NONEQUILIBRIUM QUANTUM STATISTICAL MECHANICS AND THERMODYNAMICS*

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Abstract

The purpose of this work is to discuss recent progress in deriving the fundamental laws of thermodynamics (0^{th}, 1^{st} and 2^{nd}-law) from *nonequilibrium quantum statistical mechanics*. Basic thermodynamic notions are clarified and different *reversible* and *irreversible* thermodynamic processes are studied from the point of view of quantum statistical mechanics. Special emphasis is put on new adiabatic theorems for steady states *close to* and *far from* equilibrium, and on investigating cyclic thermodynamic processes using an extension of *Floquet* theory.

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Chapter 1

Introduction

There are numerous examples of many-particle systems in Nature, such as atoms and molecules in gases, fluids, superfluids, solids and plasmas, electrons in conductors and semi-conductors, nuclear matter in neutron stars, and the quark-gluon plasma. It is both fascinating and intriguing that *all* these different systems, when in thermal equilibrium, are theoretically described by very *general* and *universal* physical laws in the thermodynamic limit. The main aim of thermodynamics is to define appropriate physical quantities, the so called *state quantities*, which characterize the macroscopic properties of many-particle systems in thermal equilibrium, and to relate these quantities to each other through *universally* valid equations, independent of the specificity and microscopics of the physical models. However, the laws of thermodynamics have been generally viewed as *empirical theorems* or axioms. The problem to derive the 0^{th}, 1^{st}, 2^{nd} (and 3^{rd}) law, from kinetic theory and non-equilibrium statistical mechanics has been studied since the late 19^{th} century, with contributions by many distinguished theoretical physicists including Maxwell, Boltzmann, Gibbs and Einstein. In this work, we discuss some recent results concerning our own attempts to derive thermodynamics from non-equilibrium quantum statistical mechanics (NEQSM) and to bring the problem just described closer to a satisfactory solution. These are necessary steps towards understanding irreversibility and the emergence of macroscopic *classical* behavior, such as thermodynamics, from more *fundamental* (and *time-reversal invariant*) microscopic laws, such as quantum mechanics.

1.1 Summary of results

The main new results in this work are:

- Extending the positive commutator method together with a suitable Virial Theorem to prove the property of return to equilibrium (RTE) for a class of systems composed of a small quantum system coupled to non-relativistic fermionic and bosonic reservoirs, such as a spin impurity interacting with magnons in a magnet or a *quantum dot* interacting with electrons in a metal.

- Studying isothermal processes of a finitely extended, driven quantum system in contact with an infinite heat bath from the point of view of quantum statistical mechanics. Notions like heat flux, work and entropy are defined for trajectories of states close to, but distinct from states of joint thermal equilibrium. In this context, a theorem characterizing *reversible* isothermal processes as *quasi-static* processes (*isothermal theorem*) is proven. Corollaries of the latter concern changes of entropy and free energy in reversible isothermal processes and the 0^{th} law of thermodynamics. We also specialize to the specific example of a small system coupled to a fermionic reservoir, and obtain an explicit estimate on the rate of convergence to the instantaneous equilibrium states in the quasi-static limit.

- Proving a novel adiabatic theorem for generally (non)normal and unbounded generators of time evolution, and applying this theorem to the study of adiabatic evolution of states close to non-equilibrium steady states (NESS).

- Studying cyclic processes of a finitely extended, periodically driven quantum system coupled to several reservoirs from the point of view of quantum statistical mechanics, and proving the convergence of the state of the system to a time-periodic state by extending Floquet theory to non-equilibrium quantum statistical mechanics. Positivity of entropy production and Carnot's formulation of the second law of thermodynamics follow from the definite sign of relative entropy and the existence of the large time limit.

Together with extending some known techniques to prove return to equilibrium and clarifying basic notions in thermodynamics based on nonequilibrium quantum statistical mechanics, this work addresses novel questions which are important in understanding the emergence of the laws of thermodynamics. As far as we know, studying reversible isothermal processes, the adiabatic evolution of nonequilibrium steady states, and cyclic thermodynamic processes from the point of view of quantum statistical mechanics have not been attempted before in the literature.

1.2 Methods

The main methods used in this thesis are the following.

- Algebraic formulation of quantum statistical mechanics.

- Spectral analysis techniques: Mourre theory and complex deformation techniques.

- Spectral approach to RTE using the standard Liouvillain.
- Spectral approach to NESS using the C-Liouvillian.
- Spectral approach to cyclic thermodynamic processes using the so called Floquet Liouvillean.
- Generalization of adiabatic theorems in non-equilibrium quantum statistical mechanics.

1.3 Organization

The organization of this thesis is as follows. In chapter 2, after reviewing the basic laws and notions of thermodynamics, we present an overview of the derivation of these laws from non-equilibrium quantum statistical mechanics (NEQSM). In chapter 3, we discuss the mathematical framework, which is the algebraic formulation of quantum statistical mechanics [BR,Ha]. We review relevant concepts, such as the standard Liouvillean, KMS states, C^* and W^*-dynamical systems and their perturbations, and we introduce new notions such as *instantaneous* equilibrium states. The presentation in this chapter is meant to be concrete, but a mathematically more elegant and powerful, yet more abstract, presentation is given in an appendix to this chapter. In chapter 4, we list all the model quantum systems we consider in this thesis as paradigms of thermodynamic systems, together with the assumptions on these model systems. An appendix to this chapter discusses some consequences of these assumptions. In chapter 5, we prove the property of return to equilibrium for a class of quantum mechanical systems composed of a *small* system coupled to a reservoir of non-relativistic bosons or fermions, by extending the positive commutator method developed in [M1, M2, FM1, FM2, FMS]. Technical proofs in this chapter are relegated to an appendix. In chapter 6, we extensively discuss a paradigm of a thermodynamic system that we consider in the following chapters: a two-level system coupled to n fermionic reservoirs. We present the method of complex deformations developed in [JP1,2,3] and extend it to the study of *time-dependent* Liouvilleans. We also present the C-Liouvillean, and discuss how it relates to non-equilibrium steady states. In chapter 7, we study isothermal processes of a small system diathermally coupled to a single reservoir, and we state and prove the *isothermal theorem*. We define notions like heat flux, work and entropy for trajectories of states close to, but distinct from states of joint thermal equilibrium. We also prove a theorem characterizing *reversible* isothermal processes as *quasi-static* processes (*isothermal theorem*), and we discuss corollaries concerning the changes of entropy and free energy in reversible isothermal processes and the 0^{th} law of thermodynamics. In chapter 8, we prove a novel adiabatic theorem for generators of time evolution which are not necessarily normal or bounded. We also discuss two applications of this theorem in non-equilibrium quantum statistical mechanics: an adiabatic theorem for states close to non-equilibrium steady states, and a concrete example of the isothermal theorem with an explicit rate of convergence to the *quasi-static limit*. Another important application of this theorem is an adiabatic theorem for quantum resonances.[A-SF3] In chapter 9, we investigate cyclic thermodynamic processes from the point of view of quantum statistical mechanics. We introduce a new Liouvillean, the Floquet Liouvillean, which generates dynamics on a suitable Banach space when the perturbation is time periodic, and we relate the time-periodic state to which the system converges to a zero-energy resonance of the Floquet Liouvillean. In principle, we can compute the entropy production per cycle (which is positive) and the difference between the degree of efficiency η and η^{rev} to arbitrary orders in the coupling, for small enough coupling.

Chapter 2

Thermodynamics and nonequilibrium quantum statistical mechanics: an overview

This chapter offers a brief overview of the progress made towards deriving the fundamental laws of thermodynamics from non-equilibrium quantum statistical mechanics. New results which are stated here without proof are carefully and thoroughly discussed in the following chapters. Along the way, we clarify certain basic notions, such as thermodynamic systems, heat baths, different thermodynamic processes, the meaning of heat energy and the rather special and *important* role of relative entropy. The discussion at this stage is necessarily *heuristic*. However, various terms and notions appearing in this section are precisely defined in the following chapters. Before presenting this overview, we briefly recall some basic thermodynamics.

2.1 Thermodynamics

2.1.1 Basic concepts and ideas of thermodynamics

The purpose of thermodynamics is to describe the average properties of macroscopically extended matter close to a state of thermal equilibrium, with small spatial and temporal variations. (Gravitational effects are usually neglected.) Typical thermodynamic systems are formed of $10^{23} - 10^{28}$ particles, and describing the system microscopically by solving the corresponding Hamilton equations or Schrödinger equation is an impossible task. Instead, one is interested in describing emergent properties, such as the average energy per particle, using few macroscopically observable quantities, such as the volume V of the system, the total energy E, and the magnetization M. These macroscopic quantities, which can be measured simultaneously and with precision, are called *thermodynamic observables* or *state quantities*. One identifies all microstates having the same thermodynamic observables with one macrostate.

An *isolated system* is a macroscopically large thermodynamic system without any kind of contact or interaction with its *environment*. For such a system, the measured values of the thermodynamic observables are stationary, that is, time-independent. It is an observed fact that the state of an isolated system (as time $t \to \infty$) approaches asymptotically a stationary *equilibrium state*, with precise values of thermodynamic observables. (This is the equilibrium postulate for isolated systems, which is part of the 0^{th} law of thermodynamics, and which plays an important role in thermodynamics.)

Thermodynamic systems can be approximately infinite. Physically interesting states of infinitely extended systems are their equilibrium states. Although realistic systems are large but finite, if one waits long enough and one looks at a macroscopically large subset of this system, these systems behave locally as infinite ones.

Let N be the number of elements in a complete family of independent thermodynamic observables of a thermodynamic system Σ, which can be measured simultaneously and with precision. Their measured values specify a point $X \in \Gamma^{\Sigma}$, where $\Gamma^{\Sigma} \subset \mathbf{R}^N$. A thermodynamic observable is a real- valued function on Γ^{Σ}, and every $X \in \Gamma^{\Sigma}$ corresponds to an equilibrium state. The space Γ^{Σ} of equilibrium states of Σ is a connected convex subset of $\mathbf{R}^N$.

One may couple two thermodynamic systems, 1 and 2, through local interactions. Initially, when the two systems are uncoupled, the state space is the Cartesian product $\Gamma^1 \times \Gamma^2$. When one allows interaction between 1 and 2, some symmetries of 1 and 2 are broken, and the new family of thermodynamic observables and the space of equilibrium states, $\Gamma^{1\vee 2}$, of the coupled system depends on the type of couplings or contacts between 1 and 2.

We now discuss the notion of a *thermodynamic process*, which plays a central role in thermodynamics.

Let $(X_1, X_2) \in \Gamma^1 \times \Gamma^2$ be the initial uncoupled equilibrium state of $1 \vee 2$ at time t_0. One or both systems can be approximately infinite. If one turns on a coupling between 1 and 2 at time t_0, one is interested in knowing the state of the coupled system at time $t_0 + T$, as $T \to \infty$. Let $\gamma(t)$ be the microstate of the coupled system. When at least one system, 1 or 2, is finite, the 0^{th} law of thermodynamics claims that $\gamma(t) \to X_{12} \in \Gamma^{1\vee 2}$, as time $t \to \infty$. Thermodynamics specifies the mapping $\Gamma^1 \times \Gamma^2 \ni (X_1, X_2) \to X_{12} \in \Gamma^{1\vee 2}$ only when the nature of the contact between 1 and 2 is known. There are two conceivable processes

$$(X_1, X_2) \to X_{12} \ ,$$
$$X_{12} \to (X_1, X_2) \ .$$

When $X_{12} \to (X_1, X_2)$ is not possible, we say that $(X_1, X_2) \to X_{12}$ is *irreversible*. In contrast, a thermodynamic process $\{X(t)\}_{t_0 \le t < \infty}$ of Σ is *reversible* if $X(t_0) = X_i, \lim_{t \to \infty} X(t) = X_f$, and $X(t) \in \Gamma^{\Sigma}, \forall t > t_0$. In such processes, infinitesimal changes of variables happen slowly as compared to some typical relaxation time of the system, and the real state of the system at time t will be infinitesimally close to the *instantaneous equilibrium state* $X(t)$.

Thermodynamic observables correspond to constants of motion of a system, or equivalently to symmetries of the system. The space of equilibrium states Γ consists of the total spectrum of all thermodynamic observables. For each symmetry which is conserved in a thermodynamic process, there corresponds a thermodynamic observable whose value is constant in time. One can hence classify thermodynamic processes from the point of view of symmetries. A contact or coupling will correspond to a perturbation of subsystems which breaks one or more of their symmetries.

A *thermal contact* (diathermal wall) between a thermodynamic system Σ and a thermal reservoir $\mathcal{R}$ is an interaction which leaves all symmetries of Σ invariant except for time-translation invariance. It leaves all the thermodynamic observables of Σ invariant except for its energy.

Similarly, one can define a thermal contact between two thermodynamic systems Σ_1 and Σ_2 as an interaction which preserves all the symmetries of Σ_1 and Σ_2 except for time-translation invariance: It leaves all the thermodynamic observables of Σ_1 and Σ_2 invariant except for their energies.

2.1.2 The laws of thermodynamics

In this subsection, we recall the fundamental laws of thermodynamics (0^{th}, 1^{st}, and 2^{nd} law), which form the axiomatic foundation of thermodynamics.* We are interested in the physical properties of a thermodynamic system Σ, which are described by a finite number N of independent thermodynamic observables, $\xi_1, \cdots, \xi_N$.

The 0^{th}-law

There are several parts to the zeroth law.

(i) Consider an isolated thermodynamic system, Σ, which is approximately infinite. The state of Σ converges to an equilibrium state as time $t \to \infty$. Each equilibrium state of Σ corresponds to a point X in a connected convex subset $\Gamma^{\Sigma} \subset \mathbf{R}^N$.

(ii) A (weaker) form of the 0^{th} law says that there exist, for all practical purposes infinitely, large thermodynamic systems, that return to equilibrium when isolated. One calls such systems thermal reservoirs or heat baths.

(iii) Two thermal reservoirs $\mathcal{R}_1$ and $\mathcal{R}_2$ are said to be equivalent ($\mathcal{R}_1 \sim \mathcal{R}_2$) *iff* no energy flows between $\mathcal{R}_1$ and $\mathcal{R}_2$ when a diathermal contact is established between them. Then we say that the two reservoirs $\mathcal{R}_1$ and $\mathcal{R}_2$ are at the same temperature (ie, they are in *thermal equilibrium* with each other). Furthermore,

*We will not discuss the third law of thermodynamics.

given three thermal reservoirs $\mathcal{R}_1, \mathcal{R}_2$ and $\mathcal{R}_3$ such that $\mathcal{R}_1 \sim \mathcal{R}_2$ and $\mathcal{R}_2 \sim \mathcal{R}_3$, then $\mathcal{R}_1 \sim \mathcal{R}_3$, ie, all reservoirs have the same temperature (transitivity of the property of thermal equilibrium).

(iv) When one brings a finite thermodynamic system Σ in thermal contact with a thermal reservoir $\mathcal{R}$ and waits for an infinitely long time, the state of the coupled system will be an equilibrium state at the temperature of the reservoir.

(v) Moreover, if one removes the contact between Σ and $\mathcal{R}$ quasi-statically, the final state of Σ will be the (Gibbs) equilibrium state at the temperature of the reservoir, while the final state of the reservoir is identical to its initial state.

The 1^{st}-law

For each finite thermodynamic system, there exists a thermodynamic observable U, the internal energy, which has a definite value in each state in Γ^{Σ}; (U is unique up to an additive constant). For a thermodynamic process γ in which one brings Σ in contact with a thermal reservoir $\mathcal{R}$, the *heat energy* exchange $\Delta Q(\gamma)$ is a well-defined quantity which depends not only on the initial point $X_i = \partial_i \gamma$ and the final point $X_f = \partial_f \gamma$, but on the whole trajectory γ. † The difference

$$\Delta A(\gamma) := U(X_f) - U(X_i) - \Delta Q(\gamma) ,$$

is the *work* done on Σ.

Before stating the 2^{nd} law of thermodynamics, we need to introduce the notion of a heat engine.

A *heat engine* is a finite thermodynamic system that works periodically in time and that is brought in contact with at least two inequivalent thermal reservoirs or with its environment. After one cycle, the system returns to its initial state, ie, $\partial_i \gamma = \partial_f \gamma$. Let $\Delta Q(\gamma)$ be the total heat exchange between the heat engine and the thermal reservoirs in one cycle. Since the internal energy of the heat engine is the same at the beginning and at the end of each cycle, the 1^{st} law says that $\Delta Q(\gamma)$ has to be converted into work done by the heat engine on its environment.

One makes the following (scaling) postulate on heat engines: The size of a heat engine can be enlarged or reduced by a scale factor $\lambda > 0$. Consider a heat engine Σ with a space of equilibrium states Γ^{Σ}. Then

$$\Gamma^{\Sigma^{\lambda}} := \{X \in \mathbf{R}^N : \lambda^{-1} X \in \Gamma^{\Sigma}\} ,$$

is the space of equilibrium states of the heat engine Σ^{λ}. To a cycle γ of Σ, there corresponds a cycle γ^{λ} of Σ^{λ} such that

$$U(\lambda X) = \lambda U(X), \ \Delta Q(\gamma^{\lambda}) = \lambda \Delta Q(\gamma) .$$

†If $\Delta Q > 0$, heat energy flows from $\mathcal{R}$ to Σ (we say $\mathcal{R}$ is hotter than Σ), and if $\Delta Q < 0$ heat flows from Σ to $\mathcal{R}$ (we say $\mathcal{R}$ is colder than Σ).

We are now in a position to state one formulation of the second law of thermodynamics.

The 2^{nd}-law

There does not exist any heat engine that converts *all* the heat energy it receives from thermal reservoirs into work done on its environment.

Now consider a heat engine Σ connected to two thermal reservoirs $\mathcal{R}_1$ and $\mathcal{R}_2$, such that, in one cycle γ, it gains a heat energy ΔQ_1 from $\mathcal{R}_1$ and it gives a heat energy ΔQ_2 to $\mathcal{R}_2$. The heat engine performs work if $\Delta Q_1 - |\Delta Q_2| = \Delta Q_1 + \Delta Q_2 > 0$. In this case, the thermal reservoir $\mathcal{R}_1$ is called the hot reservoir, while $\mathcal{R}_2$ is called the cold reservoir.

It follows from the above formulation of the second law of thermodynamics, that if there exists a heat engine that uses $\mathcal{R}_1$ as a hot reservoir and $\mathcal{R}_2$ as a cold one, then there does not exist any heat engine that uses $\mathcal{R}_2$ as a hot reservoir and $\mathcal{R}_1$ as a cold one. This fact can be used to define an *empirical* temperature Θ : the temperature Θ_1 of $\mathcal{R}_1$ is higher than the temperature Θ_2 of $\mathcal{R}_2$ if there exists a heat engine Σ that uses $\mathcal{R}_1$ as a hot reservoir and $\mathcal{R}_2$ as a cold one.

A heat engine is said to be *reversible* (or a Carnot machine) if, in a time-reversed cycle, it can work as a heat pump: During a cycle γ^-, it takes heat ΔQ_2 from $\mathcal{R}_2$ and gives heat ΔQ_1 to $\mathcal{R}_1$. In this case, the environment must supply the work per cycle $\Delta A = \Delta Q_1 - |\Delta Q_2|$. Reversible heat engines are idealizations of realistic systems.

Define the *degree of efficiency* of a heat engine Σ as the ratio of the work done per cycle and the heat it gains from the hot reservoir in one cycle,

$$\eta^{\Sigma} := \frac{\Delta A}{\Delta Q_1} = \frac{\Delta Q_1 + \Delta Q_2}{\Delta Q_1} = 1 + \frac{\Delta Q_2}{\Delta Q_1} \ .$$

It follows from the second law of thermodynamics that among all heat engines with the same hot and cold reservoirs, the reversible engine has the highest efficiency η^{rev}. One can use this fact to define an absolute temperature T for a thermal reservoir $\mathcal{R}$, such that

$$\eta^{rev} = \frac{T_1 - T_2}{T_1} \ .$$

The fact that $\eta^{\Sigma} \leq \eta^{rev}$ implies that

$$\frac{\Delta Q_1}{T_1} + \frac{\Delta Q_2}{T_2} \leq 0 \ ,$$

with equality when γ is reversible.

This result can be generalized to the case when Σ is connected to n thermal reservoirs $\mathcal{R}_1, \cdots, \mathcal{R}_n$ with temperatures $T_1 > \cdots > T_n$. In this case,

$$\sum_{i=1}^{n} \frac{\Delta Q_i}{T_i} \leq 0 \ ,$$

with equality when the cyclic process is reversible. Taking the limit $n \to \infty$ gives

$$\oint_\gamma \frac{\delta Q}{T} \leq 0 ,$$

with equality when γ is reversible.

Consider $\gamma \in \Gamma^\Sigma$, a reversible cyclic process of Σ, and parametrize its curve in Γ^Σ by (the time) $\tau \in [t_0, \infty)$. We assume that

$$\dot{\gamma}(\tau) := \lim_{h \searrow 0} \frac{1}{h}(\gamma(\tau + h) - \gamma(\tau))$$

exists for all $\tau \in [t_0, \infty)$.

Denote by γ_t the subprocess $\{\gamma(\tau)\}_{t_0 \leq \tau \leq t}$ from $X_i = \gamma(t_0)$ to $\gamma(t) \in \Gamma^\Sigma$. From the first law of thermodynamics, $\Delta Q(\gamma_t)$ is a well-defined quantity. For $h > 0$,

$$\Delta Q(\gamma_{t+h}) - \Delta Q(\gamma_t) = h \cdot K(t) + O(h^2) ,$$

where we (assume) $K(t)$ is continuous in t. For every point $X \in \Gamma^\Sigma$, and each vector $Z \in \mathbf{R}^N$, there exists a subprocess γ_t of a reversible cyclic process γ of Σ, such that

$$\gamma(t) = X \,; \dot{\gamma}(t) = cZ ,$$

where $c \in \mathbf{R}$. One can use the functional $\Delta Q(\gamma_t)$ over a reversible subprocess $\gamma_t \in \Gamma^\Sigma$ to define a 1-form $\delta Q(\gamma(t))$ with the property that[‡]

$$\dot{\gamma}(t) \cdot \delta Q(\gamma(t)) = \lim_{h \searrow 0} \frac{1}{h}(\Delta Q(\gamma_{t+h}) - \Delta Q(\gamma_t)) = K(t) .$$

The internal energy U of Σ is a state function, ie, a function over Γ^Σ. Denote by dU the 1-form over Γ^Σ with components equal to the gradients of U. We define the work 1-form to be

$$\delta A := dU - \delta Q .$$

Let $X_1, \cdots, X_N$ be the coordinates of Γ^Σ. Then one can write

$$\delta A = \sum_{i=1}^N a_i(X) dX_i ,$$

where $a_i(X), i = 1, \cdots, N$, are called the work coefficients. They are intensive quantities, meaning that under rescaling, $a_i(\lambda X) = a_i(X), i = 1, \cdots, N$.[§]

[‡]One needs to make these arguments mathematically accurate. For further details and references, see for example [LY].

[§]Quantities ξ with the property that under rescaling $\xi(\lambda X) = \lambda \xi(X), \lambda > 0$, are called extensive, such as internal energy U and heat Q, while quantities with the property that $\xi(\lambda X) = \xi(X)$ are called intensive, such as the temperature T and work coefficients.

Using the fact that

$$\oint_{\gamma^{rev}} \frac{\delta Q}{T} = 0,\ \forall\, \gamma^{rev} \subset \Gamma^{\Sigma},$$

and the convexity of Γ^{Σ}, one can define a state function S, the *entropy*, over Γ^{Σ} such that

$$dS = \frac{\delta Q}{T}\ .$$

This gives the following identity

$$dU = TdS + \delta A\ ,$$

for reversible changes of state.

Consider $\gamma : X_i \to X_f$ a thermodynamic process of an isolated system Σ, such that $X_{i,f} \in \Gamma^{\Sigma}$. It follows from the definition of entropy and the fact that $\oint_{\gamma} \frac{\delta Q}{T} \leq 0$ that

$$S(X_f) \geq S(X_i)\ .$$

Together with the scaling postulate and the connectivity and convexity of Γ^{Σ}, one can show that the entropy S is concave. For $\lambda \in (0,1)$,

$$S(\lambda X_1 + (1-\lambda)X_2) \geq \lambda S(X_1) + (1-\lambda)S(X_2)\ .$$

There are several equivalent formulations of the second law of thermodynamics, which we list here.

(i) *Clausius* (1854). When one connects two thermal reservoirs $\mathcal{R}_1$ and $\mathcal{R}_2$ through a thermal contact, heat flows either from $\mathcal{R}_1$ to $\mathcal{R}_2$, or from $\mathcal{R}_2$ to $\mathcal{R}_1$. The opposite direction of the flow is not possible.

(ii) *Carnot* (1824). For a heat engine Σ, $\eta^{\Sigma} \leq \eta^{rev}$.

(iii) *Caratheodory* (1873-1950). In an arbitrarily small neighborhood of each equilibrium state X of an isolated system Σ, there are equilibrium states X' of Σ that are not accessible from X via reversible and adiabatic paths (for a mathematically rigorous discussion, see for example [Boy]).

It follows that for an isolated thermodynamic system, the entropy of the equilibrium state is maximal (extremal principle for entropy).

2.2 Quantum description of thermodynamic systems, heat baths and processes

We start with a brief review of the quantum theory of thermodynamic systems and heat baths which are expounded in chapter 3, and then discuss different types of thermodynamic processes. This will clarify certain notions that are needed in the ensuing discussion and will help to fix our notation.

A thermodynamic system Σ is a quantum mechanical system confined to a compact region Λ of physical space $\mathbf{R}^3$. The pure states of Σ are rays in a separable Hilbert space $\mathcal{H}^\Sigma$, and its mixed states correspond to density matrices ρ, which are positive, self-adjoint operators that have unit trace and that belong to $\mathcal{L}^1(\mathcal{H}^\Sigma)$, the two sided ideal of trace-class operators in the space of bounded operators $\mathcal{B}(\mathcal{H}^\Sigma)$ of $\mathcal{H}^\Sigma$. Since ρ is positive, $k = \rho^{\frac{1}{2}}$ belongs to $\mathcal{L}^2(\mathcal{H}^\Sigma) =: \mathcal{K}^\Sigma$, the two sided ideal of Hilbert-Schmidt operators in $\mathcal{B}(\mathcal{H}^\Sigma)$ which is isomorphic to $\mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma$. The kinematics of Σ is encoded in a C^*-algebra $\mathcal{O}^\Sigma$ such that $\mathcal{O}^\Sigma \subseteq \mathcal{B}(\mathcal{H}^\Sigma)$. The dynamics is generated by a family of (*generally time dependent*) Hamiltonians, $H^\Sigma(t) = H^\Sigma(\lambda_t)$, where λ_t are time-dependent parameters. The time-dependent Hamiltonians are self-adjoint and semi-bounded operators acting on $\mathcal{H}^\Sigma$. In the Heisenberg picture, the time evolution of an operator $a \in \mathcal{O}^\Sigma$ is $\alpha_t^\Sigma(a) = U^\Sigma(t)^* a U^\Sigma(t)$, where $U^\Sigma(t)$ is a unitary operator that satisfies $\partial_t U^\Sigma(t) = -iH^\Sigma(t)U^\Sigma(t)$ and $U^\Sigma(t=0) = 1$ (in units where $\hbar = 1$). In certain cases, α_t^Σ defines a *-automorphism on $\mathcal{O}^\Sigma$. In the Schrödinger picture, the time-evolution of an element $k \in \mathcal{K}^\Sigma$ is given by $k_t := \alpha_{-t}^\Sigma(k) = U^\Sigma(t)kU^\Sigma(t)^*$. The generator of the dynamics on $\mathcal{K}^\Sigma$ is the Liouvillean or thermal Hamiltonian $\mathcal{L}^\Sigma = ad_{H^\Sigma}$, which can be shown to be selfadjoint on a dense core of $\mathcal{K}^\Sigma$ (see chapter 3 for an extensive discussion of Liouvilleans). The time evolution of an element $k \in \mathcal{K}^\Sigma$ is given by $k_t = \widetilde{U}^\Sigma(t)k$, where $\widetilde{U}^\Sigma$ satisfies the equation $\partial_t\widetilde{U}^\Sigma(t) = -i\mathcal{L}^\Sigma(t)\widetilde{U}^\Sigma(t)$ and $\widetilde{U}^\Sigma(t=0) = 1$. Since $\mathcal{L}^2(\mathcal{H}^\Sigma)$ is a Hilbert space, one may study the spectrum of $\mathcal{L}^\Sigma(t)$ using the available methods of spectral theory, even in the thermodynamic limit $\Lambda \nearrow \mathbf{R}^3_\pm$.

A heat bath, or reservoir, $\mathcal{R}$, is the thermodynamic limit ($\Lambda \nearrow \mathbf{R}^3_\pm$) of an increasing family $\mathcal{R}_\Lambda$ of thermodynamic systems. The kinematics of the reservoir is encoded in the C^*-algebra $\mathcal{O}^\mathcal{R} := \overline{\bigvee_{\Lambda\nearrow\mathbf{R}^3_\pm} \mathcal{O}^{\mathcal{R}_\Lambda}}$, where $\overline{(\cdot)}$ denotes the norm closure. When $\mathcal{R}$ is isolated, we assume that its state is a *KMS* state on $\mathcal{O}^\mathcal{R}$ at some inverse temperature $\beta_\mathcal{R} = (k_BT^\mathcal{R})^{-1} > 0$ and chemical potentials $\mu = (\mu_1, \ldots, \mu_m)$, which correspond to conserved charges $\mathbf{Q} = (Q_1, \ldots, Q_m)$ affiliated to $(\mathcal{O}^\mathcal{R})'$. The expectation value of an operator $a \in \bigvee_{\Lambda\nearrow\mathbf{R}^3_\pm} \mathcal{O}^{\mathcal{R}_\Lambda}$ at equilibrium is

$$\omega^\mathcal{R}_{\beta,\mu}(a) = \lim_{\Lambda\nearrow\mathbf{R}^3_\pm} Tr(\mathsf{P}_{R_\Lambda} a)\ ,$$

where $\mathsf{P}_{\mathcal{R}_\Lambda} = \frac{1}{Z^{\mathcal{R}_\Lambda}_{\beta,\mu}} e^{-\beta[H^{\mathcal{R}_\Lambda} - \mu\cdot\mathbf{Q}_\Lambda]}$, $e^{-\beta[H^{\mathcal{R}_\Lambda} - \mu\cdot\mathbf{Q}_\Lambda]}$ is assumed to be trace-class, and $Z^{\mathcal{R}_\Lambda}_{\beta,\mu} = Tr(e^{-\beta[H^{\mathcal{R}_\Lambda} - \mu\cdot\mathbf{Q}_\Lambda]})$.

The dynamics of the coupled system, $\Sigma \vee \mathcal{R}$, (*before taking the thermodynamic limit*) is generated by the Hamiltonian $H(t) \equiv H^{\Sigma\vee\mathcal{R}}(t) := H^\Sigma(t) + H^\mathcal{R}$, where $H^\Sigma(t) = H_0^\Sigma(\lambda_t) + g(t)V^{\Sigma\vee\mathcal{R}}$. If P_0 is the initial state of the system at time $t = 0$, then the true state of the system at time t is $\mathsf{P}_t = U(t)\mathsf{P}_0U(t)^* =: \alpha_{-t}^{\Sigma\vee\mathcal{R}}(\mathsf{P}_0)$; it satisfies the Liouville equation $\dot{\mathsf{P}}_t = -i[H(t), \mathsf{P}_t]$. Let the reference state at time t be

$\mathsf{P}_t^\beta := Z_{\beta,\mu}(t)^{-1} e^{-\beta[H(t)-\mu\cdot\mathbf{Q}^{\Sigma\vee\mathcal{R}}]}$. A key problem in quantum statistical mechanics is establishing the existence of the thermodynamic limit of the above quantities.

$$\rho_t(\cdot) = \lim_{TD} Tr(\mathsf{P}_t \cdot) \ , \ (\textit{real state}) \tag{2.1}$$

$$\omega_t^\beta(\cdot) = \lim_{TD} Tr(\mathsf{P}_t^\beta \cdot) \ , \ (\textit{instantaneous equilibrium state}) \tag{2.2}$$

$$\rho_t^\Sigma := \rho_t|_{\mathcal{O}^\Sigma \otimes \mathbf{1}^\mathcal{R}} \ , \ (\textit{restriction to small system}) \tag{2.3}$$

and the existence of the thermodynamic limit of the dynamics α_t^g, where "$\lim_{TD}$" denotes the thermodynamic limit for $\mathcal{R}$. We will not discuss this problem; for results see [GNS, HHW, AWo,AWy,Rob,BR,Ru1].

Equivalently, one may work directly in the thermodynamic limit using the GNS construction, as explained in chapter 3.

2.3 Thermodynamic processes

We roughly sketch what we mean by different thermodynamic processes before considering specific ones later. In the example of a small system Σ coupled to reservoirs, the choice of $\{H^\Sigma(t)\}$ determines the trajectory of states $\{\rho_t^\Sigma\}$ of Σ, alternatingly in contact with $0, 1, 2, \cdots, n$ heat baths. Isothermal processes correspond to diathermal contacts of Σ to a single heat bath (or equivalently heat baths with the same temperature). Diathermal contacts preserve all extensive quantities except for the internal energy U^Σ of Σ. Circular processes, in which $\gamma_{t_i} = \gamma_{t_f}$, correspond to the case when $H^\Sigma(t + t_*) = H^\Sigma(t)$, for $t_* < \infty$. Adiabatic processes correspond to Σ isolated, and reversible processes to $\rho_t \simeq \omega_t^\beta$.

2.4 Return to equilibrium

We start with the example of an irreversible isothermal process. We will show in chapter 3 that the KMS state at inverse temperature β of a quantum mechanical system, assuming that it exists, corresponds to the simple zero eigenvalue of the *standard* Liouvillean $\mathcal{L}$, while the rest of the latter's spectrum is continuous. Hence, the study of the property of return to equilibrium is equivalent to the analysis of the spectrum of $\mathcal{L}$. In the following discussion, consider a small system Σ with finitely many degrees of freedom coupled to a single reservoir $\mathcal{R}$, and work directly in the thermodynamic limit.

Return to Equilibrium: Under suitable hypotheses, such as sufficient smallness of the coupling constant g, Fermi's golden rule, appropriate infra-red behavior of the coupling, and $\int^\infty dt \|(\mathcal{L}_t - \mathcal{L}_\infty)(\mathcal{L}_\infty + i)^{-1}\| < \infty$, one may prove the property of return to equilibrium for a class of systems $\Sigma \vee \mathcal{R}$: for an initial state of ρ_0 normal *to* $\rho_0^\Sigma \otimes \omega_\beta^{\mathcal{R}}$*,* $\lim_{t\to\infty}\rho_t(a) = \omega_\beta^\infty(a),\ \forall a \in \mathcal{O}^{\Sigma\vee\mathcal{R}}$*, where* ω_β^∞ *is the equilibrium state of the coupled system for* $t \to \infty$*, with convergence that may be exponentially fast in time for suitably chosen operators* a*.*

Using methods from spectral theory, the property of return to equilibrium has been established for a variety of quantum mechanical systems: complex deformation techniques for the spin-boson system [JP1,JP2], Feshbach map and RG for a small system coupled to a thermal reservoir of photons [BFS], and an extension of Mourre's positive commutator method together with a suitable Virial Theorem for a small system coupled to a thermal bath. [M1,FM1] All these results are based on important insights of [HHW]. (PC methods used in studying return to equilibrium have been extended to studying thermal ionization of atoms and molecules in the radiation field. [FM2,FMS])

Part of the 0^{th}-law of thermodynamics asserts that when a reservoir $\mathcal{R}$, with temperature $T^{\mathcal{R}}$, is locally perturbed, it always returns to the same unique equilibrium state after a long time. If a quantum system $\Sigma \vee \mathcal{R}$ possesses the property of return to equilibrium, the state of the coupled system will be an equilibrium state at $T^{\mathcal{R}}$ as $t \to \infty$. Moreover, if the contact between $\mathcal{R}$ and Σ is removed, then $\mathcal{R}$ returns to the same equilibrium state $\omega_\beta^{\mathcal{R}}$ after a long time. The remaining part of the 0^{th} law will be discussed later.

Proving the property of RTE for simple, yet physically relevant models, will be discussed extensively in chapter 5; (see also chapter 6).

