon \end{aligned}$$

which concludes the proof of the lemma.

**Lemma 4.22 (Behaviour of the spectral gap of $\Lambda^{(\lambda,\eta)}$).**
*For all $(\lambda,\eta) \in \mathbb{R}\times\mathbb{R}$,*

$$\min\left\{ |\mathrm{Re}\{p\}| : p \in \sigma\left(\Lambda^{(\lambda,\eta)}\right)\backslash\{0\}\right\} \geq C_{4.22}\lambda^2,$$

*with $C_{4.22} > 0$ being a constant only depending on $H_{\mathrm{Lamb}}$, $H_{\mathrm{p}}$, and $\mathfrak{L}_d$.*

*Proof.* We define the function

$$g(\lambda,\eta) := \lambda^{-2}\min\left\{ |\mathrm{Re}\{p\}| : p \in \sigma(\Lambda^{(\lambda,\eta)})\backslash\{0\}\right\}$$

on the set $\mathbb{R}\backslash\{0\}\times\mathbb{R}$. Observe that $g(\lambda,\eta)$ only depends on the ratio $\eta/\lambda^2$ and is strictly positive, by Theorems 4.30 and 4.35. Indeed,

$$g(\lambda,\eta) = \min\left\{ |\mathrm{Re}\{p\}| : p \in \sigma\left(\left(\frac{\eta}{2\lambda^2}\mathfrak{L}_{\mathrm{p}} + \mathfrak{L}_{\mathcal{R}}\right)\Big|_{\tilde{\mathfrak{H}}_\varepsilon^{(0,0)}}\right)\backslash\{0\}\right\}$$

with $\tilde{\mathfrak{H}}_\varepsilon^{(0,0)}$ being an invariant subspace of $\Lambda^{(\lambda,\eta)}$, and $\mathfrak{L}_{\mathcal{R}}$ is the generator of a Markov CP and $C_0$ semigroup satisfying Assumption (B), whereas $\mathfrak{L}_{\mathrm{p}} := -i[H_{\mathrm{p}},\cdot]$ (cf. (4.26)) with $H_{\mathrm{p}} = H_{\mathrm{p}}^*$ and $\mathrm{Tr}\left(H_{\mathrm{p}}\right) = 0$. Their sum must be a relaxing Markov CP and $C_0$ semigroup, by Theorems 4.30 and 4.35. By Kato's perturbation theory, for some constants $c, r > 0$, $g(\lambda,\eta) \geq c$ whenever $\eta < r\lambda^2$. Using again Kato's perturbation theory and Theorem 4.35, $\varkappa \mapsto g(\varkappa^{-\frac{1}{2}},1)$ is a strictly positive continuous function on the interval $[r,r']$ for any finite constant $r' > r$. By compactness of the interval $[r,r']$, it follows that

$$\min\left\{g(\varkappa^{-\frac{1}{2}},1) \mid \varkappa \in [r,r']\right\} > 0.$$

So, it remains to prove that $g(\lambda,\eta) \geq c'$ whenever $\eta > r'\lambda^2$ for some constants $c' > 0$ and sufficiently large $r'$. Note that

$$\sigma(\Lambda^{(0,\eta)}) = \sigma\big(\left.\tilde{\Lambda}^{(0,\eta)}\right|_{\tilde{\mathfrak{H}}_0^{(0,0)}}\big) \subset i\mathbb{R}.$$

Thus, as $\tilde{\mathfrak{H}}_0^{(0,0)}$ is an invariant space of $\tilde{\Lambda}^{(0,\eta)}$, by Kato's perturbation theory for the discrete spectrum, the limit

$$\lim_{\varkappa\to\infty} g(\varkappa^{-\frac{1}{2}},1) \in [0,\infty) \tag{4.69}$$

exists and satisfies

$$\lim_{\varkappa\to\infty} g(\varkappa^{-\frac{1}{2}},1) \geq \min\left\{|\mathrm{Re}\{p\}| : p \in \sigma\left(\sum_{\varepsilon\in\frac{\eta}{2}\sigma([H_{\mathrm{p}},\cdot])} \mathbf{1}_\varepsilon\mathfrak{L}_{\mathcal{R}}\mathbf{1}_\varepsilon\right)\backslash\{0\}\right\}, \tag{4.70}$$

where $\mathbf{1}_\varepsilon$ denotes the spectral projection of $[H_{\mathrm{p}},\cdot]$. They are well defined as $H_{\mathrm{p}}$ is selfadjoint. By (4.27), we note that

$$\sum_{\varepsilon\in\frac{\eta}{2}\sigma([H_{\mathrm{p}},\cdot])} \mathbf{1}_\varepsilon\mathfrak{L}_{\mathcal{R}}\mathbf{1}_\varepsilon = \sum_{\varepsilon\in\frac{\eta}{2}\sigma([H_{\mathrm{p}},\cdot])} \mathbf{1}_\varepsilon\mathfrak{L}_d\mathbf{1}_\varepsilon - \sum_{\varepsilon\in\frac{\eta}{2}\sigma([H_{\mathrm{p}},\cdot])} \mathbf{1}_\varepsilon i[H_{\mathrm{Lamb}},\cdot]\mathbf{1}_\varepsilon. \tag{4.71}$$

Using Lemma 4.21, the first sum on the r.h.s. of this equality is the generator of a Markov CP and $C_0$ semigroup satisfying Assumption (B). The second sum is the generator of the continuous one-parameter group

$$\begin{aligned}
&\exp\left(t\sum_{\varepsilon\in\frac{\eta}{2}\sigma([H_{\mathrm{p}},\cdot])}\mathbf{1}_\varepsilon\left(-i\left[H_{\mathrm{Lamb}},\cdot\right]\right)\mathbf{1}_\varepsilon\right)\\
=\;&\lim_{\lambda\downarrow 0}\exp\left\{it\frac{\eta}{2\lambda^2}\left[H_{\mathrm{p}},\cdot\right]\right\}\exp\left\{-it\left(\frac{\eta}{2\lambda^2}\left[H_{\mathrm{p}},\cdot\right]+\lambda^2\left[H_{\mathrm{Lamb}},\cdot\right]\right)\right\},
\end{aligned}$$

by Theorem 4.33. As a limit of a product of automorphisms, which are Markov and CP, the right hand side is also Markov and CP. Thus, the operator (4.71) is also the generator of a Markov CP and $C_0$ semigroup satisfying Assumption (B) and, by (4.70) and Theorem 4.35,

$$\lim_{\varkappa\to\infty} g(\varkappa^{-\frac{1}{2}},1)\in(0,\infty).$$

In other words, for some constants $c'>0$ and sufficiently large $r'>r$, $g(\lambda,\eta)\geq c'$. □

We now conclude by the proof of Theorem 4.13, that is, for any $\varepsilon\in(0,1)$,

$$\left\|e^{\alpha\Lambda^{(\lambda,\eta)}}-e^{alphaP_0^{(\lambda,\eta)}G^{(\lambda,\eta)}P_0^{(\lambda,\eta)}}\right\|\leq C_\varepsilon\left|\lambda\right|^{2(1-\varepsilon)}, \tag{4.72}$$

where the constant $C_\varepsilon\in(0,\infty)$ does not depend on $\lambda$, $\eta$, and $\alpha$.

**Corollary 4.23.** *There are constants $D<\infty$, $C_1,C_2>0$ independent of $\eta$, $\lambda$, such that, for $\lambda$ sufficiently small,*

$$\begin{aligned}
&\limsup_{\tilde\alpha\to\infty}\left\|e^{\alpha\Lambda^{(\lambda,\eta)}}-e^{\tilde\alpha\Lambda^{(\lambda,\eta)}}\right\|\leq De^{-\alpha C_1\lambda^2},\\
&\limsup_{\tilde\alpha\to\infty}\left\|e^{\alpha P_0^{(\lambda,\eta)}G^{(\lambda,\eta)}P_0^{(\lambda,\eta)}}-e^{\tilde\alpha P_0^{(\lambda,\eta)}G^{(\lambda,\eta)}P_0^{(\lambda,\eta)}}\right\|\leq D\mathrm{e}^{-\alpha C_2\lambda^2},
\end{aligned}\tag{4.73}$$

*and*

$$\limsup_{\alpha\to\infty}\left\|\exp\left(\alpha\Lambda^{(\lambda,\eta)}\right)-\exp\left(\alpha P_0^{(\lambda,\eta)}G^{(\lambda,\eta)}P_0^{(\lambda,\eta)}\right)\right\|\leq D\lambda^2$$

*for all $\alpha\geq 0$.*

*Proof.* Note that, by Lemma 4.22, for some $c\in(0,\infty)$ independent of $\lambda$ and $\eta$,

$$\begin{aligned}
&\exp\left(\alpha\Lambda^{(\lambda,\eta)}\right)-\exp\left(\tilde\alpha\Lambda^{(\lambda,\eta)}\right)\\
=\;&\lim_{L\to\infty}\int_{-L}^{L}\left(\mathrm{e}^{(ix-c\lambda^2)\alpha}-\mathrm{e}^{(ix-c\lambda^2)\alpha}\right)\left(ix-c\lambda^2+\Lambda^{(\lambda,\eta)}\right)^{-1}dx,\\
&\exp\left(\alpha P_0^{(\lambda,\eta)}G^{(\lambda,\eta)}P_0^{(\lambda,\eta)}\right)-\exp\left(\tilde\alpha P_0^{(\lambda,\eta)}G^{(\lambda,\eta)}P_0^{(\lambda,\eta)}\right)\\
=\;&\lim_{L\to\infty}\int_{-L}^{L}\left(\mathrm{e}^{(ix-c\lambda^2)\alpha}-\mathrm{e}^{(ix-c\lambda^2)\alpha}\right)\left(ix-c\lambda^2+P_0^{(\lambda,\eta)}G^{(\lambda,\eta)}P_0^{(\lambda,\eta)}\right)^{-1}dx
\end{aligned}$$

and

$$\lim_{\tilde{\alpha}\to\infty} \exp\left(\tilde{\alpha}\Lambda^{(\lambda,\eta)}\right) - \exp\left(\tilde{\alpha}P_0^{(\lambda,\eta)}G^{(\lambda,\eta)}P_0^{(\lambda,\eta)}\right) = c\lambda^2$$
$$\cdot \int_0^1 e^{2\pi ix}\left[\left(\Lambda^{(\lambda,\eta)} - c\lambda^2 e^{2\pi ix}\right)^{-1} - \left(P_0^{(\lambda,\eta)}G^{(\lambda,\eta)}P_0^{(\lambda,\eta)} - c\lambda^2 e^{2\pi ix}\right)^{-1}\right]dx$$

Observe that

$$\begin{aligned}
& \lim_{L\to\infty}\int_{-L}^{L}(e^{(ix-c\lambda^2)\tilde{\alpha}} - e^{(ix-c\lambda^2)\alpha})(ix - c\lambda^2 + \Lambda^{(\lambda,\eta)})^{-1}dx \\
= & \lim_{L\to\infty}\int_{-L}^{L}\frac{(e^{(ix-c\lambda^2)\tilde{\alpha}} - e^{(ix-c\lambda^2)\alpha})}{(ix-c\lambda^2)^2}(ix - c\lambda^2 + \Lambda^{(\lambda,\eta)})^{-1}(\Lambda^{(\lambda,\eta)})^2dx \\
= & \lambda^{-2}\lim_{L\to\infty}\int_{-L}^{L}\frac{(e^{(ix-c)\lambda^2\tilde{\alpha}} - e^{(ix-c)\lambda^2\alpha})}{(ix-c)^2}((ix-c)\lambda^2 + \Lambda^{(\lambda,\eta)})^{-1}(\Lambda^{(\lambda,\eta)})^2dx
\end{aligned}$$

and

$$\begin{aligned}
& \lim_{L\to\infty}\int_{-L}^{L}(e^{(ix-c\lambda^2)\tilde{\alpha}} - e^{(ix-c\lambda^2)\alpha})(ix - c\lambda^2 + P_0^{(\lambda,\eta)}G^{(\lambda,\eta)}P_0^{(\lambda,\eta)})^{-1}dx \\
= & \lambda^{-2}\lim_{L\to\infty}\int_{-L}^{L}\frac{(e^{(ix-c)\lambda^2\alpha} - e^{(ix-c)\lambda^2\alpha})}{(ix-c)^2} \\
& ((ix-c)\lambda^2 + P_0^{(\lambda,\eta)}G^{(\lambda,\eta)}P_0^{(\lambda,\eta)})^{-1}(P_0^{(\lambda,\eta)}G^{(\lambda,\eta)}P_0^{(\lambda,\eta)})^2dx.
\end{aligned}$$

Hence, as

$$\left\|\Lambda^{(\lambda,\eta)}\right\|, \left\|P_0^{(\lambda,\eta)}G^{(\lambda,\eta)}P_0^{(\lambda,\eta)}\right\| = \mathcal{O}(\lambda^2),$$

it suffices to show that for some finite constant $C$ not depending on $\eta$ and $\lambda$,

$$\begin{aligned}
C\lambda^{-2} & \geq \left\|\left((ix-c)\lambda^2 + P_0^{(\lambda,\eta)}G^{(\lambda,\eta)}P_0^{(\lambda,\eta)}\right)^{-1}\right\|, \qquad (4.74) \\
C\lambda^{-2} & \geq \left\|\left((ix-c)\lambda^2 + \Lambda^{(\lambda,\eta)}\right)^{-1}\right\|, \\
C & \geq \left\|(-c\lambda^2 e^{2\pi iy} + P_0^{(\lambda,\eta)}G^{(\lambda,\eta)}P_0^{(\lambda,\eta)})^{-1} - (-c\lambda^2 e^{2\pi iy} + \Lambda^{(\lambda,\eta)})^{-1}\right\|
\end{aligned}$$

for all $x \in \mathbb{R}$ and all $y \in [0,1]$. Observe that

$$\left\|\Lambda^{(\lambda,\eta)} - P_0^{(\lambda,\eta)}G^{(\lambda,\eta)}P_0^{(\lambda,\eta)}\right\| = \mathcal{O}(\lambda^4).$$

□

Assuming that the inequalities

$$\begin{aligned}
\left\|\left(-c\lambda^2 e^{2\pi iy} + P_0^{(\lambda,\eta)}G^{(\lambda,\eta)}P_0^{(\lambda,\eta)}\right)^{-1}\right\| & \leq C\lambda^{-2}, \qquad (4.75) \\
\left\|\left(-c\lambda^2 e^{2\pi iy} + \Lambda^{(\lambda,\eta)}\right)^{-1}\right\| & \leq C\lambda^{-2},
\end{aligned}$$

hold, for some $C < \infty$ and all $y \in [0,1]$, and by using the second resolvent equation one gets the third inequality in (4.74). Similarly, by using Neumann series for perturbations of resolvents and assuming that the first inequalities in (4.74) and (4.75) hold we obtain the corresponding second inequalities (up to a pre-factor), if $\lambda$ is sufficiently small. Thus, it remains to prove that the third inequalities in (4.74) and (4.75) are satisfied. Note that these are equivalent to

$$\begin{aligned} \left\| \left( -c e^{2\pi i y} + \mathcal{L}_{\mathcal{R}} + \varkappa \mathcal{L}_P \right)^{-1} \right\| &\leq C, \\ \left\| \left( (ix - c) + \mathcal{L}_{\mathcal{R}} + \varkappa \mathcal{L}_P \right)^{-1} \right\| &\leq C, \end{aligned} \tag{4.76}$$

by using Neumann series for perturbation of resolvents, with by $\varkappa := \frac{\eta}{\lambda^2}$ and recalling $\varkappa \in [-\varkappa_0, \varkappa_0]$ for some prefixed, finite $\varkappa_0$, by Assumption (MP). By Lemma 4.22 and by using Neumann series for perturbations of resolvents, the maps $g_1 : [0,1] \times [-\varkappa_0, \varkappa_0] \to \mathbb{R}$, $g_1 : [-N, N] \times [-\varkappa_0, \varkappa_0] \to \mathbb{R}$ defined by

$$\begin{aligned} g_1(y, \varkappa) \quad : &= \left\| \left( -c e^{2\pi i y} + \mathcal{L}_{\mathcal{R}} + \varkappa \mathcal{L}_P \right)^{-1} \right\|, \\ g_2(x, \varkappa) \quad : &= \left\| \left( (ix - c) + \mathcal{L}_{\mathcal{R}} + \varkappa \mathcal{L}_P \right)^{-1} \right\|, \end{aligned}$$

are continuous. Hence, by compactness, the inequalities (4.76) hold for some finite constant $C$ depending only on $N$. Furthermore, for $N$ sufficiently large, from simple arguments Neumann series it follows, finally, that the second inequality in (4.76) holds for all $(x, \varkappa) \in (\mathbb{R} \backslash [-N, N]) \times [-\varkappa_0, \varkappa_0]$.

*Proof of Theorem 4.13.* Note that the semigroups

$$\left\{ \exp\left( \alpha \Lambda^{(\lambda,\eta)} \right) \right\}_{\alpha \geq 0} \quad \text{and} \quad \left\{ \exp\left( \alpha P_0^{(\lambda,\eta)} G^{(\lambda,\eta)} P_0^{(\lambda,\eta)} \right) \right\}_{\alpha \geq 0}$$

are bounded, uniformly in $\lambda, \eta$, as the first one is a CP semigroup and the second one is the restriction of $\{\mathcal{T}_\alpha\}_{\alpha \geq 0}$, see (4.42). Thus, Duhamel's formula yields the inequality

$$\begin{aligned} &\left\| \exp\left( \alpha \Lambda^{(\lambda,\eta)} \right) - \exp\left( \alpha P_0^{(\lambda,\eta)} G^{(\lambda,\eta)} P_0^{(\lambda,\eta)} \right) \right\| \\ \leq \; & C_{10} \alpha \left\| P_0^{(\lambda,\eta)} G^{(\lambda,\eta)} P_0^{(\lambda,\eta)} - \Lambda^{(\lambda,\eta)} \right\| \end{aligned} \tag{4.77}$$

for some constant $C_{10} < \infty$ independent of $\lambda$, $\eta$, and $\alpha$. For some constant $C_{11} < \infty$, observe that

$$\left\| P_0^{(\lambda,\eta)} G^{(\lambda,\eta)} \right\| \leq C_{11} \lambda^2 \quad \text{and} \quad \left\| G^{(\lambda,\eta)} P_0^{(0,0)} \right\| \leq C_{11} \lambda^2,$$

using $P_0^{(0,0)} G^{(0,0)} = 0$. Hence, we combine these last upper bounds with (4.54) and the triangle inequality to get that

$$\begin{aligned} \left\| P_0^{(\lambda,\eta)} G^{(\lambda,\eta)} P_0^{(\lambda,\eta)} - \Lambda^{(\lambda,\eta)} \right\| &= \left\| P_0^{(\lambda,\eta)} G^{(\lambda,\eta)} P_0^{(\lambda,\eta)} - P_0^{(0,0)} G^{(\lambda,\eta)} P_0^{(0,0)} \right\| \\ &\leq C_{12} \lambda^4, \end{aligned} \tag{4.78}$$

with $C_{12} < \infty$. By (4.77), it follows that

$$\left\| e^{\alpha \Lambda^{(\lambda,\eta)}} - e^{\alpha P_0^{(\lambda,\eta)} G^{(\lambda,\eta)} P_0^{(\lambda,\eta)}} \right\| \leq C_{13} \alpha \lambda^4 \tag{4.79}$$

with $C_{13} < \infty$. We finally infer from (4.79) and Corollary 4.23 that

$$\left\| e^{\alpha \Lambda^{(\lambda,\eta)}} - e^{\alpha P_0^{(\lambda,\eta)} G^{(\lambda,\eta)} P_0^{(\lambda,\eta)}} \right\| \leq C_{17} \max \left\{ x\lambda^4, \lambda^2 + \mathrm{e}^{-xC_{18}\lambda^2} \right\}, \tag{4.80}$$

for all $x \geq 0$, where the constants $C_{18}, C_{17} \in (0, \infty)$ do not depend on $\lambda$, $\eta$, and $\alpha$. Taking

$$x = |\lambda|^{2(1-\varepsilon)-4}$$

in (4.80) we obtain (4.72) for sufficiently small $\lambda$. □

## 4.4 The Generalised Einstein Coefficients

For any initial density matrix $\rho \in \mathfrak{H}_{\mathrm{at}}$, the final (approximate) density matrix $P_{\mathfrak{D}}(\tilde{\rho}_\infty)$ of the atom restricted to the block diagonal subspace $\mathfrak{D}$ of $\mathfrak{H}_{\mathrm{at}}$ is attained according to the solution $\{\rho_{\mathfrak{D}}(\alpha)\}_{\alpha \geq 0}$ of the pre–master equation, see Theorems 4.8, 4.15 (ii), 4.16, and Corollary 4.19, provided that $\mathfrak{B}$ is the restriction of a generator of a (CP) Markov semigroup. We assume this to be the case in this section, either by Proposition 4.17 or other means, see Remark 4.18. Disregarding this for a moment, we could have computed this final density matrix as the stationary density matrix of some "phenomenological Pauli–equation", similar to the Pauli–equations found in the literature. The dynamics described by this phenomenological Pauli–equation is *in general quite different* from the time evolution of the density matrix $\{\rho_{\mathfrak{D}}(\alpha)\}_{\alpha \geq 0}$, which corresponds up to small errors to the real dynamics $\{P_{\mathfrak{D}}\rho_{\mathrm{at}}(t)\}_{t \geq 0}$ of the atom, see again Theorem 4.8. Nevertheless, both dynamics lead to the same density matrix $P_{\mathfrak{D}}(\tilde{\rho}_\infty)$ in the limit $t \to \infty$. The coefficients of such Pauli–equations, called here *generalised Einstein coefficients*, satisfy strong constrains, named here *generalised Einstein relations*, which encode a balance condition for the final density matrix $P_{\mathfrak{D}}(\tilde{\rho}_\infty)$, see Corollary 4.19. Therefore, the aim of this section to set up more precise the notion of Pauli–equation and to analyse the structure of its generator.

For this purpose, define first the positive cone

$$\mathfrak{D}^+ := \mathcal{B}^+(\mathbb{C}^d) \cap \mathfrak{D} = \mathrm{conv} \left\langle \bigcup_{k=1}^{N} \mathcal{B}^+(\mathcal{H}_k) \right\rangle$$

of block–diagonal density matrices of the atom. Here $\mathcal{B}^+(\mathfrak{h})$ denotes the set of positive operators on a Hilbert space $\mathfrak{h}$ and conv $\langle \mathfrak{m} \rangle$ stands for the convex hull of the set $\mathfrak{m}$. Observe that $\mathfrak{D}^+$ is an invariant cone of the semigroup $\{\hat{\tau}_t^{(\lambda,0)}\}_{t \geq 0}$, see (4.39).

We next define the maps $A_{j,k}, B_{j,k}$ from $\mathcal{B}(\mathcal{H}_k)$ to $\mathcal{B}(\mathcal{H}_j)$, respectively, by

$$\begin{aligned} B_{j,k} \quad &: \quad = \frac{\eta^2}{4\lambda^2} \, P_{jj} \, \mathfrak{B} \, P_{kk}, \\ A_{j,k} \quad &: \quad = \lambda^2 \, P_{jj} \, \mathfrak{L}_{\mathcal{R}} \, P_{kk} \, , \end{aligned}$$

with $P_{jk}$ defined by (4.66). From the proof of Proposition 4.17 we recall that $B_{j,k}$ equals $B_{j,k} = 0$ for all $j \in \{2, \ldots, N-1\}$ or $k \in \{2, \ldots, N-1\}$, and

$$\begin{aligned}
\forall \rho &\in \mathcal{B}(\mathcal{H}_1) : B_{N,1}(\rho) = \frac{\eta^2}{4\lambda^2}\left( (\mathfrak{L}_{\mathcal{R}})^{-1}(h_{\mathrm{p}}\rho)\, h_{\mathrm{p}}^* + h_{\mathrm{p}}\, (\mathfrak{L}_{\mathcal{R}})^{-1}\left(\rho h_{\mathrm{p}}^*\right)\right), \\
\forall \rho &\in \mathcal{B}(\mathcal{H}_N) : B_{1,N}(\rho) = \frac{\eta^2}{4\lambda^2}\left( (\mathfrak{L}_{\mathcal{R}})^{-1}\left(h_{\mathrm{p}}^*\rho\right) h_{\mathrm{p}} + h_{\mathrm{p}}^*\, (\mathfrak{L}_{\mathcal{R}})^{-1}(\rho h_{\mathrm{p}})\right), \\
\forall \rho &\in \mathcal{B}(\mathcal{H}_1) : B_{1,1}(\rho) = -\frac{\eta^2}{4\lambda^2}\left( h_{\mathrm{p}}^*\, (\mathfrak{L}_{\mathcal{R}})^{-1}(h_{\mathrm{p}}\rho) + (\mathfrak{L}_{\mathcal{R}})^{-1}\left(\rho h_{\mathrm{p}}^*\right) h_{\mathrm{p}}\right), \\
\forall \rho &\in \mathcal{B}(\mathcal{H}_N) : B_{N,N}(\rho) = -\frac{\eta^2}{4\lambda^2}\left( h_{\mathrm{p}}\, (\mathfrak{L}_{\mathcal{R}})^{-1}\left(h_{\mathrm{p}}^*\rho\right) + (\mathfrak{L}_{\mathcal{R}})^{-1}(\rho h_{\mathrm{p}})\, h_{\mathrm{p}}^*\right).
\end{aligned}$$

Here, $(\mathfrak{L}_{\mathcal{R}})^{-1}$ is the Laplace–Transform

$$(\mathfrak{L}_{\mathcal{R}})^{-1} := \int_0^\infty P_{\mathfrak{D}}^{\perp}\, \mathrm{e}^{s\mathfrak{L}_{\mathcal{R}}}\, P_{\mathfrak{D}}^{\perp}\, \mathrm{d}s\,.$$

Physically, the map

$$A := \sum_{j,k} A_{j,k} = \lambda^2 \mathfrak{L}_{\mathcal{R}} P_{\mathfrak{D}}$$

from $\mathfrak{H}_{\mathrm{at}}$ to $\mathfrak{H}_{\mathrm{at}}$ describes the dynamics of the fermion field–atom system in absence of an electromagnetic field (pump). In other words, the "coefficient" $A_{j,k}$ has to be interpreted as the *spontaneous (quantum) transition* rate of populations from the atomic level $j$ to the atomic level $k$. The second map

$$B := \sum_{j,k} B_{j,k} = \frac{\eta^2}{4\lambda^2}\mathfrak{B}$$

from $\mathfrak{H}_{\mathrm{at}}$ to $\mathfrak{H}_{\mathrm{at}}$ describes the contribution of the pump to the final density matrix and the "coefficient" $B_{j,k}$ is interpreted as the effective *stimulated transition rate* of populations from the atomic level $j$ to the atomic level $k$ at the final density matrix.

We now remark that $A_{j,k}$ and $B_{j,k}$ map the positive cone $\mathcal{B}^+(\mathcal{H}_k)$ to the positive cone $\mathcal{B}^+(\mathcal{H}_j)$ for all $j, k \in \{1, \ldots, N\}$ because $A$ and $B$ generate CP $C_0$ semigroups. In many situations, for instance, in presence of symmetries, it turns out that $A_{j,k}$ and $B_{j,k}$ define maps from $K_k \subset \mathcal{B}^+(\mathcal{H}_k)$ to $K_j \subset \mathcal{B}^+(\mathcal{H}_j)$ where $K_j$ and $K_k$ are sub-cones. The smaller the dimension of such cones is, the more classical is the description of the final state via the transition rates $A_{j,k}$ and $B_{j,k}$. It can even happen that the dimension of all $K_j$, $j \in \{1, \ldots, N\}$, can be chosen to be one. In this case we get the usual classical phenomenological description with parameters given as functions of microscopic quantities.