2.5 Heat energy and entropy of thermodynamic systems

Some of the observed thermodynamic quantities during a thermodynamic process γ of a system formed of Σ coupled to n reservoirs $\mathcal{R}_i, i = 1, \cdots, n$, are the internal energy U^Σ of Σ and the heat energy Q^Σ transferred from the heat baths $\mathcal{R}_i$ to Σ. The 1^{st}-law of thermodynamics asserts the existence of functionals

$$\begin{aligned} U^\Sigma\ &: \Gamma^\Sigma \ni \gamma_. \to u^\Sigma(\gamma_.) \\ \Delta Q^\Sigma_{\mathcal{R}_i}\ &: \gamma \to \Delta Q^\Sigma_{\mathcal{R}_i}(\gamma)\ , \end{aligned}$$

and relates, for an arbitrary processes γ,

$$\Delta A^\Sigma(\gamma) := \Delta U^\Sigma - \Delta Q^\Sigma(\gamma)\ ,$$

where ΔA^Σ is the work performed on Σ during γ.

Indeed, from the quantum theory of thermodynamic systems and heat baths, the above quantities have explicit definitions. For simplicity of exposition, let the reservoirs be finite, and take the thermodynamic limit of well-defined quantities later.

The internal energy of Σ is defined by $U^{\Sigma}(t) := \rho_t(H^{\Sigma}(t))$, and the rate of change of heat energy is given by

$$\begin{aligned}\frac{\delta Q(t)}{dt} &:= -\sum_{i=1}^{n} \frac{d}{dt}\rho(H^{\mathcal{R}_i}) = -i\sum_{i=1}^{n} \rho_t([H(t), H^{\mathcal{R}_i}]) \\ &= i\sum_{i=1}^{n} \rho_t([H^{\mathcal{R}_i}, gV^{\Sigma\vee\mathcal{R}_i}(t)]) =: \sum_{i=1}^{n} \frac{\delta Q^{\mathcal{R}_i}(t)}{dt} \ ,\end{aligned}$$

where $\delta(\cdot)$ denotes the *imperfect* or *inexact* differential of $(\cdot)$. It follows that $\dot{U}^{\Sigma}(t) - \frac{\delta Q(t)}{dt} = \rho_t(\dot{H}^{\Sigma}(t)) =: \frac{\delta A(t)}{dt}$. The thermodynamic limit of the above relationship is well defined. This is nothing but the expression of the 1^{st}-law of thermodynamics.

Define the (relative) entropy of Σ as

$$\begin{aligned}S^{\Sigma}(t) &:= -k_B \lim_{TD} Tr(\mathsf{P}_t[\log \mathsf{P}_t - \sum_i \log \mathsf{P}^{\mathcal{R}_i}]) \\ &= -k_B \lim_{TD} Tr(\mathsf{P}_t[\log \mathsf{P}_t + \sum_j \{\beta_i(H^{\mathcal{R}_i} - \mu_i \cdot Q^{\mathcal{R}_i}) + \log Z^{\mathcal{R}_i}\}]) \ .\end{aligned}$$

The usefulness of this definition will become apparent soon. Since $Tr(B\log B) \geq Tr(B\log A) + Tr(B - A)$ for A and B positive, self-adjoint, and bounded operators, the relative entropy of Σ has a definite sign for all $t \in \mathbf{R}$,[¶]

$$S^{\Sigma}(t) \leq 0 \ .$$

An important property of relative entropy is its strong subadditivity (see [LR]).

Both $Tr\mathsf{P}_t \log \mathsf{P}_t$ and $Tr\mathsf{P}_t \log Z^{\mathcal{R}_i}$ are time-independent. Moreover, $Tr\mathsf{P}_t\mu_i Q^{\mathcal{R}_i}$ is time-independent for diathermal contacts. Therefore, the rate of change of entropy is

$$\begin{aligned}\dot{S}^{\Sigma}(t) &= -\sum_i \frac{1}{T_i}\frac{d\rho_t(H^{\mathcal{R}_i})}{dt} \\ &= \sum_i \frac{1}{T_i}\frac{\delta Q^{\mathcal{R}_i}(t)}{dt} \ .\end{aligned}$$

Note that if the rate of entropy production $\mathcal{E} = -\lim_{t\to\infty} \dot{S}^{\Sigma}(t)$ exists, then $\mathcal{E} \geq 0$ due to the fixed sign of $S^{\Sigma}(t)$. The last statement implies the second law of thermodynamics in the formulation of Clausius.

2.6 Isothermal processes and the isothermal theorem

The question we want to address in this section is what characterizes *reversible isothermal processes*. Careful statement of results in this section together with de-

[¶]Proof of a more general trace inequality will be given in chapter 7.

tailed proofs are given in chapter 7.

Suppose a system $\Sigma \vee \mathcal{R}$ has the property of return to equilibrium. What happens if this system is slowly perturbed after return to equilibrium, for example, by *quasi-statically* removing the contact between $\mathcal{R}$ and Σ?

Again consider the system $\Sigma \vee \mathcal{R}$ directly in the thermodynamic limit, such that the standard Liouvillean $\mathcal{L}_g^\tau(t) := \mathcal{L}_g(s)$, where the rescaled time is $s := \frac{t}{\tau}$. Assume $\mathcal{L}_g(s)$ have a common dense domain for all $s \in I$, where $I \subset \mathbf{R}$ is a compact interval. Moreover, assume that for all $s \in I$, $(\mathcal{L}_g(s)+i)^{-1}$ is differentiable in s, $\mathcal{L}_g(s)\frac{d}{ds}(\mathcal{L}_g(s)+i)^{-1}$ is uniformly bounded, $\sigma_{pp}(\mathcal{L}_g(s)) = \{0\}$ and $\sigma(\mathcal{L}_g(s))\backslash\{0\} = \sigma_c(\mathcal{L}_g(s))$, and that the projection onto the eigenstate corresponding to the zero eigenvalue of $\mathcal{L}_g(s)$, $P(s) = |\Omega_{\beta,g}(s)\rangle\langle\Omega_{\beta,g}(s)|$, is twice differentiable in s for almost all $s \in I$. Note that $P(s)$ corresponds to the instantaneous equilibrium state, or reference state, $\omega_\beta^{\tau s}$ at time $t = \tau s$. We are interested in the quasi-static limit $\tau \to \infty$. Physically, this limit corresponds to $\tau \gg \tau_R$, where τ_R is the relaxation time.

(Isothermal Theorem): Under these hypotheses, $\rho_{\tau s}(a) = \omega_{\tau s}^\beta(a) + o(1)$, as $\tau \to \infty$, $\forall a \in \mathcal{O}^\Sigma \otimes \mathcal{O}^\mathcal{R}$ and $\forall s \in I$, where $I \subset \mathbf{R}$ is an arbitrary compact interval.

To get a better estimate on the rate of convergence in the quasi-static limit, we need further information about the spectrum of the standard Liouvillian $\mathcal{L}_g(s)$. With additional hypotheses that allow one to apply complex deformation techniques, the rate of convergence is shown to be $O(\tau^{-1})$ in chapter 8. These hypotheses can be verified in classes of quantum mechanical systems, such as those for which the property of return to equilibrium has been established.

We now sketch several consequences of this theorem which will clarify the notions of heat energy and reversibilty in isothermal thermodynamic processes and emphasize the role of relative entropy. Further details can be found in chapter 7 and in [A-SF3].

Without loss of generality, assume that the small system Σ is coupled through diathermal contacts to a single reservoir $\mathcal{R}$, which will be treated as finite first before taking the thermodynamic limit. From the discussion of the previous section, we know that in an isothermal process

$$\dot{U}^\Sigma(t) = \frac{\delta Q(t)}{dt} + \frac{\delta A(t)}{dt} \; ,$$
$$\dot{S}^\Sigma(t) = \frac{1}{T^\mathcal{R}}\frac{\delta Q}{dt}(t) \; .$$

Consider an isothermal process of $\Sigma \vee \mathcal{R}$ from $t_0 = \tau s_0$ till $t_1 = \tau s_1$, for s_0 and s_1 fixed, $\tau \to \infty$, and where the initial state ω^β is independent of s for $s < s_0$. The following holds.

(i) *Reversible isothermal processes are equivalent to "quasi-static" isothermal processes for $\tau \gg \tau_R$.*

This is a standard *assumption* in *equilibrium thermodynamics*. Moreover, the definition of entropy in the latter setting is

$$\begin{aligned}
S^{\Sigma}_{rev}(t) &= -\lim_{TD} k_B Tr(\mathsf{P}^{\beta}_t[\log \mathsf{P}^{\beta}_t - \log \mathsf{P}^{\mathcal{R}}]) \\
&= \lim_{TD}[k_B\omega_\beta(\beta H^{\Sigma}(t)) + k_B \log \frac{Z_\beta(t)}{Z^{\mathcal{R}}}] \\
&= \lim_{TD}[\frac{1}{T^{\mathcal{R}}}(U^{\Sigma}_{rev} - F^{\Sigma})] ,
\end{aligned}$$

where $F^{\Sigma}(t) = -k_B \log \frac{Z_\beta(t)}{Z^{\mathcal{R}}}$ is the free energy of Σ, and k_B is Boltzmann's constant . Using the isothermal theorem, one may replace $\omega^{\beta}_{\tau s}$ by $\rho_{\tau s}$ up to an error term that vanishes in the quasi-static limit, and hence, in the thermodynamic limit,

$$\begin{aligned}
T^{\mathcal{R}}\Delta S^{\Sigma}_{rev} &= \omega^{\beta}_{\tau s}(H^{\Sigma}(s_1)) - \omega^{\beta}_{\tau s}(H^{\Sigma}(s_0)) - \int_{s_0}^{s_1} ds\omega^{\beta}_{\tau s}(\dot{H}^{\Sigma}(s)) \\
&= \Delta U^{\Sigma} - \Delta A + o(1) \\
&= \Delta Q + o(1) ,
\end{aligned}$$

where we made use of the isothermal theorem in the second step and the 1^{st}-law of thermodynamics in the last step. We have just sketched the proof of the following claim, which asserts the equivalence of the definition of entropy in equilibrium statistical mechanics and relative entropy in non-equilibrium quantum statistical mechanics, in the quasi-static limit.

(ii) $\Delta S^{\Sigma}_{rev} = \Delta S^{\Sigma} + o(1)$ *as* $\tau \to \infty$.

(iii) Furthermore, if one slowly removes the contact between $\mathcal{R}$ and Σ, the state of Σ will be the *Gibbs* state at inverse temperature $\beta_{\mathcal{R}}$, independently of the diathermal contacts.

This is part of the 0^{th}*-law of thermodynamics: If* $H^{\Sigma}(t) \to H^{\Sigma}_{\infty} \in \mathcal{O}^{\Sigma}$*, i.e.* $g(t) \to 0$ *as* $t \to \infty$*, then* $\rho_{\tau s}$ *tends to the Gibbs state at temperature* $T^{\mathcal{R}}$ *for* H^{Σ}_{∞} *as* $\tau \to \infty$ *and* $s \to \infty$*.*

2.7 Clausius' and Carnot's formulation of the 2^{nd}-law

As discussed in the previous section, there are several equivalent formulations of the 2^{nd}-law of thermodynamics. A standard consequence of the 2^{nd}-law is the existence of the absolute temperature $T_{\mathcal{R}} > 0$ of a reservoir $\mathcal{R}$ and the entropy functional

$$S^{\Sigma}_{rev} : \Gamma^{\Sigma} \ni \gamma. \to S^{\Sigma}_{rev}(\gamma.) ,$$

where Γ^{Σ} are the equilibrium states of Σ sampled in a reversible thermodynamic process.

When two or more reservoirs, with an initial state ρ_0, are coupled , the convergence to a non-equilibrium steady state (NESS) $\rho^{NESS} := w^* - \lim_{t\to\infty} \rho_0 \circ \alpha_t$ (or more weakly $w^* - \lim_{T\to\infty} \frac{1}{T}\int_0^T \rho_0 \circ \alpha_t dt$) has been proven recently in several examples using different approaches: [FMUe,Ru2,3] use algebraic scattering theory where one has to establish the existence of scattering endomorphisms. The latter is based on the work of [He,Rob]. On the other hand, [JP3] relates the NESS to the zero energy resonance of the adjoint of the so called C-Liouvillean. In the latter setting we prove an adiabatic theorem for states close to non-equilibrium steady states using a novel adiabatic theorem and complex deformation techniques in chapter 8.

Consider a thermodynamic system Σ coupled to heat baths $\mathcal{R}_1, \cdots, \mathcal{R}_n$, where $n \geq 2$. We have shown that, for diathermal contacts,

$$
\begin{aligned}
&-\infty < S^{\Sigma}(t) \leq 0 \,, \\
&\dot{S}^{\Sigma}(t) = \sum_i \frac{1}{T_i}\frac{\delta Q^{\mathcal{R}_i}(t)}{dt} \,.
\end{aligned}
$$

(NESS and Clausius) Assume that $H^{\Sigma}(t) \to H^{\Sigma}_{\infty} \in \mathcal{O}^{\Sigma} \otimes \mathcal{O}^{\mathcal{R}}$, as $t \to \infty$. If $\rho_t \to_{t\to\infty} \rho^{NESS}$, then

$$
\begin{aligned}
&i) \sum_{i=1}^{n} \frac{\delta Q^{\mathcal{R}_i}}{dt} \to 0 \\
&ii) \dot{S}^{\Sigma}(t) \to -\mathcal{E} \leq 0 \\
&iii) \lim_{t\to\infty} \sum_{i=1}^{n} \frac{1}{T_i}\frac{\delta Q^{\mathcal{R}_i}}{dt} = -\mathcal{E} \leq 0 \,,
\end{aligned}
$$

where $\mathcal{E}$ is the entropy production rate. A direct consequence is the following:

i) and iii) imply Clausius' formulation of the 2^{nd}-law.

Now consider a cyclic thermodynamic process such that $H^{\Sigma}(t+\tau_*) = H^{\Sigma}(t)$, where the period $\tau_* < \infty$, and assume, without loss of generality, that the number of reservoirs is $n = 2$. This is an example of a *heat engine* or a *heat pump*. Let $\omega^p_t := \lim_{N\to\infty} \rho_{t+N\tau_*}$. For small enough coupling between the two reservoirs, one can prove using a norm-convergent Dyson-Schwinger series that ω^p_t is periodic in time t with period τ_*, and that the change in entropy per cycle is $-\int_0^{t_*} dt\dot{S} = -\Delta S \geq 0$.[FMUe,FMSUe] We also prove convergence to a time-periodic state by relating the latter to the zero-energy resonance of the so called *Floquet Liouvillean* in chapter 9.

After one period,

$$\Delta u^{\Sigma} = 0 ,$$
$$\frac{\Delta Q^{\mathcal{R}_1}}{T_1} + \frac{\Delta Q^{\mathcal{R}_2}}{T_2} = \Delta S \leq 0 .$$

If the engine does work, $\Delta A = \Delta Q^{\mathcal{R}_1} + \Delta Q^{\mathcal{R}_2} \geq 0$. Suppose that $T_1 \geq T_2$, then *Clausius* implies that $\Delta Q^{\mathcal{R}_1} \geq 0$. The following is nothing but *Carnot's* formulation of the 2^{nd}-law of thermodynamics.

(Carnot)Assume that $T_1 > T_2$. Then

$$\begin{aligned} 0 \leq \eta^{\Sigma} := \frac{\Delta A}{\Delta Q^{\mathcal{R}_1}} &= 1 + \frac{\Delta Q^{\mathcal{R}_2}}{\Delta Q^{\mathcal{R}_1}} \\ &\leq 1 - \frac{T_2}{T_1} := \eta^{rev} . \end{aligned}$$

It is important to note that this result follows *only* from the sign of relative entropy and the existence of time periodic states in the large time limit. Moreover, the difference $\eta^{rev} - \eta^{\Sigma}$ can be explicitly computed in terms of the entropy production per cycle (see remark in chapter 9 and [FMUe]).

We conclude by mentioning that, recently, transport phenomena have been rigorously investigated from the point of view of quantum statistical mechanics. Transport phenomena between two reservoirs formed of free fermions at different temperatures/chemical potentials and coupled through bounded local interactions has been studied in [FMUe]. Together with showing the convergence of the coupled system to a NESS using scattering theory and establishing strict positivity of entropy production, they show that the Onsager reciprocity relations hold to first non-trivial order. Furthermore, [JOP] study linear response theory from the point of view of the algebraic formulation of quantum statistical mechanics and prove the Green-Kubo formula and Onsager reciprocity relations for heat fluxes generated by temperature gradients.

Chapter 3

Mathematical framework: algebraic formulation of NEQSM

For the sake of simplicity, we opt for a concrete discussion of the algebraic formulation of quantum statistical mechanics, while deferring a mathematically more elegant, yet more abstract, discussion of it to Appendix 1.[BR, Sa, DJP]

3.1 Quantum description of finite thermodynamic systems

Consider a quantum system confined to a compact region of physical space. Its pure states are unit rays in a separable Hilbert space $\mathcal{H}^\Sigma$, and its mixed states are described by density matrices ρ, which are positive trace-class operators such that $Tr(\rho) = 1$. The kinematical algebra of observables is a C^*-subalgebra $\mathcal{O}^\Sigma \subseteq \mathcal{B}(\mathcal{H}^\Sigma)$, where $\mathcal{B}(\mathcal{H}^\Sigma)$ is the set of bounded operators on $\mathcal{H}^\Sigma$. The dynamics is generated by a semi-bounded, self-adjoint operator H^Σ, the Hamiltonian, such that the time evolution of an operator $A \in \mathcal{O}^\Sigma$ is given in the Heisenberg picture by

$$\alpha^t_\Sigma(A) = e^{itH^\Sigma} A e^{-itH^\Sigma} \ , \tag{3.1}$$

assuming that $\alpha^t_\Sigma(A) \in \mathcal{O}^\Sigma$ for every $A \in O^\Sigma$.

One may represent the algebra $\mathcal{O}^\Sigma$ on the space of Hilbert-Schmidt operators, which is a Hilbert space. (In fact, the latter is a Hilbert algebra.) Consider the two-sided ideal of trace-class operators $\mathcal{L}^1(\mathcal{H}^\Sigma)$, and the two-sided ideal of Hilbert-Schmidt operators $\mathcal{L}^2(\mathcal{H}^\Sigma) = \mathcal{K}$. (An operator $k \in \mathcal{K}$ if $Tr(k^*k) < \infty$.) $\mathcal{K}$ is a Hilbert space with scalar product

$$\begin{aligned} \langle\cdot|\cdot\rangle : \mathcal{K} \times \mathcal{K} &\to \mathbf{C} \\ (\sigma, k) &\to \langle\sigma, k\rangle := Tr(\sigma^* k) \ . \end{aligned}$$

Given $\rho \in \mathcal{L}^1(\mathcal{H}^\Sigma)$ and positive, then $k := \rho^{1/2} \in \mathcal{K}$. Suppose the system is initially described by a density matrix ρ. The expectation value of an observable $A \in \mathcal{O}^\Sigma$ is

$$\langle A \rangle_\rho := Tr(\rho A) \ . \tag{3.2}$$

Its expectation value after a time t is given by

$$\begin{aligned}
\langle \alpha_\Sigma^t(A) \rangle_\rho &= Tr(\rho e^{iH^\Sigma t} A e^{-iH^\Sigma t}) \\
&= Tr(kk^* e^{iH^\Sigma t} A e^{-iH^\Sigma t}) \\
&= Tr((e^{-iH^\Sigma t} k e^{iH^\Sigma t})^* A (e^{-iH^\Sigma t} k e^{iH^\Sigma t})) \\
&= Tr(\alpha_\Sigma^{-t}(k)^* A \alpha_\Sigma^{-t}(k)) \ ;
\end{aligned}$$

hence, $k_t := \alpha_\Sigma^{-t}(k) = e^{-iH^\Sigma t} k e^{iH^\Sigma t}$ in the Schrödinger picture. Let $\mathcal{L}^\Sigma := ad_H^\Sigma$, which is a selfadjoint operator defined on $\mathcal{D}$, a dense domain in $\mathcal{K}$. (For example, $\mathcal{D} = span|\psi_i\rangle\langle\psi_j|$, where $\{\psi_i\}_i$ is the orthonormal basis in $\mathcal{H}^\Sigma$ such that $H^\Sigma|\psi_i\rangle = E_i|\psi_i\rangle$.) It follows that

$$k_t = e^{-i\mathcal{L}^\Sigma t} k \ . \tag{3.3}$$

The operator $\mathcal{L}^\Sigma$ is called the Liouvillean or thermal Hamiltonian.

A selfadjoint operator Q is said to be affiliated with the commutant $(\mathcal{O}^\Sigma)'$ if all the spectral projections of Q belong to $(\mathcal{O}^\Sigma)'$. Typically, a conserved charge of Σ corresponds to a selfadjoint operator Q affiliated to $(\mathcal{O}^\Sigma)'$, such that all the spectral projections of Q commute with all the spectral projections of H^Σ.

According to the Gibbs Ansatz, the equilibrium state of Σ at inverse temperature $\beta > 0$ and chemical potential $\mu \in \mathbf{R}$ is described by the density matrix

$$\mathsf{P}_\beta^\Sigma := \frac{e^{-\beta(H^\Sigma - \mu Q)}}{Z_\beta^\Sigma} \ , \tag{3.4}$$

where $Z_\beta^\Sigma := Tr(e^{-\beta(H^\Sigma - \mu Q)})$ is a normalization factor.

The expectation value of an operator $A \in \mathcal{O}^\Sigma$ in equilibrium is given by

$$\omega_\beta^\Sigma(A) := Tr(\mathsf{P}_\beta^\Sigma A) \ . \tag{3.5}$$

We list some of the main properties of the equilibrium state.

(i) *Time-translation invariance.* It follows from equations (3.5), (3.1), and the cyclicity of the trace that $\omega_\beta^\Sigma(\alpha_\Sigma^t(A)) = \omega_\beta^\Sigma(A)$.

(ii) *Kubo-Martin-Schwinger (KMS) condition.*

$$\omega_\beta^\Sigma(A\alpha_\Sigma^t(B)) = \omega_\beta^\Sigma(\alpha_\Sigma^{t-i\beta}(B)A) \ , \tag{3.6}$$

for $A, B \in \mathcal{O}^\Sigma$. This follows from (3.5), cyclicity of the trace, and the fact that Q is affiliated with $(\mathcal{O}^\Sigma)'$ such that its spectral projections commute with the spectral projections of H^Σ,

$$\begin{aligned}
\omega_\beta^\Sigma(A\alpha_\Sigma^t(B)) &= Tr(\mathsf{P}_\beta^\Sigma A\alpha_\Sigma^t(B)) \\
&= Tr(e^{-\beta(H^\Sigma - Q)} A e^{iH^\Sigma t} B e^{-iH^\Sigma t})/Z_\beta^\Sigma \\
&= Tr(e^{-\beta(H^\Sigma - Q)} e^{iH^\Sigma t + \beta H^\Sigma} B e^{-iH^\Sigma t - \beta H^\Sigma} A)/Z_\beta^\Sigma \\
&= Tr(\mathsf{P}_\beta^\Sigma \alpha_\Sigma^{t-i\beta}(B)A)/Z_\beta^\Sigma \\
&= \omega_\beta^\Sigma(\alpha_\Sigma^{t-i\beta}(B)A) \ .
\end{aligned}$$

There are two representations of the algebra $\mathcal{O}^\Sigma$ on the Hilbert space of Hilbert-Schmidt operators $\mathcal{K}$. The left representation $l[\mathcal{O}^\Sigma]$ is defined by

$$l[A]k = Ak \ , \tag{3.7}$$

for any $A \in O^\Sigma$ and $k \in \mathcal{K}$. A dual representation which commutes with $l[\mathcal{O}^\Sigma]$ is given by the right representation

$$r[A]k = kA^* \ , \tag{3.8}$$

for any $A \in \mathcal{O}^\Sigma$ and $k \in \mathcal{K}$. Note that $r[AB] = r[A]r[B]$ and $r[zA] = \overline{z}r[A]$, for $A, B \in \mathcal{O}^\Sigma$ and $z \in \mathbf{C}$.

In fact, one may show that $\mathcal{K}$ is isomorphic to $\mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma$. Introduce the isomorphism

$$\begin{aligned}
I_C : \mathcal{K} &\to \mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma \\
|\psi\rangle\langle\varphi| &\to \psi \otimes C^\Sigma \varphi \ ,
\end{aligned}$$

where $\psi, \varphi \in \mathcal{H}^\Sigma$, and C^Σ is an antiunitary involution on $\mathcal{H}^\Sigma$ (i.e., $(C^\Sigma)^2 = 1$ and $(C^\Sigma\psi, C^\Sigma\varphi) = (\varphi, \psi)$, where $(\cdot, \cdot)$ denotes the scalar product in $\mathcal{H}^\Sigma$). By looking at $I_C l[A]k$ and $I_C r[A]k$, for $A \in \mathcal{O}^\Sigma$ and $k \in \mathcal{K}$, one may show that

$$l[A] = A \otimes \mathbf{1} \ , \tag{3.9}$$

$$r[A] = \mathbf{1} \otimes C^\Sigma A C^\Sigma \ , \tag{3.10}$$

on $\mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma$. Both $l[\mathcal{O}^\Sigma]$ and $r[\mathcal{O}^\Sigma]$ can be related to each other, but we will defer this discussion to the more general case of infinite systems.

3.2 Quantum description of a thermal reservoir

In this section, we will discuss the quantum description of an infinitely extended thermal reservoir or heat bath $\mathcal{R}$. One may regard the heat bath or reservoir $\mathcal{R}$ as the limit of a sequence of thermodynamic systems confined to compact regions of physical space $\{\Lambda_i\}_{i=1}^{\infty}$, such that $\Lambda_i \subseteq \Lambda_j$ for $i < j$ and $\lim_{i\to\infty} \Lambda_i = \mathbf{R}^3_{\pm}$. Denote by $\mathcal{O}^{\Lambda_i}$ the kinematical algebra of Λ_i, then we will assume that $\mathcal{O}^{\Lambda_i} \subseteq \mathcal{O}^{\Lambda_j}$ if $i < j$. The kinematical algebra of *observables* in the thermodynamic limit is $\mathcal{O}^{\mathcal{R}} := \overline{\bigvee_{i\in\mathbf{N}} \mathcal{O}^{\Lambda_i}}$, where $\overline{(\cdot)}$ denotes the norm closure.

We make the following assumptions, which need to be verified in specific physical models (such as those considered in chapter 4; see also [BR]), regarding the existence of the time evolution and equilibrium states in the thermodynamic limit. Let $\mathcal{O}^{\infty} := \bigvee_{i\in\mathbf{N}} \mathcal{O}^{\Lambda_i}$.*

(A1) *Existence of dynamics.* We assume that

$$n - \lim_i \alpha^t_{\Lambda_i}(A) =: \alpha^t_{\mathcal{R}}(A) \, , \tag{3.11}$$

exists for all $A \in \mathcal{O}^{\infty}$, $t \in \mathbf{R}$, and $\{\alpha^t_{\mathcal{R}}\}_{t\in\mathbf{R}}$ is a one-parameter group of $*$-automorphisms on $\mathcal{O}^{\mathcal{R}}$. Note that $\alpha^t_{\mathcal{R}}$ need not be norm continuous, as in the case of bosonic reservoirs where it is only σ-weakly continuous (see Appendix 1).

(A2) *Existence of equilibrium states.* For $A \in \mathcal{O}^{\infty}$, consider the sequence of equilibrium expectation values $\omega^{\Lambda_i}_{\beta}$ at inverse temperatures $\beta > 0$. We assume existence of the limit of a suitable (sub)sequence $\omega^{\Lambda_i}_{\beta}(\cdot)$ as $i \to \infty$. The limiting equilibrium state $\omega^{\mathcal{R}}_{\beta}$ is $\alpha^t_{\mathcal{R}}$-invariant

$$\omega^{\mathcal{R}}_{\beta}(\alpha^t_{\mathcal{R}}(A)) = \omega^{\mathcal{R}}_{\beta}(A) \, , \tag{3.12}$$

for $A \in \mathcal{O}^{\mathcal{R}}$ and $t \in \mathbf{R}$. Moreover, it satisfies the KMS condition, which says that, for A, B in a suitable (sub)algebra of $\mathcal{O}^{\mathcal{R}}$,

$$\omega^{\mathcal{R}}_{\beta}(A\alpha^t_{\mathcal{R}}(B)) = \omega^{\mathcal{R}}_{\beta}(\alpha^{t-i\beta}_{\mathcal{R}}(B)A) \, . \tag{3.13}$$

We will state the KMS condition more carefully. Let

$$F_{AB}(t) := \omega^{\mathcal{R}}_{\beta}(A\alpha^t_{\mathcal{R}}(B)) \, , \tag{3.14}$$

$$G_{AB}(t) := \omega^{\mathcal{R}}_{\beta}(\alpha^t_{\mathcal{R}}(B)A) \, , \tag{3.15}$$

where $A \in \mathcal{O}^{\mathcal{R}}$ and $B \in O^0$. The KMS condition is equivalent to saying that $F_{AB}(t)$ is the boundary value of the function $F_{AB}(z)$, which is analytic in the

*There are several ensembles in statistical mechanics: the microcanonical ensemble, where the number of particles and energy are fixed, the canonical ensemble where the number of particles in the system is fixed while the energy varies, and the macrocanonical ensemble where both the number of particles and the energy are allowed to vary. Although different for finite systems, in the thermodynamic limit the three ensembles are equivalent.

strip $S_\beta := \{z \in \mathbf{C} : 0 < Imz < \beta\}$, bounded and continuous on its boundary, with

$$\lim_{\eta \nearrow \beta} F_{AB}(t + i\eta) = G_{AB}(t) \ . \tag{3.16}$$

(Equivalently, $G_{AB}(z)$ is analytic in the strip $S_{-\beta} := \{z \in \mathbf{C} : -\beta < Imz < 0\}$, bounded and continuous on its closure, such that $\lim_{\eta \nearrow \beta} G_{AB}(t - i\eta) = F_{AB}(t)$.) Let $\mathcal{O}^0$ be a dense subalgebra of $\mathcal{O}^{\mathcal{R}}$ which is invariant under $\alpha^t_{\mathcal{R}}$,

$$\mathcal{O}^0 := \{A_f = \int dt \alpha^t_{\mathcal{R}}(A) f(t) : A \in O^{\mathcal{R}} \text{and} \widetilde{f} \in C^\infty_0(\mathbf{R})\} \ , \tag{3.17}$$

where $\widetilde{f}$ is the Fourier transform of f. It follows from (3.12) and (3.13) that

$$\omega^{\mathcal{R}}_\beta(A^* B) = \omega^{\mathcal{R}}_\beta(\alpha^{-i\beta/2}_{\mathcal{R}}(B)(\alpha^{-i\beta/2}_{\mathcal{R}}(A))^*) \ , \tag{3.18}$$

for $A, B \in \mathcal{O}^0$. Using (3.13) and the Cauchy-Schwartz inequality, one may show that

$$\mathcal{N} := \{A \in \mathcal{O}^{\mathcal{R}} : \omega^{\mathcal{R}}_\beta(A^* A) = 0\} \tag{3.19}$$

is a two-sided ideal of $\mathcal{O}^{\mathcal{R}}$. In particular, if $\mathcal{O}^{\mathcal{R}}$ is simple (i.e., if $\mathcal{O}^{\mathcal{R}}$ does not contain any two-sided ideal except $\{0\}$ and itself), then $\omega^{\mathcal{R}}_\beta(A^* A) = 0 \Rightarrow A = 0$.

In order to do computations and to prove theorems in a concrete setting, it is useful to have a representation of $\mathcal{O}^{\mathcal{R}}$ on a certain Hilbert space. This is provided by the *GNS* (Gel'fand-Naimark-Segal) construction.

Assume there exists a countable subspace $\widetilde{\mathcal{O}} \subset \mathcal{O}^{\mathcal{R}}$ such that, $\forall A \in \mathcal{O}^{\mathcal{R}}$, there exists a sequence $\{A_i\}_{i \in \mathbf{N}} \subset \widetilde{\mathcal{O}}$ with the property that

$$\lim_{i \to \infty} \omega^{\mathcal{R}}_\beta((A - A_i)^*(A - A_i)) = 0 \ . \tag{3.20}$$

GNS. The *GNS* construction associates to the data $(\mathcal{O}^{\mathcal{R}}, \alpha^t_{\mathcal{R}}, \omega^{\mathcal{R}}_\beta)$ a Hilbert space $\mathcal{H}_\beta$, a representation π_β of $\mathcal{O}^{\mathcal{R}}$ on $\mathcal{H}_\beta$, a vector $\Omega_\beta \in \mathcal{H}_\beta$, which is cyclic for $\pi_\beta[\mathcal{O}^{\mathcal{R}}]$, and a continuous one-parameter group of unitary operators $\{e^{-i\mathcal{L}t}\}_{t \in \mathbf{R}}$, where $\mathcal{L}$ is selfadjoint on $\mathcal{H}_\beta$, such that, for all $A \in \mathcal{O}^{\mathcal{R}}$,

$$\omega^{\mathcal{R}}_\beta(A) = \langle \Omega_\beta | \pi_\beta(A) \Omega_\beta \rangle \ ; \tag{3.21}$$

$$\pi_\beta[\alpha^t_{\mathcal{R}}(A)] = e^{i\mathcal{L}t} \pi_\beta[A] e^{-i\mathcal{L}t} \ ; \tag{3.22}$$

$$\mathcal{L}\Omega_\beta = 0 \ . \tag{3.23}$$

To construct $\mathcal{H}_\beta$, Ω_β, π_β and $\mathcal{L}$, let, for all $A \in \mathcal{O}^{\mathcal{R}}$, $[A] := A \ mod \mathcal{N}$, where the two-sided ideal $\mathcal{N}$ has been defined in (3.19). Define on the linear quotient space $\widetilde{\mathcal{H}} := \mathcal{O}^{\mathcal{R}}/\mathcal{N}$ the scalar product

$$\langle [A] | [B] \rangle := \omega_\beta^{\mathcal{R}}(A^* B) \ . \tag{3.24}$$

The Hilbert space $\mathcal{H}_\beta$ is the completion (the closure in the norm induced by the scalar product defined in (3.24)) of $\widetilde{\mathcal{H}}$. Note that since $\widetilde{\mathcal{O}}$ is countable, $\mathcal{H}_\beta$ is separable. Let $\Omega_\beta := [1]$, and define $\pi_\beta : \mathcal{O}^{\mathcal{R}} \to \mathcal{B}(\mathcal{H}_\beta)$ by

$$\pi_\beta(A)[B] := [AB] \ , \tag{3.25}$$

which extends by continuity to $\mathcal{H}_\beta$. The one-parameter unitary group on $\mathcal{H}_\beta$ is defined by

$$e^{-i\mathcal{L}t}[A] := [\alpha_{\mathcal{R}}^t(A)] \ , \tag{3.26}$$

for $A \in \mathcal{O}^{\mathcal{R}}$. Unitarity follows from the fact that $\omega_\beta^{\mathcal{R}}$ is invariant under $\alpha_{\mathcal{R}}^t$, and, by Stone's theorem, the generator of the dynamics is selfadjoint because $e^{-i\mathcal{L}t}$ is strongly continuous on a separable Hilbert space.

Modular operator and modular conjugation. Assume that Ω_β is separating for $\pi_\beta(\mathcal{O}^{\mathcal{R}})$ (i.e., $\pi_\beta(A)\Omega_\beta = 0 \Rightarrow \pi_\beta(A) = 0$), and define the unbounded antilinear operator $\mathcal{S}$ on $\pi_\beta(\mathcal{O}^0)$ such that

$$\mathcal{S}(\pi_\beta(A)\Omega_\beta) := \pi_\beta(A^*)\Omega_\beta \ , \tag{3.27}$$

for $A \in \mathcal{O}^0$. We shall call this operator the modular operator, which is well-defined since Ω_β is cyclic and separating for $\pi_\beta(\mathcal{O}^0)$.

Moreover, define the modular conjugation operator J on $\pi_\beta(\mathcal{O}^0)$ such that

$$J(\pi_\beta(A)\Omega_\beta) := \mathcal{S}\pi_\beta(\alpha_{\mathcal{R}}^{-i\beta/2}(A))\Omega_\beta = \pi_\beta(\alpha_{\mathcal{R}}^{i\beta/2}(A^*))\Omega_\beta \ , \tag{3.28}$$

for $A \in \mathcal{O}^0$. Some of the properties of the modular conjugation are the following.

(i) $Je^{-i\mathcal{L}t} = e^{-i\mathcal{L}t}J$. Since $\mathcal{O}^0$ is dense in $\mathcal{O}^{\mathcal{R}}$, and Ω_β is cyclic, it suffices to show that $Je^{-i\mathcal{L}t}\pi_\beta(A)\Omega_\beta = e^{-i\mathcal{L}t}J\pi_\beta(A)\Omega_\beta$, for $A \in \mathcal{O}^0$.

$$\begin{aligned} Je^{-i\mathcal{L}t}\pi_\beta(A)\Omega_\beta &= J\pi_\beta(\alpha_{\mathcal{R}}^t(A))\Omega_\beta \\ &= \mathcal{S}\pi_\beta(\alpha_{\mathcal{R}}^{t-i\beta/2}(A))\Omega_\beta \\ &= \pi_\beta(\alpha^{t+i\beta/2}(A^*))\Omega_\beta \\ &= e^{-i\mathcal{L}t}\pi_\beta(\alpha_{\mathcal{R}}^{i\beta/2}(A^*))\Omega_\beta \\ &= e^{-i\mathcal{L}t}J\pi_\beta(A)\Omega_\beta \ . \end{aligned}$$

(ii) $\langle J\pi_\beta(A)\Omega_\beta | J\pi_\beta(B)\Omega_\beta \rangle = \langle \pi_\beta(B)\Omega_\beta | \pi_\beta(A)\Omega_\beta \rangle$, for $A, B \in \mathcal{O}^0$.

$$
\begin{aligned}
\langle J\pi_\beta(A)\Omega_\beta | J\pi_\beta(B)\Omega_\beta &= \langle \alpha_{\mathcal{R}}^{i\beta/2}(A^*)\Omega_\beta | \alpha_{\mathcal{R}}^{i\beta/2}(B^*)\Omega_\beta \\
&= \omega_\beta^{\mathcal{R}}(\alpha_{\mathcal{R}}^{-i\beta/2}(A)\alpha_{\mathcal{R}}^{i\beta/2}(B^*)) \\
&= \omega_\beta^{\mathcal{R}}(\alpha_{\mathcal{R}}^{-i\beta/2}(B^*)\alpha_{\mathcal{R}}^{-i\beta/2}(A)) \\
&= \omega_\beta^{\mathcal{R}}(B^*A) \\
&= \langle \pi_\beta(B)\Omega_\beta | \pi_\beta(A)\Omega_\beta \rangle \ .
\end{aligned}
$$

(iii) The dual representation defined by $\pi_\beta^\# = J\pi_\beta J$ commutes with π_β (i.e., $\pi_\beta^\#(\mathcal{O}^{\mathcal{R}}) \subset \pi_\beta(\mathcal{O}^{\mathcal{R}})'$). It is enough to look at $\pi_\beta^\#(A)\pi_\beta(B)\pi_\beta(C)\Omega_\beta$, for $A, B, C \in \mathcal{O}^0$.

$$
\begin{aligned}
\pi_\beta^\#(A)\pi_\beta(B)\pi_\beta(C)\Omega_\beta &= J\pi_\beta(A)J\pi_\beta(BC)\Omega_\beta \\
&= J\pi_\beta(A)\pi_\beta(\alpha_{\mathcal{R}}^{i\beta/2}(C^*B^*))\Omega_\beta \\
&= \pi_\beta(\alpha_{\mathcal{R}}^{i\beta/2}(\alpha_{\mathcal{R}}^{-i\beta/2}(BC)A^*))\Omega_\beta \\
&= \pi_\beta(BC\alpha^{i\beta/2}(A^*))\Omega_\beta \\
&= \pi_\beta(B)J\pi_\beta(A)\pi_\beta(\alpha_{\mathcal{R}}^{i\beta/2}(C^*))\Omega_\beta \\
&= \pi_\beta(B)\pi_\beta^\#(A)\pi_\beta(C)\Omega_\beta \ .
\end{aligned}
$$

The claim follows by continuity. Note that, with our assumptions, one may show that $(\pi_\beta(\mathcal{O}^{\mathcal{R}}))'' = (\pi_\beta^\#(\mathcal{O}^{\mathcal{R}}))'$ (see for example [HHW]).

(iv) Note that

$$J = \mathcal{S}e^{\beta\mathcal{L}/2} = e^{-\beta\mathcal{L}/2}\mathcal{S}.$$

The polar decomposition of $\mathcal{S}$ is

$$\mathcal{S} = Je^{-\beta\mathcal{L}/2} = e^{\beta\mathcal{L}/2}J \ ,$$

$|\mathcal{S}| = e^{-\beta\mathcal{L}/2}$ and $J = \mathcal{S}|\mathcal{S}|^{-1}$.

(v)

$$e^{it\mathcal{L}}\pi_\beta^\#(A)e^{-it\mathcal{L}} = \pi_\beta^\#(\alpha_{\mathcal{R}}^t(A)) \ ,$$

where $A \in \mathcal{O}^{\mathcal{R}}$. This follows from the definition of ${\pi_\beta}^\#$ and (i).

(vi) Suppose that ψ is an eigenvector of $\mathcal{L}$ with eigenvalue λ, and that $J\psi = \psi$. Then $\lambda = 0$.

$$\lambda\psi = \mathcal{L}\psi = \mathcal{L}J\psi = -J\mathcal{L}\psi = -J\lambda\psi = -\overline{\lambda}\psi$$

and hence $\lambda + \overline{\lambda} = 0$. However, $\lambda \in \mathbf{R}$ since $\mathcal{L}$ is selfadjoint, and therefore $\lambda = 0$.

(vii) It follows from the definition of J and the fact that $\Omega_\beta = [1]$ that $J\Omega_\beta = \Omega_\beta$.

3.3 Return to equilibrium

Part of the zeroth law of thermodynamics is that equilibrium states of reservoirs are stable under local perturbations, and that the system returns to equilibrium if the perturbation is such that it satisfies some conditions (see chapters 5 and 6).

In the thermodynamic limit, the KMS state at inverse temperature β of a quantum mechanical system, assuming that it exists, corresponds to the simple zero eigenvalue of the Liouvillean $\mathcal{L}$, while the rest of the latter's spectrum is continuous (see, for example [JP2]).[†]

Return to equilibrium

(i) Consider a state ω normal to the equilibrium state ω_β at inverse temperature β, and suppose that zero is a simple eigenvalue of the Liouvillian $\mathcal{L}$, such that the spectrum of $\mathcal{L}$ away from zero is continuous. Then the system possesses the property of return to equilibrium in the ergodic sense,

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T dt\omega(\alpha^t(A)) = \omega_\beta(A) , \tag{3.29}$$

for $A \in \mathcal{O}$.

(ii) Moreover, if the spectrum of $\mathcal{L}$ away from zero is absolutely continuous, then the system possesses the property of return to equilibrium in the mixing sense

$$\lim_{t\to\infty} \omega(\alpha^t(A)) = \omega_\beta(A) , \tag{3.30}$$

for $A \in \mathcal{O}$.

Proof. To a state ω normal to ω_β, one associates a density matrix $\rho = \sum_n p_n|\psi_n\rangle\langle\psi_n|$, such that $\sum_n p_n = 1$ and $\psi_n \in \mathcal{H}_\beta$. Since any vector $\psi_n \in \mathcal{H}_\beta$ can be approximated by a sequence of vectors $\psi_n^m = \pi_\beta(A_n^m)\Omega_\beta$, $A_n^m \in \mathcal{O}^0$, it is enough to prove

$$w - \lim_{T\to\infty} \frac{1}{T}\int_0^T \langle\pi_\beta(B)\Omega_\beta|\pi_\beta(\alpha^t(A))\pi_\beta(C)\Omega_\beta\rangle = \omega_\beta(B^*C)\omega_\beta(A) , \tag{3.31}$$

for case (i), and

$$w - \lim_{t\to\infty} \langle\pi_\beta(B)\Omega_\beta|\pi_\beta(\alpha^t(A))\pi_\beta(C)\Omega_\beta\rangle = \omega_\beta(B^*C)\omega_\beta(A) , \tag{3.32}$$

for case (ii).

For the first case (i), we use the fact that

$$w - \lim_{T\to\infty} \frac{1}{T}\int_0^T dte^{\pm i\mathcal{L}t} = |\Omega_\beta\rangle\langle\Omega_\beta| , \tag{3.33}$$

[†]The Liouvillean $\mathcal{L}$ depends on the inverse temperature β, but we suppress this dependence where there is no confusion.

and the KMS condition,

$$\begin{aligned}
&\lim_{T\to\infty}\frac{1}{T}\int_0^T dt\langle\pi_\beta(B)\Omega_\beta|\pi_\beta(\alpha^t(A))\pi_\beta(C)\Omega_\beta\rangle\\
&=\lim_{T\to\infty}\frac{1}{T}\int_0^T dt\langle\Omega_\beta|\pi_\beta(B^*)\pi_\beta(\alpha^t(A))\pi_\beta(C)|\Omega_\beta\rangle\\
&=\lim_{T\to\infty}\frac{1}{T}\int_0^T dt\langle\Omega_\beta|\pi_\beta(\alpha^{-i\beta}(C))\pi_\beta(B^*)e^{i\mathcal{L}t}\pi_\beta(A)|\Omega_\beta\rangle\\
&=\langle\Omega_\beta|\pi_\beta(\alpha^{-i\beta}(C))\pi_\beta(B)|\Omega_\beta\rangle\langle\Omega_\beta|\pi_\beta(A)\Omega_\beta\rangle\\
&=\omega_\beta(B^*C)\omega_\beta(A).
\end{aligned}$$

Case (ii) similarly follows using

$$w-\lim_{t\to\infty}e^{\pm i\mathcal{L}t}=|\Omega_\beta\rangle\langle\Omega_\beta|\ , \tag{3.34}$$

and the KMS condition.

□

We have reduced proving the property of return to equilibrium to showing that zero is a simple eigenvalue of the standard Liouvillian $\mathcal{L}$, while the rest of the spectrum away from zero is continuous. Since $\mathcal{H}_\beta$ is a Hilbert space, we can make use of the available spectral methods to prove RTE.

3.4 Perturbation of the equilibrium state

In this section, we discuss perturbation of the KMS equilibrium state. To simplify the discussion, we will consider bounded perturbations as in [Ar1]. For the unbounded case, look at the appendix, where the proof is based on the perturbation of W^*-dynamical systems, as discussed in [DJP].

Suppose the Hamiltonian of the system is perturbed by a local bounded perturbation $V\in\mathcal{O}$. The perturbed dynamics is given by the Dyson series expansion

$$\alpha_V^t(A):=\sum_{n=0}^{\infty}i^n\int_0^t dt_1\int_0^{t_1}dt_2\cdots\int_0^{t_{n-1}}dt_n[\alpha^{t_n}(V),\cdots[\alpha^{t_1}(V),\alpha^t(A)]\cdots]\ , \tag{3.35}$$

for $A\in\mathcal{O}$. This defines a one-parameter group $\{\alpha_V^t\}_{t\in\mathbf{R}}$ on $\mathcal{O}$, and α_V^t can be unitarily implemented on the GNS representation

$$\pi_\beta[\alpha_V^t(A)]=e^{it(\mathcal{L}+\pi_\beta(V))}\pi_\beta(A)e^{-it(\mathcal{L}+\pi_\beta(V))}\ . \tag{3.36}$$

Note that one may add to $(\mathcal{L}+\pi_\beta(V)$ an element $W\in\pi_\beta(\mathcal{O})^\#$. Furthermore,

$$\begin{aligned}
\pi_\beta^\#[\alpha_V^t(A)]&=J\pi_\beta(\alpha_V^t(A))J\\
&=Je^{it(\mathcal{L}+\pi_\beta(V)+W)}J\pi_\beta^\#(A)Je^{-it(\mathcal{L}+\pi_\beta(V)+W)}J\\
&=e^{it(\mathcal{L}-\pi_\beta^\#(V)-JWJ)}\pi_\beta^\#(A)e^{-it(\mathcal{L}-\pi_\beta^\#(V)-JWJ)}\ .
\end{aligned}$$

Imposing that the left representation and its dual have the same generator of dynamics gives

$$\mathcal{L}_V = \mathcal{L} + \pi_\beta(V) - \pi_\beta^{\#}(V) + Z \ ,$$

where $Z \in (\pi_\beta(\mathcal{O})' \cap \pi_\beta^{\#}(\mathcal{O})')$. Without loss of generality, set $Z = 0$. The *standard* Liouvillian is hence given by

$$\mathcal{L}_V = \mathcal{L} + \pi_\beta(V) - \pi_\beta^{\#}(V) \ . \tag{3.37}$$

Note that $J\mathcal{L}_V = -\mathcal{L}_V J$. One may also find an expression for the perturbed (α_V^t, β)-KMS state, noting that Ω_β is in the domain of the unbounded operators $e^{-\beta(\mathcal{L}+\pi_\beta(V))/2}$ and $e^{\beta(\mathcal{L}+\pi_\beta(V))/2}$.

The expectation value of an operator $A \in \mathcal{O}$ in the perturbed equilibrium state is

$$\omega_\beta^V(A) := \langle \Omega_\beta^V | \pi_\beta(A) \Omega_\beta^V \rangle \ , \tag{3.38}$$

where

$$\begin{aligned} \Omega_\beta^V &:= (Z_\beta^V)^{-\frac{1}{2}} e^{-\beta(\mathcal{L}+\pi_\beta(V))/2} \Omega_\beta \\ &= (Z_\beta^V)^{-\frac{1}{2}} \sum_{n=0}^{\infty} \int_0^{\beta/2} d\tau_1 \int_0^{\tau_1} d\tau_2 \cdots \int_0^{\tau_{n-1}} d\tau_n \pi_\beta(\alpha^{\tau_n}(V)) \cdots \pi_\beta(\alpha^{\tau_1}(V)) \Omega_\beta \ , \end{aligned}$$

after Wick rotating ($it \to \tau$), and $Z_\beta^V := \omega_\beta(e^{-\beta(\mathcal{L}+\pi_\beta(V))})$ is a normalization factor so that $\langle \Omega_\beta^V | \Omega_\beta^V \rangle = 1$. Note that we can also write

$$\Omega_\beta^V = (Z_\beta^V)^{-\frac{1}{2}} e^{\beta(\mathcal{L}-\pi_\beta^{\#}(V))/2} \Omega_\beta \ ; \tag{3.39}$$

$$J\Omega_\beta^V = \Omega_\beta^V \ , \tag{3.40}$$

$$\text{and } \mathcal{L}_{\mathrm{V}} \Omega_\beta^{\mathrm{V}} = 0. \tag{3.41}$$

3.5 Instantaneous equilibrium states

Now suppose the perturbation $V = V(t) \in \mathcal{O}$ is time-dependent. We define the *instantaneous* equilibrium states $\omega_{\beta,t}^V$ by

$$\omega_{\beta,t}^V(\cdot) := \langle \Omega_\beta^V(t) | \pi_\beta(\cdot) \Omega_\beta^V(t) \rangle \ , \tag{3.42}$$

where

$$\Omega_\beta^V(t) := (Z_{\beta,t}^V)^{-\frac{1}{2}} e^{-\beta(\mathcal{L}+\pi_\beta(V(t)))/2} \Omega_\beta \ , \tag{3.43}$$

and

$$Z_{\beta,t}^V := \omega_\beta(e^{-\beta(\mathcal{L}+\pi_\beta(V(t)))}) \ . \tag{3.44}$$

Note that, for each $t \in \mathbf{R}$,

$$\mathcal{L}_V(t) \Omega_{\beta,t}^V = 0 \ ,$$

and

$$J\Omega_{\beta,t}^V = \Omega_{\beta,t}^V.$$

These states will be useful in characterizing *reversible* isothermal processes (see chapter 7).

3.6 Appendix 1: Basics of operator algebras

3.6.1 Banach algebras

Consider an associative algebra $\mathcal{U}$ over a field $\mathcal{F}$ (which might be $\mathbf{R}$ or $\mathbf{C}$), with a norm $||\cdot||$ such that $\mathcal{U}$ is a Banach space. The algebra $\mathcal{U}$ is called a Banach algebra if $||AB|| \leq ||A||\,||B||$, for any $A, B \in \mathcal{U}$. We say $\mathcal{U}$ is unital if it contains the unit element $\mathbf{1}$. An example of a Banach algebra is the space of bounded operators on a Banach space with the operator norm.

The spectrum of $A \in \mathcal{U}$ is $\sigma(A) := \{\lambda \in \mathbf{C} : A - \lambda\mathbf{1} \text{ is not invertible in } \mathcal{U}\}$, and its spectral radius is $r(A) := \sup\{|\lambda| : \lambda \in \sigma(A)\} = \lim_{n\to\infty} ||A^n||^{\frac{1}{n}} = \inf_n ||A^n||^{\frac{1}{n}}$.

In order to discuss C^*-algebras, we need to introduce the notion of an adjoint operator. An adjoint operator in an algebra over $\mathbf{C}$ is an anti-linear map $A \to A^*$, such that $(A^*)^* = A$ and $(AB)^* = B^*A^*$, for any $A, B \in \mathcal{U}$. A C^*-algebra $\mathcal{U}$ is a Banach algebra over $\mathbf{C}$ such that $\|A^*A\| = \|A\|^2$. In particular, $\|A^*\| = \|A\|$. If $\mathcal{U}$ is a C^*-algebra without the unit element, one can extend the algebraic structure by adjoining the unit element, such that the norm on the extended algebra $\mathcal{U}_{un} := \mathbf{C}1 \oplus \mathcal{U}$ is given by $\|\alpha\mathbf{1} + A\| := \sup_{B\in\mathcal{U}\,;\|B\|=1} \|\alpha B + AB\|$, where $\alpha \in \mathbf{C}$ and $A \in \mathcal{U}$. One may also show that a C^*-algebra $\mathcal{U}$ is isomorphic to an algebra $\mathcal{O}$ of bounded operators on a complex Hilbert space $\mathcal{H}$, such that $\mathcal{O}$ is selfadjoint ($\mathcal{O}^* = \mathcal{O}$) and closed in the operator norm topology. For all practical purposes, we will consider the latter to be the definition of a C^*-algebra.

3.6.2 Positive elements

An element A of a C^*-algebra $\mathcal{O}$ is said to be positive ($A \geq 0$) if $A = A^*$ and $\sigma(A) \geq 0$, or equivalently, $A = B^*B$ for some $B \in \mathcal{O}$.

3.6.3 States

A continuous linear functional ρ on a C^*-algebra $\mathcal{O}$ is a state if $\rho \geq 0$ (ie, for positive $A \in \mathcal{O}$, $\rho(A) \geq 0$), and $||\rho|| = 1$. If $\mathcal{O}$ is unital and $\rho \geq 0$, then $||\rho|| = 1$ iff $\rho(\mathbf{1}) = 1$. A state on a C^*-algebra $\mathcal{O}$ has a unique extension to a state on $\mathcal{O}_{un}$. The set $E(\mathcal{O})$ of all states on $\mathcal{O}$ is a convex subset of the dual of $\mathcal{O}$. In particular, if $\mathcal{O}$ is unital, $E(\mathcal{O})$ is compact in the w^*-topology of the dual.

3.6.4 Representations

A representation of a C^*-algebra $\mathcal{O}$ is a pair $(\mathcal{H}, \pi)$, where $\mathcal{H}$ is a complex Hilbert space and π is a morphism of $\mathcal{O}$ to the C^*-algebra $\mathcal{B}(\mathcal{H})$ of bounded operators on $\mathcal{H}$. The representation π is said to be faithful if, for $A \in \mathcal{O}$, $\pi(A) = 0 \Rightarrow A = 0$.

A cyclic representation of $\mathcal{O}$ is a triple $(\mathcal{H}, \pi, \Omega)$, where $\Omega \in \mathcal{H}$ such that $||\Omega|| = 1$ and $\pi(\mathcal{O})\Omega$ is dense in $\mathcal{H}$.

3.6.5 Groups of automorphisms

A morphism $g : \mathcal{O} \to \mathcal{O}$ that has an inverse g^{-1} is called an automorphism. We say that a state ρ is invariant under a group of automorphisms G if $\rho(gA) = \rho(A) \forall g \in G$ and $A \in \mathcal{O}$.

3.6.6 GNS construction

If $(\mathcal{H}, \pi, \Omega)$ is a cyclic representation of a C^*-algebra $\mathcal{O}$, then $A \to \rho(A) := \langle \Omega | \pi(A) \Omega \rangle$ defines a state on $\mathcal{O}$. The converse is also true, and it is known as the GNS construction.

Let G be a group of automorphisms of the C^*-algebra $\mathcal{O}$ and ρ a corresponding G-invariant state on $\mathcal{O}$. Then there is a cyclic representation $(\mathcal{H}_\rho, \pi_\rho, \Omega_\rho)$ of $\mathcal{O}$ such that

$$\pi_\rho(gA) = U_\rho(g) \pi_\rho(A) U_\rho(g)^{-1} \, , U_\rho(g) \Omega_\rho = \Omega_\rho \, , \tag{3.45}$$

for all $g \in G$ and $A \in \mathcal{O}$. The data $(\mathcal{H}_\rho, \pi_\rho, \Omega_\rho)$ are unique up to unitary equivalence.

Proof. Assume $\mathcal{O}$ is unital (adjoin the unit element if necessary), and let $\mathcal{N} = \{A \in \mathcal{O} : \rho(A^* A) = 0\}$, and $[\cdot] : \mathcal{O} \to \mathcal{O}/\mathcal{N}$, the quotient map. Using the Cauchy-Schwarz inequality, one may show that $\mathcal{N}$ is a two-sided ideal in $\mathcal{O}$. Define the scalar product over $\mathcal{O}/\mathcal{N}$ by

$$\langle [A] | [B] \rangle = \rho(A^* B).$$

The Hilbert space $\mathcal{H}_\rho$ is the completion of $\mathcal{O}/\mathcal{N}$ with respect to this scalar product. Moreover,

$$\begin{aligned} \pi_\rho(A)[B] &:= [AB] \, ; \\ \Omega_\rho &:= [1] \, ; \\ U_\rho(g)[A] &:= [gA] \, , \end{aligned}$$

for $g \in G$ and $A, B \in \mathcal{O}$. □

3.6.7 Pure and ergodic states

Let E_G be the set of states which are G-invariant. It is a convex set. The extremal points of this set are the so-called G-ergodic states. In particular, if G is reduced to the identity on $\mathcal{O}$, E_G reduces to E, and its extremal points are pure states. Moreover, ρ is ergodic iff the only bounded operators on $\mathcal{H}_\rho$ commuting with $U_\rho(G)$ are multiples of the identity, ie, $\pi_\rho(\mathcal{O}) \vee U_\rho(G)$ is irreducible.

3.6.8 von Neumann algebras

Commutant

Let $\mathcal{B}(\mathcal{H})$ be the algebra of all bounded operators on a complex Hilbert space $\mathcal{H}$ and $\mathbf{1}$ the identity operator on $\mathcal{H}$. The commutant of a set $\mathcal{U} \subset \mathcal{B}(\mathcal{H})$ is $\mathcal{U}' := \{A \in \mathcal{B}(\mathcal{H}) : B \in \mathcal{U} \Rightarrow [A, B] = 0\}$. If the commutant $\mathcal{U}'$ consists of multiples of the identity, then $\mathcal{U}$ is irreducible. Let $\mathcal{U}'' := (\mathcal{U}')'$, the double commutant of $\mathcal{U}$.

A selfadjoint algebra $\mathcal{M}$ of $\mathcal{B}(\mathcal{H})$ is a von Neumann algebra if it satisfies one of the following *equivalent* conditions:

(1) $\mathbf{1} \in \mathcal{M}$ and $\mathcal{M}$ is closed in the strong operator topology.

(2) $\mathbf{1} \in \mathcal{M}$ and $\mathcal{M}$ is closed in the weak operator topology.

(3) $\mathcal{M} = \mathcal{M}''$.

For all practical purposes, it is useful to think of a von Neumann algebra $\mathcal{M}$ as a unital C^*-algebra on a Hilbert space. Let $\mathcal{U}$ be a selfadjoint subset of $\mathcal{B}(\mathcal{H})$. Then $\mathcal{U}'$ is a von Neumann algebra, and the double commutant $\mathcal{U}''$ is the smallest von Neumann algebra containing $\mathcal{U}$.

A von Neumann algebra $\mathcal{M}$ is called a factor if $\mathcal{M} \cap \mathcal{M}' = \lambda \mathbf{1}$, where $\lambda \in \mathbf{C}$. Factors are classified into three main types (I,II,III). We will not go into the discussion of the classification of factors, because it is beyond this review appendix.

(A von Neumann algebra is called a *concrete* W^*-algebra. An equivalent, yet abstract, definition of a W^*-algebra is given by [Sa], whereby a W^*-algebra is a C^*-algebra with a predual (see following subsection).)

3.6.9 Predual and normal states

Let $\mathcal{M}$ be a von Neumann algebra on a Hilbert space $\mathcal{H}$. Linear functionals ω on $\mathcal{M}$ of the form $A \to \omega(A) = \sum_n (\psi_n, A\varphi_n)$, where $\sum_n ||\psi_n||^2 < \infty$, $\sum_n ||\varphi_n||^2 < \infty$, form a closed subspace $\mathcal{M}_*$ of the Banach dual $\mathcal{M}^*$ of $\mathcal{M}$. $\mathcal{M}_*$ is called the predual of $\mathcal{M}$. The dual of $\mathcal{M}_*$ is $\mathcal{M}$ in the duality

$$(A, \omega) \in \mathcal{M} \times \mathcal{M}_* \to \omega(A) \ .$$

The predual of $\mathcal{B}(\mathcal{H})$ can be identified with the Banach space $\mathcal{L}^1(\mathcal{H})$ of trace-class operators on $\mathcal{H}$ using the duality

$$(A, \rho) \in \mathcal{B}(\mathcal{H}) \times \mathcal{L}^1(\mathcal{H}) \to Tr(\rho A) \ .$$

States in the predual are called normal: A state ω on $\mathcal{M}$ is normal iff there is a density matrix ρ (a positive trace-class operator with unit trace) such that $\omega(\cdot) = Tr_{\mathcal{H}}(\rho \cdot)$.

Cyclic and separating vectors

Let $\mathcal{M}$ be a von Neumann algebra on a Hilbert space $\mathcal{H}$. A vector $\Omega \in \mathcal{H}$ is cyclic if $\mathcal{M}\Omega$ is dense in $\mathcal{H}$. One says that Ω is separating if $A\Omega = 0 \Rightarrow A = 0$. Note that Ω cyclic for $\mathcal{M}$ is equivalent to Ω separating for $\mathcal{M}'$.

Suppose that $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ is the GNS construction associated with a von Neumann algebra $\mathcal{M}$ and a state ω. Then $\pi_\omega(\mathcal{M})$ is again a von Neumann algebra. Moreover, if ω is faithful (ie, $\omega(A^*A) = 0 \Rightarrow A = 0$, for $A \in \mathcal{M}$), then Ω_ω is separating for $\pi_\omega(\mathcal{M})$. In particular, π_ω is an isomorphism. W^*-algebras are $*$-isomorphism classes of von Neumann algebras.

3.6.10 Tomita-Takesaki theory

Consider the von Neumann algebra $\mathcal{M}$, with cyclic and separating vector Ω on $\mathcal{M}$. Since $\mathcal{M}'' = \mathcal{M}$, it follows that Ω is also cyclic and separating for $\mathcal{M}'$. Define the operators S and S' by

$$\begin{aligned} SA\Omega &:= A^*\Omega \,, A \in \mathcal{M} \;; \\ S'B\Omega &:= B^*\Omega \,, B \in \mathcal{M}' \;. \end{aligned}$$

Both S and S' are closable, and denote their closures by the same symbols. One can show that there is a unique positive operator, the modular operator Δ, and a unique anti-linear operator, the modular conjugation operator J, such that $S = J\Delta^{1/2}$ and $S' = J\Delta^{-1/2}$.

The Tomita-Takesaki theorem says that

$$J\mathcal{M}J = \mathcal{M}' \,, \Delta^{it}\mathcal{M}\Delta^{-it} = \mathcal{M} \,,$$

for $t \in \mathbf{R}$.

3.6.11 Modular automorphism group and the modular condition

Let ω be a faithful normal state on the von Neumann algebra $\mathcal{M}$, and $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ the corresponding GNS representation. Moreover, let Δ be the modular operator associated with the pair $(\pi_\omega, \Omega_\omega)$. (von Neumann algebras with a faithful state are called σ-finite.) One may show that there is a σ-weakly continuous one-parameter group $t \to \sigma_t^\omega$ of $*$-automorphisms of $\mathcal{M}$ defined by

$$\sigma_t^\omega(A) := \pi_\omega^{-1}(\Delta^{it}\pi_\omega(A)\Delta^{-it}).$$

This is the modular automorphism group associated with $(\mathcal{M}, \omega)$. The modular condition is

$$\begin{aligned}\langle \Delta^{1/2}\pi_\omega(A)\Omega_\omega|\Delta^{1/2}\pi_\omega(B)\Omega_\omega\rangle &= \langle J\pi_\omega(A^*)\Omega_\omega|J\pi_\omega(B^*)\Omega_\omega\rangle \\ &= \langle \pi_\omega(B^*)\Omega_\omega|\pi_\omega(A^*)\Omega_\omega\rangle \ .\end{aligned}$$

The pair $(\sigma_\omega^t, \mathcal{M})$ is called a W^*-dynamical system. We will discuss perturbations of W^*-dynamical systems in the following subsection.

3.6.12 Standard form of W^*-dynamical systems

A W^*-algebra in a standard form is a quadruple $(\mathcal{M}, \mathcal{H}, J, \mathcal{H}^+)$, where $\mathcal{H}$ is a Hilbert space, $\mathcal{M} \subset \mathcal{B}(\mathcal{H})$ is a concrete W^*-algebra, J is an antiunitary involution on $\mathcal{H}$, and $\mathcal{H}^+$ is a self-dual cone in $\mathcal{H}$ such that

(1) $J\mathcal{M}J = \mathcal{M}'$;

(2) $JAJ = A^*$ for A in the center of $\mathcal{M}$;

(3) $J\psi = \psi$ for $\psi \in \mathcal{H}^+$;

(4) $AJA\mathcal{H}^+ \subset \mathcal{H}^+$ for $A \in \mathcal{M}$.

If $\mathcal{M}$ is an abstract W^*-algebra, and if $\pi : \mathcal{M} \to \mathcal{B}(\mathcal{H})$ is an injective unital representation and $(\pi(\mathcal{M}), \mathcal{H}, J, \mathcal{H}^+)$ is a standard form, then we say that $(\pi, \mathcal{H}, J, \mathcal{H}^+)$ is its standard representation.

Suppose $\mathcal{M}$ has a faithful state ω, $\pi : \mathcal{M} \to \mathcal{B}(\mathcal{H})$ the corresponding GNS representation with cyclic vector Ω, and $\mathcal{H}^+ := \{\pi(A)J\pi(A)\Omega : A \in \mathcal{M}\}^{cl}$. Then $\mathcal{H}^+$ is a self-dual cone and $(\pi, \mathcal{H}, J, \mathcal{H}^+)$ is a standard representation of $\mathcal{M}$. Moreover, every W^*-algebra $\mathcal{M}$ possesses at least one standard representation. If $(\pi_1, \mathcal{H}_1, J_1, \mathcal{H}_1^+)$ and $(\pi_2, \mathcal{H}_2, J_2, \mathcal{H}_2^+)$ are two standard representations of $\mathcal{M}$, then there exists a unique unitary operator $W : \mathcal{H}_1 \to \mathcal{H}_2$ such that

$$\begin{aligned}W\pi_1(A) &= \pi_2(A)W \ , \\ W\mathcal{H}_1^+ &= \mathcal{H}_2^+ \ , \\ WJ_1 &= J_2W \ .\end{aligned}$$

(For a proof of these results, see for example [BR].)

From now on we will fix the standard form $(\mathcal{M}, \mathcal{H}, J, \mathcal{H}^+)$. For a vector $\Omega \in \mathcal{H}$, we associate the corresponding state ω_Ω such that

$$\omega_\Omega(A) := \langle \Omega|A\Omega\rangle \ ,$$

where $A \in \mathcal{M}$. Note that ω_Ω is a normal positive functional on $\mathcal{M}$. The following hold.

(1) The mapping $\mathcal{H}^+ \ni \Omega \to \omega_\Omega \in \mathcal{M}_*^+$ is a bijection, where $\mathcal{M}_*^+$ is the predual of $\mathcal{M}$ formed of positive linear functionals.

(2) If $\Psi, \Phi \in \mathcal{H}^+$, then

$$||\Psi - \Phi||^2 \leq ||\omega_\Psi - \omega_\Phi|| \leq ||\Psi - \Phi|| \, ||\Psi + \Phi|| \ .$$

(3) If $\Omega \in \mathcal{H}^+$, then Ω is cyclic $\Leftrightarrow$ Ω is separating $\Leftrightarrow$ ω_Ω is faithful.

Suppose that $t \to \alpha^t$ is a W^*-dynamics on $\mathcal{M}$ and let $U(\alpha^t)$ be the standard unitary operator corresponding to α^t. Then there exists a unique selfadjoint operator $\mathcal{L}$ such that $U(\alpha^t) = e^{i\mathcal{L}t}$ and $e^{i\mathcal{L}t}\mathcal{H}^+ \subset \mathcal{H}^+$. This operator is called the *standard* Liouvillean of α^t. Furthermore, $\{\omega_\Phi : \Phi \in \mathcal{H}^+ \cap Ker\mathcal{L}\} = \{\omega \in \mathcal{M}_*^+ : \omega$ is α^t-invariant $\}$. It follows that

(1) $dim\ Ker\mathcal{L} = 1 \Leftrightarrow$ there exists one normal α^t-invariant state ;

(2) $dim\ Ker\mathcal{L} = 0 \Leftrightarrow$ there are no normal α^t-invariant states.

3.6.13 Perturbation of W^*-dynamical systems

Perturbation of the W^*-dynamics

Consider a W^*-algebra $\mathcal{M} \subset \mathcal{B}(\mathcal{H})$ with W^*-dynamics implemented by a selfadjoint operator $\mathcal{L}$, and a Hamiltonian perturbation V, which is a selfadjoint operator affiliated to $\mathcal{M}$. We will make the following sufficient assumptions to prove the existence of the perturbed dynamics.

(A1) $\mathcal{L} + V$ is essentially selfadjoint on $\mathcal{D}(\mathcal{L}) \cap \mathcal{D}(V)$.

Proposition A1.1. Let $\alpha_V^t(A) := e^{it(\mathcal{L}+V)}Ae^{-it(\mathcal{L}+V)}$ for $A \in \mathcal{M}$, and suppose (A1) holds. Then

(i) α_V^t is a W^*-dynamics on $\mathcal{M}$;

(ii) if the perturbation V is bounded, then

$$\alpha_V^t(\cdot) = \sum_{n\geq 0} i^n \int_{0\leq t_n\leq\cdots\leq t_1\leq t} [\alpha^{t_n}(V), [\cdots[\alpha^{t_1}(V), \alpha^t(\cdot)]\cdots]dt_1\cdots dt_n \ .$$

Since L and V are selfadjoint, and $L+V$ is essentially selfadjoint on $\mathcal{D}(L)\cap\mathcal{D}(V)$, the proof of the above proposition follows from the Trotter product formula [RS1]

$$\alpha_V^t(A) = s - \lim_{n\to\infty}(e^{it\mathcal{L}/n}e^{itV/n})^n(A)(e^{-it\mathcal{L}/n}e^{-itV/n})^n \ ,$$

where $A \in \mathcal{M}$. Since $e^{\pm itV/n} \in \mathcal{M}$, $\alpha_V^t(A) \in \mathcal{M}$. Therefore, α_V^t is a W^*-dynamics. Claim (ii) is nothing but a Dyson series expansion when the perturbation is bounded.

Perturbation of the standard Liouvillean

Suppose that $(\mathcal{M}, \mathcal{H}, J, \mathcal{H}^+)$ is a standard form of a W^*-algebra, and define the standard Liouvillean as $\mathcal{L}_V := \mathcal{L} + V - JVJ$. We will make the following assumption.

(A2) $\mathcal{L}_V$ is essentially selfadjoint on $\mathcal{D}(\mathcal{L}) \cap \mathcal{D}(V) \cap \mathcal{D}(JVJ)$.

Proposition A1.2. Suppose that (A1) and (A2) hold. Then

(i) $\alpha_V^t(A) = e^{it\mathcal{L}_V} A e^{-it\mathcal{L}_V}$;

(ii) $e^{\pm i\mathcal{L}_V t}\mathcal{H}^+ \subset \mathcal{H}^+$.