Therefore we define a simple notion for invariance of sub-cones $\{K_k\}_{k=1}^N$ which ensures that $A_{j,k}$ and $B_{j,k}$ map $K_k$ to $K_j$:

**Definition 4.24 (Invariant family of cones).**
A family $\{K_k\}_{k=1}^N$ of sub-cones $K_k \subset \mathcal{B}^+(\mathcal{H}_k)$ is an invariant family whenever

$$K := \mathrm{conv}\left\langle \bigcup_{k=1}^{N} K_k \right\rangle$$

is invariant under the action of the semigroups $\left\{e^{tA}\right\}_{t\geq 0}$ and $\left\{e^{tB}\right\}_{t\geq 0}$.

By the Trotter product formula, observe that the subset $K$ defined in this definition is also invariant under the action of the semigroups $\left\{e^{t(A+B)}\right\}_{t\geq 0}$. Furthermore, the invariance of the family $\{K_k\}_{k=1}^N$ yields

$$\forall j,k \in \{1,\ldots,N\} : \quad A_{j,k}(K_k), B_{j,k}(K_k) \subset K_j.$$

In other words, $A_{j,k}$ and $B_{j,k}$ map, in this case, $K_k$ to $K_j$. One trivial example of an invariant family is given by taking $K_k = \mathcal{B}^+(\mathcal{H}_k)$ for all $k \in \{1,\ldots,N\}$.

The Pauli–equation reads now:

$$\forall t \geq 0,\ j \in \{1,\ldots,N\} : \ \frac{d}{dt}\rho_j(t) = \sum_{k=1}^{N} \left(A_{j,k} + B_{j,k}\right)\rho_k(t),\ \ \rho_j(0) = \rho_j \in K_j. \tag{4.81}$$

The unique solution of this initial value problem satisfies $\{\rho_j(t)\}_{t\geq 0} \subset K_j$. Here the initial values $\{\rho_j\}_{j=1}^N$ comes from the initial density matrix $\rho \in \mathfrak{H}_{\mathrm{at}}$ via the definition

$$\forall j \in \{1,\ldots,N\} : \qquad \rho_j := \mathbf{1}\left[H_{\mathrm{at}} = E_j\right]\ \rho\ \mathbf{1}\left[H_{\mathrm{at}} = E_j\right].$$

**Remark 4.25.**
The discussion above shows that $B = \eta^2 F(A)$, i.e., $B$ is proportional to the intensity of the pumping (monochromatic) light $\eta^2$ and proportional to a fixed function $F(A)$ of the spontaneous transition rates $A$. Einstein has derived this kind of relation, called here Einstein AB–relations, for an atom interacting with a (broad–band, i.e., non–monochromatic) radiation field in his famous paper [Ein16] from phenomenological considerations about the expected final state of the atomic populations and the asymptotics of the light intensity at large wave–numbers (Maxwell distribution). Note that $F$ strongly depends on the specific setting. Hence, the function $F$ appearing in the present paper cannot be compared to the one appearing in Einstein's works. However, the fact that the stimulated coefficients only depends on light intensity and the spontaneous coefficient, seems to be universal. We stress that this property is directly derived, here, from a microscopic quantum mechanical description of the system under consideration in rigorous way and not from phenomenological assumptions.

Einstein gives in his works a relation between the stimulated transition rates $B_{j,k}$ and $B_{k,j}$: Denoting the degeneracy of the $j$th atomic level by $n_j$, he obtained the equations

$$\forall j,k \in \{1,\ldots,N\} : \qquad n_k B_{j,k} = n_j B_{k,j},$$

called here Einstein BB–relations. Let $p_j$ denote the population in the $j$th atomic level and define the stimulated flux from the $k$th to $j$th atomic level by $f_{j,k} := B_{j,k} p_k$. Then the Einstein BB–relations for transition rates reads

$$\forall j,k \in \{1,\dots,N\}: \qquad p_j n_k f_{j,k} - p_k n_j f_{k,j} = 0. \tag{4.82}$$

Consider the sub-cones

$$\forall j \in \{1,\dots,N\}: \qquad K_j^0 := \mathbb{R}_0^+ \, \mathbf{1}\left[H_{\mathrm{at}} = E_j\right] \subset \mathcal{B}^+(\mathcal{H}_j).$$

In our setting it turns out that a variant of BB–relations (4.82) for fluxes holds, at least for density matrices in the sub-cone

$$K^0 := \mathrm{conv}\left\langle \bigcup_{k=1}^{N} K_k^0 \right\rangle.$$

In this context and for any density matrix $\rho \in \mathfrak{H}_{\mathrm{at}}$, the population in the $j$th atomic level is naturally defined to be

$$p_j(\rho) := \mathrm{Tr}\left(\rho_j\right) \geq 0$$

for all $j \in \{1,\dots,N\}$. Similarly, for all $j,k \in \{1,\dots,N\}$,

$$f_{j,k}(\rho) := \mathrm{Tr}\left(B_{j,k}(\rho)\right) = \mathrm{Tr}\left(B_{j,k}(\rho_k)\right)$$

represents the stimulated flux from the $j$th to the $k$th atomic level with respect to the density matrix $\rho \in \mathfrak{H}_{\mathrm{at}}$.

**Lemma 4.26 (BB–Relations for states in $K^0$).**
*For any $\rho \in K^0$, the Einstein BB–relations for the flux hold:*

$$p_j(\rho) n_k f_{j,k}(\rho) - p_k(\rho) n_j f_{k,j}(\rho) = 0.$$

*Proof.* Clearly,

$$n_j \rho_j = p_j(\rho) \mathbf{1}\left[H_{\mathrm{at}} = E_j\right].$$

Thus the assertion follows from the equation

$$\mathrm{Tr}\left(B_{j,k}(\mathbf{1}\left[H_{\mathrm{at}} = E_k\right])\right) = \mathrm{Tr}\left(B_{k,j}(\mathbf{1}\left[H_{\mathrm{at}} = E_j\right])\right). \qquad \square$$

Let $j,k = 1,N$, because in the other cases the flux vanishes and there is nothing to prove. Observe that

$$\begin{aligned} B_{1,N}(\mathbf{1}\left[H_{\mathrm{at}} = E_N\right]) &= \frac{\eta^2}{4\lambda^2}\left(\left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}\left(h_{\mathrm{p}}\right) h_{\mathrm{p}}^* + h_{\mathrm{p}}\left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}\left(h_{\mathrm{p}}^*\right)\right), \\ B_{N,1}(\mathbf{1}\left[H_{\mathrm{at}} = E_1\right]) &= \frac{\eta^2}{4\lambda^2}\left(\left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}\left(h_{\mathrm{p}}^*\right) h_{\mathrm{p}} + h_{\mathrm{p}}^*\left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}\left(h_{\mathrm{p}}\right)\right). \end{aligned}$$

From the cyclicity of the trace,

$$\begin{aligned} \mathrm{Tr}\left(B_{1,N}(\mathbf{1}\left[H_{\mathrm{at}} = E_N\right])\right) &= \frac{\eta^2}{4\lambda^2}\mathrm{Tr}\left(h_{\mathrm{p}}\left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}\left(h_{\mathrm{p}}^*\right) + \left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}\left(h_{\mathrm{p}}\right) h_{\mathrm{p}}^*\right) \\ &= \frac{\eta^2}{4\lambda^2}\mathrm{Tr}\left(\left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}\left(h_{\mathrm{p}}^*\right) h_{\mathrm{p}} + h_{\mathrm{p}}^*\left(\mathfrak{L}_{\mathcal{R}}\right)^{-1}\left(h_{\mathrm{p}}\right)\right) \\ &= \mathrm{Tr}\left(B_{N,1}(\mathbf{1}\left[H_{\mathrm{at}} = E_1\right])\right). \end{aligned}$$

Observe that for $\eta = 0$ the final density matrix $P_{\mathfrak{D}}(\tilde{\rho}_\infty)$ is an element of the cone $K_0$. More precisely, it is in this case the Gibbs state of $H_{\mathrm{at}}$. Thus from the Lemma above, the uniqueness of $P_{\mathfrak{D}}(\tilde{\rho}_\infty)$ and Kato's perturbation theory for non–degenerated eigenvectors the (asymptotic) BB–relations follow for the NESS at weak pump, in general.

**Corollary 4.27 (BB-relations at weak pump).**
*For some $C \in (0, \infty)$ and all $(\eta, \lambda) \in \mathbb{R}^2$,*

$$\left| p_j(\rho_\infty) d_k f_{jk}(P_{\mathfrak{D}}(\tilde{\rho}_\infty)) - p_k(P_{\mathfrak{D}}(\tilde{\rho}_\infty)) d_j f_{kj}(P_{\mathfrak{D}}(\tilde{\rho}_\infty)) \right| \leq C \frac{\eta^2}{\lambda^4}.$$

## 4.5 Appendix

For the convenience of the reader, we give in Section 4.5.1 a short review on completely positive (CP) semigroups on Banach spaces, focussing on the results relevant for our analysis.

### 4.5.1 Completely positive semigroups

In open quantum systems, one usually studies the restricted dynamics on the small quantum system of the time evolution of the full, composite system (the atom and one fermion reservoir in our case), that typically is, a small quantum object in interaction with macroscopic systems, i.e., reservoirs. This restriction on the time evolution formally defines at any fixed time a map $\mathcal{C}$ within the set of density matrices of the small system. This is pedagogically explained in [AL07, Section 1.2.1]. As explained in [AL07, Section 1.2.2], such maps usually share similar mathematical properties, which refer to the so–called *completely positive (CP)* maps defined as follows.

**Definition 4.28 (Completely positive maps).**
A positive map $\mathcal{C} \in \mathcal{B}(\mathcal{B}(\mathcal{X}))$ acting on the set $\mathcal{B}(\mathcal{X})$ of bounded operators on a Hilbert space $\mathcal{X}$ is called completely positive (CP) if the extended map $\mathcal{C} \otimes \mathbf{1}_{\mathcal{B}(\mathbb{C}^n)}$ is positive for any $n \in \mathbb{N}$. If $\mathcal{C}$ is unital, i.e., $\mathcal{C}(\mathbf{1}_{\mathcal{X}}) = \mathbf{1}_{\mathcal{X}}$, then the operator $\mathcal{C}$ is called a Markov map.

Then completely positive CP semigroups are simply semigroups which are CP maps for all times:

**Definition 4.29 (Completely positive semigroups).**
A semigroup $\{\mathcal{C}_t\}_{t \geq 0} \subset \mathcal{B}(\mathcal{B}(\mathcal{X}))$, with $\mathcal{X}$ being a Hilbert space, is CP if the map $\mathcal{C}_t$ is CP for any $t \in \mathbb{R}^+$. If $\mathcal{C}_t$ is unital for any $t \in \mathbb{R}^+$, then $\{\mathcal{C}_t\}_{t \geq 0}$ is called Markov.

From now on until the end of Section 4.5.1, $\mathcal{X}$ is always a $n$–dimensional Hilbert space. We denote by $\mathcal{B}_2(\mathcal{X}) \equiv \mathcal{B}(\mathcal{X})$ the Hilbert space of Hilbert–Schmidt operators with scalar product

$$\langle A, B \rangle_{\mathcal{B}_2(\mathcal{X})} := \mathrm{Tr}_{\mathcal{X}}(A^* B), \qquad A, B \in \mathcal{B}_2(\mathcal{X}).$$

In the special case where a semigroup $\{\mathcal{C}_t\}_{t\geq 0} \subset \mathcal{B}(\mathcal{B}_2(\mathcal{X}))$ acts on $\mathcal{B}_2(\mathcal{X})$, we can define its (unique) *adjoint semigroup* $\{\mathcal{C}_t^\dagger\}_{t\geq 0} \subset \mathcal{B}(\mathcal{B}_2(\mathcal{X}))$ as usual via the equations

$$\forall t \geq 0: \quad \langle \mathcal{C}_t^\dagger(A), B\rangle_{\mathcal{B}_2(\mathcal{X})} = \langle A, \mathcal{C}_t(B)\rangle_{\mathcal{B}_2(\mathcal{X})}, \qquad A, B \in \mathcal{B}_2(\mathcal{X}).$$

Note that a Markov CP and $C_0$ semigroup $\{\mathcal{C}_t\}_{t\geq 0}$ defines a $C_0$ semigroups $\{\mathcal{C}_t^\dagger\}_{t\geq 0}$ which *preserves the trace*. In this case, $\{\mathcal{C}_t^\dagger\}_{t\geq 0}$ is also called a Markov CP and $C_0$ semigroup. Generators of Markov CP and $C_0$ semigroups $\{\mathcal{C}_t\}_{t\geq 0}$ and $\{\mathcal{C}_t^\dagger\}_{t\geq 0}$ can then be characterised in the finite dimensional case (cf. [GKS76, Theorem 2.2]):

**Theorem 4.30 (Generators of CP Markov semigroups, dim $\mathcal{X} = n$–I).** *The operator* $\mathrm{L} \in \mathcal{B}(\mathcal{B}_2(\mathcal{X}))$ *is the generator of a Markov CP and* $C_0$ *semigroup* $\{\mathcal{C}_t\}_{t\geq 0}$ *if and only if*

$$\mathrm{L}(A) = i[\mathrm{h}, A] + \frac{1}{2}\sum_{j,k=1}^{n^2-1} \mathrm{c}_{j,k}\left\{[\mathrm{V}_k^*, A]\,\mathrm{V}_j + \mathrm{V}_k^*\,[A, \mathrm{V}_j]\right\}, \qquad A \in \mathcal{B}_2(\mathcal{X}), \tag{4.83}$$

*where* $\mathrm{h} = \mathrm{h}^* \in \mathcal{B}_2(\mathcal{X})$ *satisfies* $\mathrm{Tr}_{\mathcal{X}}(\mathrm{h}) = 0$, $\{\mathrm{V}_j\}_{j=1}^{n^2-1} \subset \mathcal{B}_2(\mathcal{X})$ *is an orthonormal family* $\{\mathrm{V}_j\}_{j=1}^{n^2-1} \subset \mathcal{B}_2(\mathcal{X})$ *such that* $\mathrm{Tr}_{\mathcal{X}}(\mathrm{V}_j) = 0$ *for all* $j \in \{1, \cdots, n^2-1\}$, *and* $\left\{\mathrm{c}_{j,k}\right\}_{1\leq j,k\leq n^2-1} \geq 0$ *forms a complex positive matrix. Additionally, the adjoint semigroup* $\{\mathcal{C}_t^\dagger\}_{t\geq 0}$ *is the* $C_0$ *(or* $C_0^*$*), trace preserving semigroup with generator equal to*

$$\mathrm{L}^\dagger(A) = -i[\mathrm{h}, A] + \frac{1}{2}\sum_{j,k=1}^{n^2-1} \mathrm{c}_{j,k}\left\{\left[\mathrm{V}_j, A\mathrm{V}_k^*\right] + \left[\mathrm{V}_j A, \mathrm{V}_k^*\right]\right\}, \qquad A \in \mathcal{B}_2(\mathcal{X}).$$

Note that [GKS76, Theorem 2.2] refers to the adjoint generator $\mathrm{L}^\dagger$ and not the generator L, which is deduced from $\mathrm{L}^\dagger$ as in [AL07, Eq. (40)]. Moreover, [GKS76, Theorem 2.2] seems to indicate only one direction in Theorem 4.30. However, a close look at its proof [GKS76, Proof of theorem 2.2.] shows both directions.

**Remark 4.31.** Observe that Theorem 4.30 implies that $\mathrm{L} + i[\tilde{\mathrm{h}}, \cdot]$, with $\tilde{\mathrm{h}} = \tilde{\mathrm{h}}^* \in \mathcal{B}_2(\mathcal{X})$ satisfying $\mathrm{Tr}_{\mathcal{X}}(\tilde{\mathrm{h}}) = 0$ and L being the generator of any Markov CP and $C_0$ semigroup $\{\mathcal{C}_t\}_{t\geq 0}$, generates also a Markov CP and $C_0$ semigroup. This observation is used several times in the paper.

It is useful to also have a more compact expression of generators of (CP) and (CP) Markov semigroups. From [DF06, Sect. 4.3] we take

**Theorem 4.32 (Generators of CP Markov semigroups, dim $\mathcal{X} = n$–II).**

An operator $M \in \mathcal{B}(\mathcal{B}(\mathcal{X}))$ is the generator of a CP semigroup iff there is a completely positive map $\Xi \in \mathcal{B}(\mathcal{B}(\mathcal{X}))$ and an operator $\Delta \in \mathcal{B}(\mathcal{X})$ such that

$$M = \underset{\rightarrow}{\Delta} + \underset{\leftarrow}{\Delta^*} + \Xi. \tag{4.84}$$

$M \in \mathcal{B}(\mathcal{B}(\mathcal{X}))$ the generator of a CP Markov semigroup iff it is the generator of a CP semigroup and $M(1) = 0$.

We also use a well–known fact about *spectral averaging*, which has a close relation to general weak coupling limit results, [Dav74, Dav80]. We use a special version appropriate for the applications we have in mind.

**Theorem 4.33 (Spectral averaging).**

Let $\mathfrak{X}$ be a finite dimensional complex vector space and $\{\exp(itL)\}_{t\in\mathbb{R}}$ be a one–parameter group of isometries. Then, for any $X \in \mathcal{B}(\mathfrak{X})$,

$$X^\sharp := \sum_{e\in\sigma(L)} \mathbf{1}[L=e]\, X\mathbf{1}[L=e] := \lim_{t\to\infty} t^{-1}\int_0^t ds\, e^{-isL}Xe^{isL},$$

and

$$\lim_{\lambda\to 0} e^{-\frac{itL}{\lambda}} e^{i\frac{t(L-i\lambda X)}{\lambda}} = e^{tX^\sharp},$$

uniformly on compact intervals $[0,T]$.

A crucial feature of certain Markov CP and $C_0$ semigroups $\{\mathcal{C}_t\}_{t\geq 0} \subset \mathcal{B}(\mathcal{B}_2(\mathcal{X}))$ used in our paper is the *relaxing* property defined as follows:

**Definition 4.34 (Relaxing semigroups, dim $\boldsymbol{\mathcal{X}} = n$).**
A Markov CP and $C_0$ semigroup $\{\mathcal{C}_t\}_{t\geq 0} \subset \mathcal{B}(\mathcal{B}_2(\mathcal{X}))$ is called relaxing if there is a unique trace–one and positive $\rho_\infty \in \mathcal{B}_2(\mathcal{X})$, i.e., a density matrix $\rho_\infty$, such that, for any density matrix $\rho \in \mathcal{B}_2(\mathcal{X})$,

$$\lim_{t\to\infty} \mathcal{C}_t^\dagger(\rho) = \rho_\infty.$$

In other words, a relaxing, Markov CP and $C_0$ semigroup has a unique invariant equilibrium state. Moreover, this state can be approximated for large times via the density matrix $\mathcal{C}_t^\dagger(\rho)$ for any initial state with density matrix $\rho$. Spohn [Spo77, Theorem 2] gave in 1977 a characterisation of relaxing semigroups which turns out to be pivotal in our study:

**Theorem 4.35 (Condition for a Markov CP semigroup to be relaxing).**
*Let $\{\mathcal{C}_t\}_{t\geq 0} \subset \mathcal{B}(\mathcal{B}_2(\mathcal{X}))$ be a Markov CP and $C_0$ semigroup with generator* L *given by Theorem 4.30. If $\{\mathrm{V}_j\}_{j=1}^{n^2-1} \subset \mathcal{B}_2(\mathcal{X})$ is a family of self–adjoint operators on $\mathcal{X}$ and the bi–commutant*

$$\left(\{\mathrm{V}_j\}_{j=1}^{n^2-1}\right)'' = \mathcal{B}_2(\mathcal{X}) \equiv \mathcal{B}(\mathcal{X}) \ , \tag{4.85}$$

*then $\{\mathcal{C}_t\}_{t\geq 0}$ is relaxing. In particular,* 0 *is a non–degenerated eigenvalue of* L *and*

$$\min\{\mathrm{Re}\{w\} \mid w \in \sigma(L)\backslash\{0\}\} > 0.$$

As explained after Assumption (B), the condition (4.85) is a non–commutative version of the irreducibility of classical Markov chains.

Let $\{\Gamma_t\}_{t\in\mathbb{R}^+}$, $\Gamma_t \in \mathcal{B}(\mathcal{B}(\mathcal{H}))$ be a continuous Markov CP semigroup and $\omega$ be a stationary state, i.e. $\omega = \omega\circ\Gamma_t$, $\forall t \in \mathbb{R}^+$, w.r.t. $\{\Gamma_t\}_{t\in\mathbb{R}^+}$. Assume that $\omega$ is a faithful state of the $C^*$-algebra $\mathcal{B}(\mathcal{H})$ and denote the corresponding GNS representation with $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$. There exists a continuous contraction semigroup $\left\{e^{-itL}\right\}_{t\in\mathbb{R}^+}$ on $\mathcal{H}_\omega$ such that

$$\pi_\omega\left(\Gamma_t\left(A\right)\right)\Omega_\omega = e^{itL}\pi_\omega\left(A\right)\Omega_\omega.$$

We conclude this section with the definition of the *detailed balance condition*, see [Ali76, FGKV77, FGKV78].

**Definition 4.36 (Detailed Balance Condition).** $L = L_{\mathrm{Re}} + iL_{\mathrm{Im}}$ be the unique decomposition, such that $L_{\mathrm{Re}}, L_{\mathrm{Im}}$ are selfadjoint operators. $\{\Gamma_t\}_{t\in\mathbb{R}^+}$ satisfies the *detailed balance condition* w.r.t. $\omega$ iff

$$\pi_\omega\left(\alpha_t\left(A\right)\right)\Omega_\omega = e^{itL_{\mathrm{Re}}}\pi_\omega\left(A\right)\Omega_\omega$$

defines a continuous group $\{\alpha_t\}_{t\in\mathbb{R}}$ of automorphisms of the $C^*$-algebra $\mathcal{B}\left(\mathcal{H}\right)$.

**Remark 4.37.** It can be shown that the detailed balance condition implies that

$$\pi_\omega\left(\zeta_t\left(A\right)\right)\Omega_\omega = e^{-tL_{\mathrm{Im}}}\pi_\omega\left(A\right)\Omega_\omega$$

defines a Markov CP continuous semigroup $\{\zeta_t\}_{t\in\mathbb{R}^+}$, [FGKV77]. In particular,

$$L_{\mathrm{Re}}\left(\Omega_\omega\right) = 0 = L_{\mathrm{Im}}\left(\Omega_\omega\right).$$

# CHAPTER 5

# Time–dependent $C$–Liouvilleans

This chapter provides the construction of time–dependent $C$–Liouvilleans, whose autonomous counterparts have been invented in [JP02]. The construction is a natural extension of the autonomous $C$–Liouvilleans. However, it is to our knowledge not contained in the literature. We will make use of the notions and notations introduced in [BPW11a].

Assume that the initial state $\omega_0$ is of the form

$$\omega_0 = \mathfrak{g}_{\mathrm{at}} \otimes \omega_{\mathcal{R}}, \tag{5.1}$$

i.e., $\omega_{\mathrm{at}} = \mathfrak{g}_{\mathrm{at}}$ is the Gibbs state. Let $(\mathfrak{H}, \pi, \Omega_{\mathfrak{g}})$ be its GNS representation. Note that $\mathfrak{H} := \mathfrak{H}_{\mathrm{at}} \otimes \mathfrak{H}_{\mathcal{R}}$, $\pi := \pi_{\mathrm{at}} \otimes \pi_{\mathcal{R}}$ and $\Omega_{\mathfrak{g}} := \Omega_{\mathrm{at},\mathfrak{g}} \otimes \Omega_{\mathcal{R}}$, where $(\mathfrak{H}_{\mathrm{at}}, \pi_{\mathrm{at}}, \Omega_{\mathrm{at},\mathfrak{g}})$ and $(\mathfrak{H}_{\mathcal{R}}, \pi_{\mathcal{R}}, \Omega_{\mathcal{R}})$ are the GNS representation of $\mathfrak{g}_{\mathrm{at}}$ and $\omega_{\mathcal{R}}$, respectively. An important property of the initial state is that $\omega_0$ is faithful. In particular, $\pi$ is injective.

For simplicity, $\pi(A)$ and $\pi(\mathcal{V})$ are denoted by $A$ and $\mathcal{V}$, respectively. Moreover, the cyclic vector $\Omega_{\mathfrak{g}}$ of the GNS representation is in this case separating for $\mathfrak{M}$, i.e., $A\Omega_{\mathfrak{g}} = 0$ implies $A = 0$. Indeed, $\omega_0$ is a $(\beta, \tau)$–KMS state, where $\{\tau_t\}_{t\in\mathbb{R}}$ is the one–parameter group of $*$–automorphisms on $\mathcal{V}$ defined by (1.11), see also [BR87, Corollary 5.3.9]. The weak closure of the $C^*$–algebra $\pi(\mathcal{V})$ is a von Neumann algebra denoted by $\mathfrak{M} := \mathcal{V}''$. The state $\omega_0$ on $\mathcal{V}$ extends uniquely to a normal state on the von Neumann algebra $\mathfrak{M}$ and $\{\tau_t\}_{t\in\mathbb{R}}$ also extends uniquely to a $\sigma$–weakly continuous $*$–automorphism group on $\mathfrak{M}$, see [BR87, Corollary 5.3.4]. Both extensions are again denoted by $\omega_0$ and $\{\tau_t\}_{t\in\mathbb{R}}$, respectively. Because $\omega_0$ is, in this case, invariant with respect to $\{\tau_t\}_{t\in\mathbb{R}}$, there is a unique unitary representation $\{U_t\}_{t\in\mathbb{R}}$ of $\{\tau_t\}_{t\in\mathbb{R}}$, i.e.,

$$\forall t \in \mathbb{R},\ A \in \mathfrak{M}: \qquad \tau_t(A) = U_t A U_t^*,$$

such that $U_t\Omega_{\mathfrak{g}} = \Omega_{\mathfrak{g}}$. As $t \mapsto \tau_t$ is $\sigma$–weakly continuous, the map $t \mapsto U_t$ is strongly continuous. Therefore, the unitary group $\{U_t\}_{t\in\mathbb{R}}$ is generated by a selfadjoint operator $L$, $U_t = \mathrm{e}^{itL}$. In particular, $\Omega_{\mathfrak{g}} \in \mathrm{Dom}(L)$ and $L$ annihilates $\Omega_{\mathfrak{g}}$, i.e. $L\Omega_{\mathfrak{g}} = 0$. Moreover, $L$ is related to the generator $\delta$ of the group $\{\tau_t\}_{t\in\mathbb{R}}$ by the following relations: We have

$$\{A\Omega : A \in \mathrm{Dom}(\delta)\} \subset \mathrm{Dom}(L) \subset \mathfrak{H} \tag{5.2}$$

and

$$\forall A \in \mathrm{Dom}(\delta) : \qquad L(A\Omega) = \delta(A)\,\Omega. \tag{5.3}$$

Now, if the faithful state $\omega_{\mathrm{at}}$ is not the Gibbs state $\mathfrak{g}_{\mathrm{at}}$ in (5.1) then the GNS representation of $\omega_0$ is also given by $(\mathfrak{H}, \pi, \Omega)$ where $\Omega = \Omega_{\mathrm{at}} \otimes \Omega_{\mathcal{R}}$ for some $\Omega_{\mathrm{at}} \in \mathfrak{H}_{\mathrm{at}}$. In other words, the von Neumann algebra $\mathfrak{M}$, the corresponding extension of the $*$–automorphism group $\{\tau_t\}_{t\in\mathbb{R}}$ does not depend on the initial state $\omega_{\mathrm{at}}$ of the atom. So, we assume from now on that

$$\omega_0 := \omega_{\mathrm{at}} \otimes \omega_{\mathcal{R}}$$

for any faithful state $\omega_{\mathrm{at}}$.

The (Tomita–Takesaki) modular objects of the pair $(\mathfrak{M}, \Omega_{\mathfrak{g}})$ are important for our further analysis. We write $\Delta$, $J$, and

$$\mathcal{P} := \overline{\{AJA\Omega_{\mathfrak{g}} \ : \ A \in \mathfrak{M}\}}$$

respectively for the modular operator, the modular conjugation and the natural positive cone of the pair $(\mathfrak{M}, \Omega_{\mathfrak{g}})$. Observe that $\Omega = AJA\Omega_{\mathfrak{g}} \in \mathcal{P}$ with

$$A = \rho_{\mathrm{at}}^{1/4}\rho_{\mathfrak{g}}^{-1/4} \otimes \mathbf{1}_{\mathfrak{H}_{\mathcal{R}}},$$

where $\rho_{\mathfrak{g}}$ is the density matrix (1.12) of the Gibbs state $\mathfrak{g}_{\mathrm{at}}$. Additionally, $\Omega$ is a cyclic vector for any faithful initial state $\omega_{\mathrm{at}}$ of the atom and hence, by [BR87, Proposition 2.5.30], it is also separating for $\mathfrak{M}$.

Standard results from Tomita–Takesaki theory (cf. [BR87, Corollary 2.5.32] and [BR96, Chapt. 5]) show that the generator $L$ of the unitary group $\{U_t\}_{t\in\mathbb{R}}$ satisfies

$$\forall t \in \mathbb{R} : \qquad LJ + JL = 0, \qquad \mathrm{e}^{itL}\mathcal{P} \subset \mathcal{P}, \qquad \Delta = \mathrm{e}^{-\beta L}. \tag{5.4}$$

Here, $L$ refers to as the *standard Liouvillean* of the $*$–automorphism group $\{\tau_t\}_{t\in\mathbb{R}}$.

In our setting, however, the free dynamics is perturbed by the pump and the atom–reservoir interaction. Altogether, this leads to a perturbation $W_t$ of the standard Liouvillean $L$. For time–independent perturbations of the generator $\delta$ of the dynamics $\{\tau_t\}_{t\in\mathbb{R}}$ (on $\mathcal{V}$) of the form $i[W,\cdot]$ with some self–adjoint $W \in \mathcal{V}$, one has

$$\forall t \in \mathbb{R} : \qquad \tau_t^W(A) = \mathrm{e}^{it(L+W)}A\mathrm{e}^{-it(L+W)} \in \mathfrak{M}, \qquad A \in \mathcal{V}\,, \tag{5.5}$$

where $\{\tau_t^W\}_{t\in\mathbb{R}}$ is the strongly continuous $*$–automorphism group on $\mathcal{V}$ generated by $\delta + i[W,\cdot]$. Analogously as above, $\{\tau_t^W\}_{t\in\mathbb{R}}$ defines a $\sigma$–weakly continuous group on whole $\mathfrak{M}$. In general, the operator $L + W$ does neither annihilate $\Omega_{\mathfrak{g}}$ nor satisfies

$$(L+W)\,J + J\,(L+W) = WJ + JW = 0.$$

It is known, [BR87, Corollary 2.5.32], that there is an operator $L_W$, the standard Liouvillean of the dynamics $\{\tau_t^W\}_{t\in\mathbb{R}}$, satisfying $[L_W, J] = 0$ together with

$$\forall t \in \mathbb{R} : \qquad \tau_t^W(A) = \mathrm{e}^{itL_W}A\mathrm{e}^{-itL_W}, \qquad A \in \mathfrak{M}\,,$$

use [BR87, Corollary 2.5.32] and the $\sigma$–weakly continuity of the map $t \mapsto \tau_t^W$. Indeed, $L_W$ equals $L + W$ up to an element of the commutant $\mathfrak{M}' = J\mathfrak{M}J$ of the von Neumann algebra $\mathfrak{M}$. To find it explicitly, it suffices to solve the equation

$$[W + JAJ, J] = 0$$

for $A \in \mathfrak{M}$. Straightforward computations show that $A = W$ is one solution. Using additionally the uniqueness of the standard Liouvillean $L_W$, one can verify that

$$L_W = L + W - JWJ ,$$

is the only solution.

The operator $L_W$ does not necessarily annihilate $\Omega_\mathfrak{g}$ or some prescribed vector $\Omega \in \mathcal{P}$. In general, $L_W$ only annihilates $\Omega_W \in \mathcal{P}$, the vector representing the unique $(\beta, \tau^W)$–KMS state normal to $\omega_0$. In other words, the standard Liouvillean $L_W$ anti–commutes with the modular conjugation $J$, but has the drawback of not having $\Omega_\mathfrak{g}$ in its kernel. A way to get around this problem is presented in [JP02, Section 2.2] where the notion of $C$–Liouvilleans, $\mathcal{L}$, is introduced. It is constructed such that $\mathcal{L}\Omega = 0$ for any fixed $\Omega \in \mathcal{P}$. In our case, we face the problem that the dynamics is non–autonomous and the standard Liouvillean $L_{W_t}$ is time–dependent. Using the $C$–Liouvilleans construction of [JP02, Section 2.2] we can design the time–depending Liouvillean of the non–autonomous dynamics such that $\mathcal{L}_t\Omega = 0$. This is a very useful property for the analysis of the dynamics.

Therefore, we now extend the definition of $C$–Liouvilleans [JP02, Section 2.2] to non–autonomous evolutions. First, the time–dependent, self-adjoint perturbation $\{W_t\}_{t\in\mathbb{R}} \subset \mathcal{V}$ should define a family of symmetric derivations

$$\delta_{W_t} := \delta + i[W_t, \cdot]$$

for all $t \in \mathbb{R}$, which generates a strongly continuous two–parameter family $\{\tau_{t,s}\}_{t\geq s}$ of automorphisms of $\mathcal{V}$, similar to the autonomous case (5.5). Recall that a symmetric derivation $\delta$ is an operator acting on a $C^*$–algebra where its domain is a dense sub–$*$–algebra and which satisfies on its domain

$$\delta(A)^* = \delta(A^*) \quad \text{and} \quad \delta(AB) = \delta(A)B + A\delta(B).$$

To this end, we use a standard result on non–autonomous Cauchy problems.

**Proposition 5.1 (Non-autonomous dynamics–I).**
*Let $\{\delta_t\}_{t\in\mathbb{R}}$ be a family of symmetric derivations having the same dense domain $\mathrm{Dom}(\delta_t) \equiv \mathcal{D} \subset \mathcal{V}$. Assume that, for all $A \in \mathcal{D}$, $\{\delta_t(A)\}_{t\in\mathbb{R}} \in C^1(\mathbb{R}, \mathcal{V})$ and for each $t \in \mathbb{R}$, $\delta_t$ generates a strongly continuous one–parameter group of automorphisms. Then, there is a unique evolution family $\{\tau_{t,s}\}_{t\geq s}$ of automorphisms solving on $\mathcal{D}$ the non–autonomous evolution equations*

$$\forall t > s : \quad \partial_t\tau_{t,s} = \delta_t\tau_{t,s} , \quad \partial_s\tau_{t,s} = -\tau_{t,s}\delta_s , \quad \tau_{s,s} := \mathbf{1} .$$

*If $\{\delta_t\}_{t\in\mathbb{R}}$ is periodic with period $T > 0$, then*

$$\forall t \geq s,\ k \in \mathbb{Z} : \quad \tau_{t,s} = \tau_{t+kT,s+kT}.$$

*Proof.* By Theorem 5.11 (iv) there is a unique evolution family $\{\tau_{t,s}\}_{t\geq s}$ solving the non–autonomous evolution equations stated in the proposition. By using the representation in Theorem 5.11 (iii) and the fact that $\delta_t$ generates a group of automorphisms for any $t \in \mathbb{R}$, it follows that $\{\tau_{t,s}\}_{t\geq s}$ is also a family of automorphisms. The $T$–periodicity of $\{\tau_{t,s}\}_{t\geq s}$ results from Theorem 5.11 (iii). □

Observe that the conditions of Proposition 5.1 are satisfied by $\{\delta_{W_t}\}_{t\geq 0}$ as soon as $\{W_t\}_{t\in\mathbb{R}} \in C^1(\mathbb{R}, \mathcal{V})$:

**Lemma 5.2 (Non–autonomous $C^*$–dynamics–II).**
*Assume that $\{W_t\}_{t\in\mathbb{R}} \in C^1(\mathbb{R}_0^+, \mathcal{V})$ and $W_t = W_t^*$ for all $t \in \mathbb{R}$. Then, $\{\delta_{W_t}\}_{t\in\mathbb{R}}$ is a family of symmetric derivations having the same dense domain*

$$\mathrm{Dom}(\delta_{W_t}) = \mathrm{Dom}(\delta) \subset \mathcal{V}.$$

*Moreover, for all $A \in \mathcal{V}$, $\{\delta_{W_t}(A)\}_{t\in\mathbb{R}} \in C^1(\mathbb{R}, \mathcal{V})$ and for each $t \in \mathbb{R}$, $\delta_{W_t}$ generates a strongly continuous one–parameter group of automorphisms.*

*Proof.* Since $\{W_t\}_{t\in\mathbb{R}} \subset \mathcal{V}$, it is clear that $\{\delta_{W_t}\}_{t\geq 0}$ defines a family of symmetric derivations having the same dense domain $\mathrm{Dom}(\delta)$. Also, the assumption $\{W_t\}_{t\in\mathbb{R}} \in C^1(\mathbb{R}, \mathcal{V})$ directly implies $\{\delta_{W_t}(A)\}_{t\in\mathbb{R}} \in C^1(\mathbb{R}, \mathcal{V})$ for all $A \in \mathcal{V}$. Moreover, as $\delta_{W_t}$ is a bounded symmetric derivation, it generates a $*$–automorphism group $\{\xi_r^{W_t}\}_{r\in\mathbb{R}}$ for any $t \in \mathbb{R}$. Then, using the Lie–Trotter formula [EN00, Chap. III, Corollary 5.8], for any $t \in \mathbb{R}_0^+$, the strong limit

$$\forall r \in \mathbb{R}: \quad \tau_r^{W_t} := \mathrm{s-}\lim_{n\to\infty} \left\{ \left( \tau_{r/n} \xi_{r/n}^{W_t} \right)^n \right\}$$

defines a $*$–automorphism group $\{\tau_r^{W_t}\}_{r\in\mathbb{R}}$ with generator $\delta_{W_t}$. □

The construction of [JP02, Section 2.2] starts with the definition of the linear space

$$\mathcal{O} := \{A\Omega : A \in \mathcal{V}\} \subset \mathfrak{H}.$$

Let $\iota$ be the map from $\mathcal{V}$ to $\mathcal{O}$ defined by $\iota(A) := A\Omega$. This map is an isomorphism of the linear space $\mathcal{V}$ and $\mathcal{O}$ because $\Omega$ is a separating vector for $\mathfrak{M}$. In particular, $\|A\Omega\|_\infty := \|A\|$ defines a norm on the space $\mathcal{O}$ and $\iota$ is an isometry with respect to this norm. Thus, $(\mathcal{O}, \|\cdot\|_\infty)$ is a Banach space. Any element $A \in \mathcal{V}$ also defines a bounded operator on $\mathcal{O}$ by left multiplication, i.e., $A(B\Omega) := (AB)\Omega$. Moreover, we define a strongly continuous two–parameter family $\{T_{t,s}\}_{t\geq s}$ acting on $\mathcal{O}$ by

$$\forall t \geq s: \quad T_{t,s} := \iota \circ \tau_{t,s} \circ \iota^{-1}. \tag{5.6}$$

In particular, since $\{\tau_{t,s}\}_{t\geq s}$ is a family of automorphisms, the operator $T_{t,s}$ has a bounded inverse and we observe that

$$\forall t \geq s: \quad T_{t,s}(\Omega) = \Omega \quad \text{and} \quad T_{t,s} A T_{t,s}^{-1} = \tau_{t,s}(A). \tag{5.7}$$

We would like now to extend the two–parameter family $\{T_{t,s}\}_{t,s\in\mathbb{R}_0^+}$ to $\mathfrak{H}$. To this end, following [JP02, Eq. 2.5] we directly define the time–dependent $C$–Liouvillean as follows:

**Definition 5.3 (Time–dependent $C$–Liouvillean).**
The time–dependent $C$–Liouvillean is defined by

$$\mathcal{L}_t = L + W_t - J\Delta^{1/2} W_t \Delta^{-1/2} J \tag{5.8}$$

for any $t \in \mathbb{R}$.

Note that the term

$$V_t := W_t - J\Delta^{1/2} W_t \Delta^{-1/2} J \in \mathcal{B}(\mathcal{O}) \tag{5.9}$$

implements the commutator $[W_t, \cdot]$ on $\mathcal{O}$ for any $t \in \mathbb{R}$, i.e. for any $A \in \mathcal{V}$,

$$[W_t, A]\Omega = W_t A\Omega - (W_t A^*)^* \Omega \tag{5.10}$$

and using $J\Delta^{1/2} A\Omega = A^*\Omega$ we also deduce that

$$J\Delta^{1/2} W_t \Delta^{-1/2} J A\Omega = (W_t A^*)^* \Omega.$$

In particular,

$$\left\| J\Delta^{1/2} W_t \Delta^{-1/2} J \right\|_{\mathcal{B}(\mathcal{O})} = \|W_t\| < \infty \tag{5.11}$$

and

$$\forall t \in \mathbb{R} : \quad \mathcal{L}_t \Omega = 0. \tag{5.12}$$

Note that the topology induced by the norm $\|\cdot\|_\infty$ on $\mathcal{O}$ is finer than the topology w.r.t. the Hilbert space norm on the corresponding subspace of $\mathfrak{H}$. In particular, the boundedness of the operator

$$J\Delta^{1/2} W_t \Delta^{-1/2} J$$

as an operator on $\mathfrak{H}$ is unclear, in spite of (5.11). Therefore, for every $t \in \mathbb{R}$, we assume some sufficient conditions on the operator family $\{V_t\}_{t\in\mathbb{R}}$ like its boundedness, in order to extend later the two–parameter family $\{T_{t,s}\}_{t\geq s}$ to the Hilbert space $\mathfrak{H}$.

**Lemma 5.4 (Extension of $\{T_{t,s}\}_{t\geq s}$-I).**
*Let $\{V_t\}_{t\geq 0} \in C^1(\mathbb{R}, \mathcal{B}(\mathfrak{H}))$. Then, there is an evolution family $\{U_{t,s}\}_{t\geq s} \subset \mathcal{B}(\mathfrak{H})$ solving on* $\mathrm{Dom}\,(L)$ *the non–autonomous evolution equations*

$$\forall t > s : \quad \partial_t U_{t,s} = i\mathcal{L}_t U_{t,s}\ , \quad \partial_s U_{t,s} = -iU_{t,s}\mathcal{L}_s\ , \quad U_{s,s} := \mathbf{1}.$$

*Moreover, for any $t \geq s$, $U_{t,s}$ possesses a bounded inverse $U_{t,s}^{-1}$. If $\{W_t\}_{t\in\mathbb{R}}$ is periodic with period $T > 0$, then*

$$\forall t \geq s,\ k \in \mathbb{Z} : \quad U_{t,s} = U_{t+kT,s+kT}.$$

*Proof.* The existence of the evolution family $\{U_{t,s}\}_{t\geq s}$ solving on $\mathrm{Dom}\,(L)$ the non–autonomous evolution equation stated in the lemma is a direct consequence of Theorem 5.11. To prove that $U_{t,s}$ has a bounded inverse $U_{t,s}^{-1}$, we note that it suffices to prove that $U_{t,s}^{-1} \in \mathcal{B}(\mathfrak{H})$ exists for small times $|t-s|>0$, by the cocycle property. To this end, we use Corollary 5.12 together with the observation that $\mathrm{e}^{i(t-s)L}$ is unitary and the bound

$$\left\| \int_s^t U_{t,r} V_r \mathrm{e}^{i(r-s)L} \mathrm{d}r \right\| \leq \frac{1}{2}$$

for sufficiently small $|t-s|>0$. Therefore, the Neumann series explicitly gives $U_{t,s}^{-1} \in \mathcal{B}(\mathfrak{H})$. If $\{W_t\}_{t\in\mathbb{R}}$ is $T$–periodic, then $\{U_{t,s}\}_{t\geq s}$ is also $T$–periodic, by Theorem 5.11 (iii). □

Combining this with Theorem 5.1 and Lemma 5.2, we deduce that the evolution family $\{U_{t,s}\}_{t\geq s}$ is the unique continuous extension of the two–parameter family $\{T_{t,s}\}_{t\geq s}$ to the Hilbert space $\mathfrak{H}$:

**Proposition 5.5 (Extension of $\{T_{t,s}\}_{t\geq s}$–II).**
*Assume that $\{W_t\}_{t\geq 0} \in C^1(\mathbb{R}, \mathcal{V})$ and $\{V_t\}_{t\geq 0} \in C^1(\mathbb{R}, \mathcal{B}(\mathfrak{H}))$. Then, the evolution family of Lemma 5.4 satisfies $U_{t,s}\Omega = \Omega$ and*

$$\forall t \geq s,\ A \in \mathcal{V}: \quad \tau_{t,s}(A) = U_{t,s} A U_{t,s}^{-1}$$

*In particular, $\{\tau_{t,s}\}_{t\in\mathbb{R}}$ also extends uniquely to a $\sigma$–weakly continuous $*$–automorphism evolution family on $\mathfrak{M}$.*

*Proof.* Note first that $U_{t,s}\Omega = \Omega$ is a direct consequence of (5.12) and Lemma 5.4. Using the isometry between $\mathcal{O}$ and $\mathcal{V}$, $\{T_{t,s}(A\Omega)\}_{t\geq s} \in C^1([s,\infty), \mathcal{O})$ for any $s \in \mathbb{R}$ and every $A \in \mathrm{Dom}(\delta)$, as $\{\tau_{t,s}(A)\}_{t\geq s} \in C^1([s,\infty), \mathrm{Dom}(\delta))$ with respect to the norm on $\mathcal{V}$, by Propositions 5.1 and 5.13. Computing its derivative with respect to $t \geq 0$ by using the non–autonomous evolution equation of Proposition 5.1 together with (5.6), (5.2)–(5.3), and (5.10) we obtain that

$$\partial_t T_{t,s}(A\Omega) = \delta_{W_t}(\tau_{t,s}(A))\,\Omega = i\mathcal{L}_t(T_{t,s}(A\Omega)) \tag{5.13}$$

for all $t > s$ and $A \in \mathrm{Dom}(\delta)$. Meanwhile, since

$$\forall A \in \mathcal{V}: \quad \|A\Omega\| \leq \|A\| = \|A\Omega\|_\infty, \tag{5.14}$$

$\{T_{t,s}(A\Omega)\}_{t\geq s} \in C^1([s,\infty), \mathrm{Dom}(L))$ with respect to the norm on $\mathfrak{H}$ and (5.13) also holds in the norm of $\mathfrak{H}$. By Proposition 5.1, it follows that

$$\forall A \in \mathrm{Dom}(\delta): \quad U_{t,s}(A\Omega) = T_{t,s}(A\Omega) := \tau_{t,s}(A)\,\Omega. \tag{5.15}$$

By density, for any $A \in \mathcal{V}$, there is a sequence $\{A_n\}_{n=1}^\infty \subset \mathrm{Dom}(\delta)$ converging in $\mathcal{V}$ to $A$. We infer from (5.14) that this sequence $\{A_n\}_{n=1}^\infty$ also converges to $A$ in the sense of $\mathfrak{H}$. On the one hand, by continuity of $U_{t,s}$ in $\mathfrak{H}$,

$$\lim_{n\to\infty} U_{t,s}(A_n\Omega) = U_{t,s}(A\Omega).$$

On the other hand, using (5.15) and the continuity of $T_{t,s}$ in $\mathcal{O}$, one gets

$$\lim_{n\to\infty} U_{t,s}(A_n\Omega) = \lim_{n\to\infty} T_{t,s}(A_n\Omega) = T_{t,s}(A\Omega).$$

As a consequence, $U_{t,s}|_{\mathcal{O}} = T_{t,s}$. In particular, from the uniqueness of the inverse we obtain $U_{t,s}^{-1}|_{\mathcal{O}} = T_{t,s}^{-1}$. We then use (5.7) to deduce that

$$\forall t \geq s,\ A \in \mathcal{V},\ x \in \mathcal{O}: \quad \tau_{t,s}(A)\, x = U_{t,s} A U_{t,s}^{-1}(x) \ .$$

By density of $\mathcal{O}$ in $\mathfrak{H}$, we arrive at the final assertion of the proposition

$$\forall t \geq s,\ A \in \mathcal{V}: \quad \tau_{t,s}(A) = U_{t,s} A U_{t,s}^{-1} \ . \qquad \square$$

The use of $C$–Liouvilleans is advantageous because of the presence of only one evolution operator in the dynamics described by

$$\forall A \in \mathfrak{M}: \quad U_{t,s} A U_{s,t} \Omega = U_{t,s} A \Omega.$$

In particular, it establishes a direct relation to the *Lindbladian*, which is an operator defined on the von Neumann algebra $\mathfrak{M}$. Observe also that $\mathcal{L}_t$ is not anymore selfadjoint and can thus be dissipative.

## Appendix to Chapter 5

In this appendix we gather some standard results for non–autonomous Cauchy problems for the convenience of the reader. Let $\mathcal{X}$ be a Banach space, and $J \subseteq \mathbb{R}$ an interval of $\mathcal{X}$. We refer to [Paz83, Kat93, EN00, Sch04] as references of the results presented below. Consider the *non–autonomous Cauchy problem* (nCP),

$$\text{(nCP)} \begin{cases} \frac{d}{dt} u(t) = A_t u(t) + f(t) \quad (t \in J), \\ u(s) = x, \end{cases} \tag{5.16}$$

where $\{A_t\}_{t\in\mathbb{R}}$ is a family of closed operators on $\mathcal{X}$ and $f \in L^1_{\mathrm{loc}}(J, X)$. The homogeneous (nCP), where $f \equiv 0$, is denoted by $(\mathrm{nCP})_0$. We start with $(\mathrm{nCP})_0$ and focus only on the $(\mathrm{nCP})_0$ of *hyperbolic type*, where the $A_t$ are generators of $C_0$–semigroups. The *parabolic* $(\mathrm{nCP})_0$ addresses the case in which $A_t$ generates an *analytic semigroup* and much stronger results on the well–posedness are known in this case. We start with the general notion of well–posedness.

**Definition 5.6 (Well–posedness).** The problem $(\mathrm{nCP})_0$ is called *well–posed* if there are dense subspaces $\mathcal{Y}_s \subseteq \mathcal{X}$, with $\mathcal{Y}_s \subseteq \mathrm{Dom}(A_s)$, $\forall s \in J$, such that for each $x \in \mathcal{Y}_s$ there is a unique solution $u = u(\cdot, s, x) \in C^1([s,\infty) \cap J, X)$ of $(\mathrm{nCP})_0$, with $u(t) \in \mathcal{Y}_t$, $\forall t \in [s,\infty) \cap J$. Moreover, if $s_n \to s$ and $x_n \to x$ in $\mathcal{X}$, with $(s_n)_{n\in\mathbb{N}} \subset J$, $x_n \in \mathcal{Y}_{s_n}$, $x \in \mathcal{Y}_s$, then

$$\hat{u}(t, s_n, x_n) \to \hat{u}(t, s, x),$$

in $\mathcal{X}$ uniformly for $t$ in compact subsets of $J$. Here, $\hat{u}(t,r,y) := u(t,r,y)$ if $t \geq r$ and $\hat{u}(t,r,y) := y$, for $t \leq r$ and $y \in \mathcal{Y}_r$.

If a $(\mathrm{nCP})_0$ is well-posed, we define

$$U_{t,s} x := u(t,s,x), \quad t \geq s,\ t,s \in J,\ x \in \mathcal{Y}_s.$$

$U_{t,s}$ naturally extends to $\mathcal{X}$ and the extension, denoted by the same symbol, satisfies:

1. The cocycle–, or Chapman–Kolmogorov property

$$\forall t \geq r \geq s,\ t,r,s \in J: \quad U_{t,s} = U_{t,r} U_{r,s}\ U_{s,s} = \mathbb{1}.$$

2. Moreover, for $t \geq s$, $t,s \in J$, the map

$$(t,s) \mapsto U_{t,s}$$

   is strongly continuous.

**Definition 5.7 (Evolution family).**
A family $\mathcal{U} := \{U_{t,s}\}_{t \geq s, t,s \in J} \subset \mathcal{B}(\mathcal{X})$ of bounded operators on $\mathcal{X}$ is called *evolution family* if it satisfies 1. and 2. If $(\mathrm{nCP})_0$ is well–posed, we say that $\mathcal{U}$ solves $(\mathrm{nCP})_0$ or that $A_{(\cdot)}$ *generates* $\mathcal{U}$.

In particular, we are interested in the non–autonomous evolution equations for which $\mathcal{Y}_s \equiv \mathcal{Y}$, where $\mathcal{Y}$ is some dense subspace of $\mathcal{X}$,

$$\forall t > s,\ x \in \mathcal{Y}: \quad \partial_t \{U_{t,s} x\} = A_t \{U_{t,s} x\}, \quad U_{s,s} := \mathbf{1}. \tag{5.17}$$

The standard results providing well-posedness in this case are due to Kato, [Kat53, Kat70, Kat73].

Standard sufficient conditions for the existence of an evolution family $\mathcal{U}$ solving the non–autonomous evolution equation (5.17) includes the notion of Kato quasi–stability.

**Definition 5.8 (Kato quasi-stability).**
For $t \in \mathbb{R}$, let $A_t$ be the generator of a $C_0$ semigroup $\{S_t(s)\}_{s \geq 0} \subset \mathcal{B}(\mathcal{X})$. The family $\{A_t\}_{t \in \mathbb{R}}$ is called *quasi–stable* with stability constants $\mu \in \mathbb{R}$ and $M \in [1, \infty)$ if

$$\left\| \prod_{j=1}^{n} S_{t_j}(s_j) \right\| \leq M \exp\left( \mu \sum_{j=1}^{n} s_j \right)$$

for all $s_j \geq 0$ with $j \in \{1, \cdots, n\}$, and all reals $t_1 \leq ... \leq t_n$.

This property is stable w.r.t. bounded perturbations [Paz83, Theorem 2.3]:

**Theorem 5.9 (Kato quasi-stability and bounded perturbation).**
*Let $\{A_t\}_{t \in \mathbb{R}}$ be a quasi–stable family of generators of $C_0$ semigroups on $\mathcal{X}$ with stability constants $\varsigma \in \mathbb{R}$ and $M \in [1, \infty)$. Then, for any uniformly bounded family $\{B_t\}_{t \in \mathbb{R}} \subset \mathcal{B}(\mathcal{X})$, $\|B_t\| \leq K < \infty$, $\{A_t + B_t\}_{t \in \mathbb{R}}$ is quasi–stable family of generators of $C_0$ semigroups on $\mathcal{X}$ with stability constants $\mu' = \mu + MK$ and $M' = M$.*

A family $\{A_t\}_{t \in \mathbb{R}}$ of generators of a $C_0$ semigroup generates an approximating evolution family defined as follows:

**Definition 5.10 (Approximating evolution family).**
For any family $\{A_t\}_{t \in [0,T]}$ of generators of $C_0$ semigroups, $\{S_t(s)\}_{s \geq 0}$ and all $n \in \mathbb{N}$, a two parameter family $\{U_{t,s,n}\}_{t \geq s \geq 0}$ is called *approximating evolution family* iff

$$U_{t,s,n} := S_{t_{j,n}}(t-s),$$

for all $t_{j,n} \leq s \leq t \leq t_{j+1,n}$ and

$$U_{t,s,n} := S_{t_{k,n}}\left(t - t_{k,n}\right)\left[\prod_{j=l+1}^{k-1} S_{t_{j,n}}\left(\frac{T}{n}\right)\right] S_{t_{l,n}}\left(t_{l,n} - s\right)$$

for all $k \geq l$, $t_{l,n} \leq s \leq t_{l+1,n}$, $t_{k,n} \leq s \leq t_{k+1,n}$. Here, $t_{j,n} := (j/n)\,T$ for $j \in \{0, \cdots, n\}$.

Kato provided in [Kat53] conditions under which the approximating evolution family $\{U_{t,s,n}\}_{t \geq s \geq 0}$ converges strongly to an evolution family, which is a solution of $(\mathrm{nCP})_0$, [Paz83, Theorem 4.8].