Proof. Note first that $e^{itJVJ} = Je^{-itV}J \in \mathcal{M}'$. Since $\mathcal{D}(\mathcal{L}) \cap \mathcal{D}(V) \subset \mathcal{D}(\mathcal{L}+V)$, it follows that $\mathcal{D}(\mathcal{L}) \cap \mathcal{D}(V) \cap \mathcal{D}(JVJ) \subset \mathcal{D}(\mathcal{L}+V) \cap \mathcal{D}(JVJ)$. Now, (i) follows from the fact that $\mathcal{L}_V$ is essentially selfadjoint on $\mathcal{D}(\mathcal{L}+V) \cap \mathcal{D}(JVJ)$ and the Trotter product formula $e^{it\mathcal{L}_V} = s - \lim_{n\to\infty}(e^{it(\mathcal{L}+V)/n}e^{-itJVJ/n})^n$. Moreover, since e^{itV} and e^{-itJVJ} commute, $e^{it(V-JVJ)} = e^{itV}Je^{itV}J$. Hence, $e^{it(V-JVJ)}\mathcal{H}^+ \subset \mathcal{H}^+$. The latter together with $e^{it\mathcal{L}}\mathcal{H}^+ \subset \mathcal{H}^+$ imply (ii). □

Relative entropy

Let $\mathcal{M}$ be a W^*-algebra, and ψ, φ be two functionals in $\mathcal{M}_*^+$ with representation vectors Ψ, Φ respectively. Before discussing relative entropy, we need to recall the definition of the relative modular operator. Define the operator $S_{\Phi,\Psi}$ by $S_{\Phi,\Psi}A\Psi := A^*\Phi$. The relative modular operator is $\Delta_{\Phi,\Psi} = S_{\Phi,\Psi}^* S_{\Phi,\Psi}$.

Denote by $Ent(\psi|\varphi)$ the relative entropy of ψ, φ as defined by Araki in [Ar2]. (We will follow the sign convention as in [BR].)

$$Ent(\psi|\varphi) = \begin{cases} \langle \Psi | \log \Delta_{\Phi,\Psi}\Psi \rangle \text{ if } S_\psi \leq S_\varphi \\ -\infty \text{ otherwise} \end{cases} . \tag{3.46}$$

Proposition A1.3.

$$Ent(\psi|\varphi) = \lim_{t\downarrow 0} t^{-1}(\|\Delta_{\Phi,\Psi}^{t/2}\Psi\|^2 - \|\Psi\|^2)$$

.

Proof. We will only sketch the main steps of the proof. The claim follows from the spectral theorem, the monotone convergence theorem, and the fact that $\log x = \lim_{t\downarrow 0}(x^t - 1)$, monotonically on the intervals $x \in [0,1], [1,\infty)$. □

Let $\mathcal{M}_1$ and $\mathcal{M}_2$ be two W^*-algebras. A map $\gamma : \mathcal{M}_1 \to \mathcal{M}_2$ is a Schwartz map iff $\gamma(\mathbf{1}) = 1$ and $\gamma(A^*A) \geq \gamma(A^*)\gamma(A)$.

Theorem A1.3 (Uhlmann's monotinicity theorem).

Let ψ_i, φ_i be normal states on $\mathcal{M}_i, i = 1, 2$, and $\gamma : \mathcal{M}_1 \to \mathcal{M}_2$ a Schwartz map such that $\psi_2 \circ \gamma = \psi_1$ and $\varphi_2 \circ \gamma = \varphi_1$. Then

$Ent(\psi_2|\varphi_2) \leq Ent(\psi_1|\varphi_1)$.(see [Uh,Do,Ar2])

Proof. We prove this result in a standard concrete setting (which is equivalent to the abstract setting). Let $(\mathcal{M}_i, \mathcal{H}_i, J_i, \mathcal{H}_i^+)$ be the standard form of $\mathcal{M}_i, i = 1, 2$, $\gamma : \mathcal{M}_1 \to \mathcal{M}_2$ a Schwartz map, and $\psi_i \in \mathcal{M}_{i,*}^+, i = 1, 2$ with corresponding representation vectors Ψ_i such that $\psi_2\gamma = \psi_1$. Furthermore, let $\mathcal{D}_1 = \mathcal{M}_1\Psi + (\mathcal{M}_1\Psi)^\perp$, and $T : \mathcal{D}_1 \to \mathcal{H}_2$ a linear map defined by

$$T(A\Psi_1 + \Theta_1) := \gamma(A)\Psi_2 \ ,$$

for $A \in \mathcal{M}_1, \Theta_1 \in (\mathcal{M}_1\Psi_1)^\perp$. Since $\gamma(\mathbf{1}) = 1$ and $T\Psi_1 = \Psi_2$, T is well defined and extends to a contraction from $\mathcal{H}_1$ to $\mathcal{H}_2$. The claim of the theorem follows from the interpolation estimate for the relative modular operator

$$\|\Delta_{\Phi,\Psi}^{t/2}\Psi_2\| \leq \|\Delta_{\Phi,\Psi_1}^{t/2}\Psi_1\| \ , 0 \leq t \leq 1,$$

together with

$$Ent(\psi|\varphi) = \lim_{t\downarrow 0}(\|\Delta_{\Phi,\Psi}^{t/2}\Psi\| - \|\Psi\|^2.$$

□

A direct corollary of this theorem is the following.

Corollary A1.4.

Let $\mathcal{N} \subset \mathcal{M}$ be W^*-algebras with common identity element, $\psi, \varphi \in \mathcal{M}_*^+$, and $|_\mathcal{N}$ is the restriction to $\mathcal{N}$. Then $Ent_\mathcal{M}(\psi|\varphi) \leq Ent(\psi|_\mathcal{N}|\phi|_\mathcal{N})$.

Perturbation of KMS states

Consider $(\mathcal{M}, \mathcal{H}, J, \mathcal{H}^+)$ a W^*-algebra in the standard form, α^t a W^*-dynamics, and ω a faithful (α^t, β)-KMS state, with $\beta > 0$. In this subsection we discuss the existence of the perturbed KMS state for a large class of *unbounded* perturbations.

We first prove its existence for bounded perturbations and then extend the proof to unbounded perturbations.

Theorem A1.5 (Bounded perturbation).

Suppose V is a bounded perturbation. Then we have the following:

(i) $\Omega \in \mathcal{D}(e^{-\beta(\mathcal{L}+V)/2})$.

Let $\Omega_V := e^{-\beta(\mathcal{L}+V)/2}\Omega$ and $\omega_V(A) := \langle\Omega_V|A\Omega_V\rangle$, for $A \in \mathcal{M}$.

(ii) $\Omega_V \in \mathcal{H}^+$ and is cyclic and separating.

(iii) ω_V is an (α_V^t, β)-KMS state.

(iv) The Peierls-Bogoliobov inequality holds

$$e^{-\beta\langle\Omega|V\Omega\rangle/2} \leq \|\Omega_V\|.$$

(v) The Golden-Thompson inequality holds

$$\|\Omega_V\| \leq \|e^{-\beta V/2}\Omega\|.$$

Sketch of the proof. Although these results have been obtained in [Ar1], we follow the proof of [DJP] which can be extended to unbounded perturbations. The first step is to prove (i)-(v) for analytic perturbations, which approximate bounded perturbations, and then extend the proof to bounded perturbations. Suppose V is analytic, and let $E_V(t) := e^{it(\mathcal{L}+V)}e^{-it\mathcal{L}}$. The latter has an analytic continuation to an entire function $z \to E_V(z)$, and $\Omega \in \mathcal{D}(e^{iz(\mathcal{L}+V)})$ for all $z \in \mathbf{C}$. In particular, $\Omega_V = E_V(i\beta/2)\Omega$. Furthermore, $E_V(i\beta/2) = E_V(i\beta/4)\alpha^{i\beta/4}(E_V(i\beta/4)^*)$, and hence

$$\begin{aligned}\Omega_V &= E_V(i\beta/4)\alpha^{i\beta/4}E_V(i\beta/4)^*\Omega \\ &= E_V(i\beta/4)JE_V(i\beta/4)\Omega\,.\end{aligned}$$

Therefore, $\Omega_V \in \mathcal{H}^+$ for analytic V.

The relation $S_\Omega E_V(i\beta/2)^* A\Omega = A^*\Omega_V = S_{\Omega_V,\Omega}A\Omega$, for $A \in \mathcal{M}$, implies that the relative modular operator

$$\begin{aligned}\Delta_{\Omega_V,\Omega} &= S^*_{\Omega_V,\Omega}S_{\Omega_V,\Omega} \\ &= E_V(i\beta/2)\Delta_\Omega E_V^*(i\beta/2) \\ &= e^{-\beta(\mathcal{L}+V)}\,.\end{aligned}$$

Hence, $\log\Delta_{\Omega_V,\Omega} = \log\Delta_\Omega - \beta V$. Let $\widetilde{V} := V + \beta^{-1}\log\|\Omega_V\|^2$, and $\Omega_{\widetilde{V}} := \Omega_V/\|\Omega_V\|$. Since $\log\Delta_{\Omega_{\widetilde{V}},\Omega} = \log\Delta_\Omega - \beta\widetilde{V}$, it follows that $Ent(\omega|\omega_V) = -\beta\omega(\widetilde{V})$. The latter together with the inequality $Ent(\omega|\omega_V) \leq 0$ imply that $e^{-\beta\langle\Omega|V\Omega\rangle/2} \leq \|\Omega_V\|$, which is the Peierls-Bogoliubov inequality.

We still want to show the Golden-Thompson inequality in the case of analytic perturbations. Consider $\mathcal{N}$ an abelian von Neumann subalgebra of $\mathcal{M}$ generated by V.

$$\begin{aligned}\log\|\Omega_V\|^2 &= Ent(\omega_V|\omega) - \beta\omega_V(V) \\ &\leq Ent(\omega_V|_{\mathcal{N}}|\omega|_{\mathcal{N}}) - \beta\omega_V(V)\,,\end{aligned}$$

where the last inequality follows from Uhlmann's monotinicity theorem. Using the estimate $Ent(\psi|\varphi) + \psi(V) \leq \log(\varphi(e^V))$ (which follows from the fact that e^V commutes with $\Delta_{\Phi,\Psi}$ and $\log x \leq x - 1$) and the last inequality, it follows that

$$\log\|\Omega_V\|^2 \leq \log\omega(e^{-\beta V}) = \log\|e^{-\beta V/2}\Omega\|^2\,,$$

and hence $\|\Omega_V\| \leq \|e^{-\beta V/2}\Omega\|$.

Now, extend the proof of the above statements to bounded operators. Suppose $V \in \mathcal{M}$ is selfadjoint, then there is a sequence of selfadjoint α-analytic elements V_n such that $V_n \to V$ strongly as $n \to \infty$. As a consequence, $\mathcal{L} + V_n \to \mathcal{L} + V$ and $\mathcal{L}_{V_n} \to \mathcal{L}_V$ in the strong resolvent sense, while $e^{-\beta(\mathcal{L}+V_n)/2}$ converges to $e^{-\beta(\mathcal{L}+V)/2}$ in the weak sense. □

The above theorem can be extended to unbounded perturbations, but we need to make one additional assumption.

(A3) $\|e^{-\beta V/2}\Omega\| < \infty$.

Theorem A1.6.

Assume (A1), (A2) and (A3). Then

(i) $\Omega \in \mathcal{D}(e^{-\beta(\mathcal{L}+V)/2})$.

(ii) $\Omega_V \in \mathcal{H}^+$ and Ω_V is cyclic and separating.

(iii) ω_V is a (α_V, β)-KMS state.

(iv) The Peierls-Bogoliubov inequality holds

$$e^{-\beta\langle\Omega|V\Omega\rangle/2} \leq \|\Omega_V\|.$$

(v) The Golden-Thompson inequality holds

$$\|\Omega_V\| \leq \|e^{-\beta V/2}\Omega\|.$$

Proof. Consider the sequence of bounded operators $V_n := \Xi_{[-n,n]}(V)V$, where $\Xi_{[-n,n]}$ is the spectral projection of V on the interval $[-n, n]$. The proof holds for V_n as in the bounded case. Moreover, $\mathcal{L} + V_n \to \mathcal{L} + V$ in the strong resolvent sense, and so does $\mathcal{L}_{V_n} \to \mathcal{L}_V$. The proof follows for V by taking the limit $n \to \infty$. □

Chapter 4

A *Zoo* of models

In this chapter, we carefully list several physically relevant models that are paradigms of thermodynamic systems. We study thermodynamic processes of these models in the following chapters, so the reader may opt to skip this chapter only to return to it when needed.

4.1 Model $A1$: a small quantum system coupled to a reservoir of non-relativistic bosons

Consider a quantum mechanical system composed of a small system Σ, with a finite dimensional Hilbert space, weakly coupled to a large infinitely extended reservoir $\mathcal{R}$ of non-relativistic Bosons.

The Hilbert space of the small system is $\mathcal{H}^\Sigma = \mathbf{C}^d$, and the kinematical algebra of observables is $\mathcal{O}^\Sigma = \mathcal{M}(\mathbf{C}^d)$, the matrix algebra on $\mathbf{C}^d$. Its dynamics is generated by the Hamiltonian H^Σ, such that $H^\Sigma \phi_i = E_i \phi_i, \phi_i \in \mathcal{H}^\Sigma, i = 0, \cdots, d-1$, and $E_0 \leq E_1 \leq \cdots \leq E_{d-1}$. In the Heisenberg picture, the time-evolution of an operator $A \in \mathcal{O}^\Sigma$ is given by

$$\alpha_t^\Sigma(A) := e^{iH^\Sigma t} A e^{-iH^\Sigma t} , t \in \mathbf{R} . \tag{4.1}$$

For inverse temperature $0 < \beta < \infty$, the (α_t^Σ, β)-KMS state is given by

$$\omega_\beta^\Sigma(\cdot) := \frac{Tr(e^{-\beta H^\Sigma} \cdot)}{Tr(e^{-\beta H^\Sigma})} , \tag{4.2}$$

where the trace is taken over $\mathcal{H}^\Sigma$, assuming $e^{-\beta H^\Sigma}$ is trace-class for $\beta > 0$.

The large system $\mathcal{R}$ is infinitely extended and is described by a free non-relativistic bosonic gas. Its state is taken to be the equilibrium state at inverse temperature $\beta > 0$. Let

$$L_0^2 := L^2(\mathbf{R}^3, d^3k) \cap L^2(\mathbf{R}^3, |k|^{-2} d^3k) , \tag{4.3}$$

and denote by $\mathcal{W}(L_0^2)$ the Weyl algebra over L_0^2 (see Appendix 2). The latter is the C^*-algebra generated by the Weyl operators $W(f), f \in L_0^2$, which satisfy

$$W(f)W(g) = e^{-\frac{i}{2}Im(f,g)}W(f+g) = e^{-iIm(f,g)}W(g)W(f) \ , \tag{4.4}$$

and $W(f)^* = W(-f), W(0) = 1$, such that the brackets $(\cdot,\cdot)$ denote the scalar product on $L^2(\mathbf{R}^3, d^3k)$. The state of the large system is described by the (α_t^f, β)-KMS state ω_β^f on $\mathcal{W}(L_0^2)$. It is quasi-free and completely determined by the two-point function

$$\omega_\beta^f(a^*(k)a(k')) = \frac{\delta(k-k')}{e^{\beta\omega(k)}-1} \ , \tag{4.5}$$

where a and a^* are the annihilation and creation operators satisfying the commutation relations

$$[a^\#(k), a^\#(k')] = 0 \tag{4.6}$$

$$[a(k), a^*(k)] = \delta(k-k') \ , \tag{4.7}$$

$\omega(k) = k^2$ the non-relativistic dispersion relation, and δ is the Dirac distribution.

The dynamics of the uncoupled reservoir is given by

$$\alpha_t^f(W(f)) = W(e^{it\omega}f) \ . \tag{4.8}$$

(Note that the latter is not norm continuous (see Appendix 1).)

Let

$$\rho(k) := \frac{1}{e^{\beta\omega(k)}-1} > 0 \ , \tag{4.9}$$

and

$$a(f) := \int d^3k f(k)a(k) \ , a^*(f) := \int d^3k f(k)a^*(k) \ . \tag{4.10}$$

According to [ArWo], the GNS representation of the free bosonic reservoir on the Hilbert space $\mathcal{F}_+ \otimes \mathcal{F}_+$ is given by the following:

$$\Omega_\beta^f = \Omega \otimes \Omega \tag{4.11}$$

$$\pi_\beta^f(a(f)) := a(\sqrt{1+\rho}f) \otimes \mathbf{1} + \mathbf{1} \otimes a^*(\sqrt{\rho}\overline{f}) \ , \tag{4.12}$$

$$(\pi_\beta^f)^\#(a(f)) := a^*(\sqrt{\rho}f) \otimes \mathbf{1} + \mathbf{1} \otimes a(\sqrt{1+\rho}\overline{f}) \ , \tag{4.13}$$

where Ω is the vacuum state in the bosonic Fock space $\mathcal{F}_+$, Ω_β^f is the vector representation of ω_β^f, and $(\bar{\cdot})$ stands for complex conjugation. One may check by direct computation that

$$\langle\Omega_\beta^f|\pi_\beta^f(a^*(k)a(k'))\Omega_\beta^f\rangle = \langle\Omega_\beta^f|(\pi_\beta^f)^\#(a^*(k)a(k'))\Omega_\beta^f\rangle = \rho(k)\delta(k-k') = \omega_\beta^f(a^*(k)a(k')) \ . \tag{4.14}$$

The Liouvillean of the bosonic reservoir on $\mathcal{F}_+ \otimes \mathcal{F}_+$ is

$$\mathcal{L}^f = \int dk\omega(k)[\pi^f_\beta(a^*(k)a(k)) - (\pi^f_\beta)^\#(a^*(k)a(k))] \, . \tag{4.15}$$

Introduce the map $\tau_\beta : L^2_0 \to L^2(\mathbf{R} \times S^2, du \times d\sigma)$ such that

$$(\tau_\beta f)(u,\sigma) = \begin{cases} \sqrt{\frac{1+\rho(u)}{2}} u^{1/4} f(u,\sigma), & u \geq 0 \\ \sqrt{\frac{\rho(-u)}{2}} (-u)^{1/4} e^{i\phi} \overline{f}(-u,\sigma), & u < 0 \end{cases} , \tag{4.16}$$

where $u = k^2$ and $f \in L^2_0$ is represented in polar coordinates. The freedom in choosing the phase ϕ will be used to impose continuity at $u = 0$, as we shall see later. Now, using the isomorphism between $L^2(\mathbf{R}^3) \oplus L^2(\mathbf{R}^3)$ and $L^2(\mathbf{R} \times S^2)$ (the latter is the so called *glued* Hilbert space), map $\mathcal{F}_+(L^2_0) \otimes \mathcal{F}_+(L^2_0) \to \mathcal{F}_+(L^2(\mathbf{R} \times S^2))$, such that Ω^f_β is mapped to the vacuum state of $\mathcal{F}_+(L^2(\mathbf{R} \times S^2))$ and $\mathcal{L}^f = d\Gamma(u)$, the second quantization of the operator of multiplication by $u \in \mathbf{R}$ (see Appendix 2 for the construction of the *glued* Hilbert space).

One may specify the interaction between Σ and $\mathcal{R}$ in a representation-independent way in terms of a suitable $*$-automorphism group α^t_g on the C^*-algebra $\mathcal{B}(\mathcal{H}^\Sigma) \otimes \mathcal{W}(L^2_0)$, where g is a perturbation parameter and let $\alpha^t_0 := \alpha^\Sigma_t \otimes \alpha^f_t$, the free dynamics (see [FM1]). However, for the sake of simplicity, we specify the interaction directly on the GNS Hilbert space. The (α^t_0, β)-KMS state is

$$\omega^0_\beta = \omega^\Sigma_\beta \otimes \omega^f_\beta \, , \tag{4.17}$$

on the algebra $\mathcal{U} = \mathcal{B}(\mathcal{H}^\Sigma) \otimes \mathcal{W}(L^2_0)$. The representation Hilbert space is

$$\mathcal{H} = \mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma \otimes \mathcal{F}_+ \, , \tag{4.18}$$

such that $\mathcal{F}_+ = \mathcal{F}_+(L^2(\mathbf{R} \times S^2, du \times d\sigma))$ is the bosonic Fock space over $L^2(\mathbf{R} \times S^2)$. The cyclic vector in the GNS construction representing ω^0_β in $\mathcal{H}$ is

$$\Omega^0_\beta = \Omega^\Sigma_\beta \otimes \Omega^f_\beta \, , \tag{4.19}$$

where Ω^f_β is the vacuum vector in $\mathcal{F}_+$, and

$$\Omega^\Sigma_\beta = (Tr(e^{-\beta H^\Sigma}))^{-1/2} \sum_{j=0}^{d-1} e^{-\beta E_j/2} \varphi_j \otimes \varphi_j \, , \tag{4.20}$$

with φ_j the eigenvector of H^Σ corresponding to the eigenvalue E_j.

Let $\varphi(h) = \frac{a^*(h)+a(h)}{\sqrt{2}}$, for $h \in L^2(\mathbf{R} \times S^2)$. The representation map $\pi_\beta : \mathcal{B}(\mathcal{H}^\Sigma) \otimes \mathcal{W}(L^2_0) \to \mathcal{B}(\mathcal{H})$ is given by the product

$$\pi_\beta := \pi^\Sigma \otimes \pi^f_\beta \, , \tag{4.21}$$

with

$$\pi^{\Sigma}(A) := A \otimes \mathbf{1}^{\Sigma} , \tag{4.22}$$

$$\pi^{f}_{\beta}(W(f)) := e^{i\varphi(\tau_\beta f)} , \tag{4.23}$$

for $A \in \mathcal{B}(\mathcal{H}^{\Sigma})$ and $f \in L^2_0$.

The interacting dynamics is generated by the *standard* Liouvillean, as seen in Chapter 3, which is given by

$$\mathcal{L}_g := \mathcal{L}_0 + gI , \tag{4.24}$$

where $\mathcal{L}_0 := \mathcal{L}^{\Sigma} + \mathcal{L}^{f}$, $\mathcal{L}^{\Sigma} = H^{\Sigma} \otimes \mathbf{1}^{\Sigma} - \mathbf{1}^{\Sigma} \otimes H^{\Sigma}$, $\mathcal{L}^{f} = d\Gamma(u), u \in \mathbf{R}$, g is a coupling constant, and the interaction I is given by

$$I = \sum_{\alpha} \{ G_\alpha \otimes \mathbf{1}^{\Sigma} \otimes \varphi(\tau_\beta(g_\alpha)) - \mathbf{1}^{\Sigma} \otimes C^{\Sigma} G_\alpha C^{\Sigma} \otimes \varphi(\tau_\beta(e^{-\beta u/2} g_\alpha)) \} . \tag{4.25}$$

Here G_α are bounded selfadjoint operators on $\mathcal{H}^{\Sigma}$, $g_\alpha \in L^2_0$ are the form factors, and C^{Σ} is the antilinear operator of complex conjugation on $\mathcal{H}^{\Sigma}$.

The corresponding interacting W^*-dynamics is defined by the one parameter group of $*$-automorphisms (see Appendix 1)

$$\alpha^{t}_{g}(\cdot) := e^{it\mathcal{L}_g}(\cdot)e^{-it\mathcal{L}_g} , \tag{4.26}$$

on the von Neumann algebra

$$\mathcal{M}_\beta := \pi_\beta(\mathcal{B}(\mathcal{H}^{\Sigma}) \otimes \mathcal{W}(L^2_0))'' \subset \mathcal{B}(\mathcal{H}) , \tag{4.27}$$

where $''$ denotes the double-commutant (weak closure). The pair $(\mathcal{M}_\beta, \alpha^t_\beta)$ defines a W^*-dynamical system. Let $N := d\Gamma(1)$, the number operator. We will often make use of the following relative bounds (see Appendix 2)

$$\|I(N+1)^{-1/2}\|, \|(N+1)^{-1/2} I\| < C(1 + 1/\beta) , \tag{4.28}$$

where C is a constant independent of the inverse temperature β.

In order to prove the existence of the perturbed dynamics and KMS state (together with the selfadjointness of $\mathcal{L}_g$ as a consequence of the Glimm-Jaffe-Nelson theorem; see also Appendix 2) and to apply a suitable Virial theorem together with a PC estimate to study the spectrum of the standard Liouvillian, we make the following assumptions.

(A1.1) *Smoothness of the form factors.*

The form factors are given by $g_\alpha(u, \sigma) = u^p \widetilde{g_\alpha}(u, \sigma)$, where $p = 1/4, 3/4, 5/4$ or $> 11/4$, and $\widetilde{g_\alpha}$ is such that, for fixed α and σ, the map $u \to \widetilde{g_\alpha}(u, \sigma)$ is C^3 on $(0, \infty)$, and

$$\|\partial^i_u \widetilde{g_\alpha}\|_{L^2(\mathbf{R} \times S^2)} < \infty , \tag{4.29}$$

for $i = 0, 1, 2, 3$. If $p = 1/4, 3/4$ or $5/4$, then the limits

$$\partial_u^i \widetilde{g}_\alpha(0,\sigma) := \lim_{u \to 0^+} \partial_u^i \widetilde{g}_\alpha(u,\sigma) \tag{4.30}$$

exist for $i = 0, 1, 2$, and there exists $\phi_0 \in \mathbf{R}$ such that

$$e^{-i\phi_0} \partial_u^i \widetilde{g}_\alpha(0,\sigma) \in \mathbf{R}, i = 0, 1, 2 \; . \tag{4.31}$$

Furthermore, we assume that for $p = 1/4, 3/4$, $\partial_u \widetilde{g}_\alpha(0,\sigma) = 0$. As mentioned before, one may use the freedom in choosing the phase ϕ (in the glued Hilbert space) to impose continuity of g at $u = 0$. For $p = 1/4$, choose $\phi = 2\phi_0 + \pi$, while for other admissible values of p, choose $\phi = 2\phi_0$.

The physical relevance of this assumption will be apparent in chapter 5, when we discuss proving the property of return to equilibrium for this model using the positive commutator method and a suitable Virial theorem. The analysis in chapter 5 involves estimating $\|gI(N+1)^{-1/2}\|$, which depends on β through the interaction I. It turns out that one has to be careful in taking the limit $\beta \to \infty$ in the infra-red singular regime $p = 1/4$. Moreover, we will need to estimate the norm of the difference between the interacting and the non-interacting KMS states, and hence to find an upper bound on the expectation value of the number operator N in the interacting KMS state $\Omega_{\beta,g}$. In a suitable infra-red regime $p \geq 1/4$, we expect the KMS-equilibrium states of the non-interacting and interacting systems to be close to each other for small enough g, which will turn out to be independent of β for $p > 1/4$, but which will go to zero in the limit $\beta \to \infty$ for $p = 1/4$. Furthermore, we will need to control multiple commutators of $\mathcal{L}_g$ with the dilatation generator $A_f = d\Gamma(i\partial_u)$ (defined in section 5.1) in order to prove a suitable Virial theorem (Theorem 5.5, chapter 5). In particular, the third commutator of the interaction I with A_f needs to be well-defined and relatively $N^{1/2}$-bounded. This is satisfied if

$$\partial_u^j \tau_\beta(g_\alpha) \;\text{ is continuous in } u \in \mathbf{R} \text{ for } j = 0, 1, 2, \text{ and} \tag{4.32}$$

$$\partial_u^j \tau_\beta(g_\alpha) \in L^2(\mathbf{R} \times S^2) \;\text{ for } j = 0, 1, 2, 3. \tag{4.33}$$

One can verify that (4.32), (4.33) follow from (A1.1). Let p and ϕ_0 be as in assumption (A1.1). Then, for $p = 3/4, 5/4$, $p > 11/4$, we choose $\phi = 2\phi_0$, while for $p = 1/4$, we choose $\phi = \pi + 2\phi_0$.

(A1.2) *Fermi Golden Rule condition.*

Assume that

$$\min_{E_m \neq E_n} \int_{S^2} d\sigma \Big| \sum_\alpha (\phi_m, G_\alpha \phi_n) g_\alpha(|E_m - E_n|, \sigma) \Big|^2 > 0 \; . \tag{4.34}$$

This assumption pertains to the positivity of the level-shift operator, and it can be verified in specific physical models, such as a spin impurity interacting with (free) magnons in a magnet (see Appendix 2). Physically, it guarantees that the probability of absorption and emission processes of field quanta does not vanish to second order in perturbation theory.

4.2 Model $A2$: spin impurity interacting with magnons in a magnet

In this section we discuss a concrete physical model corresponding to the earlier model.

Consider a ferromagnet, say a cubic lattice $\mathbf{Z}^3$, with lattice spacing a. Its Hamiltonian is given by

$$H = H_{spin} + H_{wave} = -J\sum_{\langle ij\rangle} \hat{S}_i\hat{S}_j - \sum_i j(i)\vec{s_0}\hat{S}_i \ , \tag{4.35}$$

where $i \in \mathbf{Z}^3$, $J > 0$. The first term corresponds to the interaction between neighbouring spins, and the second term corresponds to the interaction between the spins and a spin impurity. The spin operators satisfy the commutation relation

$$[\hat{S}_i^\alpha, \hat{S}_j^\beta] = i\epsilon^{\alpha\beta\gamma}\delta_{ij}\hat{S}_i^\gamma \ , \tag{4.36}$$

where $\alpha, \beta, \gamma = 1, 2, 3$. One may write the Hamiltonian as

$$H = -J\sum_{\langle ij\rangle}\{\frac{1}{2}(\hat{S}_i^+\hat{S}_j^- + \hat{S}_i^-\hat{S}_j^+) + \hat{S}_i^3\hat{S}_j^3\} - \sum_i j(i)\{\frac{1}{2}(s_0^+\hat{S}_i^- + s_0^-\hat{S}_i^+) + s_0^3\hat{S}_i^3\} \ , \tag{4.37}$$

where $\hat{S}_i^+ = \hat{S}_i^1 + i\hat{S}_i^2$ and $\hat{S}_i^- = \hat{S}_i^1 - i\hat{S}_i^2$ are the raising and lowering operators respectively. Using the Holstein-Primakoff transformation, one may write the above expression in terms of bosonic creation and annihilation operators a^*, a:

$$\hat{S}_i^+ = (2S)^{1/2}(1 - \frac{a_i^*a_i}{2s})^{1/2}a_i \ , \tag{4.38}$$

$$\hat{S}_i^- = (2S)^{1/2}a_i^*(1 - \frac{a_i^*a_i}{2s})^{1/2} \ , \tag{4.39}$$

$$\hat{S}_i^3 = S - a_i^*a_i \ , \tag{4.40}$$

where S denotes the spin of the system. Regard $a_i^*a_i$ as a perturbation of S, such that $\hat{S}_i^+ \approx (2S)^{1/2}a_i$ and $\hat{S}_i^- \approx (2S)^{1/2}a_i^*$. Substituting back in the total Hamiltonian,

$$H \approx -nNJS^2 - s_0^3 j_0 M + 2JSn\sum_i a_i^*a_i - \sum_{\langle ij\rangle} JS(a_ia_j^* + a_i^*a_j) - \sum_i j_i\sqrt{\frac{S}{2}}(s_0^+a_i^* + s_0^-a_i) \ , \tag{4.41}$$

where $M = \sum_i j_i s_0^3 (S - a_i^* a_i)$, n the number of nearest neighbors (which is 6 in case of a cubic lattice), N is the total number of spins, and $j_0 = \sum_i j_i$.

For a cubic lattice, take the Fourier transform of the annihilation and creation operators $a_i = \frac{1}{\sqrt{N}} \sum_k e^{-ik\cdot i} b_k$ and $a_i^* = \frac{1}{\sqrt{N}} \sum_k e^{ik\cdot i} b_k^*$. One may check that as a direct consequence of the commutation relations $[a_i^\#, a_j^\#] = 0$ and $[a_i, a_j^*] = \delta_{ij}$, $[b_k^\#, b_{k'}^\#] = 0$ and $[b_k, b_{k'}^*] = \delta_{kk'}$.

The total Hamiltonian for $a|k| \ll 1$ becomes

$$H \approx -nNJS^2 - s_0^3 j_0 M + JS \sum_k a^2 k^2 b_k^* b_k - \sqrt{\frac{S}{2N}} \sum_i \sum_k \{ j_i (s_0^+ e^{ik\cdot i} b_k^* + s_0^- e^{-ik\cdot i} b_k) \} ,$$

and in the continuum limit $\sum_k \to \frac{V}{(2\pi)^3} \int d^3k$, $\sum_i \to \frac{1}{V} \int dx$, where V is the volume of the system,

$$H \approx -nNJS^2 - s_0^3 j_0 M + \frac{JSV}{(2\pi)^3} \int d^3k k^2 b_k^* b_k - \frac{1}{(2\pi)^3} \sqrt{\frac{S}{2N}} \int d^3k (\hat{j}(k) s_0^+ b_k^* + \bar{\hat{j}}(k) s_0^- b_k) \tag{4.42}$$

$$= H_{pp} + H_c + I \ , \tag{4.43}$$

where

$$\hat{j}(k) = \int dx j(x) e^{ik\cdot x} \ ,$$
$$H_{pp} = -nNJS^2 - s_0^3 j_0 M \ on \ \mathbf{C}^2,$$
$$H_c = \frac{JSV}{(2\pi)^3} \int d^3k k^2 b_k^* b_k \ on \ \mathcal{F}_+;$$
$$I = -\frac{1}{(2\pi)^3} \sqrt{\frac{S}{2N}} \int d^3k (\hat{j}(k) s_0^+ b_k^* + \bar{\hat{j}}(k) s_0^- b_k) =: \int d^3k (G(k) b^*(k) + \overline{G}(k) b(k)) \ on \ \mathbf{C}^2 \otimes \mathcal{F}_+.$$

Using the Pauli matrices $s_0^i, i = 1, 2, 3$, it follows that

$$H_{pp} = diag(-nNJS^2 - j_0 M, -nNJS^2 + j_0 M)$$

See remark after Proposition A2.2 for an explicit expression of the level-shift operator for this model.

4.3 Model B: a *quantum dot* coupled to a reservoir of non-relativistic fermions

Consider a quantum mechanical system, say a quantum dot, composed of a small system Σ with a finite dimensional Hilbert space coupled to an infinitely extended reservoir $\mathcal{R}$ of free non-relativistic fermions.*

We assume that the small system can trap finitely many fermions. Its pure states are given by vectors in $\mathbf{C}^d$. Interpret $(1, 0, \cdots, 0)$ as the ground state (no fermions trapped by the quantum dot), $(0, 1, \cdots, 0)$ as the first excited state (one fermion trapped by the quantum dot), and so on, and assume that the Hamiltonian is given by

$$H^\Sigma = diag(E_0, E_1, \cdots, E_{d-1}) \ . \tag{4.44}$$

Introduce the raising and lowering operators (which are $d \times d$ matrices and which correspond to adding or removing an electron in the quantum dot)

$$c_+ = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ 1 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots \\ \vdots & & & \\ 0 & \cdots & 1 & 0 \end{pmatrix} , \tag{4.45}$$

and

$$c_- = (c_+)^* \ . \tag{4.46}$$

They raise and lower the energy level by one. For $A \in \mathcal{B}(\mathbf{C}^d)$, the dynamics is given by

$$\alpha_t^\Sigma(A) := e^{itH^\Sigma} A e^{-itH^\Sigma} \ . \tag{4.47}$$

Initially, before the systems are coupled together, the state of the fermionic reservoir is the KMS equilibrium state at inverse temperature $\beta \in [\beta_0, \beta_*]$, $0 < \beta_0 < \beta_*$, and chemical potential $\nu \in \mathbf{R}$.

Let $\mathbf{h} := L^2(\mathbf{R}^3, d^3x)$ be the Hilbert space of a single fermion with h its energy operator on $\mathbf{h}$. The fermionic creation and annihilation operators $b^*(f), b(f), f \in \mathbf{h}$, on the antisymmetric Fock space $\mathcal{F}_-(\mathbf{h})$ satisfy the CAR relations

$$\{b^\#(f), b^\#(g)\} = 0 \ , \tag{4.48}$$

$$\{b(f), b^*(g)\} = (f, g)\mathbf{1} \ , \tag{4.49}$$

for $f, g \in L^2(\mathbf{R}^3)$. Unlike in the bosonic case, it follows from the CAR relations that $b^\#$ are bounded, since $\|b^\#(f)\| = \|f\|$ for $f \in \mathbf{h}$.