**Theorem 5.11 (Well-posedness of $(\mathrm{nCP})_0$).**
*Let $\{A_t\}_{t\in\mathbb{R}}$ be a quasi–stable family of generators of $C_0$ semigroups on $\mathcal{X}$ with stability constants $\mu \in \mathbb{R}$ and $M \in [1, \infty)$. If $\mathrm{Dom}\,(A_t) = \mathcal{Y} \subset \mathcal{X}$ and, for all $x \in \mathcal{Y}$, $\{A_t x\}_{t\in\mathbb{R}} \in C^1(\mathbb{R}, \mathcal{X})$, then there is an evolution family $\mathcal{U}$ satisfying the following properties:*
(i) $\|U_{t,s}\| \leq M\mathrm{e}^{\mu(t-s)}$ *and $U_{t,s}\mathcal{Y} \subset \mathcal{Y}$ for all $t \geq s$.*
(ii) *For all $T \geq t \geq s$, $U_{t,s}\mathcal{Y} \subset \mathcal{Y}$ and for any $x \in \mathcal{Y}$ the map $(t, s) \mapsto U_{t,s}x \in (\mathcal{Y}, \|\cdot\|_{\mathcal{Y}})$ is continuous, where $\|\cdot\|_{\mathcal{Y}}$ is the graph norm of $A_0$.*
(iii) *$\{U_{t,s,n}\}_{t\geq s}$ converges strongly to $\{U_{t,s}\}_{t\geq s}$.*
(iv) *It is the unique evolution family solving* $(\mathrm{nCP})_0$*, i.e., $U_{s,s} := \mathbf{1}$ and, for all $x \in \mathcal{Y}$,*

$$\begin{aligned} \forall t \quad &\geq \quad s: \quad \partial_t^+ U_{t,s}x = A_t U_{t,s}x \; . \\ \forall t \quad &> \quad s: \quad \partial_s U_{t,s}x = -A_s U_{t,s}x \; . \end{aligned}$$

**Corollary 5.12.**
*Let $A_t := A + B_t$ with $A$ being the generator of a $C_0$ semigroup on $\mathcal{X}$ and $\{B_t\}_{t\in\mathbb{R}} \in C^1(\mathbb{R}, \mathcal{B}(\mathcal{X}))$. Then, there is a unique evolution family $\{U_{t,s}\}_{t\geq s} \subset \mathcal{B}(\mathcal{X})$ satisfying (i)–(iv) of Theorem 5.11 and*

$$\forall t \geq s: \quad U_{t,s} = \mathrm{e}^{(t-s)A} + \int_s^t U_{t,r}B_r\mathrm{e}^{(r-s)A}\mathrm{d}r$$

*in the strong sense.*

We close with a result for the *in-homogenous* (nCP), where $f \neq 0$. In this case the following theorem holds, [Paz83, Theorem 5.3].

**Theorem 5.13 (Well-posedness of (nCP)).**
*Assume $f \in C^1(\mathbb{R}, \mathcal{X})$ and the assumption of Theorem 5.11. Then, the* (nCP) *(5.16) has a unique $C^1$–solution equal to*

$$u\,(t) = U_{t,s}x + \int_s^t U_{t,r}f\,(r)\,\mathrm{d}r\;,$$

*where $\{U_{t,s}\}_{t\geq s} \subset \mathcal{B}(\mathcal{X})$ is the evolution family satisfying (i)–(iv) of Theorem 5.11.*

## 5.1 Bibliography


[AGF10] A. Aspect, G. Grynberg, and C. Fabre, *Introduction to quantum optics*, vol. XXIX, Cam. Univ. Press, 2010.

[AJP06a] S. Attal, A. Joye, and C.-A. Pillet (eds.), *Open quantum systems i: The Hamiltonian approach*, Lecture Notes in Mathematics, vol. 1880, Springer-Verlag, 2006.

[AJP06b] S. Attal, A. Joye, and C.-A. Pillet (eds.), *Open quantum systems ii: The Markovian approach*, Lecture Notes in Mathematics, vol. 1881, Springer-Verlag, 2006.

[AJP06c] S. Attal, A. Joye, and C.-A. Pillet (eds.), *Open quantum systems iii: Recent developments*, Lecture Notes in Mathematics, vol. 1882, Springer-Verlag, 2006.

[AL07] R. Alicki and K. Lendi, *Quantum dynamical semigroups and applications*, Lecture Notes in Phys., vol. 286, Springer, 2007.

[Ali76] R. Alicki, *On the detailed balance condition for non-Hamiltonian systems*, Rep. on Math. Phys. **2** (1976), 249–258.

[AS95] G. Alli and G.L. Sewell, *New methods and structures in the theory of the multi-mode Dicke laser model*, J. Math. Phys. **36** (1995), 5598–5626.

[Bag02] F. Bagarello, *Relations between the Hepp-Lieb and the Alli-Sewell laser models*, Ann. Henri Poincaré **3** (2002), 983–1002.

[BD09] L. Bruneau and J. Derezinski, *Thermal relaxation of a QED cavity*, J. Stat. Phys. (2009).

[BFS00] V. Bach, J. Fröhlich, and I. M. Sigal, *Return to equilibrium*, J. Math. Phys. **41** (2000), no. 6, 3985–4060.

[BMPS11] V. Bach, M. Merkli, W. Pedra, and I.M. Sigal, *Control of decoherence*, in preparation (2011).

[BMS08] G. Berman, M. Merkli, and I.M. Sigal, *Resonance theory of decoherence and thermalization*, Ann. of Phys. **323** (2008), 373–412.

[BPW11a] J.-B. Bru, W. Pedra, and M. Westrich, *Characterisation of the quasi-stationary state of an impurity driven by monochromatic light I - The effective theory*, in preparation (2011).

[BPW11b] ———, *Characterisation of the quasi-stationary state of an impurity driven by monochromatic light II - Microscopic foundations*, in preparation (2011).

[BR87] O. Bratteli and D. Robinson, *Operator algebras and quantum statistical mechanics 1*, 2 ed., Text and Monographs in Physics, Springer-Verlag, Berlin, 1987.

[BR96] ______, *Operator algebras and quantum statistical mechanics 2*, 2 ed., Text and Monographs in Physics, Springer-Verlag, Berlin, 1996.

[Dav74] E. B. Davies, *Markovian master equations*, Commun. Math. Phys. **39** (1974), 91–110.

[Dav75] ______, *Markovian master equations III*, Markovian Master Equations III **XI** (1975), 265–273.

[Dav76] ______, *Markovian master equations II*, Math. Ann. **219** (1976), 147–158.

[Dav80] E.B. Davies, *One parameter semigrops*, Academic Press, 1980.

[DF06] J. Derezinski and R. Früboes, *Fermi Golden Rule and Open Quantum Systems*, Open Quantum Systems III, vol. 1882, Springer Verlag, 2006, pp. 67–116.

[Ein16] A. Einstein, *Zur Quantentheorie der Strahlung*, Verh. d. deutschen phys. Gesellschaft **13** (1916).

[EN00] K.-J. Engel and R. Nagel, *One-parameter semigroups for linear evolution equations*, 1 ed., Graduate Texts in Mathematics, no. 194, Springer-Verlag, New York, 2000.

[FGKV77] A. Frigerio, V. Gorini, A. Kossakowski, and M. Verri, *Quantum detailed balance and kms condition*, Comm. Math. Phys. **57** (1977), 97–110.

[FGKV78] ______, *Erratum: Quantum detailed balance and KMS condition*, Comm. Math. Phys. **60** (1978), 96.

[GKS76] V. Gorini, A. Kossakowski, and E.C.G. Sudarshan, *Completely positive dynamical semigroups of n-level systems*, J. of Math. Phys. **17** (1976), 821–825.

[Hep74] K. Hepp, *The classical limit for quantum mechanical correlation functions*, Commun. math. Phys. **35** (1974), 265–277.

[HL73] K. Hepp and E.H. Lieb, *Phase transitions in reservoir-driven open systems with applications to lasers and superconductors*, Helv. Phys. Acta **46** (1973), 573–603.

[JP96] V. Jakšić and C. A. Pillet, *On a model for quantum friction III: Ergodic properties of the spin-boson system*, Commun. Math. Phys. **178** (1996), no. 3, 627–651.

[JP02] ______, *Non-equilibrium steady states of finite quantum systems coupled to thermal reservoirs*, Comm. Math. Phys. **226** (2002), 131–162.

[JZK$^+$03] E. Joos, H. D. Zeh, C. Kiefer, D. J. W. Giulini, J. Kupsch, and I.-O. Stamatescu, *Decoherence and the appearance of a classical world in quantum theory*, Springer, 2003.

[Kat53] T. Kato, *Integration of the equation of evolution in a Banach space*, J. Math. Soc. Japan **5** (1953), 208–234.

[Kat70] ______, *Linear evolution equations of 'hyperbolic' type*, J. Math. Soc. Japan **17** (1970), 241–258.

[Kat73] ______, *Linear evolution equations of 'hyperbolic' type ii*, J. Math. Soc. Japan **25** (1973), 648–666.

[Kat76] T. Kato, *Perturbation theory of linear operators*, 2 ed., Grundlehren der mathematischen Wissenschaften, vol. 132, Springer-Verlag, 1976.

[Kat93] T. Kato, *Abstract evolution equations, linear and quasilinear, revisited*, Functional Analysis and Related Topics (H. Komatsu, ed.), Lecture Notes Math., vol. 1540, Springer, 1993, pp. 103–125.

[MMS07] M. Merkli, M. Mück, and I.M. Sigal, *Theory of non-equilibrium stationary states as a theory resonances. existence and properties of NESS*, Ann. Henri Poincaré **8** (2007), 1539–1593.

[Paz83] A. Pazy, *Semigroups of linear operators and applications to partial differential equations*, 2 ed., Springer, New York, 1983.

[Sch04] R. Schnaubelt, *Asymptotic behaviour of parabolic nonautonomous evolution equations*, Functional Analytic Methods for Evolution Equations (M. Iannelli, R. Nagel, and S. Piazzera, eds.), Springer, 2004, pp. 401–472.

[Sim93] B. Simon, *The statistical mechanics of lattice gases*, Princeton Series in Physics, vol. 1, Princeton University Press, Princeton, NJ, 1993.

[Spo77] H. Spohn, *An algebraic condition for the approach to equilibrium of an open n–level system*, Lett. in Math. Phys. **2** (1977), 33–38.

[SY68] E. Snitzer and C.G. Young, *Lasers*, A Series of Advances, vol. 2, Edward Arnold, London, 1968.

[Wes08] M. Westrich, *Asymptotisch offene Quantensysteme*, Master's thesis, Universität Hamburg, II. Inst. f. Th. Physik, 2008, in German.

# Part IV

# Towards a Dynamical Renormalisation Group

CHAPTER 6

# Towards a Dynamical Renormalisation Group

V. BACH, J. S. MØLLER, M. WESTRICH

**Abstract**

In this paper we provide a detailed analysis of the long time dynamics of a spin boson model, restricted to low field energies. Assuming dilation analytic coupling functions, an effective generator for the atomic- and low energy photon degrees of freedom is derived. The effective generator is obtained as the unique solution of an implicit operator equation. We provide quantitative bounds on the approximation of the full dynamics by the effective dynamics. In the weak coupling limit regime, our result reproduces the well known results by Davies.

## 6.1 Introduction

We study the long time dynamics of an open quantum system consisting of a two–level atom weakly coupled to the environment, which is modelled by a massless boson field at zero temperature. Assuming dilation analyticity of the Hamiltonian, we derive an effective generator for the evolution of the atomic- and low energy photon degrees of freedom and provide quantitative errors in the coupling constant. In the weak coupling limit our result reproduces the well known results of Davies, [Dav74, Dav75, Dav76], for our model. We neither require Fermi golden rule nor an infrared regularisation. For the type of model we investigate, it is expected that the weak coupling limit in the sense of Davies cannot be extended to times beyond the van Hove timescale. Our paper is a first step to develop a renormalisation group analysis that provides for a given timescale $\tau_n = tg^{n+\epsilon}$, for a fixed $\epsilon \in [0,1)$, $n \in \mathbb{N}$, $n \geq 2$, an effective generator $H_{\mathrm{at}} + \mathfrak{T}_g^{(n)}(H_{\mathrm{f}})$ for the evolution of atomic- and low energy field degrees of freedom, as well as quantitative error bounds. The effective operator is obtained as the unique solution of an implicit operator equation.

The general strategy of this paper is to restrict to low momentum modes the complex deformed Hamiltonian dynamics of the full system and to analyse this object using the inverse (vector–valued) Laplace transform. The inverse Laplace transform expresses $C_0$–semigroups in terms of the resolvent of their generator. In spectral regions far from the unperturbed eigenstates, we obtain exponentially decaying error terms. For regions close to the unperturbed eigenvalues, we analyse the restricted resolvent by means of the Feshbach map. Estimates on the distance of a given contour to the spectrum of the unperturbed Hamiltonian allow to reduce the analysis to an "effective" Feshbach map. The residue theorem yields the effective dynamics, and its generator is determined by the "zeros" of the effective Feshbach map.

Our work is inspired by works on resonances over the past 30 years. Let

$$H_g := H_0 + gW,$$

where $H_0$ is assumed to be selfadjoint, $W$ is a relatively $H_0$–bounded perturbation of $H_0$. Then, assume that $\lambda$ is an eigenvalue of $H_0$ with finite multiplicity. It is known, that excited eigenvalues may be unstable if a perturbation is switched on and it is possible to estimate the decay of matrix elements,

$$\begin{aligned} (\psi, f(H_g)e^{-itH_g}\psi) &= \left(1+\mathcal{O}\left(g^2\right)\right)e^{-it\lambda(g)} + b\left(t,g\right), \ \mathrm{Im}\left(\lambda\left(g\right)\right) > 0, \\ \left|b\left(t,g\right)\right| &\leq o\left(g^2\right)\left(1+t\right)^{-n}, \quad n \in \mathbb{N},\ t \geq 0, \end{aligned} \tag{6.1}$$

provided Fermi's golden rule holds and the resolvent, $\left(H_g - z\right)^{-1}$, is sufficiently regular with respect to some auxiliary operator $A$. For our model, the resolvent is even analytic in a strip around the real axis with respect to the conjugation with the group generated by $A$. In the context of regular perturbation theory there are strong results on the decay rate of the resonances. These results usually assume a deformation analyticity of the Hamiltonian $H_g$, in order to separate the essential from the discrete spectrum. The first result which provided rigorous estimates on the decay law of resonances states is due to Hunziker, [Hun90]. He proves a relation of the type (6.1), but the error term $b\left(t,g\right)$ decays as $(1+t)^{-n}$ for any $n \in \mathbb{N}$. For finite regularity, i.e. if finitely many commutators of $\left(H_g - z\right)^{-1}$ and $A$ exist, Cattaneo, Graf and Hunziker proved in [CGH06] a similar result as Hunziker, but the decay of $b\left(t,g\right)$ is then related to the degree of regularity and does not hold for any $n \in \mathbb{N}$ any longer. Both results, [Hun90] and [CGH06], depend on the function $f\left(\cdot\right)$, which localises the group $e^{-itH_g}$ to a small interval around the eigenvalue $\lambda$. For a different choice of $f$, namely assuming that $f$ is of Gevrey class, Rama and Klein proved recently, [KR10], that for an abstract dilation analytic model that $b\left(t,g\right)$ is almost exponentially decaying,

$$\left|b\left(t,g\right)\right| \leq \mathcal{O}\left(g^2\right)e^{-Ct^{\frac{1}{a}}}, \quad C \leq ac^{\frac{1}{a}},$$

for any $a > 1$, $c > 0$ and $g$ sufficiently small. They also point out, that for semibounded Hamiltonians $H_g$, the absolute value of the matrix element (6.1) cannot be exponentially decaying. Namely, if (6.1) is exponentially bounded, i.e.

$$\left|(\psi, f(H_g)e^{-itH_g}\psi)\right| \leq Ce^{-C't}, \quad C, C' > 0,$$

a Payley–Wiener argument implies $\psi = 0$. Finally, in the case of finite temperature, Jaksic and Pillet used in [JP95, JP96a, JP96b] a complex deformation technique, a complex translation, which allows to deform Liouvilleans such that the discrete spectrum is separated from the essential spectrum, even if the reservoir arises from a massless field. In this vein, the problem becomes tractable by regular perturbation theory, whereas this is not possible for the generator of dilations.

In the context of singular perturbation theory, more specifically in massless quantum field theoretic models, resonances have first been analysed by Bach, Fröhlich and Sigal, [BFS98a]. Their analysis is based on the *isospectral Feshbach map*. The Feshbach map has as an intrinsic feature a reduction of state space. An iteration based on an repeated decimation of the state space leads to the construction of a *renormalisation group analysis*, which provides an algorithm to localise the resonance to arbitrary precision, [BFS98b, BCFS03]. The first result to determine the decay rate of (6.1) for dilation analytic, massless, quantum field theoretic models has been established in [BFS99], using a single step Feshbach map analysis. The result proved there is of the same type as the result by Hunziker, [Hun90]. In a more recent paper Hasler, Herbst and Huber proved also a lower bound on the decay rate of (6.1). Their analysis is also based on the Feshbach map, see [HHH08].

For open quantum systems one is interested in finding an effective evolution for the entire "small system", i.e. the atom. Assume that $H_0$ has $N$ eigenvalues with finite multiplicity, $E_\ell$, with spectral projections $P_\ell$, $\ell = 1, \ldots, N$. Moreover let $P_\ell W P_\ell = 0$, for $\ell = 1, \ldots, N$. If

$$\begin{aligned} M_\ell &:= P_\ell W \overline{P}_\ell \left( (E_\ell + i0)\, \overline{P}_\ell - H_0 \overline{P}_\ell \right)^{-1} \overline{P}_\ell W P_\ell \\ &:= \lim_{\epsilon \searrow 0} P_\ell W \overline{P}_\ell \left( (E_\ell + i\epsilon)\, \overline{P}_\ell - H_0 \overline{P}_\ell \right)^{-1} \overline{P}_\ell W P_\ell, \end{aligned}$$

exists for $\ell = 1, \ldots, N$, we define the *level shift operator (LSO)*, as

$$M := -i \sum_{\ell=1}^{N} P_\ell W \overline{P}_\ell \left( (E_\ell + i0)\, \overline{P}_\ell - H_0 \overline{P}_\ell \right)^{-1} \overline{P}_\ell W P_\ell. \tag{6.2}$$

There are several notions of *Fermi golden rule (FGR)*, depending on the problem one has in mind. Following [DF06], there are three types of FGR involving the LSO:

1. **Analytic Fermi golden rule:** $H_0 P + g^2 M$, $P := \sum_{\ell=1}^{N} P_\ell$, predicts up to an error $o\left(g^2\right)$ the location and multiplicity of the resonances and eigenvalues of $H_g$ in a neighbourhood of the spectrum of $H_0$, $\sigma\left(H_0\right)$, for small $|g|$.

2. **Spectral Fermi golden rule:** The intersection

$$\sigma\left(H_0 P + g^2 M\right) \cap \mathbb{R},$$

predicts the possible location of eigenvalues of $H_g$, for small $|g| \neq 0$.

3. **Dynamical Fermi golden rule:** The semigroup

$$\left\{\exp\left(-it\left(H_0 P + g^2 M\right)\right)\right\}_{t\geq 0},$$

describes approximately the reduced dynamics $PX(t)P$, for small $|g|$.

The dynamical Fermi golden rule has first been rigorously established by Davies, [Dav74, Dav75, Dav76] in form of a *weak coupling limit (WCL)*. Davies proved under mild assumptions

$$\lim_{g\to 0} e^{i\tau g^{-2} H_0 P} P e^{-i\tau g^{-2} H_g} P = e^{-i\tau M}. \tag{6.3}$$

Note, that the time has been subject to a rescaling, i.e. the weak coupling limit refers to a timescale where

$$\tau = tg^2, \tag{6.4}$$

which is sometimes referred to as the *van Hove timescale*. Results beyond this timescale are scarce, but see [Kos00] for the analysis of an explicitly solvable model.

Finally, in the context of positive temperature, Jaksic and Pillet proved, using *translation analyticity* facilitated by a novel method now usually referred to as *Jaksic–Pillet glueing*,

$$(\Psi, e^{-itH_g}\Phi) = (A\Psi, e^{-it\left(H_{\mathrm{at}} + \sum_{n=1}^{\infty} g^{2n} M^{(2n)}\right)} B\Phi) + \mathcal{O}\left(e^{-ct}\right),$$

for some operators $A, B$ and $t \to +\infty$, see [JP96a, Thm. 2.5]. Due to fundamental obstacles, this method cannot extended to the zero temperature case. In this case, one expects that the WCL cannot be extended to the original timescale, but one rather has to find "higher order" LSO's $M^{(n)}$, for a given timescale $\tau_n = tg^n$, $\epsilon \in [0, 1)$, $n \in \mathbb{N}$, $n \geq 2$. That is the eventual goal of our project.

This paper is organised as follows. In Section 6.1.1 we define the model and the spectral projections used in our analysis. Then, we introduce the complex dilation, provide an estimate on the numerical range of the complex dilated model and state our main result in Section 6.1.2. The proof if the main theorem is the content of Section 6.2 and finally in Section 6.3 we present heuristic ideas for an iteration of our analysis.

### 6.1.1 Definition of the model

We follow the convention of the literature, which may be found in [BCFS03]. To keep the analysis as simple as possible, we restrict ourselves to a 2-level atom described by the Hamiltonian

$$H_{\mathrm{at}} = H_{\mathrm{at}}^* \in \mathfrak{B}\left(\mathcal{H}_{\mathrm{at}}\right). \tag{6.5}$$

The corresponding Hilbert space is $\mathcal{H}_{\mathrm{at}} := \mathbb{C}^2$. The electromagnetic field will be simplified by neglecting the polarisation of the photons. The state space is then the *bosonic Fock space*

$$\mathcal{F} := \bigoplus_{n=0}^{\infty} \mathcal{S}_n \mathfrak{h}^{\otimes n}, \tag{6.6}$$

with

$$\mathfrak{h} := L^2(\mathbb{R}^3, d^3k), \tag{6.7}$$

the orthogonal projection onto the totally symmetric $n$-particle wave functions $\mathcal{S}_n$ and $\mathcal{S}_0\mathfrak{h}^{\otimes 0} = \mathbb{C} \cdot \{\Omega\}$. $\Omega$ is the vacuum vector of $\mathcal{F}$. The scalar product in $\mathcal{F}$ is defined as

$$(\Psi, \Phi) := \sum_{n=0}^{\infty} \int \prod_{j=1}^{n} d^3k_j \overline{\psi_n}(k_1, \ldots, k_n) \varphi_n(k_1, \ldots, k_n), \tag{6.8}$$

$\forall \Psi = (\psi_n)_{n\in\mathbb{N}}, \Phi = (\varphi)_{n\in\mathbb{N}} \in \mathcal{F}$. Clearly, any element in $\mathcal{F}$ may be identified by such sequences. Denote by $\mathcal{F}_{\mathrm{fin}}$ the subspace of elements $\Psi \in \mathcal{F}$ corresponding to finite sequences $\Psi = (\psi_n)_{n\in\mathbb{N}}$. Then, for $\varphi \in \mathfrak{h}$ we define $a(\varphi)\Psi =: \Phi$ as $\Phi = (\phi_n)$, with

$$\phi_n(k_1, \ldots, k_n) := \sqrt{n+1} \int d^3k \overline{\varphi}(k) \phi_{n+1}(k, k_1, \ldots, k_n) \tag{6.9}$$

and

$$a(\varphi)\Omega = 0. \tag{6.10}$$

The operator $a(\varphi)$ is closable and we denote its closure with the same symbol and call it the *annihilation operator*. The adjoint of $a(\varphi)$ with respect to the scalar product, $a^*(\varphi)$, is called the *creation operator*. Note, that $a(\varphi)$ is anti-linear in $\varphi$ and $a^*(\varphi)$ is linear, so that the symbolic notation

$$a(\varphi) = \int d^3k\, \overline{\varphi}(k)\, a(k), \quad a^*(\varphi) = \int d^3k\, \varphi(k)\, a^*(k)$$

becomes meaningful if $a(k), a^*(k)$ are interpreted as unbounded operator-valued distributions. They obey the *canonical commutation relations* (CCR)

$$[a^\sharp(k), a^\sharp(k')] = 0, \quad [a(k), a^*(k')] = \delta(k - k'). \tag{6.11}$$

Let $\omega(k) := |k|$, $k \in \mathbb{R}^3$. Then, we define $H_{\mathrm{f}}\Psi = (\phi_n)_{n\in\mathbb{N}}$, with

$$\phi_n(k_1, \ldots, k_n) := \left( \sum_{j=1}^{n} \omega(k_j) \right) \psi_n(k_1, \ldots, k_n), \; \forall \Psi \in \mathcal{F}_0. \tag{6.12}$$

The closure of $H_{\mathrm{f}}$ is self-adjoint and its spectrum consists of the positive real half–line with the simple eigenvalue 0,

$$\sigma(H_{\mathrm{f}}) = \mathbb{R}_{>0} \cup \{0\}. \tag{6.13}$$

This gives the representation

$$H_{\mathrm{f}} = \int d^3k\, a^*(k)\, \omega(k)\, a(k), \tag{6.14}$$

where the right hand side is to be understood as a weak integral. The state space of the combined system is

$$\mathcal{H} := \mathcal{H}_{\mathrm{at}} \otimes \mathcal{F}. \tag{6.15}$$

On the domain $\mathcal{H}_{\mathrm{at}} \otimes \mathcal{D}(H_{\mathrm{f}})$ one observes $H_0 := H_{\mathrm{at}} \otimes \mathbb{1} + \mathbb{1} \otimes H_f$ to be a selfadjoint operator, since $\mathcal{H}_{\mathrm{at}}$ is finite dimensional. Next, we define the coupled system. The *(Segal) field operator* is defined as

$$\phi(gG) := g \int_{\mathbb{R}^3} d^3k \, \{G(k)\, a^*(k) + G^*(k)\, a(k)\}, \tag{6.16}$$

with $G \in L^2(\mathbb{R}^3, \mathbb{C}^{2\times 2})$ and $g \geq 0$, on the dense domain $\mathcal{H}_{\mathrm{at}} \otimes \mathcal{F}_{\mathrm{fin}}$. Since $\phi(gG)$ is symmetric, it is closable. The operator $\phi(gG)$ is infinitesimally $H_0$-bounded on $\mathcal{H}_{\mathrm{at}} \otimes (\mathcal{D}(H_{\mathrm{f}}) \cap \mathcal{F}_{\mathrm{fin}})$ and thus

$$H_g := H_0 + \phi(gG) \tag{6.17}$$

is selfadjoint on the domain of $H_0$ for any choice of $g$. As a short hand we introduce the notation

$$a(gG) := g \int_{\mathbb{R}^3} d^3k \, G(k)\, a(k)\,, \;\; a^*(gG) := g \int_{\mathbb{R}^3} d^3k \, G(k)\, a^*(k). \tag{6.18}$$

We use the following spectral projections in order to reduce the field degrees of freedom. Let

$$P_\rho := \mathbf{1}[H_{\mathrm{f}} < \rho]\,, \; P_\rho^\perp := \mathbb{1} - P_\rho, \tag{6.19}$$

$$P := \mathbb{1} \otimes \mathbf{1}[H_{\mathrm{f}} < \rho]\,, \; \overline{P} := \mathbb{1} - P. \tag{6.20}$$

It will be useful to also define the following projections on the range of $P$, i.e.

$$P_{\mathrm{at},\ell} := \mathbf{1}[H_{\mathrm{at}} = E_\ell] \otimes P_\rho, \; \overline{P}_{\mathrm{at},\ell} := \mathbb{1}_{P\mathcal{H}} - P_{\mathrm{at},\ell} = \mathbf{1}[H_{\mathrm{at}} = E_\ell]^\perp \otimes P_\rho. \tag{6.21}$$

### 6.1.2 Spectral deformation and main result

Let $f \in \mathfrak{h}$ and define the unitary strongly continuous one–parameter group of dilations, $u(\cdot)$, on the space $\mathfrak{h}$ by $(u(\alpha)f)(r,\Omega) := e^{-\frac{3}{2}\alpha} f(e^{-\alpha}r, \Omega)$, using *polar coordinates*, $(r,\Omega)$. Its second quantised analogue is denoted by $U(\alpha) := \Gamma(u(\alpha))$. We will use the convenient Hilbert space $\mathfrak{h}_\omega$ consisting of all $f \in \mathfrak{h}$ such that $\|f\|_{\mathfrak{h}_\omega}^2 := \|f\|^2 + \left\|\omega^{-1/2} f\right\|^2 < \infty$. Moreover, for matrix–valued functions, like $G_\alpha$, we use the convention that the norm is the operator norm on $\mathfrak{B}(\mathbb{C}^2)$ and we write again $\|G\|_{\mathfrak{h}_\omega}$ if $G$ is matrix–valued.