The kinematical algebra of the Fermi gas $\mathcal{O}^f$ is the C^*-algebra generated by the operators $\{b^\#(f), f \in \mathbf{h}\}$ and the identity $\mathbf{1}$. The field operators are defined by $\varphi(f) = \frac{1}{\sqrt{2}}(b(f) + b^*(f))$.

The dynamics of the reservoir is specified by the Hamiltonian $H^f = d\Gamma(h)$, the second quantization of the energy operator h, such that

$$\alpha_t^f(b^\#(f)) = e^{itH^f} b^\#(f) e^{-itH^f} = b^\#(e^{ith} f) \ , \tag{4.50}$$

*Mesoscopically, electrons in a normal metal are satisfactorily described by the Landau-Fermi liquid theory. This has been argued for heuristically and proven rigorously using renormalization group analysis (see for example [CFS, FMRT, FLKT]).

and $h = u = k^2$ the non-relativistic dispersion relation.[†]

For each inverse temperature $\beta > 0$ and chemical potential $\nu \in \mathbf{R}$, there exists a unique KMS state $\omega^f_{\beta,\nu}$ on $\mathcal{O}^f$, which is a quasi-free, gauge-invariant state uniquely determined by the two-point function

$$\omega^f_{\beta,\nu}(b^*(f)b(f)) = (f, (e^{\beta(u-\nu)} + 1)^{-1} f) \ . \tag{4.51}$$

The C^*-algebra of the combined system is the tensor product algebra $\mathcal{O} = \mathcal{O}^\Sigma \otimes \mathcal{O}^f$, and the free dynamics is generated by the group of automorphisms $\alpha^0_t = \alpha^\Sigma_t \otimes \alpha^f_t$, such that, for $A \in \mathcal{O}$,

$$\alpha^0_t(A) = e^{itH_0} A e^{-iH_0} \ , \tag{4.52}$$

and $H_0 = H^\Sigma \otimes \mathbf{1}^f + \mathbf{1}^\Sigma \otimes H^f$.

Introduce the interaction between Σ and $\mathcal{R}$,

$$V = \sum_\alpha \{c_- \otimes b^*(g_\alpha) + c_+ \otimes b(g_\alpha)\} \ , \tag{4.53}$$

where $g_\alpha \in \mathbf{h}$ are the form factors. Note that V is a bounded selfadjoint perturbation ($V \in \mathcal{O}$ and $V = V^*$), and the perturbation is invariant under gauge transformations of the first kind (ie, the total number of fermions is conserved, which is expected in the nonrelativistic regime).

The dynamics of the coupled system is generated by the Hamiltonian

$$H_g := H_0 + gV \ , \tag{4.54}$$

such that

$$\alpha^g_t(A) = e^{itH_g} A e^{-itH_g} \ , \tag{4.55}$$

for $A \in \mathcal{O}$.

As in the bosonic case, we will work directly in a concrete GNS representation. Let $\hat{\Omega}_f$ be the Fock vacuum on $\mathcal{F}_-(\mathbf{h})$, N the number operator, $\theta = \Gamma(-1) = (-1)^N$, and $\rho_{\beta,\nu}(u) := (1+e^{\beta(u-\nu)})^{-1}$. Moreover, let $\mathcal{H}^f = \mathcal{F}_-(\mathbf{h}) \otimes \mathcal{F}_-(\mathbf{h})$ and $\Omega_f = \hat{\Omega}_f \otimes \hat{\Omega}_f$.

The Araki-Wyss representation π_β of $\mathcal{O}^f$ on $\mathcal{H}^f$ is defined by [ArWy]

$$\pi_\beta(b(f)) := b(\sqrt{1-\rho_{\beta,\nu}} f)) \otimes \mathbf{1}^f + \theta \otimes b^*(\sqrt{\rho_{\beta,\nu}}\, \overline{f}) \ , \tag{4.56}$$

$$\pi^\#_\beta(b(f)) := b^*(\sqrt{\rho_{\beta,\nu}} f)\theta \otimes \theta + \mathbf{1}^f \otimes \theta b(\sqrt{1-\rho_{\beta,\nu}}\, \overline{f}) \ . \tag{4.57}$$

The Liouvillean of the uncoupled system is

$$\mathcal{L}_0 = \mathcal{L}^\Sigma + \mathcal{L}^f \ , \tag{4.58}$$

[†]For non-zero chemical potential, an equivalent free dynamics of the reservoirs is generated by $d\Gamma(u-\nu)$, see for example [BR].

where $\mathcal{L}^\Sigma = H^\Sigma \otimes \mathbf{1}^\Sigma - \mathbf{1}^\Sigma \otimes H^\Sigma$ and $\mathcal{L}^f = H^f \otimes \mathbf{1}^f - \mathbf{1}^f \otimes H^f$. The *standard* Liouvillean of the coupled system is

$$\mathcal{L}_g = \mathcal{L}_0 + g\pi_\beta(V) - g\pi_\beta^\#(V) \ . \tag{4.59}$$

Associate to every function $f(u,\sigma) \in \mathbf{h} = L^2(\mathbf{R}^+, S^2)$ (in polar coordinates), two functions $f_\beta(u,\sigma), f_\beta^\#(u,\sigma) \in L^2(\mathbf{R}, S^2)$, the glued Hilbert space (with chemical potential $\nu \in \mathbf{R}$), such that

$$f_\beta(u,\sigma) := \begin{cases} \sqrt{1-\rho_{\beta,\nu}(u)}\frac{u^{1/4}}{\sqrt{2}} f(u,\sigma) \ , u \geq 0 \\ \sqrt{\rho_{\beta,\nu}(-u)}\frac{|u|^{1/4}}{\sqrt{2}} \overline{f}(-u,\sigma) \ , u < 0 \end{cases} \tag{4.60}$$

$$= \begin{cases} \frac{e^{\beta(u-\nu)/4}}{2\cosh^{1/2}(\beta(u-\nu)/2)} u^{1/4} f(u,\sigma) \ , u \geq 0 \\ \frac{e^{-\beta(|u|-\nu)/4}}{2\cosh^{1/2}(\beta(|u|-\nu)/2)} |u|^{1/4} \overline{f}(-u,\sigma) \ , u < 0 \end{cases} \ , \tag{4.61}$$

and

$$f_\beta^\#(u,\sigma) := \begin{cases} i\sqrt{\rho_{\beta,\nu}(u)}\frac{u^{1/4}}{\sqrt{2}} f(u,\sigma) \ , u \geq 0 \\ i\sqrt{1-\rho_{\beta,\nu}(-u)}\frac{|u|^{1/4}}{\sqrt{2}} \overline{f}(-u,\sigma) \ , u < 0 \end{cases} \tag{4.62}$$

$$= \begin{cases} \frac{ie^{-\beta(u-\nu)/4}}{2\cosh^{1/2}(\beta(u-\nu)/2)} u^{1/4} f(u,\sigma) \ , u \geq 0 \\ \frac{ie^{\beta(|u|-\nu)/4}}{2\cosh^{1/2}(\beta(|u|-\nu)/2)} |u|^{1/4} \overline{f}(-u,\sigma), u < 0 \end{cases} \tag{4.63}$$

$$= ie^{-\beta\frac{|u|}{u}(|u|-\nu)/2} f_\beta(u,\sigma) \tag{4.64}$$

$$= i\overline{f}_\beta(-u,\sigma) \ . \tag{4.65}$$

Map $\mathcal{F}_-(\mathbf{h}) \otimes \mathcal{F}_-(\mathbf{h}) \to \mathcal{F}_-(L^2(\mathbf{R}, S^2))$ using the isomorphism between $L^2(\mathbf{R}^+, S^2) \oplus L^2(\mathbf{R}^+, S^2)$ and $L^2(\mathbf{R}, S^2)$ (see Appendix 2 for a discussion of the glued Hilbert space $L^2(\mathbf{R}, S^2)$).

The perturbed Liouvillean acting on $\mathcal{H} = \mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma \otimes \mathcal{F}_-(L^2(\mathbf{R}, S^2))$ is given by

$$\mathcal{L} = \mathcal{L}^\Sigma + \mathcal{L}^f + gI \ , \tag{4.66}$$

where $\mathcal{L}^\Sigma$ is as before, $\mathcal{L}^f = d\Gamma(u)$, the second quantization of the operator of multiplication by $u \in \mathbf{R}$,

$$I = \sum_\alpha \{c_- \otimes \mathbf{1}^\Sigma \otimes b^*(g_{\alpha,\beta}) + c_+ \otimes \mathbf{1}^\Sigma \otimes b(g_{\alpha,\beta}) - \tag{4.67}$$

$$- \mathbf{1}^\Sigma \otimes C^\Sigma c_- C^\Sigma \otimes (i\theta b^*(g_{\alpha,\beta}^\#)) - \mathbf{1}^\Sigma \otimes C^\Sigma c_+ C^\Sigma \otimes (i\theta b(g_{\alpha,\beta}^\#))\} \ , \tag{4.68}$$

and C^Σ is the operator corresponding to complex conjugation on $\mathcal{H}^\Sigma$.

Note that the perturbed Liouvillean is selfadjoint since the perturbation is bounded and selfadjoint. Both the existence of the perturbed dynamics and the perturbed KMS state follow from the latter fact (see Appendix 1, chapter 3). We will make the following assumptions on the form factors.

(B.1) *Smoothness of the form factors.* In order to apply the Virial theorem (see Proposition 5.10, section 5.2) in the proof of RTE for this model, impose that

$$\lim_{u\to 0}\partial_u^j g_{\alpha,\beta}(u,\sigma)=0\ ,\ j=0,1,2,3. \tag{4.69}$$

This condition is satisfied if $g_\alpha(u,\sigma)=u^p\widetilde{g}_\alpha(u,\sigma)$, for $\widetilde{g}\in C^3$ on $(0,\infty)$ and $p>11/4$.

(B.2) *Fermi Golden Rule.* This condition ensures that the small system is coupled to the reservoirs,

$$\min_{E_m\neq E_n}\int_{S^2}|\sum_\alpha(\varphi_m,G_\alpha\phi_n)g_\alpha(|E_n-E_m|,\sigma)|^2>0\ . \tag{4.70}$$

This condition is translated to the positivity of the so called level-shift operator (Appendix 2).

4.4 Model C_n: a 2 level system coupled to n fermionic reservoirs

For the sake of concreteness, and without loss of generality, assume that the small system Σ is a 2 level system (as described in section 4.3), coupled to n reservoirs of free fermions,$\mathcal{R}_1,\cdots,\mathcal{R}_n$, in equilibrium at inverse temperatures $\beta_1,\cdots,\beta_n\in[\beta_0,\beta_*]$, for fixed β_0,β_*, such that $0<\beta_0<\beta_*<\infty$, and chemical potentials $\nu_1,\cdots,\nu_n$. For the sake of simplicity of exposion, we set all the chemical potentials of the reservoirs equal to $\nu\in\mathbf{R}$.[‡] We will remark on how our results change if the chemical potentials are different in due course.

The kinematical algebra of the small system Σ is $\mathcal{O}^\Sigma=\mathcal{M}(\mathbf{C}^2)$, the matrix algebra over $\mathbf{C}^2$, and its Hamiltonian is $H^\Sigma=\sigma_3$, where $\sigma_i, i=1,2,3$ are the Pauli matrices.

Each dispersive and infinitely extended reservoir $\mathcal{R}_i, i=1,\cdots,n$ is formed of free fermions, which are not necessarily non-relativistic. We make the assumption that the Hilbert space of a single fermion is $\mathbf{h}=L^2(\mathbf{R}^+;\mathcal{B})$, where $\mathcal{B}$ is some auxilliary Hilbert space, and that the single particle Hamiltonian h is the operator of multiplication by $u\in\mathbf{R}^+$. (In the previous section, $\mathcal{B}=L^2(S^2)$ and $u=k^2$.)

The kinematical algebra of the coupled system is $\mathcal{O}=\mathcal{O}^\Sigma\otimes\mathcal{O}^{\mathcal{R}_1}\otimes\cdots\otimes\mathcal{O}^{\mathcal{R}_n}$. The interaction between the small system and the fermionic reservoirs is given by a generally time-dependent perturbation

$$V(t)=\sum_i\{\sigma_-\otimes b^*(f_i(t))+\sigma_+\otimes b(f_i(t))\}, \tag{4.71}$$

[‡]We exclude the case when $\nu=2$ so that the first nontrivial terms in perturbation theory for the coupled system are second order in the coupling parameter.

where $t \in \mathbf{R}$, $\sigma_\pm = \sigma_1 \pm i\sigma_2$, the raising and lowering spin operators, and $f_i(t) \in \mathbf{h}, i = 1, \cdots, n$ are the form factors.[§]

The dynamics of the coupled system is generated by the Hamiltonian

$$H_g(t) := H_0 + gV(t) , \tag{4.72}$$

where $H_0 = H^\Sigma + H^{\mathcal{R}_1} + \cdots + H^{\mathcal{R}_n}$, such that

$$\alpha_t^g(A) = U(-t)AU(t) , \tag{4.73}$$

for $A \in \mathcal{O}$ and the propagator $U(t)$ satisfies the initial value problem

$$\begin{aligned} \partial_t U(t) &= -iH_g(t)U(t) , \\ U(0) &= 1. \end{aligned}$$

(Note that since the perturbation is bounded in the fermionic case, the perturbed time evolution can be expanded in a Dyson series (see [RS2]).)

The GNS representation of the system is similar to the one given in the previous section (Model B). (In particular, each reservoir is represented using the Araki-Wyss representation, and then mapping the latter to the glued Hilbert space representation; see Appendix 2.)

For every function $f \in L^2(\mathbf{R}^+; \mathcal{B})$, associate the functions $f_\beta, f_\beta^\# \in L^2(\mathbf{R}; \mathcal{B})$ given by

$$f_\beta(u, \sigma, t) := \begin{cases} \sqrt{1 - \rho_{\beta,\nu}(u)} f(u, \sigma, t) , & u \geq 0 \\ \sqrt{\rho_{\beta,\nu}(-u)}\ \overline{f}(-u, \sigma, t) , & u < 0 \end{cases} , \tag{4.74}$$

and

$$\begin{aligned} f_\beta^\#(u, \sigma, t) \ &:= \ \begin{cases} i\sqrt{\rho_{\beta,\nu}(u)} f(u, \sigma, t), u \geq 0 \\ i\sqrt{1 - \rho_{\beta,\nu}(-u)}\ \overline{f}(-u, \sigma, t), u < 0 \end{cases} && (4.75) \\ &= \ i\overline{f}_\beta(-u, \sigma, t). && (4.76) \end{aligned}$$

The interacting *standard* Liouvillean acting on the Hilbert space $\mathcal{H} := \mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma \otimes \mathcal{F}_-^{(1)}(L^2(\mathbf{R}; \mathcal{B})) \otimes \cdots \otimes \mathcal{F}_-^{(n)}(L^2(\mathbf{R}; \mathcal{B}))$ is

$$\mathcal{L}_g(t) = \mathcal{L}^\Sigma + \mathcal{L}^f + gI(t) , \tag{4.77}$$

where $\mathcal{L}_0 = \mathcal{L}^\Sigma + \mathcal{L}^f$, $\mathcal{L}^\Sigma = H^\Sigma \otimes \mathbf{1}^\Sigma - \mathbf{1}^\Sigma \otimes H^\Sigma, \mathcal{L}^f = \sum_i d\Gamma(u_i)$, and

$$\begin{aligned} I(t) \ &= \ \sum_{i=1}^n \{\sigma_- \otimes \mathbf{1}^\Sigma \otimes b^*(f_{i,\beta_i}(t)) + \sigma_+ \otimes \mathbf{1}^\Sigma \otimes b(f_{i,\beta_i}(t)) \\ &- \ i\mathbf{1}^\Sigma \otimes \sigma_- \otimes (-1)^{N_i} b^*(f_{i,\beta_i}^\#(t)) - i\mathbf{1}^\Sigma \otimes \sigma_+ \otimes (-1)^{N_i} b(f_{i,\beta_i}^\#(t))\} \ . \end{aligned}$$

[§]This form of interaction is invariant under gauge transformations of the first kind.

Let

$$I(\delta) := \{z \in \mathbf{C} : |Imz| < \delta\} \; ; \tag{4.78}$$
$$I^-(\delta) := \{z \in \mathbf{C} : -\delta < Imz < 0\} \; . \tag{4.79}$$

Moreover, for every function $f \in L(\mathbf{R}^+; \mathcal{B})$ associate the function $\widetilde{f} \in \mathcal{B}$ such that

$$\widetilde{f}(u,\sigma) := \begin{cases} f(u,\sigma), u \geq 0 \\ \overline{f}(|u|,\sigma), u < 0 \; , \end{cases} \tag{4.80}$$

and denote by $H^2(\delta, \mathcal{B})$ the Hardy class of all analytic functions $g : I(\delta) \to \mathcal{B}$, such that

$$\|g\|_{H^2(\delta,\mathcal{B})} := \sup_{|\theta|<\delta} \int_{\mathbf{R}} \|g(u+i\theta)\|^2_{\mathcal{B}} du < \infty \; . \tag{4.81}$$

In order to apply the method of complex translations, we make the following assumptions on the interaction.

(C_n.1) *Regularity of the form factors.*

Assume that $\exists \delta > 0$, independent of t and $i \in \{1, \cdots, n\}$, such that

$$\widetilde{f}_i(t) \in H^2(\delta, \mathcal{B}), \tag{4.82}$$

the Hardy class of analytic functions.

(C_n.2) *Fermi Golden Rule.*

Assume that

$$\sum_i \|\widetilde{f}_i(2,t)\|_{\mathcal{B}} > 0 \; , \tag{4.83}$$

for almost all $t \in \mathbf{R}$, which is another way of saying that the small system is coupled to at least one reservoir.

Note that for this model, $\sigma(\mathcal{L}^{\Sigma}) = \{E_j\}_{j=0}^3$, where $E_0 = E_1 = 0, E_2 = -2$ and $E_3 = 2$.[¶]

We make the following additional assumption which we will need in discussing C-Liouvilleans in chapter 6.

(C_n.3) *Stronger Regularity of the form factors.*

Assume that $\exists \delta > 0$, independent of t and $i \in \{1, \cdots, n\}$, such that

$$e^{-\beta_i u_i/2} \widetilde{f}_i(t) \in H^2(\delta, \mathcal{B}) \; , \tag{4.84}$$

[¶]A *concrete* example where the above assumptions are satisfied is when $\mathbf{h} = L^2(\mathbf{R}^3, d^3k), h = k^2$. In polar coordinates, $\mathcal{B} = L^2(S^2, d\sigma)$. If the form factor $f(k) = |k|^{1/2} e^{-|k|^4}$, then both assumptions (C_n.1) and (C_n.2) are satisfied.

the Hardy class of analytic functions. This assumption is stronger than $(C_n.1)$, and we shall need it in studying the spectrum of the so called C-Liouvillean using complex deformation techniques. It implies that the mapping

$$\mathbf{R} \ni r \to \Delta^{ir} V(t) \Delta^{-ir} \in \mathcal{M} \ , \tag{4.85}$$

(where $\Delta = \Delta^{\Sigma} \otimes \Delta^{\mathcal{R}_1} \otimes \cdots \otimes \Delta^{\mathcal{R}_n}$ is the modular operator of the coupled system,) has an analytic continuation to the strip $I(1/2) = \{z \in \mathbf{C} : |Imz| < 1/2\}$, which is bounded and continuous on its closure, $\forall t \in \mathbf{R}$.

$(C_n.4)$ The perturbation is constant for $t < 0$, $V(t) \equiv V(0)$, and then *slowly* changes over a time interval τ such that $V^{\tau}(t) = V(s)$, where $s = t/\tau \in [0, 1]$ is the rescaled time. We also assume that $V(s)$ is twice differentiable in $s \in [0, 1]$ as a bounded operator, such that

$$\mathbf{R} \ni r \to \Delta^{ir} \partial_s^j V(s) \Delta^{-ir} \in \mathcal{M} \ , j = 0, 1, 2 \tag{4.86}$$

has an analytic continuation to the strip $\{z \in \mathbf{C} : |Imz| < 1/2\}$, which is bounded and continuous on its closure. This follows if we assume that there exists $\delta > 0$, independent of s and $i \in \{1, \cdots, n\}$, such that

$$e^{-\beta_i u_i/2} \partial_s^j \widetilde{f}_i(s) \in H^2(\delta, \mathcal{B}) \ , \tag{4.87}$$

the Hardy class of analytic functions, for $j = 0, 1, 2$. This assumption is needed to prove an adiabatic theorem for states close to NESS (chapter 8).

$(C_n.5)$ The perturbation is constant for $t < 0$, $V(t) = V(0)$, and then *slowly* changes over a time interval τ such that $V^{\tau}(t) = V(s)$, where $s = t/\tau \in [0, 1]$ is the rescaled time. We also assume that $V(s)$ is twice differentiable in $s \in [0, 1]$ as a bounded operator. Moreover, we assume that there exists $\delta > 0$, independent of s, $i \in \{1, \cdots, n\}$, such that

$$\partial_s^j \widetilde{f}_i(s) \in H^2(\delta, \mathcal{B}) \ , \tag{4.88}$$

the Hardy class of analytic functions, for $j = 0, 1, 2$. This assumption is needed in studying an explicit example of the isothermal theorem (chapter 8).

$(C_n.6)$ The perturbation is periodic with period $\tau_* < \infty$: $V(t) = V(t + \tau_*)$. This assumption is needed to investigate cyclic thermodynamic processes (chapter 9).

4.5 Appendix 2

4.5.1 Selfadjointness of $\mathcal{L}_g$ and some relative bounds for Model A

Consider the positive operator $\Lambda = \mathrm{d}\Gamma(|u|)$ with domain $\mathcal{D}(\Lambda) = \{\psi \in \mathcal{H} : \|\Lambda\psi\| < \infty\}$ and the number operator

$$N = \mathrm{d}\Gamma(1) , \tag{4.89}$$

with domain $\mathcal{D}(N) = \{\psi \in \mathcal{H} : \|N\psi\| < \infty\}$.
Without loss of generality, assume $u(k) = k^2$.

Proposition A2.1 (Some Relative Bounds).
Let $L^2 = L^2(\mathbb{R} \times S^2)$, and $0 < \beta_0 < \infty$ be a fixed number. Then the following hold.

(i) If $f \in L^2$, then $||a(f)N^{-1/2}|| \leq ||f||_{L^2}$.

(ii) If $|u|^{-1/2} f \in L^2$, then $||a(f)\Lambda^{-1/2}|| \leq || \, |u|^{-1/2} f||_{L^2}$.

(iii) For $\psi \in \mathcal{D}(N^{1/2})$ and $\psi \in \mathcal{D}(\Lambda^{1/2})$ respectively, we have the following bounds, uniformly in $\beta \geq \beta_0$:

$$\begin{aligned} ||I\psi||^2 &\leq C \sum_\alpha ||G_\alpha|| \left(\|N^{1/2}\psi\|^2 + \|\psi\|^2 \right) , \\ ||I\psi||^2 &\leq C \sum_\alpha ||G_\alpha|| \left(\|\Lambda^{1/2}\psi\|^2 + \|\psi\|^2 \right) , \end{aligned}$$

where $C \leq C'(1 + \beta_0^{-1})$, and C' is a constant independent of β, β_0.

(iv) For $\psi \in \mathcal{D}(N^{1/2})$, any $c > 0$, and uniformly in $\beta \geq \beta_0$, one has

$$|\langle \psi, gI\psi \rangle| \leq c||N^{1/2}\psi||^2 + \frac{16g^2}{c} \sum_\alpha ||G_\alpha||^2 ||\psi||^2 \int_{\mathbb{R}^3} (1 + \beta_0^{-1} u^{-1}) |g_\alpha|^2 d^3k.$$

(v) For $\psi \in \mathcal{D}(\Lambda^{1/2})$, any $c > 0$, and uniformly in $\beta \geq \beta_0$, one has

$$|\langle \psi, gI\psi \rangle| \leq c||\Lambda^{1/2}\psi||^2 + \frac{32g^2}{c} \sum_\alpha ||G_\alpha||^2 ||\psi||^2 \int_{\mathbb{R}^3} (1 + \beta_0^{-1} u^{-1}) \frac{|g_\alpha|^2}{u} d^3k.$$

Proof. The proof is standard (see for example [BFS], [JP1,2]). As an illustration, we present the proof of (iii). We know that

$$\|I\psi\|^2 \leq \sum_\alpha 4\|G_\alpha\|^2 \left(\|a^*(g_\alpha)\psi\|^2 + \|a(g_\alpha)\psi\|^2 \right) ,$$

and using the CCR $[a^*(f), a(g)] = \langle f, g\rangle$, one gets

$$\|a^*(g_\alpha)\psi\|^2 = \langle\psi, a(g_\alpha)a^*(g_\alpha)\psi\rangle = \|a(g_\alpha)\psi\|^2 + \|g_\alpha\|_{L^2}^2\|\psi\|^2,$$

and hence $\|I\psi\|^2 \leq \sum_\alpha 8\|G_\alpha\|^2 \left(\|a(g_\alpha)\psi\|^2 + \|g_\alpha\|_{L^2}^2\|\psi\|^2\right)$. (i) and (ii) give

$$\begin{aligned}\|I\psi\|^2 &\leq 16\sum_\alpha \|G_\alpha\|^2\|g_\alpha\|_{L^2}^2 \left(\|N^{1/2}\psi\|^2 + \|\psi\|^2\right),\\ \|I\psi\|^2 &\leq 16\sum_\alpha \|G_\alpha\|^2 \left\||u|^{-1/2}g_\alpha\right\|_{L^2}^2 \left(\|\Lambda^{1/2}\psi\|^2 + \|\psi\|^2\right).\end{aligned}$$

We show that $\|g_\alpha\|_{L^2} \leq C$ and $\|\,|u|^{-1/2}g_\alpha\|_{L^2} \leq C$, uniformly in $\beta \geq \beta_0$. Note that $\|g_\alpha\|_{L^2}^2 = \int_{\mathbf{R}^3}(1+2\rho)|g_\alpha(u,\sigma)|^2 du d\sigma$, where we represented g_α in the integral in spherical coordinates, and $u(k) = k^2$. Since we have $1+2\rho = 1+2(e^{\beta u}-1)^{-1} \leq 1+2\beta^{-1}u^{-1} \leq 1+2\beta_0^{-1}u^{-1}$, uniformly in $\beta \geq \beta_0$, one has the following uniform bound in $\beta \geq \beta_0$:

$$\|g_\alpha\|_{L^2}^2 \leq 2\int_{\mathbf{R}^3}(1+\beta_0^{-1}u^{-1})|g_\alpha(k)|^2 d^3k = C < \infty. \tag{4.90}$$

Similarly, $\|\,|u|^{-1/2}g_\alpha\|_{L^2}^2 \leq 2\int_{\mathbf{R}^3}(1+\beta_0^{-1}u^{-1})u^{-1}|g_\alpha(u,\sigma)|^2 d^3k = C < \infty$, uniformly in $\beta \geq \beta_0$. It is clear from the last two estimates that C satisfies the bound indicated in the proposition. □

These relative bounds and Nelson's commutator theorem (see [RS2]) yield essential selfadjointness of the standard Liouvillian $\mathcal{L}_g$. (Essential selfadjointness of $\mathcal{L}_g$ also follows from the GJN Theorem, see Appendix 3, chapter 5.)

4.5.2 *Glued* Hilbert Space representation

Consider a reservoir of non-relativistic bosons (Model A1 discussed in section 4.1). We want to show that

$$\mathcal{F}_+(L^2(\mathbf{R}^3, d^3k)) \otimes \mathcal{F}_+(L^2(\mathbf{R}^3, d^3k)) \cong \mathcal{F}_+(L^2(\mathbf{R}\times S^2, du d\sigma)),$$

where S^2 is the unit sphere in three dimensions, $d\sigma$ is the element of the solid angle, and $u = k^2$.

For bosonic creation/annihilation operators on $\mathcal{F}_+(L^2(\mathbf{R}^3, d^3k))$,

$$a^\#(f) := \int d^3k f(k) a^\#(k),\ f \in L^2(\mathbf{R}^3, d^3k),$$

define the creation/annihilation operators on $\mathcal{F}_+(L^2(\mathbf{R}^3, d^3k)) \otimes \mathcal{F}_+(L^2(\mathbf{R}^3, d^3k))$ as

$$\begin{aligned} a_l^\#(f) &:= a^\#(f)\otimes \mathbf{1};\\ a_r^\#(f) &:= \mathbf{1}\otimes a^\#(\overline{f}), \end{aligned}$$

where $\bar{\cdot}$ corresponds to complex conjugation. An isomorphism between $\mathcal{F}_+(L^2(\mathbf{R}^3, d^3k))\otimes \mathcal{F}_+(L^2(\mathbf{R}^3, d^3k))$ and $\mathcal{F}_+(L^2(\mathbf{R}^3, d^3k) \oplus L^2(\mathbf{R}^3, d^3k))$ follows by the identification

$$a_l^\#(f_1)\cdots a_l^\#(f_m)a_r^\#(g_1)\cdots a_r^\#(g_n) = a_l^\#((f_1,0))\cdots a_l^\#((f_m,0))a_r^\#((0,g_1))\cdots a_r^\#((0,g_n)) \ ,$$

where the RHS acts on $\mathcal{F}_+(L^2(\mathbf{R}^3, d^3k)\oplus L^2(\mathbf{R}^3, d^3k))$. Now we claim that $\mathcal{F}_+(L^2(\mathbf{R}^3, d^3k)\oplus L^2(\mathbf{R}^3, d^3k))$ is isomorphic to $\mathcal{F}_+(L^2(\mathbf{R}\times S^2, dud\sigma))$. For $\phi, \psi \in \mathbf{R}$, consider the mapping

$$j_{\phi,\psi} : L^2(\mathbf{R}^3, d^3k) \oplus L^2(\mathbf{R}^3, d^3k) \ni (f, g) \to h \in L^2(\mathbf{R} \times S^2, dud\sigma) \ ,$$

such that

$$h(u,\sigma) := \begin{cases} \frac{e^{i\phi}}{\sqrt{2}} u^{1/4} f(u,\sigma) \ , u \geq 0 \\ \frac{e^{i\psi}}{\sqrt{2}} |u|^{1/4} g(|u|,\sigma) \ , u < 0 \end{cases} .$$

This mapping is an isometry, since

$$\begin{aligned} \|h\|^2_{L^2(\mathbf{R}\times S^2, dud\sigma)} &= \|(f,g)\|^2_{L^2\oplus L^2} \\ &= \int_{\mathbf{R}^+\times S^2} dud\sigma \frac{u^{1/2}}{2}|f(u,\sigma)|^2 + \int_{\mathbf{R}^+\times S^2} dud\sigma \frac{u^{1/2}}{2}|g(u,\sigma)|^2 \\ &= \int_{\mathbf{R}^+\times S^2} dkd\sigma k^2|f(k,\sigma)|^2 + \int_{\mathbf{R}^+\times S^2} dkd\sigma k^2|g(k,\sigma)|^2 \\ &= \|f\|^2_{L^2(\mathbf{R}^3, d^3k)} + \|g\|^2_{L^2(\mathbf{R}^3, d^3k)} \ , \end{aligned}$$

where we have used the fact that $u = k^2$ for the non-relativistic reservoir.

Moreover, the mapping $j_{\phi,\psi}$ is an isomorphism, since, for given $h \in L^2(\mathbf{R} \times S^2, dud\sigma)$, there exists a mapping $j^{-1}_{\phi,\psi} : h \to (f, g) \in L^2(\mathbf{R}^3, d^3k) \oplus L^2(\mathbf{R}^3, d^3k)$, such that

$$\begin{aligned} f(u,\sigma) &:= \frac{\sqrt{2}e^{-i\phi}}{u^{1/4}} h(u,\sigma), u > 0 \ , \\ g(u,\sigma) &:= \frac{\sqrt{2}e^{-i\psi}}{|u|^{1/4}} h(|u|,\sigma), u < 0 \ . \end{aligned}$$

Using the Araki-Woods representation, section 4.1, and the mapping (4.16), one may write the interaction term on $L^2(\mathbf{R} \times S^2, dud\sigma)$ as given in (4.25).

Similarly, one may construct of the *glued* Hilbert space representation for fermionic reservoirs, as in Models B and C_n, sections 4.3 and 4.4, except that one needs to use the Araki-Wyss representation for fermionic reservoirs, section 4.3 (instead of the Araki-Woods representation).

4.5.3 Feshbach map

Consider a closed operator A acting on a Hilbert space $\mathcal{H}$, and a bounded (and not necessarily orthogonal) projection P on $\mathcal{H}$ such that $Ran(P) \subset \mathcal{D}(A)$. Let $\overline{P} := 1-P$, and define

$$A_P := PAP ,$$
$$A_{\overline{P}} := \overline{P}A\overline{P} .$$

We will view $A_{\overline{P}}$ as an operator on $\overline{P}\mathcal{H}$. We will make the following assumptions.

(F1) $z \in \rho(A_{\overline{P}})$, where $\rho(A_{\overline{P}})$ is the resolvent set of $A_{\overline{P}}$ (ie, $(A_{\overline{P}} - z\mathbf{1})^{-1}$ exists and is bounded).

(F2) $\|\overline{P}(A_{\overline{P}} - z)^{-1}\overline{P}AP\| < \infty$ and $\|PA\overline{P}(A_{\overline{P}} - z)^{-1}\overline{P}\| < \infty$.

Define the Feshbach map

$$\mathcal{F}_{P,z}(A) := (P(A-z)P - PA\overline{P}(A_{\overline{P}} - z)^{-1}\overline{P}AP)|_{Ran(P)} , \qquad (4.91)$$

provided assumptions (F1) and (F2) are satisfied.

Moreover, define

$$S_{P,z} := P - \overline{P}(A_{\overline{P}} - z)^{-1}\overline{P}AP . \qquad (4.92)$$

Since $P = (1 + \overline{P}(A_{\overline{P}} - z)^{-1}\overline{P}AP)S_{P,z}$, it follows that

$$Ker(S_{P,z}) = Ker(P).$$

The following theorem establishes a very useful property of the Feshbach map, which is its isospectrality (see, for example, [BFS,BFSS]). We will use this property in discussing the level-shift operator, which is relevant in a rigorous treatment of Fermi Golden Rule (for a review, see for example [DF1,2]), and in proving the property of RTE in chapter 5.

Theorem A2.2 (Isospectrality of the Feshbach map)

Suppose (F1) and (F2) hold. Then

$$z \in \sigma_\#(A) \Leftrightarrow 0 \in \sigma_\#(\mathcal{F}_{P,z}(A)) , \qquad (4.93)$$

where $\sigma_\# = \sigma_c$ or σ_p (continuous or pure point spectrum). Moreover, the eigenfunctions of $(A-z)$ and $\mathcal{F}_{P,z}(A)$ are related by

$$Ker((A-z)S_{P,z}) = Ker(\mathcal{F}_{P,z}(A)) , \qquad (4.94)$$

and

$$P\ Ker(A-z) = Ker(\mathcal{F}_{P,z}(A)) . \qquad (4.95)$$

These imply that

$$dim\ Ker(A-z) = dim\ Ker(\mathcal{F}_{P,z}(A)) .$$

Proof.

Using the second resolvent identity and the fact that

$$A = A_P + A_{\overline{P}} + PA\overline{P} + \overline{P}AP ,$$

we have the following identities

$$(A - z)S_{P,z} = \mathcal{F}_{P,z}(A) , \tag{4.96}$$

and

$$P(A - z)^{-1}P = (\mathcal{F}_{P,z}(A))^{-1} \tag{4.97}$$

on $Ran(P)$, and

$$\begin{aligned}(A - z)^{-1} =&(\mathcal{F}_{P,z}(A))^{-1}P - (\mathcal{F}_{P,z}(A))^{-1}PA\overline{P}(A_{\overline{P}} - z)^{-1}\overline{P}\\ &- \overline{P}(A_{\overline{P}} - z)^{-1}\overline{P}AP(\mathcal{F}_{P,z}(A))^{-1} + \overline{P}(A_{\overline{P}} - z)^{-1}\overline{P}\\ &+ \overline{P}(A_{\overline{P}} - z)^{-1}\overline{P}AP(\mathcal{F}_{P,z}(A))^{-1}PA\overline{P}(A_{\overline{P}} - z)^{-1}\overline{P}\end{aligned} \tag{4.98}$$

Now, (4.96) imply (4.94). Moreover, we claim that (4.96) and (4.97) imply (4.93). If $z \in \rho(A) \cap \rho(A_{\overline{P}})$, then the LHS of (4.97) defines the inverse of $\mathcal{F}_{P,z}(A)$, and thus $0 \in \rho(\mathcal{F}_{P,z}(A))$. Next suppose that $z \in \rho(A_{\overline{P}})$ and $0 \in \rho(\mathcal{F}_{P,z}(A))$. The RHS of (4.98) defines the inverse of $(A - z)$. Therefore, (4.96) and (4.97) imply (4.93).