**Condition 6.1 (Coupling functions).**
Let $\xi_0 \in \left(0, \frac{\pi}{2}\right)$ and $G \in L^2(\mathbb{R}^3, \mathfrak{B}(\mathcal{H}_{\mathrm{at}}))$. The map $\mathbb{R} \ni \alpha \mapsto G_\alpha := u(\alpha)G$ extends to an analytic function in the strip $I(\xi_0) := \mathbb{R} + i(-\xi_0, \xi_0)$ and

$$\sup_{|\theta| < \xi_0} \|G_{\alpha + i\theta}\|_{\mathfrak{h}_\omega} < \infty. \tag{6.22}$$

Moreover,

$$G(k) = G(|k|), \quad (G(k))_{\ell\ell} = 0, \quad \forall k \in \mathbb{R}^3,\ \ell = 0, 1. \tag{6.23}$$

There is a $c_{6.1} \in \mathbb{R}_+$, such that

$$\|G(k)\| \leq \frac{c_{6.1}}{\sqrt{|k|}}, \quad \forall k \in \mathbb{R}^3. \tag{6.24}$$

Finally, assume that $\|G(k)\| \to 0$ sufficiently rapid, as $|k| \to \infty$. We refer to the sufficiently fast convergence $\|G(k)\| \to 0$ as the *ultraviolet cutoff*.

For any bounded operator $A \in \mathfrak{B}(\mathcal{H})$, we write

$$A_\alpha := U(\alpha) A U^*(\alpha),\ \alpha \in \mathbb{R}. \tag{6.25}$$

$U$ leaves the domain of $H_0$, $\mathcal{D}(H_0)$, invariant and one easily computes

$$H_{0,\alpha} = H_{\mathrm{at}} + e^{-\alpha} H_{\mathrm{f}},\ \forall \alpha \in \mathbb{R}. \tag{6.26}$$

For any $z \in \mathbb{C}$ with $|\operatorname{Arg}_\pi(z)| > \xi_0$, the resolvent, $R_\alpha(z) := (z - H_{0,\alpha})^{-1}$ extends to an analytic function of $\alpha$ in the strip $I(\xi_0)$, as a consequence of the first resolvent identity. $\operatorname{Arg}_a$ denotes the argument function with cut at $a \in (-\pi, \pi]$. For any $\alpha \in \mathbb{C}$,

$$H_{0,\alpha} = H_{\mathrm{at}} + e^{-\alpha} H_{\mathrm{f}},$$

is a closed operator on $\mathcal{H}_{\mathrm{at}} \otimes \mathcal{D}(H_{\mathrm{f}})$, as $\mathcal{H}_{\mathrm{at}}$ is finite dimensional. From the selfadjointness of $H_{\mathrm{at}}$ and $H_{\mathrm{f}}$ follows that the adjoint of $H_{0,\alpha}$ is a closed operator on $\mathcal{H}_{\mathrm{at}} \otimes \mathcal{D}(H_{\mathrm{f}})$ and

$$H_{0,\alpha}^* = H_{\mathrm{at}} + e^{-\bar{\alpha}} H_{\mathrm{f}}. \tag{6.27}$$

Since

$$\left[H_{0,\alpha}, H_{0,\alpha}^*\right] = 0$$

as a quadratic form on $\mathcal{H}_{\mathrm{at}} \otimes \mathcal{D}(H_{\mathrm{f}})$, it follows that $H_{0,\alpha}$ is a *normal* operator. Moreover, one may observe

$$\sigma(H_{0,\alpha}) = \sigma(H_{\mathrm{at}}) + e^{-\alpha}\sigma(H_{\mathrm{f}}),\ \forall \alpha \in \mathbb{C}. \tag{6.28}$$

Pick now $\xi \in I(\xi_0)$. Then, since $H_{0,\xi}$ is normal it follows from (6.28) that

$$\left\|R_\xi(z)\right\| \leq \frac{1}{\operatorname{dist}\left(z, \{E_0, E_1\} + e^{-\xi}\mathbb{R}_0^+\right)}. \tag{6.29}$$

Hille–Yosida's theorem implies that $H_{0,\xi}$ generates a contraction semigroup and as one easily observes also an analytic semigroup. Next we shall define the "analytic continuation" of the dilated field operator, $\phi(G_\alpha)$, $\alpha \in \mathbb{R}_+$. Let $\xi \in I(\xi_0)$ be as above. Then, on the domain $\mathcal{H}_{\mathrm{at}} \otimes \mathcal{F}_{\mathrm{fin}}$ we define

$$\check{\phi}(G_\xi) := \frac{1}{\sqrt{2}}\left(a\left(G_{\bar{\xi}}\right) + a^\dagger(G_\xi)\right). \tag{6.30}$$

Note, that we used $\bar{\xi}$ for the annihilation operator, $a(\cdot)$, since it is anti-linear in the argument. Hence there is a $C_\xi \in \mathbb{R}_+$, depending on $\xi$, $\|G_\xi\|_{\mathfrak{h}_\omega}$, $\left\|G_{\bar{\xi}}\right\|_{\mathfrak{h}_\omega}$, such that

$$\left\|\check{\phi}\left(G_\xi\right)\left(H_\mathrm{f}+\mathbb{1}\right)^{-\frac{1}{2}}\right\| \leq C_\xi. \tag{6.31}$$

On the domain $\mathcal{H}_\mathrm{at} \otimes \mathcal{D}\left(H_\mathrm{f}\right)$ we define the closed operator

$$H_{g,\xi} := H_{0,\xi} + \check{\phi}\left(gG_\xi\right). \tag{6.32}$$

As $\check{\phi}\left(G_\xi\right)$ is infinitesimally $H_\mathrm{f}$ bounded and $H_{0,\xi}$ generates an analytic semigroup, one may observe by [Kat76, Thm. IX.2.4] that $H_{g,\xi}$ generates also an analytic semigroup. Moreover, $\left\{H_{g,\xi}\right\}_{\xi \in I(\xi_0)}$ is an analytic family of type A. For later reference, we introduce the constants

$$\eta_0 := e^{-\mathrm{Re}(\xi)} \sin\left(\mathrm{Im}\left(\xi\right)\right), \quad \eta_1 := e^{-\mathrm{Re}(\xi)} \cos\left(\mathrm{Im}\left(\xi\right)\right). \tag{6.33}$$

**Proposition 6.2 (Numerical range of $H_{g,\xi}$).** *For any $g \in \mathbb{R}$, and $M > 1$, the numerical range of $H_{g,\xi}$, denoted by* $\mathrm{NumRan}\left(H_{g,\xi}\right)$, *is contained in*

$$\mathrm{NumRan}\left(H_{g,\xi}\right) \subseteq \mathcal{NR}\left(H_{g,\xi}\right) := \left[E_0, E_1\right] + e^{-\xi}\mathcal{K}_{\frac{M}{M-1}} + \overline{D}\left(\left|e^{\xi}\right| c^2 g^2 M\right), \tag{6.34}$$

*with*

$$\mathcal{K}_\beta := \left\{ re^{i\alpha} \middle| \, r \geq 0, \quad \alpha \in \left[-\beta, \beta\right]\right\} \tag{6.35}$$

*and*

$$\overline{D}\left(r\right) := \left\{z \in \mathbb{C} \middle| \, |z| \leq r\right\}. \tag{6.36}$$

*For $g = 0$ one has*

$$\mathrm{NumRan}\left(H_{0,\xi}\right) \subseteq \left[E_0, E_1\right] + e^{-\xi}\left[0, \infty\right). \tag{6.37}$$

*Proof.* Let $\varepsilon > 0$. Note first that

$$\left\|a\left(G_{\bar{\xi}}\right)\left(H_\mathrm{f}+\varepsilon\right)^{-\frac{1}{2}}\right\| \leq \left\|\omega^{-\frac{1}{2}} G_{\bar{\xi}}\right\|_{L^2(\mathbb{R}^3, \mathfrak{B}(\mathcal{H}_\mathrm{at}))}. \tag{6.38}$$

This implies

$$\left\|\left(H_\mathrm{f}+\varepsilon\right)^{-\frac{1}{2}} \check{\phi}\left(G_\xi\right)\left(H_\mathrm{f}+\varepsilon\right)^{-\frac{1}{2}}\right\| \leq 2\varepsilon^{-\frac{1}{2}} \left\|\omega^{-\frac{1}{2}} G_{\bar{\xi}}\right\|_{L^2(\mathbb{R}^3, \mathfrak{B}(\mathcal{H}_\mathrm{at}))}. \tag{6.39}$$

From now on we write $\|\cdot\|_{L^2}$ for $\|\cdot\|_{L^2(\mathbb{R}^3, \mathfrak{B}(\mathcal{H}_\mathrm{at}))}$ and abbreviate $c := 2\left\|\omega^{-\frac{1}{2}} G_{\bar{\xi}}\right\|_{L^2}$. Hence, for all $\psi \in \mathcal{H}_\mathrm{at} \otimes \mathcal{D}\left(H_\mathrm{f}^{\frac{1}{2}}\right)$ we obtain

$$\begin{aligned} \left|\left(\psi, \check{\phi}\left(gG_\xi\right)\psi\right)\right| &\leq \frac{gc}{\sqrt{\varepsilon}}\left(\psi, \left(H_\mathrm{f}+\varepsilon\right)\psi\right) \\ &= \frac{gc}{\sqrt{\varepsilon}}\left(\psi, H_\mathrm{f}\psi\right) + g\varepsilon^{\frac{1}{2}} c \left\|\psi\right\|^2. \end{aligned} \tag{6.40}$$

Then, for all $\psi \in \mathcal{H}_{\mathrm{at}} \otimes \mathcal{D}\left(H_{\mathrm{f}}^{\frac{1}{2}}\right)$, $\|\psi\| = 1$, we compute for the full Hamiltonian

$$\left(\psi, H_{g,\xi}\psi\right) = \left(\psi, H_{\mathrm{at}}\psi\right) + e^{-\xi}\left(1 + \zeta\left(\psi\right)\right)\left(\psi, H_{\mathrm{f}}\psi\right) + \widetilde{\zeta}\left(\psi\right), \tag{6.41}$$

where

$$\zeta\left(\psi\right) := e^{\xi}\frac{\left(\psi, \check{\phi}\left(gG_{\xi}\right)\psi\right)}{\left(\psi, \left(H_{\mathrm{f}} + \varepsilon\right)\psi\right)}, \quad \widetilde{\zeta}\left(\psi\right) := \rho\frac{\left(\psi, \check{\phi}\left(gG_{\xi}\right)\psi\right)}{\left(\psi, \left(H_{\mathrm{f}} + \varepsilon\right)\psi\right)}. \tag{6.42}$$

Note that

$$\left|\zeta\left(\psi\right)\right| \le \left|e^{\xi}\right| cg\varepsilon^{-\frac{1}{2}}, \qquad \left|\widetilde{\zeta}\left(\psi\right)\right| \le cg\varepsilon^{\frac{1}{2}}. \tag{6.43}$$

Moreover, choose $\varepsilon := \left(\left|e^{\xi}\right| cMg\right)^2$, for $M > \left(\frac{\pi}{3} - 1\right)^{-1}$,

$$\left|\mathrm{Arg}\left(1 + \zeta\left(\psi\right)\right)\right| = \left|\arctan\left(\frac{\mathrm{Im}\left(\zeta\right)}{1 + \mathrm{Re}\left(\zeta\right)}\right)\right| \le \frac{M}{M-1}. \tag{6.44}$$

Putting the estimates (6.41), (6.43) and (6.44) together, we arrive at (6.34). The case $g = 0$ is easily obtained. □

**Remark 6.3.** Note that in Proposition 6.2 for $M > \left(\frac{\pi}{3} - 1\right)^{-1}$ the opening angle of $\mathcal{K}_{\frac{M}{M-1}}$ is less than $\pi/3$, but that opening angle of $\mathcal{K}_{\frac{M}{M-1}}$ is always less than 1. Since $H_{g,\xi}$ is a normal operator for all $g \in \mathbb{R}$, it follows from Proposition 6.2 and Hille–Yosida's theorem, that $H_{g,\xi}$ generates a $C_0$–semigroup. We denote the semigroup generated by $H_{g,\xi}$ with $\left\{X\left(t\right)\right\}_{t \in \mathbb{R}_0^+}$ if $g \neq 0$ and with $\left\{Y\left(t\right)\right\}_{t \in \mathbb{R}_0^+}$ for $g = 0$. Proposition 6.2 provides also exponential bounds on the semigroups $\left\{X\left(t\right)\right\}_{t \in \mathbb{R}_0^+}$, $\left\{Y\left(t\right)\right\}_{t \in \mathbb{R}_0^+}$, namely

$$\left\|X\left(t\right)\right\| \le e^{2\left|e^{\xi}\right| c^2 g^2 M t}, \qquad \left\|Y\left(t\right)\right\| \le 1, \tag{6.45}$$

for all $t \in \mathbb{R}_0^+$.

We are now prepared to state our main result.

**Theorem 6.4.** *Let*

$$X_{g,\xi}\left(t\right) := e^{-itH_{g,\xi}}$$

*and* $\rho = g^{\mu}$, $\mu \in (0,2)$, *and pick* $\nu \in \left(0, \min\left(1, \mu^{-1} - \frac{1}{2}\right)\right)$. *There is a bounded operator,*

$$\Xi_{g,\xi}\left(H_{\mathrm{f}}\right) := \sum_{\ell=0,1} z_{\ell}\left(H_{\mathrm{f}}\right) P_{\mathrm{at},\ell} \in \mathfrak{B}\left(P\mathcal{H}\right)$$

*and bounded operators* $z_{\ell}\left(H_{\mathrm{f}}\right) \in \mathfrak{B}\left(P_{\mathrm{at},\ell}\mathcal{H}\right)$, *such that*

$$E_{\ell} + e^{-\xi}r - z_{\ell}\left(H_f\right) - g^2\widetilde{\Lambda}_{11}\left(r, z_{\ell}\left(H_f\right)\right) = 0, \quad \ell = 0, 1 \tag{6.46}$$

*where for* $\ell = 0, 1$, $r \in [0, \rho]$

$$\widetilde{\Lambda}_{\ell\ell}\left(r, z\right) := \int_0^{\infty} dk\, \frac{e^{-3\xi}k^2\left|\left(G\right)_{(1-\ell)\ell}\left(e^{-\xi}k\right)\right|^2}{E_{1-\ell} + e^{-\xi}\left(r + k\right) - z}. \tag{6.47}$$

*For any $t \in \mathbb{R}_+$,*

$$\left\| \mathbf{1}\left[H_\mathrm{f} < \rho\right] X_{g,\xi}\left(t\right) \mathbf{1}\left[H_\mathrm{f} < \rho\right] - e^{-it\Xi_{g,\xi}(H_\mathrm{f})} \right\| \\ \leq C\left(e^{-tc_\delta} + e^{c_1 g^2 \rho^\nu t}\left(\rho^{\frac{1-\nu}{2}} + g^{\frac{1}{2}} \rho^{-\frac{1}{2}\left(\nu + \frac{1}{2}\right)}\right)\right),$$

*for some $C, c_0, c_1, c_\delta \in \mathbb{R}_+$, which are independent of $g$. Moreover, for $\ell = 0, 1$, and $r \in [0, \rho]$,*

$$\Xi_{g,\xi}\left(r\right) P_{\mathrm{at},\ell} = \left(E_\ell + e^{-\xi} r - g^2 \widetilde{\Lambda}_{\ell\ell}\left(0, E_\ell\right)\right) P_{\mathrm{at},\ell} + \mathcal{O}\left(g^2 \rho\right).$$

**Remark 6.5.** (i) It is possible to relate $\widetilde{\Lambda}_{\ell\ell}\left(0, E_\ell\right)$ to objects which are $\xi$ independent. For the ground state, $\ell = 0$, this yields a correction in second order of $g$ with vanishing imaginary part $= 0$. For the excited state, $\ell = 1$, the obtained correction has a negative imaginary part, provided Fermi Golden Rule holds.
(ii) To our knowledge, the evolution of the ground state has previously not been addressed in singular perturbation theory. Note, that the error contains an exponentially growing factor, $e^{c_1 g^2 \rho^\nu t}$, which is due to contributions of the ground state. This exponential growth is however of a mild type, as it becomes constant on the van Hove timescale, where $tg^2 =$ const. as $g \to 0$.
(iii) The optimal choice of $\mu$ depends on the value of $t$. If one chooses $\mu = \frac{2}{3}$, then $\rho^{\frac{1-\nu}{2}} = g^{\frac{1}{2}} \rho^{-\frac{1}{2}\left(\nu + \frac{1}{2}\right)}$.
(iv) Our result reproduces Davies results in the weak coupling limit, but also provides quantitative bounds.

## 6.2 Effective Dynamics on the van Hove Timescale

The present section is devoted to a quantitative analysis of second order perturbation theory. There are two recurrent quantities which are important in our analysis.

**Definition 6.6 (Control quantities).** Define for any $\epsilon, \epsilon' \geq 0$ the sets

$$\mathcal{A}^{(\ell)}_{\epsilon,\epsilon'} := \overline{B_\epsilon\left(E_\ell\right)} + e^{-\xi}\left[\epsilon', \infty\right), \quad \ell = 0, 1 \tag{6.48}$$

and

$$\mathcal{A}_{\epsilon,\epsilon'} := \mathcal{A}^{(0)}_{\epsilon,\epsilon'} \cup \mathcal{A}^{(1)}_{\epsilon,\epsilon'}. \tag{6.49}$$

For any $z \in \mathbb{C} \backslash \left(\mathcal{A}_{0,0} \cap \mathcal{A}^c_{0,\rho}\right)$, $\mathcal{A}^c_{0,\rho} := \mathbb{C} \backslash \mathcal{A}_{0,\rho}$, define

$$\mathfrak{d}_\rho\left(z\right) := \left\| \frac{P}{H_0 - z} \right\|. \tag{6.50}$$

Moreover, for any $z \in \mathcal{A}_{0,\epsilon}$ set

$$\mathfrak{z}_\varepsilon\left(z\right) := \left\| \left(H_\mathrm{f} + \rho\right)^{\frac{1}{2}} \left(\frac{\mathbf{1}\left[H_\mathrm{f} \geq \varepsilon\right]}{H_0 - z}\right) \left(H_\mathrm{f} + \rho\right)^{\frac{1}{2}} \right\|, \tag{6.51}$$

provided the right hand side is finite.

**Remark 6.7.** We remark, that the notation of (6.51) does not explicitly refer to its $\rho$–dependence due to the factors $(H_{\mathrm{f}}+\rho)^{\frac{1}{2}}$. This is done to ease the notation in the upcoming estimates.

We start with the identification of the leading contribution to the dynamics generated by (6.32). From now on, we drop the $\xi$–dependence in $H_{g,\xi}$ and $H_{0,\xi}$.

**Proposition 6.8 (Effective Feshbach operator – I).** *Let $\varepsilon \in (0,\rho)$. For any $z \in \mathcal{A}_{\rho,\rho}$ define*

$$
\begin{aligned}
F_P\left(H_g - z\right) &= PH_gP - zP - g^2 PW\bar{P}\left(\bar{P}H_g\bar{P} - z\bar{P}\right)^{-1}\bar{P}WP, &(6.52)\\
\widetilde{F}_P(z) &:= PH_gP - zP - g^2\Lambda_\rho\left(H_{\mathrm{f}}, z\right), &(6.53)
\end{aligned}
$$

*with*

$$
\begin{aligned}
\Lambda_\rho\left(H_{\mathrm{f}}, z\right) \quad := \quad & \int_{\mathbb{R}^3} d^3k\, G^*_{\bar{\xi}}(k)\left(H_{\mathrm{at}} + e^{-\xi}\left(H_{\mathrm{f}} + \omega(k)\right) - z\right)^{-1} \qquad (6.54)\\
& \times G_\xi(k)\, \boldsymbol{1}\left[H_{\mathrm{f}} + \omega(k) \geq \rho\right] P.
\end{aligned}
$$

*The operators $\widetilde{F}_P(z)$ and $F_P\left(H_g - z\right)$ exist and are bounded. Set*

$$
c_{6.8} := \max_{|\xi| \leq |\xi_0|}\left\{\left\|\omega^{-\frac{1}{2}}\overline{G_{\bar{\xi}}}\right\|_{L^2(\mathbb{R}^3,\mathbb{C})}, \left\|\omega^{-\frac{1}{2}}G_\xi\right\|_{L^2(\mathbb{R}^3,\mathbb{C})}\right\} < \infty. \qquad (6.55)
$$

*If*

$$
c_{6.8}\mathfrak{z}_\rho(z)\, g < \frac{1}{2}\sqrt{\rho}, \qquad (6.56)
$$

*then there is a $C \in \mathbb{R}_+$, such that*

$$
\left\|F_P\left(H_g - z\right) - \tilde{F}_P(z)\right\| \leq C\left(\mathfrak{z}_\rho(z)\, g^2\rho + \mathfrak{z}_\rho(z)^2 g^3 \rho^{-\frac{1}{2}}\right). \qquad (6.57)
$$

*Proof.* We estimate the following terms:

$$
A_1(z) := g^2 PW\bar{P}\left(\left(\bar{P}H_g\bar{P} - z\bar{P}\right)^{-1} - \left(H_0\bar{P} - z\bar{P}\right)^{-1}\right)\bar{P}WP, \qquad (6.58)
$$

$$
\begin{aligned}
A_2(z) \quad := \quad g^2 & \int_{B_\rho(0)\times B_\rho(0)} d^3k_1 d^3k_2\, \boldsymbol{1}\left[H_{\mathrm{f}} + \omega(k_1) + \omega(k_2) \geq \rho\right]\\
& Pa^*(k_2)\, G^*_{\bar{\xi}}(k_1)\left(H_{\mathrm{at}} + e^{-\xi}\left(H_{\mathrm{f}} + \omega(k_1) + \omega(k_2)\right) - z\right)^{-1}\\
& G_\xi(k_2)\, a(k_1)\, P. \qquad (6.59)
\end{aligned}
$$

Observe that a Neumann series expansion and (6.56) yield

$$\begin{aligned}
\|A_1(z)\| &\leq \sum_{n=2}^{\infty} \left\| PW\left(\bar{R}_0(z)\, gW\right)^n P \right\| \\
&\leq 2\rho \sum_{n=2}^{\infty} g^{n+1} \left\| (H_\mathrm{f}+\rho)^{-\frac{1}{2}} W (H_\mathrm{f}+\rho)^{-\frac{1}{2}} \right\|^{n+1} \\
&\qquad \cdot \left\| (H_\mathrm{f}+\rho)^{\frac{1}{2}} \bar{R}_0(z) (H_\mathrm{f}+\rho)^{\frac{1}{2}} \right\|^{n} \\
&\leq 2\mathfrak{z}_\rho(z)^2 \rho \left( \frac{c_{6.8}g}{\sqrt{\rho}} \right)^3 \sum_{n=0}^{\infty} \left( \frac{c_{6.8}\mathfrak{z}_\rho(z)\, g}{\sqrt{\rho}} \right) \\
&\leq \frac{2\rho}{\mathfrak{z}_\rho(z)} \left( \frac{c_{6.8}\mathfrak{z}_\rho(z)\, g}{\sqrt{\rho}} \right)^3 \frac{1}{1-\frac{c_\xi \mathfrak{z}_\rho(z) g}{\sqrt{\rho}}} \\
&\leq \frac{4\rho}{\mathfrak{z}_\rho(z)} \left( \frac{c_{6.8}\mathfrak{z}_\rho(z)\, g}{\sqrt{\rho}} \right)^3 = 4c_{6.8}^3 \mathfrak{z}_\rho(z)^2 \rho^{-\frac{1}{2}} g^3,
\end{aligned} \tag{6.60}$$

where $\bar{R}_0(z) := (H_0 - z)^{-1} \bar{P}$. Moreover, let $\psi_1, \psi_2 \in \mathcal{H}$, with $\|\psi_1\| = \|\psi_2\| = 1$. Then,

$$\begin{aligned}
&|(\psi_2, A_2(z)\,\psi_1)| \\
\leq\ & 2g^2 \int_{B_\rho(0)\times B_\rho(0)} d^3k_1 d^3k_2 \, \|G_\xi^*(k_1)\| \, \|G_\xi(k_2)\| \\
&\cdot \left\| \frac{(H_\mathrm{f}+\omega(k_1)+\omega(k_2)+\rho)\, \mathbf{1}\left[H_\mathrm{f}+\omega(k_1)+\omega(k_1) \geq \rho\right]}{\left(H_\mathrm{at}+e^{-\xi}(H_\mathrm{f}+\omega(k_1)+\omega(k_2))-z\right)} \right\| \\
&\cdot \prod_{j=1}^{2} \left\| (H_\mathrm{f}+\omega(k_1)+\omega(k_2)+\rho)^{-\frac{1}{2}} a(k_j)\, P\psi_j \right\| \\
\leq\ & 2\mathfrak{z}_\rho(z)\, g^2 \int_{B_\rho(0)\times B_\rho(0)} d^3k_1 d^3k_2 \left\| G_\xi^*(k_1) \right\| \|G_\xi(k_2)\| \\
&\cdot \prod_{j=1}^{2} \left\| (H_\mathrm{f}+\omega(k_1)+\omega(k_2)+\rho)^{-\frac{1}{2}} a(k_j)\, P\psi_j \right\| \\
\leq\ & 2\mathfrak{z}_\rho(z)\, g^2 \int_{B_\rho(0)\times B_\rho(0)} d^3k_1 d^3k_2 \left\| \frac{G_\xi^*(k_1)}{\sqrt{\omega}(k_1)} \right\| \left\| \frac{G_\xi(k_2)}{\sqrt{\omega}(k_2)} \right\| \\
&\cdot \prod_{j=1}^{2} \left\| \omega^{\frac{1}{2}}(k_j)\, a(k_j)\, (H_\mathrm{f}+\rho)^{-\frac{1}{2}} P\psi_j \right\| \\
\leq\ & C\mathfrak{z}_\rho(z)\, g^2 \rho \prod_{j=1}^{2} \left( \psi_j, \frac{H_\mathrm{f}}{H_\mathrm{f}+\rho} \psi_j \right) \\
\leq\ & C\mathfrak{z}_\rho(z)\, g^2 \rho,
\end{aligned} \tag{6.61}$$

where we used the Cauchy-Schwarz inequality for the third estimate and, as a consequence of (6.24),

$$\left\| \omega^{-\frac{1}{2}} G_\xi^*(k_1) \right\|_{L^2(B_\rho(0))}, \left\| \omega^{-\frac{1}{2}} G_\xi \right\|_{L^2(B_\rho(0))} \leq C\rho.$$

□

In the following we use the inverse Laplace transform to determine the effective evolution on the van Hove timescale of

$$X(t) = \frac{1}{2\pi i} \lim_{N\to\infty} \int_{-N}^{N} dx\, e^{-i(x+ic)t} P \left(H_g - (x+ic)\right)^{-1} P, \tag{6.62}$$

where $c \in \mathbb{R}_+ = (0,\infty)$ is chosen sufficiently large. The integral is understood as a strong integral in $\mathcal{H}$. We intend to deform the contour of the integral above appropriately in several spectral regions. Let $\Gamma$ be a curve in the resolvent set of $H_g$ and define

$$\forall t \in \mathbb{R}_+ : \qquad X_\Gamma(t) := \frac{1}{2\pi i} \int_\Gamma dz\, e^{-izt} P \left(H_g - z\right)^{-1} P, \tag{6.63}$$

provided the integral exists in norm. Note, that this implies restrictions on the possible choices of $\Gamma$. Observe that for any $c' \in (-\infty, 0] \cup \{-\infty\}$,

$$\lim_{N\to\infty} \int_{c'}^{c} dy\, e^{-i(\pm N+iy)t} P \left(H_g - (\pm N + iy)\right)^{-1} P = 0.$$

Therefore, and by the analyticity of the integrand, we may always bend the domain of integration in (6.62) far from the spectral points $E_0$, $E_1$ to the lower half plane. Next we define a family of admissible paths in the complex plane, to which the domain (6.62) will be deformed, see also Figure 6.1.