It remains to show (4.95). Let $z \in \sigma_p(A)$, and $\psi \in Ker(A - z)$. Projecting $(A - z)\psi = 0$ on $Ran(P)$ and $Ran(\overline{P})$ gives

$$(A_P - z)P\psi + PA\overline{P}\psi = 0 , \tag{4.99}$$

and

$$(A_{\overline{P}} - z)\overline{P}\psi + \overline{P}AP\psi = 0 . \tag{4.100}$$

Since $z \in \rho(A_{\overline{P}})$, it follows from (4.100) that

$$\overline{P}\psi = -(A_{\overline{P}} - z)^{-1}\overline{P}AP\psi . \tag{4.101}$$

Substituting (4.101) in (4.99) gives

$$\mathcal{F}_{P,z}(A)P\psi = 0 .$$

Therefore, $P\ Ker(A - z) \subset Ker(\mathcal{F}_{P,z}(A))$. Conversely, if $\phi = P\psi \in Ker(\mathcal{F}_{P,z}(A))$, then $S_{P,z}\phi \in Ker(A - z)$ by (4.99) and (4.100). Therefore,

$$P\phi = PS_{P,z}\phi \in P\ Ker(A - z).$$

□

A further property of the Feshbach map is

$$\mathcal{F}_{P_1} \circ \mathcal{F}_{P_2} = \mathcal{F}_{P_1P_2},$$

if $[P_1, P_2] = 0$.

4.5.4 The Level-Shift Operator (LSO) and Fermi Golden Rule: a formal motivation

In this subsection, we *formally* discuss the perturbation of the point spectrum of a selfadjoint operator A (acting on a Hilbert space $\mathcal{H}$) using the Feshbach map, and we show how it relates to the so called level-shift operator (LSO) to second order in perturbation theory. Specific examples will be dealt with *rigorously* in chapters 5 and 6.

Consider a finitely degenerate eigenvalue $\lambda \in \sigma_p(A)$, with corresponding bounded projection P. Add a bounded perturbation, gW, to A,

$$A^g = A + gW,$$

and assume that $PWP = 0$ (so that the first nontrivial perturbation of λ is second order in g). Since the Feshbach map is isospectral (Theorem A2.2), we can use it to calculate the perturbation of λ. To second order in g, this is related to the level-shift operator.

Consider the Feshbach map

$$\begin{aligned}
\mathcal{F}_{P,\lambda}(A^g) &= P(A^g - \lambda)P - PA^g\overline{P}(A^g_{\overline{P}} - \lambda)^{-1}\overline{P}A^g P \\
&= -g^2 PW\overline{P}(A^g_{\overline{P}} - \lambda)^{-1}\overline{P}WP \\
&= -g^2\widetilde{\Gamma}(\lambda) + O(g^3)\ ,
\end{aligned}$$

where $\widetilde{\Gamma}(\lambda) := PW\overline{P}(A_{\overline{P}} - \lambda)^{-1}\overline{P}WP$ is the *level-shift* operator (LSO). Since $PW\overline{P} = PW$ and $\overline{P}WP = WP$, it follows that

$$\widetilde{\Gamma}(\lambda) := PW(A_{\overline{P}} - \lambda)^{-1}WP.$$

To second order in g, the real part of the shift of λ is

$$\begin{aligned}
-g^2 Re\widetilde{\Gamma}(\lambda) &= -\frac{1}{2}g^2 \lim_{\epsilon\to 0^+} PW\{(A_{\overline{P}} - \lambda + i\epsilon)^{-1} + (A_{\overline{P}} - \lambda - i\epsilon)^{-1}\}WP \\
&= -g^2 PW\mathcal{PV}(A_{\overline{P}} - \lambda)^{-1}WP\ ,
\end{aligned}$$

where $\mathcal{PV}$ stands for the Cauchy principal value. Moreover, the imaginary part of the perturbation of λ to second order in g is

$$\begin{aligned}
-g^2 Im\widetilde{\Gamma}(\lambda) &= -\frac{1}{2i}g^2 \lim_{\epsilon\to 0^+} PW\{(A_{\overline{P}} - \lambda + i\epsilon)^{-1} - (A_{\overline{P}} - \lambda - i\epsilon)^{-1}\}WP \\
&= -g^2\pi PW\delta(A_{\overline{P}} - \lambda)WP\ ,
\end{aligned}$$

where we have used the fact that $\lim_{\epsilon\to 0}\frac{\epsilon}{x^2+\epsilon^2} = \delta(x)$. This last term is related to the *Fermi Golden Rule* for quantum resonances.

To make these arguments rigorous, one uses spectral methods such as complex dilatation and RG analysis (see for example [BFS]) or complex translations (see for example [JP1,2] and chapter 6).

4.5.5 Explicit calculation of LSO

In this subsection we review some of the consequences of the *Fermi Golden Rule* condition in proving RTE. For further details, see, for example [BFSS,BFS], and previous subsection. In Models A1,A2 and B, the Liouvillean of the small system $\mathcal{L}^\Sigma = H^\Sigma \otimes \mathbf{1}^\Sigma - \mathbf{1}^\Sigma \otimes H^\Sigma$ has discrete spectrum $\sigma(\mathcal{L}^\Sigma) = \{e = E_i - E_j =: E_{ij} : E_i, E_j \in \sigma(H^\Sigma)\}$. For each eigenvalue $e \in \sigma(\mathcal{L}^\Sigma)$, the (imaginary part of the) *level-shift operator* acting on $RanP(\mathcal{L}^\Sigma = e) \subset \mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma$, is

$$\Gamma(e) = \int_{\mathbf{R}\times S^2} m^*(u,\sigma) P(\mathcal{L}^\Sigma \neq e)\delta(\mathcal{L}^\Sigma - e + u) m(u,\sigma), \tag{4.102}$$

where

$$m(u,\sigma) = \sum_\alpha \{G_\alpha \otimes \mathbf{1}^\Sigma \otimes \tau_\beta(g_\alpha(u,\sigma)) - \mathbf{1}^\Sigma \otimes C^\Sigma G_\alpha C^\Sigma \otimes \tau_\beta(e^{-\beta u/2} g_\alpha(u,\sigma))\} \,. \tag{4.103}$$

Without loss of generality, set $\alpha = 1$, and let $G \otimes \mathbf{1}^\Sigma = G_l$, $\mathbf{1}^\Sigma \otimes C^\Sigma G C^\Sigma = G_r$, $\tau_\beta(g) = g_1$, $\tau_\beta(e^{-\beta u/2} g) = g_2$. (The result can be easily generalized to arbitrary $\alpha \in \mathbf{N}$.) Note that $\Gamma(e)$ is a non-negative selfadjoint operator. The Fermi Golden Rule condition (assumptions A1.2 and B.2) is used to show the instability of embedded eigenvalues away from zero:

$$\text{for } e \neq 0, \quad \gamma_e := \inf \sigma\left(\Gamma(e) \restriction RanP(\mathcal{L}^\Sigma = e)\right) > 0, \tag{4.104}$$

while $\Gamma(0)$ has a simple eigenvalue at zero, with corresponding eigenvector the Gibbs state of the small system, Ω_β^Σ. Physically, this means that the zero eigenvalue of $\mathcal{L}_0$ survives the perturbation, but its degeneracy is lifted:

$$\gamma_0 := \inf \sigma\left(\Gamma(0) \restriction RanP(\mathcal{L}^\Sigma = 0) P^\perp_{\Omega^\Sigma_\beta}\right) > 0. \tag{4.105}$$

Here, $P_{\Omega_\beta^\Sigma}$ is the projection onto $\mathbf{C}\Omega_\beta^\Sigma$, and $P^\perp_{\Omega^\Sigma_\beta} = \mathbf{1} - P_{\Omega_\beta^\Sigma}$. In the following, we consider Models A1,2, but the result holds when the large system consists of free fermions (ie, for Model B) ;(see chapter 5).

Proposition A2.3
Assume (A1.2), and let $\Gamma_\Sigma(e) := P(\mathcal{L}^\Sigma = e)\Gamma(e)P(\mathcal{L}^\Sigma = e)$. Then the following hold.

(i) Let $e \neq 0$. Then there is a non-negative number δ_0 (independent of β, g) such that

$$\Gamma_\Sigma(e) \geq \delta_0 \inf_{\{E_{ij}\neq 0\}} \left(|E_{ij}| \int_{S^2} dS(\omega,\sigma)\, |g(|E_{ij}|,\sigma)|^2\right) P(\mathcal{L}^\Sigma = e) > 0.$$

(ii) $\Gamma_\Sigma(0)$ has a simple eigenvalue at zero, with the Gibbs state Ω_β^Σ as eigenvector:

$$\Omega_\beta^\Sigma = Z^\Sigma(\beta)^{-1/2} \sum_i e^{-\beta E_i/2} \varphi_i \otimes \varphi_i, \tag{4.106}$$

where $Z^\Sigma(\beta) = Tr_{\mathcal{H}^\Sigma}(e^{-\beta H^\Sigma})$, and the spectrum of $\Gamma_\Sigma(0)$ has a gap at zero: $(0, 2g_0 Z^\Sigma) \cap \sigma(\Gamma_\Sigma(0)) = \emptyset$.

Proof.
For $e \neq 0$, let

$$\begin{aligned}
\mathcal{N}_r^{(i)} &:= \{j | E_i - E_j = e\}, \\
\mathcal{N}_l^{(j)} &:= \{i | E_i - E_j = e\}, \\
\mathcal{N}_r &:= \cup_i \mathcal{N}_r^{(i)} = \{j | E_i - E_j = e \text{ for some } i\}, \\
\mathcal{N}_l &:= \cup_j \mathcal{N}_l^{(j)} = \{i | E_i - E_j = e \text{ for some } j\}.
\end{aligned}$$

Moreover, let P_i denote the rank-one projector onto $\mathbf{C}\varphi_i$, where $\{\varphi_i\}_{i=0}^{d-1}$, the eigenvectors of H^Σ. For $\mathcal{N} \subset \mathbf{N}$, put

$$P_\mathcal{N} := \sum_{j \in \mathcal{N}} P_j, \quad \text{and} \quad P_\mathcal{N} := 0 \text{ if } \mathcal{N} \text{ is empty.}$$

Let $E_{mn} := E_m - E_n$, and for $e \in \sigma(\mathcal{L}^\Sigma) \backslash \{0\}$, $m \in \mathcal{N}_l$ and $n \in \mathcal{N}_r$, let

$$\delta_m := \inf \sigma\Big(P_{\mathcal{N}_r^{(m)}} G P_{\mathcal{N}_r^c} G P_{\mathcal{N}_r^{(m)}} \restriction P_{\mathcal{N}_r^{(m)}}\Big) \geq 0, \tag{4.107}$$

$$\delta_n' := \inf \sigma\Big(P_{\mathcal{N}_l^{(n)}} G P_{\mathcal{N}_l^c} G P_{\mathcal{N}_l^{(n)}} \restriction P_{\mathcal{N}_l^{(n)}}\Big) \geq 0, \tag{4.108}$$

where ^{c} denotes the complement. If $e = 0$, then $\mathcal{N}_r^c = \mathcal{N}_l^c$ are empty, and $\delta_m, \delta_n' = 0$. Let $\delta_0 := \inf_{m \in \mathcal{N}_l}\{\delta_m\} + \inf_{n \in \mathcal{N}_r}\{\delta_n'\}$. From $P(\mathcal{L}^\Sigma = e) = \sum_{\{i,j: E_{ij} = e\}} P_i \otimes P_j$, one has

$$\Gamma_\Sigma(e) = \sum_{m,n} (1 - \delta_{E_{mn},e}) \sum_{\{i,j:E_{ij}=e\}} \sum_{\{k,l:E_{kl}=e\}} \int \delta(E_{mn} - e + u) P_{ij}\ m^*\ P_{mn}\ m\ P_{kl}. \tag{4.109}$$

We want to get a lower bound on $(m,n) \in \mathcal{N} \times \mathcal{N}$ by summing only over a convenient subset of $\mathcal{N} \times \mathcal{N}$. Using (4.103),

$$\begin{aligned}
&P_{ij} m^* P_{mn} m P_{kl} \\
&= P_{ij} \left(G_l \overline{g}_1 - G_r \overline{g}_2\right) P_{mn} \left(G_l g_1 - G_r g_2\right) P_{kl} \\
&= P_i G P_m G P_k \otimes P_n \delta_{jn} \delta_{nl} |g_1|^2 - P_i G P_m \otimes P_n C^\Sigma G C^\Sigma P_l \delta_{jn} \delta_{mk} \overline{g}_1 g_2 \\
&\quad - P_m G P_k \otimes P_j C^\Sigma G C^\Sigma P_n \delta_{im} \delta_{nl} \overline{g}_2 g_1 + P_m \otimes P_j C^\Sigma G C^\Sigma P_n C^\Sigma G C^\Sigma P_l \delta_{im} \delta_{mk} |g_2|^2.
\end{aligned}$$

Summing over i, j and k, l gives

$$\sum_{\{i,j:E_{ij}=e\}} \sum_{\{k,l:E_{kl}=e\}} P_{ij} m^* P_{mn} m P_{kl}$$
$$= \left(\overline{g}_1 P_{\mathcal{N}_l^{(n)}} G P_m \otimes P_n - \overline{g}_2 P_m \otimes P_{\mathcal{N}_r^{(m)}} C^\Sigma G C^\Sigma P_n \right) \cdot \text{ adjoint.}$$

For $(m, n) \in \mathcal{N}_l \times \mathcal{N}_r^c$, one has $P_{\mathcal{N}_l^{(n)}} = 0$ and $P_{\mathcal{N}_r^{(m)}} \neq 0$. For $(m, n) \in \mathcal{N}_l^c \times \mathcal{N}_r$, $P_{\mathcal{N}_l^{(n)}} \neq 0$ and $P_{\mathcal{N}_r^{(m)}} = 0$. Sum only over the disjoint union

$$(m, n) \in \mathcal{N}_l \times \mathcal{N}_r^c \,\dot{\cup}\, \mathcal{N}_l^c \times \mathcal{N}_r.$$

After some calculation gives

$$\Gamma_\Sigma(e) \geq \inf_{E_{ij} \neq 0} \left(\int_{S^2} dS \, |g_2(E_{ij}, \alpha)|^2 \right) \sum_{m \in \mathcal{N}_l} P_m \otimes C^\Sigma P_{\mathcal{N}_r^{(m)}} G \; P_{\mathcal{N}_r^c} \; G P_{\mathcal{N}_r^{(m)}} C^\Sigma$$
$$+ \inf_{E_{ij} \neq 0} \left(\int_{S^2} dS \, |g_1(E_{ij}, \alpha)|^2 \right) \sum_{n \in \mathcal{N}_r} P_{\mathcal{N}_l^{(n)}} G \; P_{\mathcal{N}_l^c} \; G P_{\mathcal{N}_l^{(n)}} \otimes P_n.$$

Moreover,

$$\int_{S^2} dS |g_{1,2}(E_{ij}, \alpha)|^2 \geq |E_{ij}| \int_{S^2} dS |g(|E_{ij}|, \alpha)|^2,$$

uniformly in $\beta \geq 1$, and together with (4.107), (4.108), it gives

$$\Gamma_\Sigma(e) \geq \inf_{E_{ij} \neq 0} \left(|E_{ij}| \int_{S^2} dS |g(E_{ij}, \alpha)|^2 \right) \left(\inf_{m \in \mathcal{N}_l} \{\delta_m\} + \inf_{n \in \mathcal{N}_r} \{\delta'_n\} \right) P(\mathcal{L}_\Sigma = e),$$

since $\sum_{m \in \mathcal{N}_l} P_m \otimes P_{\mathcal{N}_r^{(m)}} = \sum_{n \in \mathcal{N}_r} P_{\mathcal{N}_l^{(n)}} \otimes P_n = P(\mathcal{L}^\Sigma)$. This proves (i).

Consider now the case $e = 0$. An element of $RanP(\mathcal{L}^\Sigma)$ is of the form $\phi = \sum_i c_i \varphi_i \otimes \varphi_i$, with $\sum_i |c_i|^2 = 1$, so

$$\langle \phi, \Gamma(0) \phi \rangle = \sum_{m,n} (1 - \delta_{E_{mn},0}) \sum_{i,j} \overline{c}_i c_j \int \delta(E_{mn} + u) \langle \varphi_i \otimes \varphi_i, m^* P_{mn} m \varphi_j \otimes \varphi_j \rangle .$$

The fact that $\langle \varphi_m, C^\Sigma G C^\Sigma \varphi_n \rangle = \overline{\langle \varphi_m, G \varphi_n \rangle}$, implies

$$\langle \phi, \Gamma(0) \phi \rangle = \sum_{m,n} (1 - \delta_{E_{mn},0}) \int \delta(E_{mn} + u) \, |\langle \varphi_n, G \varphi_m \rangle|^2 \, |c_n g_1 - c_m g_2|^2, \qquad (4.110)$$

and hence

$$\int \delta(E_{mn} + u) |c_n g_1 - c_m g_2|^2$$
$$= \int_{\mathbf{R}^3} \left\{ \delta(E_{mn} + \omega) \left| \sqrt{1 + \rho} c_n g - \sqrt{\rho} c_m g \right|^2 + \delta(E_{mn} - \omega) \left| \sqrt{\rho} c_n g - \sqrt{1 + \rho} c_m g \right|^2 \right\}.$$

Together with (4.110), this implies

$$\langle\phi,\Gamma(0)\phi\rangle = 2\sum_{\{m,n:E_{mn}<0\}}|\langle\varphi_n,G\varphi_m\rangle|^2\,\frac{e^{\beta E_n}}{e^{-\beta E_{mn}}-1}\times\left|e^{-\beta E_m/2}c_n-e^{-\beta E_n/2}c_m\right|^2\int\delta(E_{mn}+\omega)|g|^2, \tag{4.111}$$

where we used $\delta(E_{mn}+\omega)\rho=\delta(E_{mn}+\omega)(e^{-\beta E_{mn}}-1)^{-1}$. Each term in the sum is zero if one chooses $c_n=Z_\Sigma^{-1/2}e^{-\beta E_n/2}$. Furthermore, $\langle\Omega_\beta^\Sigma,\Gamma(0)\Omega_\beta^\Sigma\rangle=0$. Since $\Gamma(0)\geq 0$, this implies that Ω_β^Σ is a zero eigenvector of $\Gamma(0)$.

We still need to estimate the spectral gap at zero. Equation (4.111) imply

$$\begin{aligned}\langle\phi,\Gamma(0)\phi\rangle &\geq 2g_0\sum_{\{m,n:E_{mn}<0\}}|e^{-\beta E_m/2}c_n-e^{-\beta E_n/2}c_m|^2\\ &= g_0\sum_{m,n}|e^{-\beta E_m/2}c_n-e^{-\beta E_n/2}c_m|^2\\ &= g_0\sum_{m,n}\left(e^{-\beta E_m}|c_n|^2+e^{-\beta E_n}|c_m|^2-e^{-\beta(E_m+E_n)/2}(\overline{c}_nc_m+c_n\overline{c}_m)\right)\\ &= g_0\Big(Z_\Sigma(\beta)+Z_\Sigma(\beta)-2\Big|\sum_m e^{-\beta E_m/2}c_m\Big|^2\Big)\\ &= 2g_0Z_\Sigma(\beta)\Big(1-\Big|\langle\Omega_\beta^\Sigma,\phi\rangle\Big|^2\Big),\end{aligned}$$

where we used $\sum_n|c_n|^2=1$. Therefore, we obtain on $RanP^\perp_{\Omega_\beta^\Sigma}$: $\Gamma(0)\geq 2g_0Z_\Sigma(\beta)$. □

Remark. As an explicit illustration of the results of the previous Proposition, consider Model A2 of a spin impurity interacting with magnons in a magnet. Recall that

$$H\approx -nNJS^2-s_0^3j_0M+\frac{JSV}{(2\pi)^3}\int d^3kk^2b_k^*b_k-\frac{1}{(2\pi)^3}\sqrt{\frac{S}{2N}}\int d^3k(\hat{j}(k)s_0^+b_k^*+\overline{\hat{j}}s_0^-b_k) \tag{4.112}$$

$$= H_{pp}+H_c+I\ , \tag{4.113}$$

where

$$\begin{aligned}\hat{j}(k) &= \int dxj(x)e^{ik\cdot x}\ ,\\ H_{pp} &= -nNJS^2-s_0^3j_0M\ ,\\ H_c &= \frac{JSV}{(2\pi)^3}\int d^3kk^2b_k^*b_k\ ;\\ I &= -\frac{1}{(2\pi)^3}\sqrt{\frac{S}{2N}}\int d^3k(\hat{j}(k)s_0^+b_k^*+\overline{\hat{j}}s_0^-b_k) =: \int d^3k(G(k)b^*(k)+\overline{G}(k)b(k))\ .\end{aligned}$$

Using the Pauli matrices $s_0^i, i = 1, 2, 3$, it follows that

$$H_{pp} = diag(-nNJS^2 - j_0M, -nNJS^2 + j_0M),$$

and hence $\sigma(\mathcal{L}^\Sigma) = \{-2j_0M, 0, 2j_0M\}$, with double degeneracy at 0. Direct computation (although lengthy) gives the following result.

(1) For $e = E_{01} = -2j_0M$,

$$\langle\varphi_0\otimes\varphi_1, \Gamma(-2j_0M)\varphi_0\otimes\varphi_1\rangle = \frac{4}{(2\pi)^5}\frac{2S}{N}|\hat{j}(-2j_0M)|^2\frac{\sqrt{2j_0M}}{e^{-2\beta j_0M} - 1} > 0\ . \tag{4.114}$$

(2) For For $e = E_{10} = 2j_0M$,

$$\langle\varphi_1\otimes\varphi_0, \Gamma(2j_0M)\varphi_1\otimes\varphi_0\rangle = \frac{4}{(2\pi)^5}\frac{2S}{N}|\hat{j}(2j_0M)|^2\frac{\sqrt{2j_0M}}{e^{2\beta j_0M} - 1} > 0\ . \tag{4.115}$$

(3) For $e = E_{11} = E_{00} = 0$,

$$\Gamma(0) = \begin{pmatrix} a & a^{\beta j_0M} \\ ae^{\beta j_0M} & ae^{2\beta j_0M} \end{pmatrix}\ , \tag{4.116}$$

where

$$a = \frac{4\pi|G_{0,1}(2j_0M)|^2\sqrt{2j_0M}}{e^{2\beta j_0M} - 1}.$$

The eigenvalues of $\Gamma(0)$ are

$$\lambda_0 = 0\ , \lambda_1 = \frac{4\pi|G_{0,1}(2j_0M)|^2\sqrt{2j_0M}(1 + e^{2\beta j_0M})}{e^{2\beta j_0M} - 1} > 0\ . \tag{4.117}$$

Chapter 5

RTE for a small quantum system coupled to non-relativistic reservoirs: PC method

In this chapter, we investigate the property of return to equilibrium (RTE) for a class of quantum systems composed of a small system with a finite dimensional Hilbert space, weakly coupled to an infinitely extended and dispersive heat bath by studying the spectrum of the corresponding standard Liouvillean. As discussed in chapter 2, this property is part of the zeroth law of thermodynamics.

In [JP1,2], RTE is proven for a class of spin-boson system (by studying the spectrum of the Liouvillian) using complex deformation techniques (see also [DJ]). The proof is not uniform in temperature. A stronger result of RTE, which is uniform in temperature, has been shown when a toy atom is coupled to the radiation field using the Feshbach map, complex dilatation, and an operator theoretic renormalization group method in [BFS]. This has been revisited again in [FM1] using Mourre's positive commutator method [M1] and a suitable Virial theorem with an explicit zero temperature limit. Similar methods have been used to investigate thermal ionization in [FM2,FMS] and to prove the stability of Bose-Einstein condensates in [M2]. We note that the approach of proving RTE using Liouvillians is based on the insights of [HHW].

In this chapter, we extend the analysis of [FM1] to proving RTE for a class of systems composed of a small system coupled to (free) non-relativistic bosonic and fermionic reservoirs under suitable assumptions on the perturbation (particularly, the form factors and *Fermi golden rule*), as discussed in chapter 4, Models A1,A2 and B. A physical example of the first model is a spin impurity coupled to (free) magnons in a magnet, while an example of the second is a *quantum dot* coupled to electrons in a metal. The three essential elements that enter in our analysis are a concrete representation of the free bosonic/fermionic reservoirs (Araki-Woods and Araki-Wyss respectively), the positive commutator method with a suitable Virial theorem, and an estimate on the norm of the difference between the KMS-equilibrium states of the non-interacting and the interacting systems (Appendix 2).

5.1 RTE for Models A1,2

The main result of this section is Theorem 5.2, which claims the property of return to equilibrium for quantum mechanical system formed of a small system with a finite dimensional Hilbert space coupled to a reservoir of free non-relativistic bosons. We refer to Model A1 in chapter 4 for relevant details and assumptions.

Proposition 5.1

Assume (A1.2) (specified in section 4.1). There is an $\epsilon_0 > 0$, independent of $\beta \geq \beta_0$ (for any β_0 fixed), such that if $0 < \epsilon < \epsilon_0$ then

$$\Pi I \frac{\epsilon}{\mathcal{L}_0^2 + \epsilon^2} I \Pi \geq \Gamma_0 \Pi - C\epsilon^{1/4}, \tag{5.1}$$

where C is a constant independent of the inverse temperature β, $\Pi = P_0 \otimes P_{\Omega_f}$, the projection onto the kernel of $\mathcal{L}_0$, and Γ_0 is a bounded operator on $\mathcal{H} = \mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma \otimes \mathcal{F}_+$, acting trivially on the last factor, $\mathcal{F}_+$, and leaving $Ker\mathcal{L}_\Sigma$ invariant. Furthermore, Γ_0 restricted to $Ker\mathcal{L}_\Sigma$ has zero as a simple eigenvalue, with Gibbs state Ω_β^Σ as eigenvector, and is strictly positive on the complement of $\mathbf{C}\Omega_\beta^\Sigma$. There is a constant $\gamma_0 > 0$, independent of $0 < \beta < \infty$, such that

$$\Gamma_0 \upharpoonright_{Ran\overline{P}_{\Omega_\beta^\Sigma}} \geq \gamma_0, \tag{5.2}$$

where, $\overline{P}_{\Omega_\beta^\Sigma} = \mathbf{1} - P_{\Omega_\beta^\Sigma}$ and $P_{\Omega_\beta^\Sigma}$ is the projection onto $\mathbf{C}\Omega_\beta^\Sigma$.

For a proof of this result (when the sum reduces to a single term and in the limit of $\epsilon \to 0$) see Appendix 2, Proposition A2.2, which can be easily generalized. One can show that,

$$\begin{aligned}&\Gamma_0 \upharpoonright_{Ran\overline{P}_{\Omega_\beta^\Sigma}} \\ &\quad \geq \min_{E_m \neq E_n} \frac{(E_m - E_m)^{\frac{1}{2}}\ Tr e^{-\beta H_\Sigma}}{|e^{-\beta E_m} - e^{-\beta E_n}|} \int_{S^2} d\sigma \left| \sum_\alpha \langle \varphi_m, G_\alpha \varphi_n \rangle\, g_\alpha\left(|E_m - E_n|, \sigma\right) \right|^2,\end{aligned}$$

and γ_0 in (5.2) is obtained by minimizing the RHS over $0 < \beta < \infty$.

Theorem 5.2(RTE1)

Suppose (A1.1) and (A1.2) (see section 4.1). Then there is a constant $g_1 > 0$, independent of $\beta \geq \beta_0$, for any $\beta_0 > 0$ fixed, such that, for

$$0 < |g| < g_1 \begin{cases} \left(1 + \log(1+\beta)\right)^{-9/2} & \text{if } p = 1/4 \\ 1 & \text{if } p > 1/4\ , \end{cases} \tag{5.3}$$

the kernel of $\mathcal{L}_g$ is spanned by the interacting KMS vector $\Omega_{\beta,g}$. (The system possesses the property of return to equilibrium in the ergodic sense.)

Remark. The analysis involves estimating $\|gI(N+1)^{-1/2}\|$, which depends on β since the interaction I does. As we shall see, one has to be careful in taking the limit $\beta \to \infty$ in the infra-red singular regime $p = 1/4$. Moreover, in order to estimate the norm of the difference between the interacting and the non-interacting KMS states, we need an upper bound on the expectation value of the number operator N in the interacting KMS state $\Omega_{\beta,g}$. In a suitable infra-red regime $p \geq 1/4$, we expect the KMS-equilibrium states of the non-interacting and interacting systems to be close to each other for small enough g, which will turn out to be independent of β for $p > 1/4$, but which will go to zero in the limit $\beta \to \infty$ for $p = 1/4$.

Proposition 5.3

Suppose (A1.1) holds, and let $P_{\Omega_{\beta,g}}$ and $P_{\Omega_{\beta,0}}$ denote the projections onto the spans of the interacting and non-interacting KMS states, $\Omega_{\beta,g}$ and $\Omega_{\beta,0}$, respectively. Then, for any $\epsilon > 0$ there is a $g_1(\epsilon) > 0$, which does not depend on $\beta > 0$, such that for

$$|g| < g_1(\epsilon) \begin{cases} \big(1+\log(1+\beta)\big)^{-1} & \text{if } p = 1/4 \\ 1 & \text{if } p > 1/4\,, \end{cases} \tag{5.4}$$

the following estimate holds,

$$\big\| P_{\Omega_{\beta,g}} - P_{\Omega_{\beta,0}} \big\| < \epsilon. \tag{5.5}$$

We discuss first the proof of Theorem 5.2. Define the conjugate operator to be $A_f = d\Gamma(i\partial_u)$, the second quantization of the *generator of energy translation*, $i\partial_u$, on $\mathcal{F}_+$ and let

$$A_0 = i\theta g \left(\Pi I \overline{R}_\epsilon^2 - \overline{R}_\epsilon^2 I \Pi \right), \tag{5.6}$$

where $\Pi = P_0 \otimes P_{\Omega_f}$, $\overline{R}_\epsilon = \overline{\Pi} R_\epsilon$, $\overline{\Pi} = \mathbf{1} - \Pi$, $R_\epsilon = (\mathcal{L}_0^2 + \epsilon^2)^{-1/2}$, and $\theta, \epsilon > 0$ are parameters to be chosen later.

Note that A_0 is a bounded operator, and the commutator $[\mathcal{L}_0, A_0]$ extends to a bounded operator with

$$\|[\mathcal{L}_g, A_0]\| \leq C \left(\frac{\theta |g|}{\epsilon} + \frac{\theta g^2}{\epsilon^2} \right). \tag{5.7}$$

Let $N = d\Gamma(\mathbf{1})$ be the number operator, and define on its domain $\mathcal{D}(N)$ the operator

$$B = N + gI_1 + i[\mathcal{L}_g, A_0], \tag{5.8}$$

where

$$I_1 = \sum_\alpha \big(G_\alpha \otimes \mathbf{1}^\Sigma \otimes \varphi(\partial_u \tau_\beta(g_\alpha)) - \mathbf{1}^\Sigma \otimes C^\Sigma G_\alpha C^\Sigma \otimes \varphi(\partial_u e^{-\beta u/2} \tau_\beta(g_\alpha)) \big). \tag{5.9}$$

(B corresponds to the quadratic form $i[\mathcal{L}_g, A_f + A_0]$ in the sense of Kato and $[\mathcal{L}^f, A_f] = N$; see [FM2].) Moreover, for any $\nu > 1$, let

$$\mathfrak{B}_\nu = \{\psi \in \mathcal{D}(N^{1/2}) : \|\psi\| = 1, \|(N+1)^{1/2}\psi\| \leq \nu\}.$$

Theorem 5.4 (Positive commutator estimate)

Suppose (A1.1) and (A1.2) (see section 4.1). Then there is a choice of the parameters ϵ and θ, and a constant $g_1(\eta) = g_1 > 0$, independent of ν and $\beta \geq \beta_0$, such that, for fixed η and β, and

$$0 < |g| < g_1 \begin{cases} \min\left(\frac{1}{1+\log(1+\beta)}, \frac{\nu^{1/\eta - 9/2}}{(1+\log(1+\beta))^\eta}\right) & \text{if } p = 1/4 \\ 1 & \text{if } p > 1/4, \end{cases} \tag{5.10}$$

the following estimate holds,

$$\overline{P}_{\Omega_{\beta,g}} B \overline{P}_{\Omega_{\beta,g}} \geq |g|^{2-\eta} \nu^{3-9\eta/2} \gamma_0 \overline{P}_{\Omega_{\beta,g}}, \tag{5.11}$$

in the sense of quadratic forms on $Ran E_\Delta(\mathcal{L}_g) \cap \mathfrak{B}_\nu$, where Δ is any interval around the origin such that $\Delta \cap \sigma(\mathcal{L}^\Sigma) = \{0\}$, $E_\Delta(\mathcal{L}_g)$ is the spectral projection, and where γ_0 is given in (5.2).

We will examine B as a quadratic form on $\mathfrak{B}_{\nu_0} \subset \mathcal{D}(N^{1/2})$. For $p > 1/4$, ν_0 is independent of $\beta \geq \beta_0$, while for $p = 1/4$, ν_0 diverges logarithmically for large β.

Theorem 5.5 (Regularity of eigenvectors and the Virial Theorem)

Assume (A1.1) (in section 4.1), and let ψ_g be an eigenvector of $\mathcal{L}_g$. Then there is a constant $C(p,\beta) < \infty$, not depending on g, such that

$$\|N^{1/2}\psi_g\| \leq C(p,\beta)|g| \, \|\psi_g\|, \tag{5.12}$$

and such that for all $\beta \geq \beta_0$ (for any $\beta_0 > 0$ fixed),

$$C(p,\beta) \leq c_1(p) \begin{cases} 1 + \log(1+\beta) & \text{if } p = 1/4 \\ 1 & \text{if } p > 1/4 \end{cases}, \tag{5.13}$$

where c_1 is independent of $\beta \geq \beta_0$. Furthermore,

$$\langle B \rangle_{\psi_g} := \langle \psi_g, B\psi_g \rangle = 0. \tag{5.14}$$

Note that the constant $C(p,\beta)$ may be expressed as

$$\|I_1(N+1)^{-1/2}\| \leq 2\sum_\alpha \|G_\alpha\| \, \|\partial_u \tau_\beta(g_\alpha)\|_{L^2} =: C(p,\beta).$$

We defer the technical proofs to Appendix 3. However, it is instructive at this point to understand them at a formal level. Formally expanding the commutator gives,

$$\langle \psi_g, [\mathcal{L}_g, A_f + A_0]\psi_g \rangle = 2i Im \langle L_g\psi_g, (A_f + A_0)\psi_g \rangle = 0. \tag{5.15}$$

Hence

$$0 \geq \langle N \rangle_{\psi_g} - \left| \langle g I_1 \rangle_{\psi_g} \right| \;\; \geq \;\; \langle N \rangle_{\psi_g} - C(p,\beta)|g| \, \|\psi_g\| \, \|N^{1/2}\psi_g\|$$
$$\geq \;\; \frac{1}{2} \langle N \rangle_{\psi_g} - \frac{1}{2} C(p,\beta)^2 g^2 \|\psi_g\|^2, \tag{5.16}$$

which yields the bound (5.12).

We need to control multiple commutators of $\mathcal{L}_g$ with $A_f + A_0$ to make the above statements rigorous. Particularly, the second and third commutator of I with the dilatation generator A_f need to be well-defined and relatively $N^{1/2}$-bounded. This is satisfied if

$$\partial_u^j \tau_\beta(g_\alpha) \;\; \text{is continuous in } u \in \mathbf{R} \text{ for } j = 0,1,2, \text{ and} \tag{5.17}$$
$$\partial_u^j \tau_\beta(g_\alpha) \in L^2(\mathbf{R} \times S^2) \;\; \text{for } j = 0,1,2,3. \tag{5.18}$$

One can verify that (5.17), (5.18) follow from (A1.1), section 4.1. Let p and ϕ_0 be as in assumption (A1.1); then, for $p = 3/4, 5/4$, $p > 11/4$, we choose $\phi = 2\phi_0$, while for $p = 1/4$, we take $\phi = \pi + 2\phi_0$.

The proof Theorem 5.2 (RTE1) follows directly from Theorems 5.4 and 5.5 by *reductio ad absurdum*, since, if for g satisfying (5.10), with $\nu = \nu_0$, there were an eigenvector $\psi_g \in Ran\overline{P}_{\Omega_{\beta,g}}$, orthogonal to $\Omega_{\beta,g}$, then

$$0 = \langle B \rangle_{\psi_g} \geq |g|^{2-\eta} \nu_0^{3-9\eta/2} \gamma_0 \,, \tag{5.19}$$

which is a contradiction, since the RHS is strictly positive. For $p = 1/4$ condition (5.10), with $\nu = \nu_0 = C[1 + \log(1+\beta)]$, gives (5.3), independently of η.

Regarding Proposition 5.3, the high-temperature result for bounded perturbation is relatively simple. For $\epsilon > 0$, $\exists \eta(\epsilon) > 0$ such that, if

$$\beta |g| < \eta(\epsilon), \tag{5.20}$$

then inequality (5.4) in Proposition 5.3 holds. A proof of this fact can be given by using the explicit expression for the perturbed KMS state (chapter 3), and using the Dyson series expansion to estimate $\|\Omega_{\beta,g} - \Omega_{\beta,0}\|$. Condition (5.20) comes from the fact that the term of order g^n in the Dyson series is given by an integral over an n-simplex of size β. This result is extended to lower temperatures and unbounded perturbation by using the decay in (imaginary) time of the field propagators, chess-board estimates and the Hölder and Peierls-Bogoliubov inequalities (see [Frö,DJP] and Appendices 1 and 3).

As for Theorem 5.4 (PC Theorem), we want to show that $\dim Ker\mathcal{L}_g = 1$. We know that $\dim Ker\mathcal{L}_g \geq 1$ since $\Omega_{\beta,g} \in Ker\mathcal{L}_g$. To prove equality, we want to show that

$$B + \delta P_{\Omega_{\beta,g}} \geq \gamma, \tag{5.21}$$

for some $\delta \geq \gamma > 0$. For $\Delta \subset \mathbf{R}$ an interval around the origin not containing any non-zero eigenvalue of the $\mathcal{L}^{\Sigma}$, we first prove (5.21) in the sense of quadratic forms on the spectral subspace of $\mathcal{L}_0$ associated with the interval Δ. Using this, we then show that

$$\overline{P}_{\Omega_{\beta,g}} B \overline{P}_{\Omega_{\beta,g}} \geq \frac{1}{2} \gamma \overline{P}_{\Omega_{\beta,g}}, \tag{5.22}$$

in the sense of quadratic forms on $Ran E_{\Delta'}(\mathcal{L}_g) \cap \mathfrak{B}_{\nu}$, where $E_{\Delta'}(\mathcal{L}_g)$ is the spectral projection of $\mathcal{L}_g$ associated to an interval Δ', an arbitrary interval properly contained in Δ.

5.2 RTE for Model B

We discuss RTE for Model B in chapter 4, section 3, composed of a small quantum system coupled to reservoir of non-relativistic fermions by using the PC method discussed in the previous section. The result is *not* uniform in temperature since there is a divergence in the derivative of the Fermi-Dirac distribution function at the chemical potential when the temperature is zero. For a result which is uniform in temperature, one may want to extend the RG analysis developed in [BFS] to this case. Since *all* of the proofs are almost identical to the previous section (and those in Appendix 3), we only sketch the main steps.

Proposition 5.6

Assume (B.2) (in section 4.3). There is an $\epsilon_0 > 0$, independent of $\beta \geq \beta_0$ (for any β_0 fixed), such that if $0 < \epsilon < \epsilon_0$ then

$$\Pi I \frac{\epsilon}{\mathcal{L}_0^2 + \epsilon^2} I \Pi \geq \Gamma_0 \Pi - C\epsilon^{1/4}, \tag{5.23}$$

where C is a constant independent of the inverse temperature β, $\Pi = P_0 \otimes P_{\Omega_f}$, the projection onto the kernel of $\mathcal{L}_0$, and Γ_0 is a bounded operator on $\mathcal{H} = \mathcal{H}^{\Sigma} \otimes \mathcal{H}^{\Sigma} \otimes \mathcal{F}_-$, acting trivially on the last factor, $\mathcal{F}_-$, and leaving $Ker \mathcal{L}^{\Sigma}$ invariant. Furthermore, Γ_0 restricted to $Ker \mathcal{L}^{\Sigma}$ has zero as a simple eigenvalue, with Gibbs state Ω_{β}^{Σ} as eigenvector, and is strictly positive on the complement of $\mathbf{C}\Omega_{\beta}^{\Sigma}$. There is a constant $\gamma_0 > 0$, independent of $0 < \beta < \infty$, such that

$$\Gamma_0 \restriction_{Ran \overline{P}_{\Omega_{\beta}^{\Sigma}}} \geq \gamma_0, \tag{5.24}$$

where, $\overline{P}_{\Omega_{\beta}^{\Sigma}} = \mathbf{1} - P_{\Omega_{\beta}^{\Sigma}}$ and $P_{\Omega_{\beta}^{\Sigma}}$ is the projection onto $\mathbf{C}\Omega_{\beta}^{\Sigma}$.

The proof is similar to that of Proposition 5.1. Explicitly,

$$\Gamma_0 \restriction_{Ran \overline{P}_{\Omega_{\beta}^{\Sigma}}} \geq \min_{E_m \neq E_n} \frac{e^{\beta E_n}}{e^{-\beta(E_m - E_n - \nu)}} \int du d\sigma \delta(E_m - E_n - u) \left| \sum_{\alpha} \langle \varphi_m, G_{\alpha} \varphi_n \rangle g_{\alpha}(|u|, \sigma) \right|^2,$$

and γ_0 in (5.24) is obtained by minimizing the RHS.

The main result of this section is the following theorem, which says that Model B (with the corresponding assumptions B.1 and B.2) possesses the property of return to equilibrium.

Theorem 5.7(RTE2)

Assume conditions (B.1) and (B.2) hold (see section 4.3). Then there is a constant $g_1 > 0$, independent of $\beta_0 \leq \beta \leq \beta_1$, for any $\beta_1 > \beta_0 > 0$ fixed such that, for

$$0 < |g| < g_1 \ , \tag{5.25}$$

the kernel of $\mathcal{L}_g$ is spanned by the interacting KMS vector $\Omega_{\beta,g}$, and the system has the property of return to equilibrium.

The proof relies on the following three propositions.

Proposition 5.8

Suppose (B.1) holds, and let $P_{\Omega_{\beta,g}}$ and $P_{\Omega_{\beta,0}}$ denote the projections onto the spans of the interacting and non-interacting KMS states, $\Omega_{\beta,g}$ and $\Omega_{\beta,0}$, respectively. Then, for any $\epsilon > 0$ there is a $g_1(\epsilon) > 0$, which does not depend on β, such that, for

$$|g| < g_1(\epsilon) \ , \tag{5.26}$$

the following estimate holds

$$\left\| P_{\Omega_{\beta,g}} - P_{\Omega_{\beta,0}} \right\| < \epsilon. \tag{5.27}$$

Since we are only interested in strictly positive temperatures, the proof of this statement follows directly from a Dyson series expansion (high-temperature result); (see remark after Theorem 5.5).

Recall $N = d\Gamma(\mathbf{1})$ is the number operator, and define on its domain $\mathcal{D}(N)$ the operator

$$B = N + gI_1 + i[\mathcal{L}_g, A_0], \tag{5.28}$$

where

$$I_1 = \sum_\alpha \left(G_\alpha \otimes \mathbf{1}^\Sigma \otimes \varphi(\partial_u g_{\beta,\alpha}) - i\mathbf{1}^\Sigma \otimes C^\Sigma G_\alpha C^\Sigma \otimes (-1)^N \varphi(\partial_u g^\#_{\beta,\alpha}) \right). \tag{5.29}$$

Proposition 5.9 (Positive commutator estimate)

Suppose (B.1) and (B.2) (in section 4.3). Then there is a choice of the parameters ϵ and θ, and a constant $g_1(\eta) = g_1 > 0$, independent of ν and $\beta \in [\beta_0, \beta_1]$, such that, for fixed η and β, and

$$0 < |g| < g_1 \tag{5.30}$$

the following estimate holds,

$$\overline{P}_{\Omega_{\beta,g}} B \overline{P}_{\Omega_{\beta,g}} \geq |g|^{2-\eta} \nu^{3-9\eta/2} \gamma_0 \overline{P}_{\Omega_{\beta,g}}, \tag{5.31}$$

in the sense of quadratic forms on $RanE_\Delta(\mathcal{L}_g) \cap \mathfrak{B}_\nu$, where Δ is any interval around the origin such that $\Delta \cap \sigma(\mathcal{L}^\Sigma) = \{0\}$, $E_\Delta(\mathcal{L}_g)$ is the spectral projection, and where γ_0 is given in (5.24).

Proposition 5.10 (Regularity of eigenvectors and the Virial Theorem)

Assume (B.1) (in section 4.3), and let ψ_g be an eigenvector of $\mathcal{L}_g$. Then

$$\langle B \rangle_{\psi_g} := \langle \psi_g, B\psi_g \rangle = 0, \tag{5.32}$$

where B has been defined in (5.28)

The proof of Theorem 5.7 follows from Propositions 5.9 and 5.10 by contradiction (similar to the proof of Theorem 5.3). Moreover, the proof of Propositions 5.9 and 5.10 is very similar to the proof of Theorems 5.4 and 5.5 (see Appendix 3).

5.3 Appendix 3

5.3.1 Proof of Theorem 5.4

Positive commutator estimate localized with respect to $\mathcal{L}_0$.

Consider the decomposition

$$\mathcal{H}^0_\Delta := RanE^0_\Delta = RanE^0_\Delta \Pi \oplus RanE^0_\Delta \overline{\Pi}, \tag{5.33}$$

where

$$\Pi = P_0 \otimes P_{\Omega_f}. \tag{5.34}$$

and where E^0_Δ is the spectral projection of $\mathcal{L}_0$ associated with the interval Δ. First, we to prove a lower bound on $E^0_\Delta \overline{\Pi}(B + \delta P_{\Omega_{\beta,g}})\overline{\Pi} E^0_\Delta$.

(Remark regarding the notation: C will denote a constant independent of $g, \theta, \epsilon, \beta \geq \beta_0 > 0$, and $C(p, \beta)$ will denote a constant independent of g, θ, ϵ, satisfying the bound given in (5.13).) We know that

$$\|E^0_\Delta \overline{\Pi}[\mathcal{L}_g, A_0]\overline{\Pi} E^0_\Delta\| \leq C\frac{\theta g^2}{\epsilon^2}\ , \tag{5.35}$$

where $\overline{\Pi} = \overline{P}_0 \otimes P_{\Omega_f} + \overline{P}_{\Omega_f}$ (and notice that $RE^0_\Delta \overline{\Pi} \subset Ran\overline{P}_{\Omega_f}$). Hence,

$$\begin{aligned} E^0_\Delta \overline{\Pi}(B + \delta P_{\Omega_{\beta,g}})\overline{\Pi} E^0_\Delta &= E^0_\Delta \overline{\Pi} N^{1/2} \left(\mathbf{1} + N^{-1/2} g I_1 N^{-1/2}\right) N^{1/2} \overline{\Pi} E^0_\Delta \\ &\quad + E^0_\Delta \overline{\Pi} \left(i[\mathcal{L}_g, A_0] + \delta P_{\Omega_{\beta,g}}\right) \overline{\Pi} E^0_\Delta \\ &\geq \frac{1}{2} E^0_\Delta \overline{\Pi} + E^0_\Delta \overline{\Pi} i[\mathcal{L}_g, A_0] \overline{\Pi} E^0_\Delta \\ &\geq \frac{1}{2}\left(1 - C\frac{\theta g^2}{\epsilon^2}\right) E^0_\Delta \overline{\Pi}, \end{aligned} \tag{5.36}$$

if

$$\|\overline{P}_{\Omega_f} N^{-1/2} g I_1 N^{-1/2} \overline{P}_{\Omega_f}\| \leq C(p,\beta)|g| < 1/2, \tag{5.37}$$

Choosing the parameters such that

$$C\frac{\theta g^2}{\epsilon^2} < 1/2, \tag{5.38}$$

it follows that

$$E^0_\Delta \overline{\Pi}(B + \delta P_{\Omega_{\beta,g}})\overline{\Pi} E^0_\Delta \geq \frac{1}{4} E^0_\Delta \overline{\Pi}. \tag{5.39}$$

In order to proceed further, we apply the Feshbach map (as was done, for example, in [BFS, BFSS]). The so called isospectrality of the Feshbach map is a very useful property which is central for our application.*

Consider the Feshbach map (with the spectral parameter $m < 1/8$), applied to

$$E^0_\Delta (B + \delta P_{\Omega_{\beta,g}}) E^0_\Delta \tag{5.40}$$

as an operator on the Hilbert space $\mathcal{H}^0_\Delta$:

$$\begin{aligned} F_{\Pi,m}(E^0_\Delta(B + \delta P_{\Omega_{\beta,g}})E^0_\Delta) &= E^0_\Delta \Pi\Big(B + \delta P_{\Omega_{\beta,g}} \\ -(B + \delta P_{\Omega_{\beta,g}}) E^0_\Delta \overline{\Pi}&\left(\overline{B + \delta P_{\Omega_{\beta,g}}} - m\right)^{-1} \overline{\Pi} E^0_\Delta (B + \delta P_{\Omega_{\beta,g}})\Big)\Pi E^0_\Delta, \end{aligned} \tag{5.41}$$

(the barred operator is understood to be restricted to the subspace $Ran E^0_\Delta \overline{\Pi} \subset \mathcal{H}^0_\Delta$). Since $\Pi I_1 \Pi = 0$, it follows that

$$\Pi B \Pi = 2\theta g^2 \Pi I \overline{R}^2_\epsilon I \Pi \geq 0. \tag{5.42}$$

First, we want to show that the second term in (5.41) is smaller than $\Pi B \Pi$. Using the fact that $\| \left(\overline{B + \delta P_{\Omega_{\beta,g}}} - m\right)^{-1} \| < 8$ for $m < \frac{1}{8}$ and (5.39), $\|\mathcal{L}_0 \overline{R}_\epsilon\| \leq 1$, $\|\overline{R}^2_\epsilon\| \leq \epsilon^{-2}$ and $\overline{\Pi} i[\mathcal{L}_g, A_0]\Pi = \theta\lambda\overline{\Pi}\mathcal{L}_g \overline{R}^2_\epsilon I \Pi$, it follows that

$$\begin{aligned} &8\|E^0_\Delta \overline{\Pi}(gI_1 + i[\mathcal{L}_g, A_0] + \delta P_{\Omega_{\beta,g}})\Pi\psi\|^2 \\ &\leq\ 16\theta^2 g^2 \|\overline{R}_\epsilon I \Pi \psi\|^2 \\ &\quad +C\left(\delta^2 \|\overline{\Pi} P_{\Omega_{\beta,g}} \Pi\|^2 + C(p,\beta) g^2 + \frac{\theta^2 g^4}{\epsilon^4}\right)\|\psi\|^2. \end{aligned} \tag{5.43}$$

It follows that

$$\begin{aligned} &\left\langle F_{\Pi,m}(E^0_\Delta(B + \delta P_{\Omega_{\beta,g}})E^0_\Delta)\right\rangle_\psi \\ &\geq\ 2\theta g^2(1 - 8\theta)\left\langle \Pi I \overline{R}^2_\epsilon I \Pi\right\rangle_\psi + \delta\|P_{\Omega_{\beta,g}}\Pi\psi\|^2 \\ &\quad -C\frac{\theta g^2}{\epsilon}\left(\frac{\epsilon}{\theta}C(p,\beta) + \frac{\theta g^2}{\epsilon^3} + \frac{\epsilon}{\theta g^2}\delta^2\|\overline{\Pi} P_{\Omega_{\beta,g}}\Pi\|^2\right)\|\psi\|^2\ , \end{aligned} \tag{5.44}$$

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*see Appendix 2, chapter 4 for a discussion and proof of the isospectrality of the Feshbach map.

for any $\psi \in \mathcal{H}^0_\Delta$. Moreover,

$$\Pi I \overline{R}^2_\epsilon I \Pi \geq \frac{1}{\epsilon}\left(\Gamma_0 - C\epsilon^{1/4}\right), \tag{5.45}$$

if $\epsilon < \epsilon_0$. Choose ϵ and θ such that

$$\theta < 1/16, \;\; \epsilon < \epsilon_0. \tag{5.46}$$

For $\psi \in Ran\Pi$,

$$\begin{aligned} \theta g^2 \left\langle I\overline{R}^2_\epsilon I + \frac{\delta}{\theta g^2} P_{\Omega_{\beta,g}} \right\rangle_\psi &\geq \frac{\theta g^2}{\epsilon}\left\langle \gamma_0 \overline{P}_{\Omega^\Sigma_\beta} + \frac{\epsilon\delta}{\theta g^2} P_{\Omega_{\beta,g}} - C\epsilon^{1/4} \right\rangle_\psi \\ &= \frac{\theta g^2}{\epsilon}\gamma_0 \left[\left(1 - C\epsilon^{1/4}/\gamma_0\right)\|\psi\|^2 + \left\langle \frac{\epsilon\delta}{\theta g^2 \gamma_0} P_{\Omega_{\beta,g}} - P_{\Omega_{\beta,0}} \right\rangle_\psi \right], \end{aligned} \tag{5.47}$$

since $P_{\Omega^\Sigma_\beta}\psi = P_{\Omega_{\beta,0}}\psi$ for $\psi \in Ran\Pi$. We choose

$$\delta \geq \frac{\theta g^2}{\epsilon}\gamma_0 \geq \frac{\theta g^2}{4\epsilon}\gamma_0 =: \gamma, \tag{5.48}$$

and

$$C\frac{\epsilon^{1/4}}{\gamma_0} < 1/4. \tag{5.49}$$

Now, from Proposition 5.3 , $\|P_{\Omega_{\beta,g}} - P_{\Omega_{\beta,0}}\| < \frac{1}{4}$ if

$$g \text{ satisfies condition (5.4) (with } \epsilon = 1/4). \tag{5.50}$$

One may use this estimate to find a lower bound for the R.H.S. of (5.47)

$$\frac{\theta g^2}{\epsilon}\gamma_0 \Big(3/4 - \|P_{\Omega_{\beta,g}} - P_{\Omega_{\beta,0}}\|\Big)\|\psi\|^2 \geq \frac{\theta g^2}{2\epsilon}\gamma_0 \;\|\psi\|^2. \tag{5.51}$$

Furthermore,

$$\|\overline{\Pi} P_{\Omega_{\beta,g}} \Pi\|^2 = \|\overline{\Pi}(P_{\Omega_{\beta,g}} - P_{\Omega_{\beta,0}})\Pi\|^2 \leq \|P_{\Omega_{\beta,g}} - P_{\Omega_{\beta,0}}\|^2 \;,$$

and with suitable bounds on the parameters ϵ, g, θ, one may choose them such that

$$C\left(\frac{\epsilon}{\theta}C(p,\beta) + \frac{\theta g^2}{\epsilon^3} + \frac{\epsilon\delta^2}{\theta g^2}\right) < \gamma_0/4. \tag{5.52}$$

Combining all of these estimates, we obtain

$$\left\langle F_{\Pi,m}(E^0_\Delta(B + \delta P_{\Omega_{\beta,g}})E^0_\Delta)\right\rangle_\psi \geq \frac{\theta g^2}{4\epsilon}\gamma_0 \;\|\psi\|^2. \tag{5.53}$$

From the isospectrality of the Feshbach map (see [BFSS,BFS]), it follows

$$E^0_\Delta(B+\delta P_{\Omega_{\beta,g}})E^0_\Delta \geq \min\left(\frac{1}{8},\frac{\theta g^2}{4\epsilon}\gamma_0\right)E^0_\Delta = \frac{\theta g^2}{4\epsilon}\gamma_0 E^0_\Delta. \tag{5.54}$$

We will use the above estimate in the following.

Positive commutator estimate localized with respect to $\mathcal{L}_g$

Denote by $0 \leq \chi_\Delta \leq 1$ a smooth function with support inside the interval Δ such that $\chi_\Delta(0) = 1$, and let $\chi^0_\Delta = \chi_\Delta(\mathcal{L}_0)$ and $\chi_\Delta = \chi_\Delta(\mathcal{L}_g)$ the operators obtained from the spectral theorem. We will show that any vector $\psi \in Ran\overline{P}_{\Omega_{\beta,g}} \cap \mathfrak{B}_\nu$, such that $\chi_\Delta\psi = \psi$, satisfies

$$\left\langle B+\delta P_{\Omega_{\beta,g}}\right\rangle_\psi = \langle B\rangle_\psi \geq \frac{\theta g^2}{8\epsilon}\gamma_0, \tag{5.55}$$

for appropriate bounds on the parameters g,ϵ and θ. One estimate from functional calculus that we use is

$$\begin{aligned}\|(1-\chi^0_\Delta)\psi\| = \|(\chi_\Delta-\chi^0_\Delta)\psi\| &\leq C|g|\ \|I(N+1)^{-1/2}\|\ \|(N+1)^{1/2}\psi\| \\ &\leq C\nu|g|, \end{aligned} \tag{5.56}$$

Decompose $\langle B\rangle_\psi$ into three terms, which we will estimate individually:

$$\begin{aligned}\langle B\rangle_\psi &= \left\langle \chi^0_\Delta(B+\delta P_{\Omega_{\beta,g}})\chi^0_\Delta\right\rangle_\psi & (5.57)\\ &\quad + \left\langle (1-\chi^0_\Delta)(B+\delta P_{\Omega_{\beta,g}})(1-\chi^0_\Delta)\right\rangle_\psi & (5.58)\\ &\quad +2\,\mathrm{Re}\left\langle (1-\chi^0_\Delta)(B+\delta P_{\Omega_{\beta,g}})\chi^0_\Delta\right\rangle_\psi . & (5.59)\end{aligned}$$

Using (5.54) and the fact that $E^0_\Delta\chi^0_\Delta = \chi^0_\Delta$, the first term is bounded from below

$$\left\langle \chi^0_\Delta(B+\delta P_{\Omega_{\beta,g}})\chi^0_\Delta\right\rangle_\psi \geq \frac{\theta g^2}{4\epsilon}\gamma_0\|\chi^0_\Delta\psi\|^2 \geq \frac{\theta g^2}{4\epsilon}\gamma_0(1-C\nu|g|)\|\psi\|^2. \tag{5.60}$$

Since $N+\delta P_{\Omega_{\beta,g}} \geq 0$ is non-negative, the second term is also bounded from below by

$$\begin{aligned}(5.58) &\geq -\left|\left\langle (1-\chi^0_\Delta)(gI_1+i[\mathcal{L}_g,A_0])(1-\chi^0_\Delta)\right\rangle_\psi\right| \\ &\geq -|g|\ \|(1-\chi^0_\Delta)\psi\|\ \|I_1(N+1)^{-1/2}\|\ \|(N+1)^{1/2}\psi\| \\ &\quad -\|[\mathcal{L}_g,A_0]\|\ \|(1-\chi^0_\Delta)\psi\|^2 \\ &\geq -C\nu^2\frac{\theta g^2}{\epsilon}\left(\frac{\epsilon}{\theta}C(p,\beta)+|g|+\frac{g^2}{\epsilon}\right). \end{aligned} \tag{5.61}$$

As for the third term, since N commutes (strongly) with χ^0_Δ and $\psi \in Ran\overline{P}_{\Omega_{\beta,g}}$, it follows that

$$\begin{aligned}&Re\left\langle (1-\chi^0_\Delta)(B+\delta P_{\Omega_{\beta,g}})\chi^0_\Delta\right\rangle_\psi \\ &\geq \delta\left\langle (1-\chi^0_\Delta)P_{\Omega_{\beta,g}}(\chi^0_\Delta-1)\right\rangle_\psi + Re\left\langle (1-\chi^0_\Delta)(gI_1+i[\mathcal{L}_g,A_0])\chi^0_\Delta\right\rangle_\psi \\ &\geq -\delta\|(1-\chi^0_\Delta)\psi\|^2 - C(p,\beta)\nu g^2\|\psi\|^2 - \left|\left\langle (1-\chi^0_\Delta)[\mathcal{L}_g,A_0]\chi^0_\Delta\right\rangle_\psi\right| . \end{aligned} \tag{5.62}$$

Moreover, $(1-\chi^0_\Delta)\Pi = 0$ and $\|(1-\chi^0_\Delta)\mathcal{L}_0^{-1}\| \le C$, and hence the last term can be estimated by

$$\begin{aligned}
&\left|\left\langle(1-\chi^0_\Delta)[\mathcal{L}_g, A_0]\chi^0_\Delta\right\rangle_\psi\right| \\
&= \theta|g| \left|\left\langle(1-\chi^0_\Delta)(gI\Pi I\overline{R}_\epsilon^2 - \mathcal{L}_g\overline{R}_\epsilon^2 I\Pi + g\overline{R}_\epsilon^2 I\Pi I)\chi^0_\Delta\right\rangle_\psi\right| \\
&\le C\nu\theta|g|\left(\frac{g^2}{\epsilon^2}+|g|\right)\|\psi\|^2 = C\nu\frac{\theta g^2}{\epsilon}\left(\frac{|g|}{\epsilon}+\epsilon\right)\|\psi\|^2. \qquad (5.63)
\end{aligned}$$

Substituting back,

$$\begin{aligned}
&\langle B\rangle_\psi \ge \qquad (5.64)\\
&\quad \frac{\theta g^2}{4\epsilon}\gamma_0\left((1-C\nu|g|) - \frac{C\nu}{\gamma_0}\left(\nu\frac{\epsilon}{\theta}C(p,\beta)+\nu|g|+\nu\frac{g^2}{\epsilon}+\frac{|g|}{\epsilon}+\epsilon\right)\right)\|\psi\|^2.
\end{aligned}$$

To arrive at inequality (5.55), choose the parameters such that

$$C\nu|g| < 1/4 \quad \text{and} \quad \frac{C\nu}{\gamma_0}\left(\nu\frac{\epsilon}{\theta}C(p,\beta)+\nu|g|+\nu\frac{g^2}{\epsilon}+\frac{|g|}{\epsilon}+\epsilon\right) < 1/4. \qquad (5.65)$$

Indeed,

$$(5.37),\ (5.38),\ (5.46),\ (5.48),\ (5.49),\ (5.50),\ (5.52),\ (5.65) \qquad (5.66)$$

can be simultaneously satisfied: If we set

$$\begin{aligned}
g &= \nu^{-9/2}g', &(5.67)\\
\epsilon &= \nu^{-3}|g'|^e, \quad \text{some } 0<e<1, &(5.68)\\
\theta &= |g'|^t, \quad \text{some } 0<t<e<1 \text{ such that } t>3e-2, &(5.69)\\
\delta &= \frac{\theta g^2}{\epsilon}\gamma_0, &(5.70)
\end{aligned}$$

there is a $g_1 > 0$, depending on e, t, but not on ν, $\beta \ge \beta_0$, such that if

$$0 < |g| < g_1 \min\left(C(p,\beta)^{-1}, \nu^{1/\eta - 9/2}C(p,\beta)^{-1/\eta}\right), \qquad (5.71)$$

where $\eta = e - t > 0$, then conditions (5.66) are satisfied.

5.3.2 Proof of Proposition 5.3

First, we use the fact that the trace-norm majorizes the operator-norm,

$$\begin{aligned}
\|P_{\Omega_{\beta,g}} - P_{\Omega_{\beta,0}}\|^2 &\le \|P_{\Omega_{\beta,g}} - P_{\Omega_{\beta,0}}\|_2^2 = 2\left(1-\left\langle\Omega_{\beta,g}, P_{\Omega_{\beta,0}}\Omega_{\beta,g}\right\rangle\right)\\
&\le 2\left\langle\Omega_{\beta,g}, \overline{P}_{\Omega^\Sigma_\beta}\Omega_{\beta,g}\right\rangle + 2\left\langle\Omega_{\beta,g}, \overline{P}_{\Omega_f}\Omega_{\beta,g}\right\rangle, \qquad (5.72)
\end{aligned}$$

since $\mathbf{1} - P_{\Omega_{\beta,0}} \le \overline{P}_{\Omega_\beta^\Sigma} + \overline{P}_{\Omega_f}$. (Recall Ω_β^Σ is the vector corresponding to the Gibbs state of Σ at inverse temperature β , and Ω_f is the vacuum vector in $\mathcal{F}_+$.) We know that

$$\left\langle \Omega_{\beta,g}, \overline{P}_\Omega \Omega_{\beta,g} \right\rangle \le \| N^{1/2} \Omega_{\beta,g} \|^2 \le c(p,\beta)^2 |g|^2, \tag{5.73}$$

where $c(p,\beta)$ satisfies (5.13). There is a $\beta_1(\epsilon) \ge \beta_0$ such that if $\beta > \beta_1(\epsilon)$ then

$$\| P_{\Omega_\beta^\Sigma} - P_{\varphi_0 \otimes \varphi_0} \| < \epsilon/2, \tag{5.74}$$

where φ_0 is the groundstate eigenvector of H^Σ and $P_{\varphi_0\otimes\varphi_0} \in \mathcal{B}(\mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma)$ is the projection onto the span of $\varphi_0 \otimes \varphi_0$. Hence

$$\| P_{\Omega_{\beta,g}} - P_{\Omega_{\beta,0}} \|^2 \le 2 \left\langle \Omega_{\beta,g}, \overline{P}_{\varphi_0\otimes\varphi_0} \Omega_{\beta,g} \right\rangle + \epsilon + 2c(p,\beta)^2 |g|^2, \tag{5.75}$$

for $\beta > \beta_1(\epsilon)$. Let

$$Q = \overline{P}_{\varphi_0} \in \mathcal{B}(\mathcal{H}^\Sigma) \tag{5.76}$$

be the projection onto the orthogonal complement of the groundstate subspace of H^Σ so that

$$\overline{P}_{\varphi_0\otimes\varphi_0} \le Q \otimes \mathbf{1}^\Sigma + \mathbf{1}^\Sigma \otimes Q. \tag{5.77}$$

Since $\left\langle \Omega_{\beta,g}, Q \otimes \mathbf{1}^\Sigma \, \Omega_{\beta,g} \right\rangle = \left\langle \Omega_{\beta,g}, \mathbf{1}^\Sigma \otimes Q \, \Omega_{\beta,g} \right\rangle = \omega_{\beta,g}(Q)$,

$$\| P_{\Omega_{\beta,g}} - P_{\Omega_{\beta,0}} \|^2 \le 4\omega_{\beta,g}(Q) + \epsilon + 2c(p,\beta)^2 |g|^2, \tag{5.78}$$

for $\beta > \beta_1(\epsilon)$.

We claim that for any $\epsilon > 0$ there exist $\beta_2(\epsilon) > 0$ and $g_1(\epsilon) > 0$ such that if $\beta > \beta_2(\epsilon)$ and $|g| < g_1(\epsilon)$ then

$$\omega_{\beta,g}(Q) < \epsilon. \tag{5.79}$$

The proof is given in a while. For now, we use (5.79) to prove Proposition 5.3. Set

$$\begin{aligned} \beta_3(\epsilon) &:= \max(\beta_1(\epsilon), \beta_2(\epsilon)), \\ g_0'(\epsilon) &:= \min\left(g_1(\epsilon), c(p,\beta)^{-1}\sqrt{\epsilon/2}, \eta(\epsilon)/\beta_3(\epsilon) \right), \end{aligned} \tag{5.80}$$

When $p > 1/4$, $c(p,\beta)$ has an upper bound which is uniform in $\beta \ge \beta_0$, and we take $g_0(\epsilon)$ to be the RHS of (5.80) with $c(p,\beta)$ replaced by this upper bound. For $p = 1/4$ we can find a $g_0(\epsilon)$, independent of $\beta > 0$, satisfying $(1+\log(1+\beta))^{-1} g_0(\epsilon) \le g_0'(\epsilon)$.

Estimate (5.78) and (5.79) give

$$\| P_{\Omega_{\beta,g}} - P_{\Omega_{\beta,0}} \|^2 \le 6\epsilon, \tag{5.81}$$

for $\beta > \beta_3(\epsilon)$. If $\beta \le \beta_3(\epsilon)$ then $\beta|\lambda| < \eta(\epsilon)$, and (5.27) follows from the high-temperature result mentioned above. This completes the proof of the theorem, given our claim (5.79).

We now turn to proving claim (5.79). Without loss of generality, we work with a finite volume approximation

$$\omega^{\Lambda}_{\beta,g}(\cdot) = \frac{Tr\left(e^{-\beta H^{\Lambda}_g}\,\cdot\right)}{Tre^{-\beta H^{\Lambda}_g}}\ , \tag{5.82}$$

of the KMS state $\omega_{\beta,g}$, where $\Lambda = [-L/2, L/2]^3 \subset \mathbf{R}^3$. The trace is taken over the Hilbert space $\mathcal{H}^{\Sigma} \otimes \mathcal{F}_{+}(L^2(\Lambda, d^3x))$. For $n = (n_1, n_2, n_3) \in \mathbb{Z}^3$, let

$$e^{\Lambda}_n(x) = L^{-3/2} e^{2\pi i n x/L},\ E^{\Lambda}_n = (\frac{2\pi}{L}|n|)^2 = (\frac{2\pi}{L})^2(n_1^2 + n_2^2 + n_3^2) \tag{5.83}$$

denote the eigenvectors and eigenvalues of the operator $-\Delta$ on $L^2(\Lambda, d^3x)$ with periodic boundary conditions at $\partial\Lambda$. We identify the basis $\{e^{\Lambda}_n\}$ of $L^2(\Lambda^3, d^3x)$ with the canonical basis of $l^2(\mathbb{Z}^3)$, and define the finite-volume Hamiltonian by

$$H^{\Lambda}_g = H^{\Sigma} + H^{\Lambda}_f + \lambda v^{\Lambda}, \tag{5.84}$$

$$v^{\Lambda} = \sum_{\alpha} G_{\alpha} \otimes \varphi(g^{\Lambda}_{\alpha}), \tag{5.85}$$

where $g^{\Lambda}_{\alpha} \in l^2(\mathbb{Z}^3)$ is given by

$$g^{\Lambda}_{\alpha}(n) = \left(\frac{2\pi}{L}\right)^{3/2} \begin{cases} g_{\alpha}\left(\frac{2\pi n}{L}\right), & n \neq 0, \\ 1, & n = 0. \end{cases} \tag{5.86}$$

and the operator

$$H^{\Lambda}_f = \mathrm{d}\Gamma(h^{\Lambda}_f), \tag{5.87}$$

acting on $\mathcal{F}_{+}(l^2(\mathbb{Z}^3))$, is the second quantization of the one-particle Hamiltonian

$$h^{\Lambda}_f e^{\Lambda}_n = \begin{cases} E^{\Lambda}_n e^{\Lambda}_n, & \text{if } n \neq (0,0,0), \\ e^{\Lambda}_n, & \text{if } n = (0,0,0). \end{cases} \tag{5.88}$$

On the complement of the zero-mode subspace h^{Λ}_f equals $-\Delta$ with periodic boundary conditions. The thermodynamic limit isn't affected by changing the action of h^{Λ}_f on finitely many modes assuming $e^{-\beta H^{\Lambda}_f}$ is trace-class. Similarly, we may modify the definition of g^{Λ}_{α} on finitely many modes without altering the thermodynamic limit. The existence of the thermodynamic limit,

$$\lim_{L\to\infty} \omega^{\Lambda}_{\beta,g}(A) = \omega_{\beta,g}(A), \tag{5.89}$$

can be proven by expanding $e^{-\beta H^{\Lambda}_g}$ into a Dyson (perturbation) series and using

$$\omega^{\Lambda}_{\beta,0}(A) = \frac{Tr\left(e^{-\beta H^{\Lambda}_0} A\right)}{Tre^{-\beta H^{\Lambda}_0}} \tag{5.90}$$

has the expected thermodynamic limit for quasi-local observables A.