**Definition 6.9 (The contour Γ).** Let $4\delta := E_1 - E_0$, $\rho = g^\mu$, $\mu \in (0,2)$, pick $\nu \in \left(0, \min\left(1, \mu^{-1} - \frac{1}{2}\right)\right)$ and $c_\ell \in \mathbb{R}_+$, $\ell = 0,1$. A curve $\Gamma \subset \mathbb{C}$, consisting of pieces $\Gamma_j$ for $j = \mathrm{le}, 0, \mathrm{m}, 1, \mathrm{ri}$, such that

$$\Gamma = \Gamma_{\mathrm{le}} \cup \Gamma_0 \cup \Gamma_{\mathrm{m}} \cup \Gamma_1 \cup \Gamma_{\mathrm{ri}} \tag{6.64}$$

and

$$\Gamma \cap \mathcal{A}_{0,0} = \emptyset, \tag{6.65}$$

is called *admissible* iff the following requirements are met. There are intervals

$$J_0 = [a_0, b_0],\ J_1 = [a_1, b_1],\ J_{\mathrm{le}} = (-\infty, 0],\ J_{\mathrm{m}} = [0,1],\ J_{\mathrm{ri}} = [0,\infty)$$

such that $\gamma_j \in C^1(J_j, \Gamma_j)$, is a continuously differentiable parametrisation of $\Gamma_j$ for $j = \mathrm{le}, 0, \mathrm{m}, 1, \mathrm{ri}$. Moreover:

1. $\gamma_{\mathrm{le}}(0) = E_0 - \delta e^{\frac{i}{2}\mathrm{Im}(\xi)}$ and
$$\gamma_{\mathrm{le}}(x) = \gamma_{\mathrm{le}}(0) + x e^{\frac{i}{2}\mathrm{Im}(\xi)}. \tag{6.66}$$
2. $\gamma_0(a_0) = \gamma_{\mathrm{le}}(0)$, $\gamma_0(b_0) = E_0 + \delta e^{-\frac{i}{2}\mathrm{Im}(\xi)}$ and
$$\mathrm{Im}(\gamma_0(x)) := c_0 g^2 \rho^\nu, \tag{6.67}$$
if
$$x \in \gamma_0^{-1}\left(\left\{ z \in \Gamma_0 \middle| \mathrm{Re}(z) \in \left[E_0 - \frac{\delta}{4}, E_0 + \frac{\delta}{4}\right]\right\}\right), \tag{6.68}$$

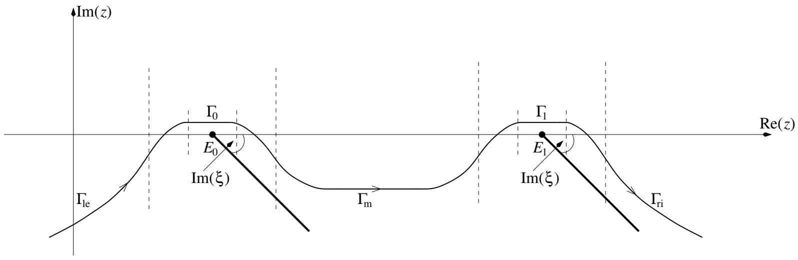


Figure 6.1: The contour Γ.

3. $\forall x \in [0,1]$,

$$\gamma_{\mathrm{m}}(x) := x\gamma_0(b_0) + (1-x)\gamma_1(a_1) \tag{6.69}$$

4. $\gamma_1(a_1) = E_1 - \delta e^{\frac{i}{2}\mathrm{Im}(\xi)}$, $\gamma_1(b_1) = E_1 + \delta e^{-\frac{i}{2}\mathrm{Im}(\xi)}$ and

$$\mathrm{Im}(\gamma_1(x)) := c_1 g^2 \rho^{\nu}, \tag{6.70}$$

   if

$$x \in \gamma_1^{-1}\left(\left\{ z \in \Gamma_1 \middle| \mathrm{Re}(z) \in \left[E_1 - \frac{\delta}{4}, E_1 + \frac{\delta}{4}\right]\right\}\right), \tag{6.71}$$

5. $\gamma_{\mathrm{ri}}(0) = E_1 + \delta e^{-\frac{i}{2}\mathrm{Im}(\xi)}$,

$$\gamma_{\mathrm{ri}}(x) := \gamma_{\mathrm{ri}}(0) + x e^{-\frac{i}{2}\mathrm{Im}(\xi)}. \tag{6.72}$$

For later reference, we introduce

$$c_\delta := \delta\left|\sin\left(\mathrm{Im}\left(\frac{\xi}{2}\right)\right)\right| > 0. \tag{6.73}$$

**Lemma 6.10 (Bounds for $\mathfrak{z}_\varepsilon$, $\mathfrak{d}_\rho$).** *Let $\varepsilon \geq 0$. For any $z \in \mathbb{C}\backslash\mathcal{A}_{0,\varepsilon}$ holds*

$$\mathfrak{z}_\varepsilon(z) \leq \left|e^{\xi}\right|\left(1 + \max_{\ell=0,1}\frac{|e^{-\xi}\rho + E_\ell - z|}{\mathrm{dist}\left(z, \mathcal{A}_{0,\varepsilon}^{(\ell)}\right)}\right). \tag{6.74}$$

*If $\varepsilon = 0$ and $z \in \Gamma_{\mathrm{le}} \cup \Gamma_{\mathrm{m}} \cup \Gamma_{\mathrm{ri}}$, then there are $c_{\Gamma_{\mathrm{lmr}}}, C_{\Gamma_{\mathrm{lmr}}} \in \mathbb{R}_+$ with*

$$\mathrm{dist}(z, \mathcal{A}_{0,0}) \geq C_{\Gamma_{\mathrm{lmr}}}\left(1+|z|^2\right)^{\frac{1}{2}} \tag{6.75}$$

$$\mathfrak{d}_\rho(z)^{-1} \geq c_{\Gamma_{\mathrm{lmr}}}\left(1+|z|^2\right)^{\frac{1}{2}} \tag{6.76}$$

*and in particular there is a $C_{6.10} \in \mathbb{R}_+$, such that*

$$\mathfrak{z}_0(z) \leq C_{6.10} < \infty, \quad \forall z \in \Gamma_{\mathrm{l}} \cup \Gamma_{\mathrm{m}} \cup \Gamma_{\mathrm{r}}. \tag{6.77}$$

*Moreover, if $\epsilon = \rho$, then there is a $\widetilde{C}_{6.10} \in \mathbb{R}_+$, depending on $\xi$, such that*

$$\forall z \in \Gamma_0 \cup \Gamma_1 : \quad \mathfrak{z}_\rho(z) \leq \widetilde{C}_{6.10} < \infty. \tag{6.78}$$

*Proof.* Let $\varepsilon \geq 0$. For any $z \in \mathbb{C}\backslash\mathcal{A}_{0,\varepsilon}$ we have

$$\begin{aligned} \mathfrak{z}_\varepsilon(z) &= \sup_{r\geq\varepsilon,\,\ell=0,1}\left|\frac{r+\rho}{E_\ell - z + e^{-\xi}r}\right| \\ &\leq \left|e^{\xi}\right| + \sup_{r\geq\varepsilon,\,\ell=0,1}\left|\frac{\rho - e^{\xi}\left(E_\ell - z\right)}{E_\ell - z + e^{-\xi}r}\right| \\ &= \left|e^{\xi}\right|\left(1+\max_{\ell=0,1}\frac{\left|e^{-\xi}\rho - E_\ell + z\right|}{\mathrm{dist}\left(z,\mathcal{A}_{0,\varepsilon}^{(\ell)}\right)}\right) < \infty. \end{aligned} \tag{6.79}$$

We consider first $z \in \Gamma_{\mathrm{ri}}$ and $\varepsilon = 0$. Observe by (6.72) that

$$\mathrm{dist}\left(z,\mathcal{A}_{0,0}\right) = |z - E_1|\sin\left(\mathrm{Im}\left(\frac{\xi}{2}\right)\right). \tag{6.80}$$

Moreover, since

$$\begin{aligned} |z - E_1|^2 &= |z|^2 + E_1^2 - 2E_1\mathrm{Re}\left(z\right) \\ &\geq |z|^2\sin^2\left(\mathrm{Arg}\left(z\right)\right) + E_1^2\sin^2\left(\mathrm{Arg}\left(z\right)\right) \end{aligned} \tag{6.81}$$

and

$$\mathrm{Arg}\left(z\right) \in \left[\mathrm{Arg}\left(E_1 + \delta e^{-\frac{i}{2}\mathrm{Im}(\xi)}\right), \mathrm{Im}\left(\frac{\xi}{2}\right)\right) \subset \left(0,\frac{\pi}{2}\right) \tag{6.82}$$

there (6.75) holds for $z \in \Gamma_{ri}$ and similarly for $z \in \Gamma_{le}$. There is a constant $C > 0$, independent of $\rho$, such that $\mathrm{dist}\left(z,\mathcal{A}_{0,0}\right) \geq C$, for any $z \in \Gamma_{\mathrm{m}}$. Since $\Gamma_{\mathrm{m}}$ is of finite length, there is a $C_{\Gamma_{\mathrm{lmr}}} > 0$, such that (6.75) holds for any $z \in \Gamma_{\mathrm{le}} \cup \Gamma_{\mathrm{m}} \cup \Gamma_{\mathrm{ri}}$. A similar consideration shows (6.76) and one may note that $\mathrm{dist}\left(z,\mathcal{A}_{0,0}\right) \leq \mathfrak{d}_\rho\left(z\right)^{-1}$.

Observe that

$$\mathrm{dist}\left(z,\mathcal{A}_{0,\rho}^{(\ell)}\right) = \left|E_\ell + \rho e^{-\xi} - z\right| \geq C\left(\xi\right)\rho, \tag{6.83}$$

for $z \in \Gamma_\ell$, $\ell = 0,1$ and a constant $C\left(\xi\right) > 0$, depending on $\xi$. In combination with (6.79) and

$$\left|e^{-\xi}\rho - E_\ell + z\right| \leq 2\left|e^{-\xi}\right|\rho + \left|E_\ell + e^{-\xi}\rho - z\right|,$$

(6.83) yields (6.78). □

Now we estimate the contributions of the regions far from the singularities near $E_0$, $E_1$ and we shall assume henceforth that $\Gamma$ is admissible.

**Theorem 6.11 (Decay estimates – regular domains).** *Let* $\Gamma_{\mathrm{lmr}} := \Gamma_{\mathrm{le}} \cup \Gamma_{\mathrm{m}} \cup \Gamma_{\mathrm{ri}}$. *For any* $t \in \mathbb{R}_+$ *we have*

$$X_{\Gamma_{\mathrm{lmr}}}\left(t\right) = X_{\Gamma_{\mathrm{l}}}\left(t\right) + X_{\Gamma_{\mathrm{m}}}\left(t\right) + X_{\Gamma_{\mathrm{r}}}\left(t\right), \tag{6.84}$$

*where*

$$X_{\Gamma_j}\left(t\right) := \frac{1}{2\pi i}\int_{\Gamma_j} dz\, e^{-izt}P\left(H_g - z\right)^{-1}P,\ t \in \mathbb{R}_+,\ j = \mathrm{l},\mathrm{m},\mathrm{r}. \tag{6.85}$$

*Then, for*

$$2gc_{6.8}C_{6.10} < \rho^{\frac{1}{2}}, \tag{6.86}$$

*there is a* $C_{6.11} \in \mathbb{R}_+$, *such that*

$$\left\| X_{\Gamma_{\mathrm{lmr}}}(t) \right\| \leq C_{6.11} e^{-c_\delta t} \left(1 + g\rho^{\frac{1}{2}}\right). \tag{6.87}$$

*Proof.* Observe,

$$X_{\Gamma_{\mathrm{lmr}}}(t) = Y_{\Gamma_{\mathrm{lmr}}}(t) + gB(t), \tag{6.88}$$

with

$$Y_{\Gamma_{\mathrm{lmr}}}(t) := \frac{1}{2\pi i} \int_{\Gamma_{\mathrm{lmr}}} dz\, e^{-izt} (H_0 - z)^{-1} P \tag{6.89}$$

and

$$B(t) := \frac{1}{2\pi i} \int_{\Gamma_{\mathrm{lmr}}} dz\, e^{-izt} (H_0 - z)^{-1} PW \left(H_g - z\right)^{-1} P. \tag{6.90}$$

Since $(H_0 - z)^{-1} P$ is holomorphic for all $z \in \mathbb{C}$ with $\mathrm{Im}(z) < -\eta_0\rho$, we obtain by Cauchy's theorem,

$$Y_{\Gamma_{\mathrm{lmr}}}(t) = Y_{\hat{\Gamma}_1 \cup \hat{\Gamma}_2}(t), \; \forall t \in \mathbb{R}_+, \tag{6.91}$$

where $\hat{\Gamma}_\ell$, $\ell = 1, 2$ are chosen such that $\mathrm{Im}(z) \leq -c_\delta \delta$, $c_\delta > 0$ as in (6.73) and $\Gamma_\ell \cup \hat{\Gamma}_\ell$ are closed curves. Thus

$$\left\| Y_{\Gamma_{\mathrm{lmr}}}(t) \right\| \leq C e^{-c_\delta t}. \tag{6.92}$$

The error term $B(t)$ is estimated as follows. By Lemma 6.10 there is $C_{\Gamma_{\mathrm{lmr}}} > 0$ a independent of $\rho$ such that

$$\forall z \in \Gamma_{\mathrm{lmr}} : \quad \mathrm{dist}\left(z, \mathcal{A}_{0,0}\right) \geq C_{\Gamma_{\mathrm{lmr}}} \left(1 + |z|^2\right)^{\frac{1}{2}} \tag{6.93}$$

and $\mathfrak{z}_0(z) \leq C_{6.10} < \infty$. Using (6.55), (6.77) and (6.76) we obtain

$$\begin{aligned}
& \left\| (H_0 - z)^{-1} PgW \left(H_g - z\right)^{-1} P \right\| \\
\leq \;& \rho \sum_{n=0}^{\infty} \left\| (H_0 - z)^{-1} P \right\|^2 \\
& \cdot \left\| (H_{\mathrm{f}} + \rho)^{-\frac{1}{2}} gW (H_{\mathrm{f}} + \rho)^{-\frac{1}{2}} \right\|^{n+1} \\
& \cdot \left\| (H_{\mathrm{f}} + \rho)^{\frac{1}{2}} (H_0 - z)^{-1} (H_{\mathrm{f}} + \rho)^{\frac{1}{2}} \right\|^{n} && (6.94) \\
\leq \;& Cg\rho^{\frac{1}{2}} \left(1 + |z|^2\right)^{-1} \sum_{n=0}^{\infty} \left( \frac{2gc_{6.8}C_{6.10}}{\sqrt{\rho}} \right)^n && (6.95) \\
\leq \;& Cg\rho^{\frac{1}{2}} \left(1 + |z|^2\right)^{-1}, && (6.96)
\end{aligned}$$

for some generic constant $C \in \mathbb{R}_+$. Therefore we conclude

$$\|gB(t)\| \leq Cg\rho^{\frac{1}{2}} \left( e^{-c_\delta t} + \int_0^\infty dr\, \frac{e^{-c_\delta (t+r)}}{1 + r^2} \right) \leq Cg\rho^{\frac{1}{2}} e^{-c_\delta t}. \tag{6.97}$$

□

Next we turn to investigate the behaviour of $X$ in the spectral regions close to the unperturbed eigenstates $E_0$ and $E_1$, which has some differences. For the region close to $E_0$ we obtain a mild exponential growth of the dynamics, which is mild in the sense that it becomes uniformly bounded on the van Hove timescale. In contrast $E_1$ may even turn into a metastable state, which decays on the van Hove timescale under generic assumptions on $G_{01}$. We investigate $X_{\Gamma_0}$ first.

**Lemma 6.12 (Spectral distance – $\Gamma_0$).** *Let $\rho = g^{\mu}$, $\mu \in (0,2)$, pick $\nu \in \left(0, \min\left(1, \mu^{-1} - \frac{1}{2}\right)\right)$ and define*

$$\widetilde{\Lambda}_{00}(0, E_0) := 4\pi \int_{\mathbb{R}^+} dw\, w^2 \left|(G)_{10}(w)\right|^2 (E_1 - E_0 + w)^{-1}. \tag{6.98}$$

*For any $z \in \Gamma_0$, $F_P(H_g - z)$ and $\widetilde{F}_P(z)$ are invertible on $P\mathcal{H}$ and there are $C_{6.12}, \widetilde{C}_{6.12} \in \mathbb{R}_+$, such that*

$$\left\| F_P\left(H_g - z\right)^{-1} \right\| \leq \frac{C_{6.12}}{g^2\rho^{\nu} + \left|z - E_0 + g^2\tilde{\Lambda}_{00}(0, E_0)\right|}, \tag{6.99}$$

*and*

$$\left\| \widetilde{F}_P(z)^{-1} \right\| \leq \frac{\widetilde{C}_{6.12}}{g^2\rho^{\nu} + \left|z - E_0 + g^2\tilde{\Lambda}_{00}(0, E_0)\right|}, \tag{6.100}$$

*provided $g^2\rho^{-1}$ is sufficiently small. Moreover for some $C \in \mathbb{R}_+$,*

$$\left\| F_P\left(H_g - z\right)^{-1} - \widetilde{F}_P(z)^{-1} \right\| \leq C\left(\rho^{1-\nu} + g\rho^{-\left(\nu + \frac{1}{2}\right)}\right) \left\| \widetilde{F}_P(z)^{-1} \right\|. \tag{6.101}$$

*Proof.* Throughout the proof $C$ denotes a generic constant in $\mathbb{R}_+$. We write, $z := x + iy$, $x, y \in \mathbb{R}$ and

$$d_\ell(r, z) := \left| e^{\xi} r - (z - E_\ell) \right|, \ \ell = 0, 1. \tag{6.102}$$

Then for any $y \in \mathbb{R}^+$ and $0 < \alpha < 1$,

$$\begin{aligned} d_\ell(r,z)^2 &= (\eta_1 r + E_\ell - x)^2 + (\eta_0 r + y)^2 \\ &\geq -\eta_1^2\left(\alpha^{-1} - 1\right) r^2 + (1-\alpha)(x - E_\ell)^2 \\ &\quad + \eta_0^2 r^2 + y^2. \end{aligned} \tag{6.103}$$

Choosing

$$\alpha = \frac{1}{1 + \frac{\eta_0^2}{2\eta_1^2}} < 1, \tag{6.104}$$

we obtain

$$d_\ell(r,z)^2 \geq \frac{\eta_0^2 r^2}{2} + (1-\alpha)\left|z - E_\ell\right|^2. \tag{6.105}$$

Note that Estimate (6.105) is not uniform in $\xi$. Thanks to our assumtion that $G_{\ell\ell} \equiv 0$, $\ell = 0, 1$, the operator $\Lambda_\rho(H_f, z)$ may be represented as the matrix

$$\Lambda_\rho(H_f, z) = \begin{pmatrix} \Lambda_{00}(H_f, z) & 0 \\ 0 & \Lambda_{11}(H_f, z) \end{pmatrix}, \tag{6.106}$$

with

$$\begin{aligned}\Lambda_{00}(H_{\mathrm{f}},z) &:= \int_{\mathbb{R}^3} d^3k \left(\overline{G_{\bar{\xi}}}\right)_{10}(k)\left(G_{\xi}\right)_{10}(k) \\ &\quad \left(E_1 + e^{-\xi}\left(H_{\mathrm{f}}+\omega(k)\right)-z\right)^{-1} \\ &\quad \mathbf{1}\left[H_{\mathrm{f}}+\omega(k)\geq\rho\right]P, \qquad (6.107)\\ \Lambda_{11}(H_{\mathrm{f}},z) &:= \int_{\mathbb{R}^3} d^3k \left(\overline{G_{\bar{\xi}}}\right)_{01}(k)\left(G_{\xi}\right)_{01}(k) \\ &\quad \left(E_0 + e^{-\xi}\left(H_{\mathrm{f}}+\omega(k)\right)-z\right)^{-1} \\ &\quad \mathbf{1}\left[H_{\mathrm{f}}+\omega(k)\geq\rho\right]P. \qquad (6.108)\end{aligned}$$

Inequality (6.105) then yields for any $r \in [\rho,\infty)$ and $z \in \mathbb{C}$ with $\mathrm{Im}(z) \in \mathbb{R}_0^+$ the bounds

$$\begin{aligned}\left\|\Lambda_{00}(H_{\mathrm{f}},z)\right\| &\leq \frac{C_0}{\left(\rho^2+|z-E_1|^2\right)^{\frac{1}{2}}}, \qquad (6.109)\\ \left\|\Lambda_{11}(H_{\mathrm{f}},z)\right\| &\leq \frac{C_1}{\left(\rho^2+|z-E_0|^2\right)^{\frac{1}{2}}}. \qquad (6.110)\end{aligned}$$

These inequalities extend to $\Gamma_0$. For the *inner part*

$$\Gamma_0 \cap \left(\left[E_0-\frac{\delta}{4},E_0+\frac{\delta}{4}\right]+i\mathbb{R}\right),$$

of $\Gamma_0$, the inequalities (6.109), (6.110) hold true. Let now $z$ be in the complement of the inner part, i.e. $z \in \Gamma_0$, $|\mathrm{Re}(z)-E_0| > \frac{\delta}{4}$. Then,

$$d_\ell(r+\omega(k),z) \geq \frac{\delta}{4}, \qquad \ell = 0,1 \qquad (6.111)$$

and hence (6.109), (6.110) hold for all $z \in \Gamma_0$. Moreover, by denoting the matrix entries of $G_\xi$, $G_{\bar{\xi}}$ with $(G_\xi)_{jk}$, $\left(G_{\bar{\xi}}\right)_{jk}$, respectively, we have

$$\widetilde{F}_P(z) = P\begin{pmatrix}\lambda_0(z,H_{\mathrm{f}}) & g\check{\phi}\left(\left(G_\xi\right)_{01}\right)\\ g\check{\phi}\left(\left(G_\xi\right)_{10}\right) & \lambda_1(z,H_{\mathrm{f}})\end{pmatrix}P.$$

with

$$\lambda_\ell(z,H_{\mathrm{f}}) := E_\ell + e^{-\xi}H_{\mathrm{f}} - z - g^2\Lambda_{\ell\ell}(H_{\mathrm{f}},z), \quad \ell = 0,1.$$

We aim at the construction of the inverse of $\tilde{F}_P(z)$ by means of the Feshbach isospectrality with projection $P_{\mathrm{at},0}$. Note that for any $z \in \Gamma_0$, $r+\omega(k) \geq \rho$,

$$d_1(r+\omega(k),z) \geq \frac{\delta}{4}. \qquad (6.112)$$

Thus, by (6.112), (6.105) and (6.110), it follows for all $z \in \Gamma_0$, that

$$\begin{aligned} \left| d_1(r,z) - g^2 \left\| \Lambda_{11}(r,z) \right\| \right| &\geq d_1(r,z) - \frac{C_1 g^2}{\rho} \\ &\geq \frac{1}{2} d_1(r,z) + \frac{\delta}{8} - \frac{C_1 g^2}{\rho} \\ &\geq \frac{1}{2} d_1(r,z). \end{aligned} \tag{6.113}$$

Therefore,

$$\widetilde{R}_1(z) := \left( E_1 + e^{-\xi} H_f P - z - g^2 \Lambda_{11}(H_f, z) \right)^{-1} \tag{6.114}$$

exists for all $z \in \Gamma_0$ on $P_{\mathrm{at},1}\mathcal{H}$ and is bounded by

$$\left\| \widetilde{R}_1(z) \right\| \leq C \delta^{-1}. \tag{6.115}$$

Hence,

$$\begin{aligned} F_{P_{\mathrm{at},0}}\left( \widetilde{F}_P(z) \right) &= E_0 + e^{-\xi} H_f P_{\mathrm{at},0} - z - g^2 \Lambda_{00}(H_f, z) \\ &\quad - g^2 P_{\mathrm{at},0} \check{\phi}\left( (G_\xi)_{01} \right) P_{\mathrm{at},1} \widetilde{R}_1(z) P_{\mathrm{at},1} \\ &\quad \cdot \check{\phi}\left( (G_\xi)_{10} \right) P_{\mathrm{at},0} \end{aligned} \tag{6.116}$$

is well–defined and we obtain the inverse of $\tilde{F}_P(z)$ by

$$\begin{aligned} \tilde{F}_P(z)^{-1} &= Q_{P_{\mathrm{at},0}}\left( \tilde{F}_P(z) \right) F_{P_{\mathrm{at},0}}\left( \widetilde{F}_P(z) \right)^{-1} Q^\sharp_{P_{\mathrm{at},0}}\left( \widetilde{F}_P(z) \right) \\ &\quad + P_{\mathrm{at},1} \tilde{R}_1(z) P_{\mathrm{at},1}, \end{aligned} \tag{6.117}$$

with

$$Q_{P_{\mathrm{at},0}}\left( \tilde{F}_P(z) \right) := P_{\mathrm{at},0} - \widetilde{R}_1(z) P_{\mathrm{at},1} \check{\phi}\left( (G_\xi)_{10} \right) P_{\mathrm{at},0}, \tag{6.118}$$

$$Q^\sharp_{P_{\mathrm{at},0}}\left( \tilde{F}_P(z) \right) := P_{\mathrm{at},0} - P_{\mathrm{at},0} \check{\phi}\left( (G_\xi)_{01} \right) P_{\mathrm{at},1} \widetilde{R}_1(z), \tag{6.119}$$

iff $F_{P_{\mathrm{at},0}}\left( \tilde{F}_P(z) \right)$ is invertible on the range of $P_{\mathrm{at},0}$. Note, that by (6.39) and

$$\left\| P_{\mathrm{at},0} \check{\phi}\left( (G_\xi)_{01} \right) P_{\mathrm{at},1} \widetilde{R}_1(z) P_{\mathrm{at},1} \check{\phi}\left( (G_\xi)_{10} \right) P_{\mathrm{at},0} \right\| \leq C \delta^{-1} \rho. \tag{6.120}$$

By Lemma 6.13 it follows for all $z \in \Gamma_0$ and all $\psi \in P_{\mathrm{at},0}\mathcal{H}$, with $\|\psi\| = 1$,

$$\left\| F_{P_{\mathrm{at},0}}\left( \widetilde{F}_P(z) \right) \psi \right\| \geq C_{6.13} \left( \left| z + g^2 \widetilde{\Lambda}_{00}(0, E_0) - E_0 \right| + g^2 \rho^\nu \right).$$

The inequality (6.100) follows now from

$$Q_{P_{\mathrm{at},0}}\left( \widetilde{F}_P(z) \right), Q^\sharp_{P_{\mathrm{at},0}}\left( \widetilde{F}_P(z) \right) = P_{\mathrm{at},0} + \mathcal{O}\left( g \rho^{\frac{1}{2}} \right) \tag{6.121}$$

and the finite length of $\Gamma_0$. It remains to prove the bound (6.99). First note that for all $z \in \Gamma_0$ by Proposition 6.8, Lemma 6.10 and (6.100)

$$\left\| \left( F_P \left( H_g - z \right) - \widetilde{F}_p \left( z \right) \right) \widetilde{F}_p \left( z \right)^{-1} \right\| \leq C \left( \rho^{1-\nu} + g\rho^{-\left(\nu + \frac{1}{2}\right)} \right). \tag{6.122}$$

Therefore, the Neumann series

$$F_p \left( H_g - z \right)^{-1} = \sum_{n=0}^{\infty} \widetilde{F}_p \left( z \right)^{-1} \left( \left( F_P \left( H_g - z \right) - \widetilde{F}_p \left( z \right) \right) \widetilde{F}_p \left( z \right)^{-1} \right)^n, \tag{6.123}$$

converges for sufficiently small $g$, and we obtain

$$\left\| F_p \left( H_g - z \right)^{-1} \right\| \leq 2 \left\| \widetilde{F}_p \left( z \right)^{-1} \right\|,$$

provided $\rho$ is sufficiently small, and thus inequality (6.99). Finally, inequality (6.101) follows from (6.122) and (6.123). ☐

Our goal is now to prove the invertibility of $F_{P_{\mathrm{at},0}} \left( \tilde{F}_P \left( z \right) \right)$.

**Lemma 6.13 (Invertibility of $F_{P_{\mathrm{at},0}} \left( \widetilde{F}_P \left( z \right) \right)$).** *Let $\rho = g^\mu$, $\mu \in (0, 2)$ and pick $\nu \in \left( 0, \min \left( 1, \mu^{-1} - \frac{1}{2} \right) \right)$. Then, for all $z \in \Gamma_0$ and all $\psi \in P_{\mathrm{at},0}\mathcal{H}$, $\|\psi\| = 1$, there is a $C_{6.13} \in \mathbb{R}_+$, such that*

$$\left\| F_{P_{\mathrm{at},0}} \left( \widetilde{F}_P \left( z \right) \right) \psi \right\| \geq C_{6.13} \left( \left| z + g^2 \widetilde{\Lambda}_{00} \left( 0, E_0 \right) - E_0 \right| + g^2 \rho^\nu \right). \tag{6.124}$$

*Proof.* We establish (6.124) in two steps. The first step addresses the inner part of $\Gamma_0$, i.e. those $z \in \Gamma_0$, for which

$$\mathrm{Re} \left( z \right) \in \left[ E_0 - \frac{\delta}{4}, E_0 + \frac{\delta}{4} \right]$$

and the second the outer part of $\Gamma_0$, i.e. $z \in \Gamma_0$ with

$$\mathrm{Re} \left( z \right) \in \mathrm{Re} \left( \Gamma_0 \right) \setminus \left[ E_0 - \frac{\delta}{4}, E_0 + \frac{\delta}{4} \right].$$

<u>*Step 1.*</u>

Let $\mathrm{Re} \left( z \right) \in \left[ E_0 - \frac{\delta}{4}, E_0 + \frac{\delta}{4} \right]$, $z \in \Gamma_0$. In order to obtain invertibility of $F_{P_{\mathrm{at},0}} \left( \widetilde{F}_P \left( z \right) \right)$, we determine the imaginary part of

$$E_0 + e^{-\xi} H_{\mathrm{f}} P_{\mathrm{at},0} - z - g^2 \Lambda_{00} \left( H_{\mathrm{f}}, z \right),$$

as the leading term. To this end, it is useful to relate $\Lambda_{00} \left( z \right)$ to a slightly different operator, which has an integrand that is analytic in $|k|$. Thus we define

$$\widetilde{\Lambda}_{00} \left( H_{\mathrm{f}}, z \right) := 4\pi \int_{\mathbb{R}^+} dk \, f_\xi \left( k \right) \left( E_1 + e^{-\xi} \left( H_{\mathrm{f}} + \omega \left( k \right) \right) - z \right)^{-1} P, \tag{6.125}$$

where

$$f_\xi \left( k \right) := e^{-3\xi} f \left( e^{-\xi} k \right), \quad f \left( k \right) := k^2 \left| \left( G \right)_{10} \left( k \right) \right|^2. \tag{6.126}$$

Note that

$$\Lambda_{00}(r,z) := 4\pi \int_{\mathbb{R}^+} dk\, f_\xi(k) \left(E_1 + e^{-\xi}(r+\omega(k)) - z\right)^{-1} \chi_{r+|k|\geq\rho}\chi_{r<\rho}.$$

Then, for any $r \in [0,\rho]$,

$$\left|\Lambda_{00}(r,z) - \widetilde{\Lambda}_{00}(r,z)\right| \leq C \int_{\mathbb{R}^3} d^3k\, \left|f_\xi(k)\right| \chi_{r+|k|<\rho} \leq C\rho^2. \tag{6.127}$$

Observe, that

$$\begin{aligned}\widetilde{\Lambda}_{00}(r,z) &= 4\pi \int_{e^{-\xi}\mathbb{R}^+} dw\, f(w) \left(E_1 + e^{-\xi}r + w - z\right)^{-1} \chi_{r<\rho} \\ &= 4\pi \int_{\mathbb{R}^+} dw\, f(w) \left(E_1 + e^{-\xi}r + w - z\right)^{-1} \chi_{r<\rho},\end{aligned}$$

by Cauchy's theorem and the sufficiently rapid decay of $f(|w|) \to 0$, as $|w| \to \infty$, due to the ultraviolet cutoff. Since $f$ is real–valued, the imaginary part of $\tilde{\Lambda}_{00}(r,z)$ is given by

$$\operatorname{Im}\left(\widetilde{\Lambda}_{00}(r,z)\right) = 4\pi \int_{\mathbb{R}^+} dw\, f(w) \frac{re^{-\operatorname{Re}(\xi)} \sin(\operatorname{Im}(\xi)) + \operatorname{Im}(z)}{\left|E_1 + e^{-\xi}r + w - z\right|^2} \chi_{r<\rho}. \tag{6.128}$$

The denominator is uniformly bounded,

$$\sup_{(r,w,z)\in[0,\rho]\times\mathbb{R}^+\times\Gamma_0} \frac{1}{\left|E_1 + e^{-\xi}r + w - z\right|^2} < \infty.$$

It follows, that for some $C > 0$,

$$\operatorname{Im}\left(\widetilde{\Lambda}_{00}(r,z)\right) \quad \geq \quad C \operatorname{Im}(z) \geq 0. \tag{6.129}$$

Now, we observe that

$$\left\| g^2 P_{\mathrm{at},0} \check{\phi}\left(\left(G_\xi\right)_{01}\right) P_{\mathrm{at},1} \widetilde{R}_1(z) P_{\mathrm{at},1} \check{\phi}\left(\left(G_\xi\right)_{10}\right) P_{\mathrm{at},0} \right\| \leq C g^2 \rho, \tag{6.130}$$

see (6.120). It is convenient to use the abbreviation

$$A_{00}(r,z) := E_0 + e^{-\xi}r - z - g^2 \widetilde{\Lambda}_{00}(r,z). \tag{6.131}$$

We next determine the shift of the energy $E_0$ by second order perturbation theory. By the fundamental theorem of calculus we have

$$\begin{aligned}A_{00}(r,z) &= E_0 - z - g^2\widetilde{\Lambda}_{00}(r,E_0) + e^{-\xi}r + g^2\left(\widetilde{\Lambda}_{00}(r,E_0) - \widetilde{\Lambda}_{00}(r,z)\right) \\ &= E_0 - z - g^2\widetilde{\Lambda}_{00}(r,E_0) + e^{-\xi}r - g^2(E_0 - z)\, h(r,z) \\ &= E_0 - z - g^2\widetilde{\Lambda}_{00}(r,E_0) + e^{-\xi}r \\ &\quad -g^2 M(r,z) + g^4 \widetilde{M}(r,z),\end{aligned} \tag{6.132}$$

where

$$\begin{aligned} M(r,z) &:= \left(E_0 - z - g^2\widetilde{\Lambda}_{00}(r,E_0)\right) h(r,z), & (6.133)\\ \widetilde{M}(r,z) &:= \widetilde{\Lambda}_{00}(r,E_0)\, h(r,z), & (6.134)\\ h(r,z) &:= \int_0^1 ds \left(\frac{d}{dz}\widetilde{\Lambda}_{00}\right)(r, z(1-s) + E_0 s). & (6.135)\end{aligned}$$

Note that

$$\sup_{r\in[0,\rho],\, z\in\Gamma_0} |h(r,z)| \le C.$$

This yields

$$\begin{aligned} A_{00}(r,z) &= \left(E_0 - z - g^2\widetilde{\Lambda}_{00}(r,E_0)\right)\left(1 - g^2 h(r,z)\right) + e^{-\xi} r + g^4 \widetilde{M}(r,z)\\ &= \left(E_0 + e^{-\xi} r - z - g^2\widetilde{\Lambda}_{00}(0,E_0)\right)\left(1 - g^2 h(r,z)\right)\\ &\quad + g^2\left(\widetilde{\Lambda}_{00}(0,E_0) - \widetilde{\Lambda}_{00}(r,E_0)\right)\left(1 - g^2 h(r,z)\right) \qquad (6.136)\\ &\quad + g^2 e^{-\xi} r h(r,z) + g^4\widetilde{M}(r,z). \end{aligned}$$

With

$$\widetilde{A}_{00}(r,z) := \left(E_0 + e^{-\xi} r - z - g^2\widetilde{\Lambda}_{00}(0,E_0)\right)\left(1 - g^2 h(r,z)\right) \qquad (6.137)$$

and

$$\left\|\widetilde{\Lambda}_{00}(0,E_0) - \widetilde{\Lambda}_{00}(r,E_0)\right\| \le C\rho, \qquad (6.138)$$

we find that (6.116) satisfies for any $\psi \in P\mathcal{H}$, $\|\psi\| = 1$,

$$\left\| F_{P_{\mathrm{at},0}}\left(\widetilde{F}_P(z)\right)\psi\right\| \ \ge\ \inf_{r\in[0,\rho]}\left|\left|\widetilde{A}_{00}(r,z)\right| - C\left(g^2\rho + g^4\right)\right|. \qquad (6.139)$$

By (6.105) we have

$$d_0\left(r, z + g^2\widetilde{\Lambda}_{00}(0,E_0)\right)^2 \ge \frac{\eta_0^2 r^2}{2} + (1-\alpha)\left|z + g^2\widetilde{\Lambda}_{00}(0,E_0) - E_0\right|^2. \qquad (6.140)$$

Moreover, for any $z \in \mathbb{C}$ with $\mathrm{Im}(z) = c_0 g^2 \rho^\nu$, $c_0 \in \mathbb{R}_+$,

$$\begin{aligned} \mathrm{Im}\left(E_0 + e^{-\xi} r - z - g^2\widetilde{\Lambda}_{00}(0,E_0)\right) &= -\mathrm{Im}(z) - \eta_0 r\\ &\quad - g^2 \underbrace{\mathrm{Im}\left(\widetilde{\Lambda}_{00}(0,E_0)\right)}_{=0}\\ &\le -\mathrm{Im}(z)\\ &\le -c_0 g^2 \rho^\nu. \qquad (6.141)\end{aligned}$$

Hence, by (6.140,6.141), follows for any $\psi \in P\mathcal{H}$, $\|\psi\| = 1$,

$$
\begin{aligned}
\left\| F_{P_{\mathrm{at},0}}\left(\widetilde{F}_P(z)\right)\psi \right\| &\geq \inf_{r\in[0,\rho]} \Big| d_0\left(r, z + g^2\widetilde{\Lambda}_{00}(0,E_0)\right)\left|1 - g^2 h(r,z)\right| \\
&\qquad - C\left(g^2\rho(1+\rho) + g^4\right)\Big| \\
&\geq \inf_{r\in[0,\rho]} \Big| \frac{\eta_0^2 r^2}{8} + \frac{(1-\alpha)}{4}\left|z + g^2\widetilde{\Lambda}_{00}(0,E_0) - E_0\right|^2 \\
&\qquad - C\left(g^2\rho\right)^2\Big|^{\frac{1}{2}} \\
&\geq \inf_{r\in[0,\rho]} \Big| \frac{\eta_0^2 r^2}{8} + \frac{(1-\alpha)}{4}\left|z + g^2\widetilde{\Lambda}_{00}(0,E_0) - E_0\right|^2 \\
&\qquad - C\left(g^2\rho\right)^2\Big|^{\frac{1}{2}} \\
&\geq \frac{(1-\alpha)}{8}\left|z + g^2\widetilde{\Lambda}_{00}(0,E_0) - E_0\right| + Cg^2\rho^\nu. \qquad (6.142)
\end{aligned}
$$

*Step 2.*
For all $z \in \mathbb{C}$, $r \in [0,\rho]$ and $\mathrm{Re}(z) \in \mathrm{Re}(\Gamma_0) \setminus \left[E_0 - \frac{\delta}{4}, E_0 + \frac{\delta}{4}\right]$,

$$
\begin{aligned}
d_0(r,z)^2 &\geq \frac{1}{2}(E_0 - x)^2 - e^{-2\mathrm{Re}(\xi)}r^2 - 2(E_0 - x)\eta_1 r + (y + \eta_0 r)^2 \\
&\geq \frac{1}{4}|E_0 - z|^2 + C\rho^{2\nu}. \qquad (6.143)
\end{aligned}
$$

This inequality extends to

$$
d_0(r,z)^2 \geq \frac{1}{8}\left|E_0 - \left(z + g^2\widetilde{\Lambda}_{00}(0,E_0)\right)\right|^2 + C\rho^{2\nu}, \qquad (6.144)
$$

by an appropriate redefinition of $C$. Thus we find for any $\psi \in P\mathcal{H}$, $\|\psi\| = 1$,

$$
\begin{aligned}
\left\| F_{P_{\mathrm{at},0}}\left(\widetilde{F}_P(z)\right)\psi \right\| &\geq \inf_{r\in[0,\rho]} \left| d_0(r,z) - Cg^2 \right| \\
&\geq \inf_{r\in[0,\rho]} \left| \frac{1}{16}\left|z + g^2\widetilde{\Lambda}_{00}(0,E_0) - E_0\right|^2 + C\rho^{2\nu} \right|^{\frac{1}{2}} \\
&\geq \frac{1}{32}\left|z + g^2\widetilde{\Lambda}_{00}(0,E_0) - E_0\right| + C\rho^\nu, \qquad (6.145)
\end{aligned}
$$

provided $g^2 < \rho^\nu$, $\rho$ small enough. This finishes the *Step 2*.
From (6.142) and (6.145) follows now (6.124). □

Lemma 6.12 sets us in the position to approximate $X_{\Gamma_0}$ by

$$
\widetilde{X}_{\Gamma_0}(t) := \frac{1}{2\pi i}\int_{\Gamma_0} dz\, e^{-izt}\widetilde{F}_p(z)^{-1}, \; t \in \mathbb{R}_+. \qquad (6.146)
$$

This is the purpose of the following proposition.

**Proposition 6.14 (Effective Feshbach operator – II).** *Let $\rho = g^{\mu}$, $\mu \in (0,2)$, and pick $\nu \in \left(0, \min\left(1, \mu^{-1} - \frac{1}{2}\right)\right)$. Then, for all $t \in \mathbb{R}_+$, there is a $C_{6.14}$*

$$\left\| X_{\Gamma_0}(t) - \widetilde{X}_{\Gamma_0}(t) \right\| \leq C_{6.14} e^{c_0 g^2 \rho^{\nu} t} \left( \rho^{\frac{1-\nu}{2}} + g^{\frac{1}{2}} \rho^{-\frac{1}{2}\left(\nu + \frac{1}{2}\right)} \right), \tag{6.147}$$

*provided $\rho^{-1} g^2$ is sufficiently small.*

*Proof.* $C$ denotes again a generic constant in $\mathbb{R}_+$. From (6.100) and (6.101) follows

$$\begin{aligned} \left\| X_{\Gamma_0}(t) - \widetilde{X}_{\Gamma_0}(t) \right\| &\leq \frac{1}{2\pi} \int_{\Gamma_0} dz \left\| e^{-itz} \left( \left( F_P \left( H_g - z \right)^{-1} - \widetilde{F}_p(z)^{-1} \right) \right) \right\| \\ &\leq C e^{c_0 g^2 \rho^{\nu} t} \left( \rho^{1-\nu} + g \rho^{-\left(\nu + \frac{1}{2}\right)} \right) \int_{\Gamma_0} dz \left\| \widetilde{F}_p(z)^{-1} \right\|. \end{aligned}$$

We split $\Gamma_0$ into the inner part defined by (6.68) and its complement in $\Gamma_0$, denoted by $\Gamma_0^c$. The inner part may be estimated by (6.100) as

$$\int_{E_0 - \frac{\delta}{4}}^{E_0 + \frac{\delta}{4}} dx \left\| \widetilde{F}_p \left( x + c_0 g^2 \rho^{\nu} \right)^{-1} \right\| \leq C \ln \left( \frac{\delta}{2 g^2 \rho^{\nu}} \right). \tag{6.148}$$

For $\Gamma_0^c$ we choose a straight line from $E_0 \pm \delta/4 + i c_0 g^2 \rho^{\nu}$ to $E_0 \pm \delta e^{\frac{i}{2}\mathrm{Im}(\xi)}$. Hence, we get similarly to (6.148) using (6.145),

$$\int_{\Gamma_0^c} dz \left\| \widetilde{F}_p(z)^{-1} \right\| \leq C \ln \left( \frac{\delta}{\rho^{\nu}} \right). \tag{6.149}$$

The elementary inequality

$$\forall \kappa \in \mathbb{R}_+, \forall r \in (0,1): \quad \ln \left( \frac{1}{r} \right) \leq \frac{1}{\kappa} r^{-\kappa},$$

yields for

$$\kappa := \frac{\min\left( \mu(1-\nu), 1 - \mu\left(\nu + \frac{1}{2}\right) \right)}{2(2 + \mu\nu)}$$

the inequality (6.147). ☐

**Remark 6.15.** We pause for a moment to comment on the relative size of the error terms in (6.147). Observe that

$$\frac{g \rho^{-\nu - \frac{1}{2}}}{\rho^{-\nu + 1}} = g \rho^{-\frac{3}{2}} = g^{1 - \frac{3}{2}\mu}.$$

Thus, if $\mu \in (2/3, 2)$, then the second term dominates the first one and vice versa for $\mu \in (0, 2/3)$. The two terms are of equal size if $\mu = 2/3$.

The next step is to write the one–parameter family $\left\{\widetilde{X}_{\Gamma_0}(t)\right\}_{t\in\mathbb{R}_+}$ as a sum

$$\widetilde{X}_{\Gamma_0}(t) = \widetilde{Y}_{\Gamma_0}(t) + o(1), \tag{6.150}$$

where

$$\begin{aligned}\widetilde{Y}_{\Gamma_0}(t) &:= \frac{1}{2\pi i}\int_{\Gamma_0} dz\, e^{-itz} F_{P_{\mathrm{at},0}}\left(\widetilde{F}_P(z)\right)^{-1} &(6.151)\\ &= \frac{1}{2\pi i}\int_{\gamma_0(a_0)}^{\gamma_0(b_0)} dx\, e^{-it(x-ic_\delta)} F_{P_{\mathrm{at},0}}\left(\widetilde{F}_P(x-ic_\delta)\right)^{-1} &(6.152)\\ &\quad+\begin{pmatrix} e^{-itz_0(H_\mathrm{f})} & 0\\ 0 & 0\end{pmatrix}.\end{aligned}$$

Provided the integral on the right hand side of (6.151) exists, we define the operator $z_0(H_\mathrm{f})$ as the solution of the implicit equation

$$E_0 + e^{-\xi} r - z - g^2\widetilde{\Lambda}_{00}(r,z) = 0,\ (r,z)\in[0,\rho]\times\overline{G_0}, \tag{6.153}$$

see (6.162). Here, $G_0$ is the interior of the compact set $\overline{G_0}$, enclosed by the curve $\Gamma_0\cup\widetilde{\Gamma}_0 = \partial G_0$, with

$$\widetilde{\Gamma}_0 := \left\{-ic_\delta + \left[E_0 - \cos\left(\mathrm{Im}\left(\frac{\xi}{2}\right)\right)\delta, E_0 + \cos\left(\mathrm{Im}\left(\frac{\xi}{2}\right)\right)\delta\right]\right\}. \tag{6.154}$$

First, we establish a refined version of (6.150).

**Lemma 6.16.** *Let $\rho = g^\mu$, $\mu\in(0,2)$ and pick $\nu\in\left(0,\min\left(1,\mu^{-1}-\frac{1}{2}\right)\right)$. Then, there is a $C_{6.16}\in\mathbb{R}_+$, such that*

$$\left\|\tilde{X}_{\Gamma_0}(t) - \tilde{Y}_{\Gamma_0}(t)\right\| \le C_{6.16}\left(g\rho^{\frac{1}{2}} + e^{-tc_\delta}\right). \tag{6.155}$$

*Proof.* Recall, that the inverse of $\widetilde{F}_p(z)$ is given by

$$\widetilde{F}_p(z)^{-1} = Q_{P_{\mathrm{at},0}}\left(\widetilde{F}_p(z)\right)\widetilde{F}_p(z)^{-1}\, Q^\sharp_{P_{\mathrm{at},0}}\left(\widetilde{F}_p(z)^{-1}\right) + \widetilde{R}_1(z), \tag{6.156}$$

with

$$\widetilde{R}_1(z) = \left(P_{\mathrm{at},1}\widetilde{F}_p(z)\,P_{\mathrm{at},1}\right)^{-1}.$$

By (6.121) we have

$$Q_{P_{\mathrm{at},0}}\left(\widetilde{F}_P(z)\right), Q^\sharp_{P_{\mathrm{at},0}}\left(\widetilde{F}_P(z)\right) = P_{\mathrm{at},0} + \mathcal{O}\left(g\rho^{\frac{1}{2}}\right),$$

for all $z\in\Gamma_0$ and moreover by (6.115)

$$\left\|\widetilde{R}_1(z)\right\| \le C\delta^{-1}.$$

This bound extends to $\overline{G}_0$ by a computation which is analogous to the one leading to (6.187) and (6.188) in Lemma 6.20. Since $\widetilde{R}_1(z)$ is holomorphic in $G_0$ we may deform the contour as

$$\frac{1}{2\pi i}\int_{\Gamma_0} dz\, e^{-itz}\widetilde{R}_1(z) = \frac{1}{2\pi i}\int_{\mathrm{Re}(\gamma_0(a_0))}^{\mathrm{Re}(\gamma_0(b_0))} dx\, e^{-it(x-ic_\delta)}\widetilde{R}_1(x-ic_\delta),$$

and hence (6.155) follows. □

We estimate now the contribution of the integral in (6.152).

**Lemma 6.17 (Spectral distance – $\widetilde{\Gamma}_0$).** *For all $z \in \widetilde{\Gamma}_0$ we have*

$$\left\| F_{P_{\mathrm{at},0}} \left( \widetilde{F}_P \left( x - ic_\delta \right) \right)^{-1} \right\| \leq C \tag{6.157}$$

*Proof.* As in the proof of Lemma 6.12, see (6.136,6.137,6.138), is

$$F_{P_{\mathrm{at},0}} \left( \widetilde{F}_P \left( z \right) \right) = \widetilde{A}_{00} \left( H_{\mathrm{f}}, z \right) + \mathcal{O} \left( \rho g^2 + g^4 \right). \tag{6.158}$$

Moreover,

$$\left| \widetilde{A}_{00} \left( r, z \right) \right|^2 = d_0 \left( r, z + g^2 \widetilde{\Lambda}_{00} \left( 0, E_0 \right) \right)^2 \geq C > 0. \tag{6.159}$$

Hence, for sufficiently small $\rho$ follows (6.157). □

Lemma 6.17 implies

$$\left\| \int_{\gamma_0(a_0)}^{\gamma_0(b_0)} dx \, e^{-it(x - ic_\delta)} F_{P_{\mathrm{at},0}} \left( \widetilde{F}_P \left( x - ic_\delta \right) \right)^{-1} \right\| \leq C e^{-tc_\delta}. \tag{6.160}$$

The construction of $z_0 \left( H_{\mathrm{f}} \right)$ is the goal of the following proposition.

**Proposition 6.18 (Construction of $z_0 \left( H_{\mathrm{f}} \right)$).** *Let $\rho = g^\mu$, $\mu \in (0,2)$, $r \in [0, \rho]$ and pick $\nu \in \left( 0, \min \left( 1, \mu^{-1} - \frac{1}{2} \right) \right)$. For sufficiently small $g$ there is a unique $z_0 \left( r \right) \in G_0$, such that for*

$$q_r \left( z \right) := E_0 + e^{-\xi} r - z - g^2 \widetilde{\Lambda}_{00} \left( r, z \right), \tag{6.161}$$

$$q_r \left( z_0 \left( r \right) \right) = 0. \tag{6.162}$$

*Moreover, the map*

$$(0, \rho) \ni r \mapsto z_0 \left( r \right) \tag{6.163}$$

*is analytic and bounded in $[0, \rho]$. In particular, $z_0$ satisfies*

$$z_0 \left( r \right) = E_0 + e^{-\xi} r - g^2 \widetilde{\Lambda}_{00} \left( 0, E_0 \right) + \mathcal{O} \left( g^2 \rho \right). \tag{6.164}$$

*Proof.* We construct first $z_0 \left( r \right)$ for a given $r \in [0, \rho]$ by Rouché's theorem and conclude the analyticity of (6.163) by the analytic implicit function theorem.

Let $r \in [0, \rho]$. Define

$$f_r \left( z \right) := E_0 + e^{-\xi} r - z - g^2 \widetilde{\Lambda}_{00} \left( r, E_0 \right), \; \forall z \in G_0. \tag{6.165}$$

For all $z \in \partial G_0$ we have

$$\begin{aligned} \left| f_r \left( z \right) - q_r \left( z \right) \right| &\leq g^2 \left| h \left( r, z \right) \right| \left| E_0 - z \right| \\ &\leq g^2 \left| h \left( r, z \right) \right| \left( \left| f_r \left( z \right) \right| \right. \\ &\qquad \left. + g^2 \left| \widetilde{\Lambda}_{00} \left( r, E_0 \right) \right| + g^2 \rho \left| e^{-\xi} \right| \right). \end{aligned} \tag{6.166}$$

Observe now, that analogously to (6.140) and (6.144) combined with (6.159)

$$|f_r(z)| \geq Cg^2\rho^\nu, \tag{6.167}$$

for all $z \in \partial G_0$. This implies for sufficiently small $g$,

$$|f_r(z) - q_r(z)| \leq Cg^2\rho^{-\nu}|f_r(z)| < |f_r(z)|, \forall z \in \partial G_0. \tag{6.168}$$

As $f_r$ and $q_r$ are analytic in $G_0$, it follows by Rouché's theorem that $q_r$ has as many zeros as $f_r$ in $G_0$, with the same multiplicity. The existence and uniqueness follows now from

$$f_r\left(E_0 + e^{-\xi}r - g^2\widetilde{\Lambda}_{00}(r, E_0)\right) = 0, \tag{6.169}$$

since

$$E_0 + e^{-\xi}r - g^2\widetilde{\Lambda}_{00}(r, E_0) \in G_0, \tag{6.170}$$

and because this is the only zero of $f_r$ in $G_0$. One easily observes that

$$(0, \rho) \times G_0 \ni (r, z) \mapsto q_r(z) \tag{6.171}$$

is analytic in both arguments and that the derivatives do not vanish for sufficiently small $g$. It follows from the analytic implicit function theorem that (6.163) is analytic. Finally, by (6.136) and (6.133,6.134,6.135) we have

$$\begin{aligned} q_r(z) \quad = \quad & \left(E_0 + e^{-\xi}r - z - g^2\widetilde{\Lambda}_{00}(0, E_0)\right)\left(1 - g^2 h(r,z)\right) \\ & + g^2\left(\tilde{\Lambda}_{00}(0, E_0) - \widetilde{\Lambda}_{00}(r, E_0)\right)\left(1 - g^2 h(r,z)\right) \\ & + g^2 e^{-\xi} r h(r,z) + g^4\widetilde{M}(r,z). \end{aligned} \tag{6.172}$$

Note, that this expression is meaningful for all $z \in G_0$. Setting $z = z_0(r)$, the left hand side vanishes and since $h(r,z)$ is uniformly bounded we have $g^2 h(r, z_0(r)) \neq 1$. Hence, we arrive at the relation (6.164). From (6.172) follows moreover that $z_1$ is bounded on $[0, \rho]$. □

Proposition 6.18 allows now to define $z_0(H_\mathrm{f})$ by functional calculus and it follows

$$q_{H_\mathrm{f}}(z_0(H_\mathrm{f})) = 0. \tag{6.173}$$

The residue theorem implies then (6.152). We summarise these results in the subsequent theorem.

**Theorem 6.19 (The effective dynamics – $\Gamma_0$).** *Let $\rho = g^\mu$, $\mu \in (0,2)$, and pick $\nu \in \left(0, \min\left(1, \mu^{-1} - \frac{1}{2}\right)\right)$. For all $t \in \mathbb{R}_+$ and sufficiently small $g$ holds*

$$\left\| X_{\Gamma_0}(t) - e^{-itz_0(H_\mathrm{f})} \right\| \leq C\left(e^{-tc_\delta} + e^{c_0 g^2\rho^\nu t}\left(\rho^{\frac{1-\nu}{2}} + g^{\frac{1}{2}}\rho^{-\frac{1}{2}\left(\nu+\frac{1}{2}\right)}\right)\right). \tag{6.174}$$

*Proof.* The inequality (6.174) readily follows from (6.152), Lemma 6.16, Proposition 6.18, (6.160) and Proposition 6.14. □

After having established an effective time evolution pertaining to the atomic level $E_0$, we now turn to the investigation of the excited state, $E_1$. To this end we start with the following lemma.

**Lemma 6.20 (Spectal distances – $\Gamma_1$).** *Let $\rho = g^{\mu}$, $\mu \in (0,2)$ and pick $\nu \in \left(0, \min\left(1, \mu^{-1} - \frac{1}{2}\right)\right)$. For any $z \in \Gamma_0$, $F_P\left(H_g - z\right)$ and $\widetilde{F}_P\left(z\right)$ are invertible on $P\mathcal{H}$ and there are $C_{6.20}, \widetilde{C}_{6.20} \in \mathbb{R}_+$, such that*

$$\left\| F_P\left(H_g - z\right)^{-1} \right\| \leq \frac{C_{6.20}}{g^2 \rho^{\nu} + |z - E_1|}, \tag{6.175}$$

*and*

$$\left\| \widetilde{F}_P\left(z\right)^{-1} \right\| \leq \frac{\widetilde{C}_{6.20}}{g^2 \rho^{\nu} + |z - E_1|}, \tag{6.176}$$

*provided $g^2 \rho^{-1}$ is sufficiently small. Moreover for some $C \in \mathbb{R}_+$,*

$$\left\| F_P\left(H_g - z\right)^{-1} - \widetilde{F}_P\left(z\right)^{-1} \right\| \leq C\left(\rho^{1-\nu} + g\rho^{-\left(\nu + \frac{1}{2}\right)}\right) \left\| \widetilde{F}_P\left(z\right)^{-1} \right\|. \tag{6.177}$$

*Proof.* $C$ denotes again a generic constant in $\mathbb{R}_+$. We start again with estimtates of $d_\ell\left(r,z\right)$. Let $r \in [0,\rho]$, $z \in \Gamma_1$, such that $\left|\mathrm{Re}\left(z\right) - E_1\right| < \frac{\delta}{4}$. Then, by definition $\mathrm{Im}\left(z\right) = c_1 g^2 \rho^{\nu}$. We compute

$$\begin{aligned}
d_1\left(r,z\right)^2 &= \left(\mathrm{Re}\left(z\right) - E_1 - \eta_1 r\right)^2 + \left(\mathrm{Im}\left(z\right) + \eta_0 r\right)^2 \\
&= \left(\mathrm{Re}\left(z\right) - E_1\right)^2 - 2\eta_1 r\left(\mathrm{Re}\left(z\right) - E_1\right) + e^{-2\mathrm{Re}(\xi)} r^2 + \mathrm{Im}\left(z\right)^2 \\
&\quad + \underbrace{2r\eta_0 \mathrm{Im}\left(z\right)}_{\geq 0} \\
&\geq \left(e^{-\mathrm{Re}(\xi)} r - \cos\left(\mathrm{Im}\left(\xi\right)\right)\left(\mathrm{Re}\left(z\right) - E_1\right)\right)^2 + \mathrm{Im}\left(z\right)^2 \\
&\quad + \left(1 - \eta_1^2\right)\left(\mathrm{Re}\left(z\right) - E_1\right)^2 \\
&\geq \left(1 - \eta_1^2\right)\left|z - E_1\right|^2 + \eta_1^2 \mathrm{Im}\left(z\right)^2 \\
&\geq C\left(\xi\right)\left(\left|z - E_1\right|^2 + \eta_1^2 c_1^2 g^4 \rho^{2\nu}\right) \\
&\geq C\left(\xi\right)\left(\left|z - E_1\right| + \eta_1 c_1 g^2 \rho^{\nu}\right)^2,
\end{aligned} \tag{6.178}$$

for some generic $\xi$–dependent $C\left(\xi\right) > 0$. Assume now $r \in [0,\rho]$, $z \in \Gamma_1$, such that $\left|\mathrm{Re}\left(z\right) - E_1\right| \geq \frac{\delta}{4}$. Then,

$$\left|\mathrm{Im}\left(z\right)\right| \leq \left|\mathrm{Re}\left(z\right) - E_1\right|.$$

Since

$$d_1\left(r,z\right) \geq \left|z - E_1\right| - \left|e^{-\xi}\right| \rho \geq \frac{1}{2}\left|z - E_1\right| + g^2 \rho^{\nu}, \tag{6.179}$$

provided $g$ is sufficiently small, the inequality (6.178) extends to $\Gamma_1$.

Next, we consider

$$\begin{aligned}
A_{11}\left(r,z\right) &:= E_1 + e^{-\xi} r - z g^2 \Lambda_{11}\left(r,z\right) && (6.180) \\
\widetilde{A}_{11}\left(r,z\right) &:= E_1 + e^{-\xi} r - z g^2 \Lambda_{11}\left(0,E_1\right), && (6.181)
\end{aligned}$$

where

$$\Lambda_{11}(r,z) := \int_0^\infty dk \, \frac{f_\xi(k)\, \chi_{k+r\geq\rho}}{E_0 + e^{-\xi}(r+k) - z} \chi_{r<\rho}, \tag{6.182}$$

and

$$f_\xi(k) := e^{-3\xi} f\left(e^{-\xi}k\right), \quad f(k) := k^2 \left|(G)_{01}(k)\right|^2. \tag{6.183}$$

Write now $a := \mathrm{Re}(z) - E_0$, $b := \mathrm{Im}(z)$. We intend to prove

$$\mathrm{dist}\left(z, \mathcal{A}_{0,0}^{(0)}\right) \geq C(\xi) > 0, \tag{6.184}$$

for all $z \in \Gamma_1$. By redefining $\tilde{r} := e^{-\mathrm{Re}(\xi)} r$, we may set for this consideration $\mathrm{Re}(\xi) = 0$. This yields

$$d_0(r,z)^2 = r^2 + a^2 + b^2 - 2\eta_1 ra + 2\eta_0 rb. \tag{6.185}$$

Observe, that this function has a minimum at

$$r_0(z) := \eta_1 a - \eta_0 b. \tag{6.186}$$

Then

$$\begin{aligned} d_0(r,z)^2 &\geq a^2 + b^2 - (\eta_1 a - \eta_0 y)^2 \\ &= \eta_0^2 a^2 + \eta_1^2 b^2 + 2\eta_0\eta_1 ab. \end{aligned} \tag{6.187}$$

Since $z \in \Gamma_1$, we have $a \geq 2\delta$ and $b > -\eta_0\delta$. Hence,

$$\begin{aligned} d_0(r,z)^2 &\geq \eta_0^2 a^2 - 2\eta_0^2\eta_1\delta a \\ &\geq a^2\eta_0^2(1-\eta_1) \\ &\geq 4\delta^2\eta_0^2(1-\eta_1) > 0. \end{aligned} \tag{6.188}$$

For any $r \in [0,\rho)$ we compute

$$\begin{aligned} \Lambda_{11}(r,z) &- \Lambda_{11}(0,E_1) \\ &= \int_0^\infty dk\, f_\xi(k) \left( \frac{\chi_{k+r\geq\rho}}{E_0 + e^{-\xi}(r+k) - z} - \frac{\chi_{k\geq\rho}}{E_0 + e^{-\xi}k - E_1} \right) \\ &= \int_0^\infty dk\, f_\xi(k)\, \chi_{k+r\geq\rho} \left( \frac{1}{E_0 + e^{-\xi}(r+k) - z} - \frac{\chi_{k\geq\rho}}{E_0 + e^{-\xi}k - E_1} \right) \\ &= \int_0^\infty dk\, \frac{f_\xi(k)\, \chi_{k+r\geq\rho}\chi_{k<\rho}}{E_0 + e^{-\xi}(r+k) - z} \\ &\quad + \int_\rho^\infty dk\, \frac{f_\xi(k)\left(z - E_1 - e^{-\xi}r\right)}{\left(E_0 + e^{-\xi}(r+k) - z\right)\left(E_0 + e^{-\xi}k - E_1\right)}. \end{aligned} \tag{6.189}$$

Hence,

$$\begin{aligned} A_{11}(r,z) &- \widetilde{A}_{11}(r,z) \\ &= -g^2\left(\Lambda_{11}(r,z) - \Lambda_{11}(0,E_1)\right) \\ &= -g^2 B_1(r,z) + g^2\left(E_1 + e^{-\xi}r - z\right) B_2(r,z) \end{aligned} \tag{6.190}$$

where

$$B_1(r,z) := \int_0^\rho dk \, \frac{f_\xi(k)\,\chi_{k+r\geq\rho}\chi_{k<\rho}}{E_0 + e^{-\xi}(r+k) - z}, \tag{6.191}$$

$$B_2(r,z) := \int_\rho^\infty dk \, \frac{f_\xi(k)}{\left(E_0 + e^{-\xi}(r+k) - z\right)\left(E_0 + e^{-\xi}k - E_1\right)}. \tag{6.192}$$

Note that by (6.188) and the definition of $f_\xi$, (6.183),

$$\forall z \in \Gamma_1,\ 0 \leq r < \rho: \quad \|B_1(r,z)\| \leq C\rho^2, \quad \|B_2(r,z)\| \leq C. \tag{6.193}$$

This leads to

$$A_{11}(r,z) = \left(E_1 + e^{-\xi}r - z\right)\left(1 + g^2 B_2(r,z)\right) - g^2 B_1(r,z), \tag{6.194}$$

and using (6.178) thus for all $z \in \Gamma_1$, $r \in [0,\rho]$:

$$\begin{aligned} |A_{11}(r,z)| &\geq \left|E_1 + e^{-\xi}r - z\right|\left(1 - Cg^2\right) - Cg^2\rho^2 \\ &\geq C\left(|E_1 - z| + g^2\rho^\nu\right). \end{aligned} \tag{6.195}$$

We again want to construct the inverse of $\widetilde{F}_P(z)$ on the range of $P$ for all $z \in \Gamma_1$ using the Feshbach isospectrality. Therefore, we define

$$\widetilde{R}_0(z) := \left(E_0 + e^{-\xi}H_\mathrm{f}P - z - g^2\Lambda_{00}(H_\mathrm{f}, z)\right)^{-1}, \tag{6.196}$$

which exists by (6.188) for all $z \in \Gamma_1$ analogously to (6.113) and is bounded by

$$\left\|\widetilde{R}_0(z)\right\| \leq C\delta^{-1}. \tag{6.197}$$

Thus,

$$\begin{aligned} &F_{P_{\mathrm{at},1}}\left(\widetilde{F}_P(z)\right) = \\ &\quad E_0 + e^{-\xi}H_\mathrm{f}P_{\mathrm{at},1} - z - g^2\Lambda_{00}(H_\mathrm{f}, z) \qquad (6.198) \\ &\quad -g^2 P_{\mathrm{at},1}\check{\phi}\left(\left(G_\xi\right)_{10}\right)P_{\mathrm{at},0}\widetilde{R}_0(z)\,P_{\mathrm{at},0}\check{\phi}\left(\left(G_\xi\right)_{01}\right)P_{\mathrm{at},1} \qquad (6.199) \end{aligned}$$

is well–defined and we obtain the inverse of $\tilde{F}_P(z)$ by

$$\begin{aligned} \tilde{F}_P(z)^{-1} &= Q_{P_{\mathrm{at},1}}\left(\tilde{F}_P(z)\right)F_{P_{\mathrm{at},1}}\left(\widetilde{F}_P(z)\right)^{-1}Q^\sharp_{P_{\mathrm{at},1}}\left(\widetilde{F}_P(z)\right) \\ &\quad + P_{\mathrm{at},0}\tilde{R}_0(z)\,P_{\mathrm{at},0}, \end{aligned} \tag{6.200}$$

with

$$Q_{P_{\mathrm{at},1}}\left(\tilde{F}_P(z)\right) := P_{\mathrm{at},1} - \widetilde{R}_0(z)\,P_{\mathrm{at},0}\check{\phi}\left(\left(G_\xi\right)_{01}\right)P_{\mathrm{at},1}, \tag{6.201}$$

$$Q^\sharp_{P_{\mathrm{at},1}}\left(\tilde{F}_P(z)\right) := P_{\mathrm{at},1} - P_{\mathrm{at},1}\check{\phi}\left(\left(G_\xi\right)_{01}\right)P_{\mathrm{at},0}\widetilde{R}_0(z), \tag{6.202}$$

iff $F_{P_{\mathrm{at},1}}\left(\tilde{F}_P(z)\right)$ is invertible on the range of $P_{\mathrm{at},1}$. The statement follows now by similar arguments as in Lemma 6.12. □

After having established the spectral distance formulas (6.175,6.176,6.177), we proceed as for $\Gamma_0$. We start with an analogue of Proposition 6.18. To this end, we introduce $G_1$ as the interior of the compact set $\overline{G_0}$, enclosed by the curve $\Gamma_1 \cup \widetilde{\Gamma}_1 = \partial G_1$, with

$$\widetilde{\Gamma}_1 := \left\{ -ic_\delta + \left[ E_1 - \cos\left(\mathrm{Im}\left(\frac{\xi}{2}\right)\right)\delta, E_1 + \cos\left(\mathrm{Im}\left(\frac{\xi}{2}\right)\right)\delta \right] \right\}. \tag{6.203}$$

**Proposition 6.21 (Construction of $z_1(H_\mathrm{f})$).** *Let $\rho = g^\mu$, $\mu \in (0,2)$, $r \in [0,\rho]$ and pick $\nu \in \left(0, \min\left(1, \mu^{-1} - \frac{1}{2}\right)\right)$. For sufficiently small $g$ there is a unique $z_1(r) \in G_1$, such that for*

$$p_r(z) := E_1 + e^{-\xi} r - z - g^2 \widetilde{\Lambda}_{11}(r,z), \tag{6.204}$$

*with*

$$\widetilde{\Lambda}_{11}(r,z) := \int_0^\infty dk \, \frac{e^{-3\xi} k^2 \left|(G)_{01}\left(e^{-\xi}k\right)\right|^2}{E_0 + e^{-\xi}(r+k) - z}, \tag{6.205}$$

*the equation*

$$p_r(z_1(r)) = 0 \tag{6.206}$$

*holds. Moreover, the map*

$$(0,\rho) \ni r \mapsto z_1(r) \tag{6.207}$$

*is analytic and bounded on $[0,\rho]$. In particular, $z_1$ satisfies*

$$z_1(r) = E_1 + e^{-\xi} r - g^2 \widetilde{\Lambda}_{11}(0, E_1) + \mathcal{O}\left(g^2 \rho\right). \tag{6.208}$$

*Proof.* Note that (6.188) implies that $\widetilde{\Lambda}_{11}(r,z)$ is analytic in $z$, uniformly in $r \in \mathbb{R}_0^+$. Define for $r \in [0,\rho]$ and $z \in \overline{G}_1$,

$$f_r(z) := E_1 + e^{-\xi} r - z - g^2 \widetilde{\Lambda}_{11}(r, E_1). \tag{6.209}$$

Then, for some generic $C \in \mathbb{R}_+$, we get similarly to (6.166), (6.167) and (6.168),

$$\begin{aligned} |p_r(z) - f_r(z)| &\leq g^2 \left|\widetilde{\Lambda}_{11}(r,z) - \widetilde{\Lambda}_{11}(r,E_1)\right| \\ &\leq g^2 \left( \sup_{z \in \overline{G}_0} \left| \frac{d}{dz} \widetilde{\Lambda}_{11}(r,z) \right| \right) |z - E_1| \\ &\leq C g^2 \left( |f_r(z)| + g^2 \left|\widetilde{\Lambda}_{11}(r,E_1)\right| + g^2 \rho \left|e^{-\xi}\right| \right) \\ &< C g^2 \rho^{-\nu} |f_r(z)|. \end{aligned} \tag{6.210}$$

Moreover, for sufficiently small $g$,

$$E_1 + e^{-\xi} r - g^2 \widetilde{\Lambda}_{11}(r, E_1) \in G_1,$$

and this is the only zero of $f_r$. Hence there is a unique $z_1(r) \in G_1$, such that

$$p_r(z_1(r)) = 0. \tag{6.211}$$

□

Again, for small $g$, the analytic implicit function theorem implies the analyticity of (6.207). Also, analogously to Proposition 6.18 one obtains (6.208) and the boundedness of $z_1$ on $[0, \rho]$.

**Remark 6.22.** (i) Note that in contrast to Proposition 6.18, the construction of $z_1$ according to Proposition 6.21 involves $\xi$–dependent objects, and thus $z_1$ depends on $\xi$.
(ii) We do not use $\operatorname{Im}\left(\widetilde{\Lambda}_{11}(r,z)\right) < -\text{const}$.

We omit now repetitions of Proposition 6.14 and Lemmata 6.16, 6.17 for $\Gamma_1$, because the same arguments can be used. Instead, we state the final result in the following theorem.

**Theorem 6.23 (The effective dynamics – $\Gamma_1$).** *Let $\rho = g^\mu$, $\mu \in (0,2)$, and pick $\nu \in \left(0, \min\left(1, \mu^{-1} - \frac{1}{2}\right)\right)$. For all $t \in \mathbb{R}_+$ and sufficiently small $g$ holds*

$$\left\| X_{\Gamma_1}(t) - e^{-itz_1(H_\mathrm{f})} \right\| \leq C\left(e^{-tc_\delta} + e^{c_1 g^2 \rho^\nu t}\left(\rho^{\frac{1-\nu}{2}} + g^{\frac{1}{2}}\rho^{-\frac{1}{2}\left(\nu+\frac{1}{2}\right)}\right)\right). \tag{6.212}$$

## 6.3 Beyond the van Hove Timescale

In this section we give a brief outlook on how to establish an iteration of our analysis. We only present heuristic ideas, not rigorous results. The regular domains, $\Gamma_{\mathrm{lmr}}$, provide exponentially decaying error bounds, which are small for any timescale $\tau_n = tg^n$, $\epsilon \in [0,1)$, $n \geq 2$, $n \in \mathbb{N}$. Therefore, we restrict the discussion to the singular domains, $\Gamma_\ell$, $\ell = 0, 1$.

The construction of the previous section is based on the replacement of

$$P\left(H_{g,\xi} - z\right)^{-1} P$$

by the Feshbach map, which in turn is approximated by $\widetilde{F}_p(z)^{-1}$. In order to obtain finer estimates, we propose to employ the spectral renormalisation group based on the (smooth) Feshbach map originally introduced by Bach, Fröhlich, and Sigal in [BFS98b] and later generalised by these and Chen in [BCFS03]. We recall from [1] that the image under the Feshbach map,

$$F_P\left(H_g - z\right) = PH_gP - zP - g^2 PW\bar{P}\left(\bar{P}H_g\bar{P} - z\bar{P}\right)^{-1}\bar{P}WP,$$

can be written as a power series in annihilation and creation operators by expanding $\left(\bar{P}H_g\bar{P} - z\bar{P}\right)^{-1}$ in a Neumann series, i.e.

$$F_P\left(H_g - z\right) = \sum_{n,m \geq 0} W_{n,m}\left(H_\mathrm{f}, z\right),$$

where $W_{n,m}(H_\mathrm{f}, z)$ is a *Wick monomial* with $n$ creation and $m$ annihilation operators. We assume the Wick monomials to be normal ordered, i.e. all creation operators are moved to the left and all annihilation operators are moved to the right, using the CCR, 6.11. Then, one can interpret $F_P\left(H_g - z\right)$ as renormalised Hamiltonian, which however depends non–linearly on $z$. This means, that one singles out a renormalised free Hamiltonian, which is formally given by

$$H_0^{(1)}(H_\mathrm{f}, z) := W_{0,0}(H_\mathrm{f}, z),$$

i.e. $PH_0P$ plus the contractions resulting from normal ordering, see [BCFS03, Thm. 3.6]. The lowest order terms in the coupling constant of the operator $H_0^{(1)}(H_\mathrm{f}, z)$ are given by

$$H_0^{(1)}(H_\mathrm{f}, z) = PH_0P - zP - g^2\Lambda_\rho(H_\mathrm{f}, z) + \mathcal{O}\left(g^4\right).$$

Therefore, the singularities in the integral,

$$Z_\rho^{(1)}(t, H_\mathrm{f}) := \frac{1}{2\pi i}\int_{\Gamma_\ell} dz\, e^{-itz}\left(H_0^{(1)}(H_\mathrm{f}, z)\right)^{-1}$$

give rise to an analogue of $\exp(-itz_\ell(H_\mathrm{f}))$, containing all orders of contractions, not only the lowest. Then, one reduces the state space of this renormalised Hamiltonian by applying the Feshbach map with projection $P^{(1)} := \mathbf{1}\left[H_\mathrm{f} < \rho^2\right]$ to the Feshbach pair

$$\left(F_P\left(H_g - z\right), H_0^{(1)}(H_\mathrm{f}, z)\right),$$

where $F_P\left(H_g - z\right)$ is now given as a normal ordered expression. Note that

$$\left[H_0^{(1)}(H_\mathrm{f}, z), \mathbf{1}\left[H_\mathrm{f} < \rho^2\right]\right] = 0.$$

For this new operator one again applies normal ordering and obtains a new renormalised Hamiltonian, whose interaction is smaller than $\rho^\alpha$, for some $\alpha > 0$, as was shown by Bach, Chen, Fröhlich, and Sigal. Therefore, we expect that the spectral distance estimates of the present paper can be improved by some power of $\rho$. Then, the contour of the first step, $\Gamma = \Gamma^{(1)}$ can be deformed to a contour, $\Gamma^{(2)}$, which is closer to the spectral points $E_\ell$, $\ell = 0, 1$. Again, we expect that the singularities in

$$Z_{\rho^2}^{(2)}(t, H_\mathrm{f}) := \frac{1}{2\pi i}\int_{\Gamma_\ell^{(2)}} dz\, e^{-itz}\left(H_0^{(2)}(H_\mathrm{f}, z)\right)^{-1}$$

yield an effective dynamics, which approximates the projected dynamics $P^{(2)}X(t)P^{(2)}$ on a larger timescale than the van Hove timescale. Eventually, we hope to establish a renormalisation group analysis of the dynamics based on an iteration of the above. The steps described above are the first in an infinite sequence which has to be controlled inductively.

We close with a remark about the normal ordering and its relation to the spectral averaging in the theory of the weak coupling limit. The weak coupling limit due to Davies involves a spectral averaging of the generator of the effective dynamics. For $A \in \mathfrak{B}(\mathcal{H}_\mathrm{at})$ one has

$$\langle A\rangle_{H_\mathrm{at}} := \lim_{T\to\infty}\frac{1}{T}\int_0^T dt\, e^{itH_\mathrm{at}}Ae^{-itH_\mathrm{at}} = \sum_\ell \mathbf{1}\left[H_\mathrm{at} = E_\ell\right]A\mathbf{1}\left[H_\mathrm{at} = E_\ell\right].$$

In our approach there are also field degrees of freedom contributing to the WCL and it is a priori not clear how the spectral averaging can be generalised to this case, [Dav80]. The Feshbach map $F_P\left(H_g - z\right)$ can be written as

$$F_P\left(H_g - z\right) = PH_0P - zP + gPW \sum_{n=0}^{\infty} \left[ \left( \frac{\overline{P}}{H_0 - z} \right) \overline{P}\left(-g\right) W \right]^n P,$$

and the normal ordering of the last term can be expressed by the formula

$$\lim_{T\to\infty} \left\{ \frac{1}{T} \int_0^T dt\, e^{itH_\mathrm{f}} gPW \sum_{n=0}^{\infty} \left[ \left( \frac{\overline{P}}{H_0 - z} \right) \overline{P}\left(-g\right) W \right]^n e^{-itH_\mathrm{f}} \right\},$$

which is a spectral averaging w.r.t. $H_\mathrm{f}$, [BCFS03].

## 6.4 Bibliography

[BCFS03] V. Bach, T. Chen, J. Fröhlich, and I. M. Sigal, *Smooth Feshbach map and operator-theoretic renormalization group methods*, J. Funct. Anal. **203** (2003), no. 1, 44–92.

[BFS98a] V. Bach, J. Fröhlich, and I. M. Sigal, *Quantum electrodynamics of confined non-relativistic particles*, Adv. in Math. **137** (1998), 299–395.

[BFS98b] ———, *Renormalization group analysis of spectral problems in quantum field theory*, Adv. in Math. **137** (1998), 205–298.

[BFS99] V. Bach, J. Fröhlich, and I. M. Sigal, *Spectral analysis for systems of atoms and molecules coupled to the quantized radiation field*, Commun. Math. Phys. **207** (1999), no. 2, 249–290.

[CGH06] L. Cattaneo, G.M. Graf, and W. Hunziker, *A general resonance theory based on Mourre's inequality*, Ann. Henri Poincaré **7** (2006), no. 3, 583–601.

[Dav74] E. B. Davies, *Markovian master equations*, Commun. Math. Phys. **39** (1974), 91–110.

[Dav75] ———, *Markovian master equations III*, Markovian Master Equations III **XI** (1975), 265–273.

[Dav76] ———, *Markovian master equations II*, Math. Ann. **219** (1976), 147–158.

[Dav80] E.B. Davies, *One parameter semigrops*, Academic Press, 1980.

[DF06] J. Derezinski and R. Früboes, *Fermi Golden Rule and Open Quantum Systems*, Open Quantum Systems III, vol. 1882, Springer Verlag, 2006, pp. 67–116.

[HHH08] D. Hasler, I. Herbst, and M. Huber, *On the lifetime of quasi-stationary states in non-relativistic QED*, Ann. Henri Poincaré **9** (2008), 1005–1028.

[Hun90] W. Hunziker, *Resonances, metastable states and exponential decay laws in perturbation theory*, Commun. Math. Phys. **132** (1990), 177–188.

[JP95] V. Jakšić and C. A. Pillet, *On a model for quantum friction. I: Fermi's golden rule and dynamics at zero temperature*, Ann. Inst. H. Poincaré **62** (1995), 47–68.

[JP96a] ______, *On a model for quantum friction. II: Fermi's golden rule and dynamics at positive temperature*, Commun. Math. Phys. **176** (1996), no. 3, 619–643.

[JP96b] ______, *On a model for quantum friction III: Ergodic properties of the spin-boson system*, Commun. Math. Phys. **178** (1996), no. 3, 627–651.

[Kat76] T. Kato, *Perturbation theory of linear operators*, 2 ed., Grundlehren der mathematischen Wissenschaften, vol. 132, Springer-Verlag, 1976.

[Kos00] Andrzej Kossakowski, *On higher order weak coupling limits i*, Open Systems and Information Dynamics **7** (2000), 201–208.

[KR10] M. Klein and J. Rama, *Almost exponential decay of quantum resonance states and Paley-Wiener type estimates in Gevrey spaces*, Ann. Henri Poincaré **11** (2010), 499–537.