We want to show that $\omega^\Lambda_{\beta,g}(Q) < \epsilon$, for Q given in (5.76), provided β and g satisfy the conditions given in our claim (5.79), *uniformly* in the size of Λ. We use the Hölder and Peierls-Bogoliubov inequalities. The Hölder inequality (for traces) reads

$$\|A_1 \dots A_n\|_1 \le \prod_{j=1}^{n} \|A_j\|_{p_j}, \tag{5.91}$$

where $1 \le p_j \le \infty$, $\sum_j p_j^{-1} = 1$, and the norms are

$$\|A\|_p = \left(Tr|A|^p\right)^{1/p}, \text{for } p < \infty, \text{ and } \|A\|_\infty = \|A\| \text{ (operator norm).} \tag{5.92}$$

The Peierls-Bogoliubov inequality says that

$$\frac{Tr\left(e^{A+B}\right)}{Tre^B} \ge \exp\left[Tr\left(Ae^B\right)/Tre^B\right], \tag{5.93}$$

which implies that

$$\frac{Tre^{-\beta H_0^\Lambda}}{Tre^{-\beta H_g^\Lambda}} \le e^{\beta|g\omega^\Lambda_{\beta,0}(v^\Lambda)|} = 1, \tag{5.94}$$

since, by (5.85), $\omega^\Lambda_{\beta,0}(v^\Lambda) = 0$.

Using the Hölder inequality,

$$\begin{aligned} \omega^\Lambda_{\beta,g}(Q) &= \frac{Tr\left(e^{-(\beta-2\tau)H_g^\Lambda} e^{-\tau H_g^\Lambda} Q e^{-\tau H_g^\Lambda}\right)}{Tre^{-\beta H_g^\Lambda}} \\ &\le \left[\frac{Tr\left\{\left(e^{-\tau H_g^\Lambda} Q e^{-\tau H_g^\Lambda}\right)^{\frac{\beta}{2\tau}}\right\}}{Tre^{-\beta H_g^\Lambda}}\right]^{\frac{2\tau}{\beta}} = \left[\frac{Tr\left\{\left(Qe^{-\frac{\beta}{2M}H_g^\Lambda}Q\right)^{2M}\right\}}{Tre^{-\beta H_g^\Lambda}}\right]^{\frac{1}{2M}}, \end{aligned} \tag{5.95}$$

where we are choosing τ s.t.

$$\frac{\beta}{2\tau} = 2M, \quad \text{for some } M \in \mathbb{N}. \tag{5.96}$$

Setting

$$v^\Lambda(t) = e^{-tH_0^\Lambda} v^\Lambda e^{tH_0^\Lambda} \tag{5.97}$$

and using the Dyson series expansion one gets

$$Qe^{-\frac{\beta}{2M}H_g^\Lambda}Q = A + B, \tag{5.98}$$

where the selfadjoint operators A and B are given by

$$
\begin{aligned}
A &= Qe^{-\frac{\beta}{2M}H_0^\Lambda}Q && (5.99)\\
B &= \sum_{n\geq 1}(-g)^n\int_{0\leq t_n\leq\ldots\leq t_1\leq\frac{\beta}{2M}} Qv^g(t_n)\cdots v^\Lambda(t_1)e^{-\frac{\beta}{2M}H_0^\Lambda}Q\ dt_1\cdots dt_n. && (5.100)
\end{aligned}
$$

Substituting (5.98) into (5.95), and using the Hölder inequality,

$$
\omega_{\beta,g}^\Lambda(Q)\leq\left[\frac{Tr\left(|A|^{2M}\right)}{Tre^{-\beta H_g^\Lambda}}\right]^{\frac{1}{2M}}+\left[\frac{Tr\left(|B|^{2M}\right)}{Tre^{-\beta H_g^\Lambda}}\right]^{\frac{1}{2M}}. \tag{5.101}
$$

Consider first the first term of (5.101). Let $\Delta=E_1-E_0>0$, the spectral gap of H^Σ. Then

$$
\begin{aligned}
\frac{Tr\left(|A|^{2M}\right)}{Tre^{-\beta H_0^\Lambda}} &= \frac{Tr_{\mathcal{H}^\Sigma}\left(Qe^{-\beta H^\Sigma}\right)}{Tr_{\mathcal{H}^\Sigma}e^{-\beta H^\Sigma}}=\frac{\sum_{j=1}^{d-1}e^{-\beta(E_j-E_0)}}{1+\sum_{j=1}^{d-1}e^{-\beta(E_j-E_0)}}\\
&\leq \sum_{j=1}^{d-1}e^{-\beta(E_j-E_0)}\leq 2\int_{E_1-E_0}^\infty e^{-\beta x}dx=2\frac{e^{-\beta\Delta}}{\beta}. && (5.102)
\end{aligned}
$$

Taking into account (5.94) and (5.96), we obtain, for $\beta\geq 1$,

$$
\left[\frac{Tr\left(|A|^{2M}\right)}{Tre^{-\beta H_g^\Lambda}}\right]^{\frac{1}{2M}}\leq 2e^{-2\tau\Delta}. \tag{5.103}
$$

To make the RHS small, take $\tau\gg\Delta^{-1}$

Consider now the second term on the RHS of (5.101). From (5.94),

$$
\frac{Tr\left(|B|^{2M}\right)}{Tre^{-\beta H_g^\Lambda}}\leq\omega_{\beta,0}^\Lambda\left(e^{\beta H_0^\Lambda}|B|^{2M}\right)=\omega_{\beta,0}^\Lambda\left(e^{\beta H_0^\Lambda}B^{2M}\right). \tag{5.104}
$$

Expanding,

$$
e^{\beta H_0^\Lambda}B^{2M}=\sum_{k_1,\ldots,k_{2M}\geq 1}T(k_1,\ldots,k_{2M}), \tag{5.105}
$$

where

$$
\begin{aligned}
T(k_1,\ldots,k_{2M}) &= (-\lambda)^{k_1+\cdots+k_{2M}}\int_0^{\frac{\beta}{2M}}dt_1^{(1)}\cdots\int_0^{t_{k_1-1}^{(1)}}dt_{k_1}^{(1)}\\
&\times\int_{\frac{\beta}{2M}}^{2\frac{\beta}{2M}}dt_1^{(2)}\cdots\int_{\frac{\beta}{2M}}^{t_{k_2-1}^{(2)}}dt_{k_2}^{(2)}\ \cdots\ \int_{(2M-1)\frac{\beta}{2M}}^{\beta}dt_1^{(2M)}\cdots\int_{(2M-1)\frac{\beta}{2M}}^{t_{k_{2M}-1}^{(2M)}}dt_{k_{2M}}^{(2M)}\\
&\times e^{\beta H_0^\Lambda}Qv^\Lambda(t_{k_1}^{(1)})\cdots v^\Lambda(t_1^{(1)})Q\ Qv^\Lambda(t_{k_2}^{(2)})\cdots v^\Lambda(t_1^{(2)})Q\times\cdots\\
&\cdots\times Qv^\Lambda(t_{k_{2M}}^{(2M)})\cdots v^\Lambda(t_1^{(2M)})Qe^{-\beta H_0^\Lambda}. && (5.106)
\end{aligned}
$$

The time variables in the integrand are ordered,

$$0 \le t_{k_1}^{(1)} \le \cdots \le t_1^{(1)} \le t_{k_2}^{(2)} \le \cdots \le t_1^{(2M)} \le \beta. \tag{5.107}$$

We want to estimate an upper bound on $|\omega_{\beta,0}^{\Lambda}(T(k_1,\ldots,k_{2M}))|$, sharp enough so that

$$\sum_{k_1,\ldots,k_{2M}\ge 1} \left|\omega_{\beta,0}^{\Lambda}(T(k_1,\ldots,k_{2M}))\right| \tag{5.108}$$

converges, and to estimate the value of the series. The expectation value of the integrand in the state $\omega_{\beta,0}^{\Lambda} = \omega_{\beta}^{\Sigma} \otimes \omega_{\beta}^{f,\Lambda}$ (see (5.90)) splits into a sum over products

$$\begin{aligned} \sum_{\alpha_1^{(1)},\ldots,\alpha_{k_1}^{(1)}} \cdots \sum_{\alpha_1^{(2M)},\ldots,\alpha_{k_{2M}}^{(2M)}} & \omega_{\beta}^{\Sigma}\left(QG_{\alpha_{k_1}^{(1)}}(t_{k_1}^{(1)})\cdots G_{\alpha_1^{(2M)}}(t_1^{(2M)})Q\right) \\ & \times \omega_{\beta}^{f,\Lambda}\left(\varphi_{\alpha_{k_1}^{(1)}}^{\Lambda}(t_{k_1}^{(1)})\cdots\varphi_{\alpha_1^{(2M)}}^{\Lambda}(t_1^{(2M)})\right), \qquad , \end{aligned} \tag{5.109}$$

where

$$\begin{aligned} G_\alpha(t) &= e^{-tH^{\Sigma}} G_\alpha e^{tH^{\Sigma}} && (5.110) \\ \varphi_\alpha^{\Lambda}(t) &= e^{-tH_f^{\Lambda}} \varphi(g_\alpha^{\Lambda}) e^{tH_f^{\Lambda}} = a^*\left(e^{-th_f^{\Lambda}} g_\alpha^{\Lambda}\right) + a\left(e^{th_f^{\Lambda}} g_\alpha^{\Lambda}\right). && (5.111) \end{aligned}$$

Using the Hölder inequality (5.91),

$$\left|\omega_{\beta}^{\Sigma}\left(QG_{\alpha_{k_1}^{(1)}}(t_{k_1}^{(1)})\cdots G_{\alpha_1^{(2M)}}(t_1^{(2M)})Q\right)\right| \le \prod_{j=1}^{2M} \|G_{\alpha_1^{(j)}}\|\cdots\|G_{\alpha_{k_j}^{(j)}}\|. \tag{5.112}$$

Since $\omega_{\beta}^{f,\Lambda}$ is a quasi-free state we can estimate the second factor in (5.109) with the help of Wick's theorem:

$$\omega_{\beta}^{f,\Lambda}\left(\varphi_{\alpha_1}^{\Lambda}(t_1)\cdots\varphi_{\alpha_{2N}}^{\Lambda}(t_{2N})\right) = \sum_{\mathcal{P}} \prod_{(l,r)\in\mathcal{P}} \omega_{\beta}^{f,\Lambda}\left(\varphi_{\alpha_l}^{\Lambda}(t_l)\varphi_{\alpha_r}^{\Lambda}(t_r)\right), \tag{5.113}$$

where the sum extends over all *contraction schemes*, i.e., decompositions of $\{1,\ldots,2N\}$ into N disjoint, ordered pairs (l,r), $l<r$. Applying the latter equation to

$$\omega_{\beta}^{f,\Lambda}\left(\varphi_{\alpha_{k_1}^{(1)}}^{\Lambda}(t_{k_1}^{(1)})\cdots\varphi_{\alpha_1^{(2M)}}^{\Lambda}(t_1^{(2M)})\right) \tag{5.114}$$

one finds that all resulting terms can be organized in *graphs* $\mathcal{G}$, constructed in the following way. (This can be done by partition the circle of circumference β into $2M$ segments parametrized by the arc length $\Delta_j = [(j-1)\frac{\beta}{2M}, j\frac{\beta}{2M}]$, $j = 1,\ldots,2M$. Putting k_j "dots" into the interval Δ_j, each dot representing a time variable $t_\cdot^{(j)} \in \Delta_j$

(increasing times are ordered according to increasing arc length). Pick any arbitrary dot in any interval and pair it with an arbitrary different dot in any interval. Then pick any unpaired dot (i.e., one not yet paired up) and pair it with any other unpaired dot. Continue this procedure until all dots in all intervals are paired. The graph $\mathcal{G}$ associated to such a pairing consists of all pairs – including multiplicity – of intervals (Δ, Δ') with the property that some dot in Δ is paired with some dot in Δ'. "Including multiplicity" means that if, say, three dots of Δ are paired with three dots in Δ', we understand that $\mathcal{G}$ contains the pair (Δ, Δ') three times.) Denote the class of all pairings $\mathcal{P}$ leading to a given graph $\mathcal{G}$ is by $C_{\mathcal{G}}$, and let

$$A_{\mathcal{P}} = \prod_{(l,r)\in\mathcal{P}} \omega_\beta^{f,\Lambda}\left(\varphi^\Lambda_{\alpha_l}(t_l)\varphi^\Lambda_{\alpha_r}(t_r)\right) \tag{5.115}$$

denote the contribution to (5.113) corresponding to the pairing $\mathcal{P}$. The value $|\mathcal{G}|$ corresponding to a graph $\mathcal{G}$ is given by

$$|\mathcal{G}| = \left|\sum_{\mathcal{P}\in C_{\mathcal{G}}} A_{\mathcal{P}}\right|. \tag{5.116}$$

It follows from (5.113), (5.115) and (5.116) that

$$\left|\omega^\Lambda_{\beta,f}\left(\varphi^\Lambda_{\alpha^{(1)}_{k_1}}(t^{(1)}_{k_1})\cdots\varphi^\Lambda_{\alpha^{(2M)}_1}(t^{(2M)}_1)\right)\right| \le \sum_{\mathcal{G}} |\mathcal{G}|. \tag{5.117}$$

In order to give an upper bound on the RHS of (5.117), one needs to estimate the imaginary-time propagators (two-point functions)

$$\begin{aligned}
&\omega_\beta^{f,\Lambda}\left(e^{-t_l H_f^\Lambda}\varphi(g^\Lambda_{\alpha_l})e^{t_l H_f^\Lambda}e^{-t_r H_f^\Lambda}\varphi(g^\Lambda_{\alpha_r})e^{t_r H_f^\Lambda}\right)\\
&= \left\langle g^\Lambda_{\alpha_r}, e^{-(\beta+t_l-t_r)h_f^\Lambda}\frac{e^{\beta h_f^\Lambda}}{e^{\beta h_f^\Lambda}-1}g^\Lambda_{\alpha_l}\right\rangle + \left\langle g^\Lambda_{\alpha_l}, e^{-(t_r-t_l)h_f^\Lambda}\frac{e^{\beta h_f^\Lambda}}{e^{\beta h_f^\Lambda}-1}g^\Lambda_{\alpha_r}\right\rangle
\end{aligned} \tag{5.118}$$

where the $g^\Lambda_{\alpha_{l,r}} \in l^2(\mathbb{Z}^3)$ are given in (5.86), and where $t_l \in \Delta_l$, $t_r \in \Delta_r$ s.t. $0 \le t_l \le t_r \le \beta$. Hence, the RHS of (5.118) is

$$\begin{aligned}
&\left(\frac{2\pi}{L}\right)^3 \sum_{n\neq(0,0,0)} \Big[\overline{g_{\alpha_r}(2\pi n/L)}g_{\alpha_l}(2\pi n/L)e^{-(\beta+t_l-t_r)E^\Lambda_n}\\
&\qquad + \overline{g_{\alpha_l}(2\pi n/L)}g_{\alpha_r}(2\pi n/L)e^{-(t_r-t_l)E^\Lambda_n}\Big] \times \frac{e^{\beta E^\Lambda_n}}{e^{\beta E^\Lambda_n}-1}\\
&+ \left(\frac{2\pi}{L}\right)^3\left[e^{-(\beta+t_l-t_r)} + e^{-(t_r-t_l)}\right]\frac{e^\beta}{e^\beta-1}.
\end{aligned} \tag{5.119}$$

In the thermodynamic limit $L \to \infty$, the sum in (5.119) converges to

$$\int_{\mathbf{R}^3} d^3k \, \left[\overline{g_{\alpha_r}(k)} g_{\alpha_l}(k) e^{-(\beta+t_l-t_r)k^2} + \overline{g_{\alpha_l}(k)} g_{\alpha_r}(k) e^{-(t_r-t_l)k^2}\right] \frac{e^{\beta k^2}}{e^{\beta k^2}-1}. \tag{5.120}$$

For arbitrary Δ_l, Δ_r and $t_l \in \Delta_l$, $t_r \in \Delta_r$,

$$|t_l - t_r| \geq d_-(\Delta_l, \Delta_r) := \frac{\beta}{2M} \begin{cases} 0, & \text{if } l = r \\ |l-r|-1, & \text{if } l \neq r \end{cases} \tag{5.121}$$

and

$$\beta - |t_l - t_r| \geq d_+(\Delta_l, \Delta_r) := \beta - \frac{\beta}{2M} \left(|l-r|+1\right). \tag{5.122}$$

Define

$$d(\Delta, \Delta') := \min(d_-(\Delta, \Delta'), d_+(\Delta, \Delta')). \tag{5.123}$$

It follows from (5.118) and (5.120), and for L large enough,

$$\begin{aligned} &\left|\omega_\beta^{f,\Lambda}\left(e^{-t_l H_f^\Lambda} \varphi(g_{\alpha_l}^\Lambda) e^{t_l H_f^\Lambda} e^{-t_r H_f^\Lambda} \varphi(g_{\alpha_r}^\Lambda) e^{t_r H_f^\Lambda}\right)\right| \\ &\qquad \leq 2 \left\langle g_{\alpha_l}^\Lambda, \frac{e^{-d(\Delta_l,\Delta_r)k^2}}{1-e^{-\beta k^2}} g_{\alpha_l}^\Lambda \right\rangle^{1/2} \left\langle g_{\alpha_r}^\Lambda, \frac{e^{-d(\Delta_l,\Delta_r)k^2}}{1-e^{-\beta k^2}} g_{\alpha_r}^\Lambda \right\rangle^{1/2}. \end{aligned} \tag{5.124}$$

Given any two intervals Δ, Δ', let

$$C(\Delta, \Delta') := 4 \max_\alpha \left\langle g_\alpha, \frac{e^{-d(\Delta,\Delta')k^2}}{1-e^{-\beta k^2}} g_\alpha \right\rangle. \tag{5.125}$$

For $L \geq C$, where C is some constant, (5.125) is a volume-independent upper bound on the (finite-volume) two-point functions arising from contractions in the graph expansion. We are now ready to give an upper bound on the RHS of (5.117). Start the procedure of pairing dots in the interval with the highest order k. Let π be a permutation of $2M$ objects, such that

$$k_{\pi(1)} \geq k_{\pi(2)} \geq \cdots \geq k_{\pi(2M)}. \tag{5.126}$$

There are $k_{l_1^{(\pi(1))}}$ possibilities of pairing the dot $t_1^{(\pi(1))}$ with some dot in an interval $\Delta_{l_1^{(\pi(1))}}$. We associate to each such pairing the value

$$k_{l_1^{(\pi(1))}} \, C(\Delta_{\pi(1)}, \Delta_{l_1^{(\pi(1))}}) \leq \sqrt{k_{\pi(1)}} \, \sqrt{k_{l_1^{(\pi(1))}}} \, C(\Delta_{\pi(1)}, \Delta_{l_1^{(\pi(1))}}), \tag{5.127}$$

where we use (5.126). Next, we pair the dot labelled by $t_2^{(\pi(1))}$ with a dot in $\Delta_{l_2^{(\pi(1))}}$ and associate to this pairing the value

$$\sqrt{k_{\pi(1)}} \, \sqrt{k_{l_2^{(\pi(1))}}} \, C(\Delta_{\pi(1)}, \Delta_{l_2^{(\pi(1))}}). \tag{5.128}$$

We continue this procedure until all dots are paired. This gives

$$\sum_{\mathcal{G}} |\mathcal{G}| \le \prod_{j=1}^{2M} (k_j)^{k_j/2} \sum_{\mathcal{G}} \prod_{(\Delta,\Delta')\in\mathcal{G}} C(\Delta,\Delta'). \tag{5.129}$$

Using that

$$|g_\alpha(k)| \le C|k|^{2p}, \tag{5.130}$$

for some constant C, and for all α, provided $|k|$ is small enough and $p > -1/4$, it follows that

$$C(\Delta,\Delta') \le C \begin{cases} d(\Delta,\Delta')^{-\frac{3}{2}-2p}, & d(\Delta,\Delta') \neq 0 \\ 1/\beta + 1, & d(\Delta,\Delta') = 0 \end{cases} \tag{5.131}$$

Moreover, using (5.123) and (5.144),

$$\sum_{\Delta'} C(\Delta,\Delta') \le \Gamma := C\left(1 + \frac{1}{\beta} + \frac{1}{p+1/4}\left(\frac{\beta}{2M}\right)^{-2p-1/2}\right) < \infty, \tag{5.132}$$

provided $p > -1/4$. Hence,

$$\sum_{\mathcal{G}} \prod_{(\Delta,\Delta')\in\mathcal{G}} C(\Delta,\Delta') \le \Gamma^{k_1+\cdots+k_{2M}}. \tag{5.133}$$

Now carry out the integral over the simplex in (5.106), and using (5.109), (5.112), (5.117), (5.129), (5.133),

$$\left|\omega^\Lambda_{\beta,0}(T(k_1,\ldots,k_{2M}))\right| \le \left(C'|g|\Gamma\frac{\beta}{2M}\right)^{k_1+\cdots+k_{2M}} \prod_{j=1}^{2M} \frac{(k_j)^{k_j/2}}{k_j!}, \tag{5.134}$$

where $C' = \sum_\alpha \|G_\alpha\|$, and where the factor $(\frac{\beta}{2M})^{k_j}\frac{1}{k_j!}$ is the volume of the simplex $\{t \le t_{k_j} \le \cdots \le t_1 \le t + \frac{\beta}{2M}\}$. Therefore, (5.108) converges for all values of g and $\beta > 0$, and

$$\left[\omega^\Lambda_{\beta,0}\left(e^{\beta H_0^\Lambda} B^{2M}\right)\right]^{\frac{1}{2M}} \le C'|g|\Gamma\frac{\beta}{2M}\sum_{k\ge 0}\left(C'|g|\Gamma\frac{\beta}{2M}\right)^k \frac{(k+1)^{\frac{k+1}{2}}}{(k+1)!}. \tag{5.135}$$

From (5.101), (5.103), (5.104), (5.139), (5.96), one obtauns, for L is large enough

$$\omega^\Lambda_{\beta,g}(Q) \le 2e^{-2\tau\Delta} + C'|g|\Gamma\tau\sum_{k\ge 0}(C'|g|\Gamma\tau)^k \frac{(k+1)^{\frac{k+1}{2}}}{(k+1)!}. \tag{5.136}$$

Choose $\beta_2(\epsilon) > 1$ such that $e^{-\beta_2(\epsilon)\Delta} < \epsilon/2$, and for $\beta \ge \beta_2(\epsilon)$, choose $\tau = \beta_2(\epsilon)/2 \le \beta/2$. From the definition of Γ, (5.142), and the relation $\frac{\beta}{2M} = 2\tau$, see (5.96), one obtains $\Gamma\tau \le C(\epsilon)$, uniformly in $\beta \ge \beta_2(\epsilon)$. Therefore $\exists g_1(\epsilon) > 0$ such that if $|g| < g_1(\epsilon)$ then the second term on the RHS of (5.140) $\le \epsilon/2$. This proves our claim (5.79).□

5.3.3 The Virial Theorem

In this section, we state two Virial theorems proven in [FM2,FMS]. Since the Theorems are applied *without* any alteration or extension, we just sketch the main steps of their proof.

We start by discussing the *Glimm-Jaffe-Nelson* condition. Consider a Hilbert space $\mathcal{H}$, a selfadjoint operator $Y \geq \mathbf{1}$ with core $\mathcal{D} \subset \mathcal{D}$, and X a symmetric operator on $\mathcal{D}$. The triple $(X, Y, \mathcal{D})$ satisfies the *GJN (Glimm-Jaffe-Nelson) Condition*, or $(X, Y, \mathcal{D})$ is a *GJN-triple*, if there is a constant $k < \infty$, such that, for all $\psi \in \mathcal{D}$:

$$\begin{aligned} \|X\psi\| &\leq k\|Y\psi\| && (5.137)\\ \pm i\left\{\langle X\psi, Y\psi\rangle - \langle Y\psi, X\psi\rangle\right\} &\leq k\left\langle \psi, Y\psi\right\rangle. && (5.138)\end{aligned}$$

Since $Y \geq \mathbf{1}$, inequality (5.137) is equivalent to

$$\|X\psi\| \leq k_1\|Y\psi\| + k_2\|\psi\|,$$

for some $k_1, k_2 < \infty$.

Theorem A3.1 (GJN commutator theorem)

If $(X, Y, \mathcal{D})$ satisfies the GJN Condition, then X determines a selfadjoint operator (again denoted by X), such that $\mathcal{D}(X) \supset \mathcal{D}(Y)$. Moreover, X is essentially selfadjoint on any core for Y, and (5.137) is valid for all $\psi \in \mathcal{D}(Y)$.

Suppose one is given a selfadjoint operator $\Lambda \geq \mathbf{1}$ with core $\mathcal{D} \subset \mathcal{H}$, and operators L, A, N, D, C_n, $n = 0, 1, 2, 3$, all symmetric on $\mathcal{D}$, and satisfying

$$\begin{aligned} \langle\varphi, D\psi\rangle &= i\left\{\langle L\varphi, N\psi\rangle - \langle N\varphi, L\psi\rangle\right\} && (5.139)\\ C_0 &= L \\ \langle\varphi, C_n\psi\rangle &= i\left\{\langle C_{n-1}\varphi, A\psi\rangle - \langle A\varphi, C_{n-1}\psi\rangle\right\}, \quad n = 1, 2, 3, && (5.140)\end{aligned}$$

where $\varphi, \psi \in \mathcal{D}$. Assume that

- $(X, \Lambda, \mathcal{D})$ satisfies the GJN Condition, for $X = L, N, D, C_n$. Consequently, all these operators determine selfadjoint operators, which we denote by the same letters.
- A is selfadjoint, $\mathcal{D} \subset \mathcal{D}(A)$, and e^{itA} leaves $\mathcal{D}(\Lambda)$ invariant.

Remark. From the invariance condition $e^{itA}\mathcal{D}(\Lambda) \subset \mathcal{D}(\Lambda)$, it follows that for some $0 \leq k, k' < \infty$, and all $\psi \in \mathcal{D}(\Lambda)$,

$$\|\Lambda e^{itA}\psi\| \leq k e^{k'|t|}\|\Lambda\psi\|. \quad (5.141)$$

(A proof can be found in [ABG], Propositions 3.2.2 and 3.2.5.)

Theorem A3.2 (First Virial Theorem)

Assume that, in addition to (5.139), (5.140), we have, in the sense of Kato on $\mathcal{D}$,

$$\begin{aligned} D &\leq kN^{1/2}, && (5.142)\\ e^{itA}C_1e^{-itA} &\leq ke^{k'|t|}N^p, \quad \text{some } 0 \leq p < \infty, && (5.143)\\ e^{itA}C_3e^{-itA} &\leq ke^{k'|t|}N^{1/2}, && (5.144) \end{aligned}$$

for some $0 \leq k, k' < \infty$, and all $t \in \mathbf{R}$. Let ψ be an eigenvector of L. Then there is a one-parameter family $\{\psi_\alpha\} \subset \mathcal{D}(L) \cap \mathcal{D}(C_1)$, s.t. $\psi_\alpha \to \psi$, $\alpha \to 0$, and

$$\lim_{\alpha \to 0} \langle \psi_\alpha, C_1\psi_\alpha \rangle = 0. \tag{5.145}$$

Remark. Formally, C_1 is the commutator $i[L, A] = i(LA - AL)$, and (5.145) as $\langle \psi, i[L, A]\psi \rangle = 0$, which is a standard way of stating the virial theorem, see also [ABG], and [GG].

The result of Theorem A3.2 is still valid if we add to the operator A a suitably small perturbation A_0:

Theorem A3.3 (Second Virial Theorem)

Suppose that we are in the situation of Theorem A3.2 and that A_0 is a bounded operator on $\mathcal{H}$ such that $RanA_0 \subset \mathcal{D}(L) \cap RanP(N \leq n_0)$, for some $n_0 < \infty$. Then $i[L, A_0] = i(LA_0 - A_0L)$ is well defined in the strong sense on $\mathcal{D}(L)$, and we have, for the same family of approximating eigenvectors as in Theorem A3.2

$$\lim_{\alpha \to 0} \langle \psi_\alpha, (C_1 + i[L, A_0])\psi_\alpha \rangle = 0. \tag{5.146}$$

Theorem A3.4 (Regularity of eigenfunctions)

Suppose C is a symmetric operator on a domain $\mathcal{D}(C)$ such that, in the sense of quadratic forms on $\mathcal{D}(C)$, we have that $C \geq \mathcal{P} - B$, where $\mathcal{P} \geq 0$ is a selfadjoint operator, and B is a bounded (everywhere defined) operator. Let ψ_α be a family of vectors in $\mathcal{D}(C)$, with $\psi_\alpha \to \psi$, as $\alpha \to 0$, and s.t.

$$\lim_{\alpha \to 0} \langle \psi_\alpha, C\psi_\alpha \rangle = 0. \tag{5.147}$$

Then $\langle \psi, B\psi \rangle \geq 0$, $\psi \in \mathcal{D}(\mathcal{P}^{1/2})$, and

$$\|\mathcal{P}^{1/2}\psi\| \leq \langle \psi, B\psi \rangle^{1/2}. \tag{5.148}$$

Concrete setting of Virial Theorem

The Hilbert space is the GNS representation $\mathcal{H} = \mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma \otimes \mathcal{F}_+(L^2(\mathbf{R} \times S^2))$. Let

$$\mathcal{D} = C_0^\infty \otimes C_0^\infty \otimes \mathcal{D}_f, \tag{5.149}$$

where

$$\mathcal{D}_f = \mathcal{F}\left(C_0^\infty(\mathbf{R} \times S^2)\right) \cap \mathcal{F}_0,$$

and $\mathcal{F}_0$ denotes the finite-particle subspace of Fock space. The operator Λ is given by

$$\begin{aligned}
\Lambda &= \Lambda^\Sigma \otimes \mathbf{1}^\Sigma + \mathbf{1}^\Sigma \otimes \Lambda^\Sigma + \Lambda^f, && (5.150)\\
\Lambda^\Sigma &= H^\Sigma P_+(H^\Sigma) + \mathbf{1}^\Sigma, && (5.151)\\
\Lambda^f &= \mathrm{d}\Gamma(u^2+1) + \mathbf{1}^f, && (5.152)
\end{aligned}$$

$P_+(H^\Sigma)$ is the projection onto the spectral interval $\mathbf{R}_+$ of H^Σ. Λ is essentially selfadjoint on $\mathcal{D}$, and $\Lambda \geq \mathbf{1}$. The operator L is the interacting Liouvillian $\mathcal{L}_g$, and

$$N = \mathrm{d}\Gamma(1) \tag{5.153}$$

is the particle number operator in $\mathcal{F}_+ \equiv \mathcal{F}_+(L^2(\mathbf{R} \times S^2))$. $X = L, N$ are symmetric operators on $\mathcal{D}$, and the symmetric operator D on $\mathcal{D}$ is given by

$$\begin{aligned}
D = \frac{ig}{\sqrt{2}} \sum_\alpha & \left\{ G_\alpha \otimes \mathbf{1}^\Sigma \otimes (-a^*(\tau_\beta(g_\alpha)) + a(\tau_\beta(g_\alpha))) \right.\\
& \left. - \mathbf{1}^\Sigma \otimes C^\Sigma G_\alpha C^\Sigma \otimes \left(-a^*(e^{-\beta u/2}\tau_\beta(g_\alpha)) + a(e^{-\beta u/2}\tau_\beta(g_\alpha))\right) \right\}. \qquad (5.154)
\end{aligned}$$

The operator A is identified by $A^f =$ and A_0 is given by $i\theta g(\Pi I \overline{R}_\epsilon^2 - \overline{R}_\epsilon^2 I \Pi)$, as before.

Some functional analysis

In this section, we collect some results which are useful in the previous analysis, particularly the first two theorems, whose proof can be found in [Frö].

Theorem A3.5 (Invariance of domain, [Frö])

Suppose $(X, Y, \mathcal{D})$ satisfies the GJN Condition, (5.137), (5.138). Then the unitary group, e^{itX}, generated by the selfadjoint operator X leaves $\mathcal{D}(Y)$ invariant, and

$$\|Ye^{itX}\psi\| \leq e^{k|t|}\|Y\psi\|, \tag{5.155}$$

for some $k \geq 0$, and all $\psi \in \mathcal{D}(Y)$.

Theorem A3.6 (Commutator expansion, [Frö])

Suppose $\mathcal{D}$ is a core for the selfadjoint operator $Y \geq \mathbf{1}$. Let $X, Z, \mathrm{ad}_X^{(n)}(Z)$ be symmetric operators on $\mathcal{D}$, where

$$\begin{aligned}\mathrm{ad}_X^{(0)}(Z) &= Z, \\ \left\langle \psi, \mathrm{ad}_X^{(n)}(Z)\psi \right\rangle &= i\left\{ \left\langle \mathrm{ad}_X^{(n-1)}(Z)\psi, X\psi \right\rangle - \left\langle X\psi, \mathrm{ad}_X^{(n-1)}(Z)\psi \right\rangle \right\},\end{aligned}$$

for all $\psi \in \mathcal{D}$, $n = 1, \ldots, M$. We suppose that the triples $(\mathrm{ad}_X^{(n)}(Z), Y, \mathcal{D})$, $n = 0, 1, \ldots, M$, satisfy the GJN Condition (5.137), (5.138), and that X is selfadjoint, with $\mathcal{D} \subset \mathcal{D}(X)$, e^{itX} leaves $\mathcal{D}(Y)$ invariant, and (5.155) holds. Then

$$\begin{aligned}e^{itX} Z e^{-itX} &= Z - \sum_{n=1}^{M-1} \frac{t^n}{n!} \mathrm{ad}_X^{(n)}(Z) \\ &\quad - \int_0^t dt_1 \cdots \int_0^{t_{M-1}} dt_M e^{it_M X} \mathrm{ad}_X^{(M)}(Z) e^{-it_M X}, \qquad (5.156)\end{aligned}$$

as operators on $\mathcal{D}(Y)$.

Two corollaries follows from (5.155).

Corollary A3.7

Suppose that the unitary group e^{itX} leaves $\mathcal{D}(Y)$ invariant, for some operator Y, and that estimate (5.155) holds. For a function χ on $\mathbf{R}$ with Fourier transform $\widehat{\chi} \in L^1(\mathbf{R})$, we define $\chi(X) = \int_{\mathbf{R}} \widehat{\chi}(s) e^{isX} ds$. If $\widehat{\chi}$ has compact support, then $\chi(X)$ leaves $\mathcal{D}(Y)$ invariant, and, for $\psi \in \mathcal{D}(Y)$,

$$\|Y\chi(X)\psi\| \leq e^{kR} \|\widehat{\chi}\|_{L^1(\mathbf{R})} \, \|Y\psi\|, \qquad (5.157)$$

for any R such that $\mathrm{supp}\widehat{\chi} \subset [-R, R]$.

Corollary A3.8

Suppose $(X, Y, \mathcal{D})$ satisfies the GJN Condition, and so do the triples $(\mathrm{ad}_X^{(n)}(Y), Y, \mathcal{D})$, for $n = 1, \ldots, M$, and for some $M \geq 1$. Moreover, assume that, in the sense of Kato on $\mathcal{D}(Y)$, $\pm \mathrm{ad}_X^{(M)}(Y) \leq kX$, for some $k \geq 0$. For $\chi \in C_0^\infty(\mathbf{R})$, a smooth function with compact support, define $\chi(X) = \int \widehat{\chi}(s) e^{isX}$, where $\widehat{\chi}$ is the Fourier transform of χ. Then $\chi(X)$ leaves $\mathcal{D}(Y)$ invariant.

Lemma A3.9

Let $\chi \in C_0^\infty(\mathbf{R})$, $\chi = F^2 \geq 0$. Suppose $(X, Y, \mathcal{D})$ satisfies the GJN condition. Suppose $F(X)$ leaves $\mathcal{D}(Y)$ invariant. Let Z be a symmetric operator on $\mathcal{D}$ such that, for some $M \geq 1$, and $n = 0, 1, \ldots, M$, the triples $(\mathrm{ad}_X^{(n)}(Z), Y, \mathcal{D})$ satisfy the GJN condition. Moreover, assume that the multiple commutators, for $n = 1, \ldots, M$, are relatively X^{2p}-bounded in the sense of Kato on $\mathcal{D}$, for some $p \geq 0$. In other words, there is some $k < \infty$, s.t. $\forall \psi \in \mathcal{D}$,

$$\|\mathrm{ad}_X^{(n)}(Z)\psi\| \leq k\left(\|\psi\| + \|X^{2p}\psi\|\right), \qquad n = 1, \ldots, M.$$

Then the commutator $[\chi(X), Z] = \chi(X)Z - Z\chi(X)$ is well defined on $\mathcal{D}$ and extends to a bounded operator.

Lemma A3.10

Suppose $(X, Y, \mathcal{D})$ is a GJN triple. Then the resolvent $(X - z)^{-1}$ leaves $\mathcal{D}(Y)$ invariant, for all $z \in \{\mathbf{C} : \ |Imz| > k\}$, for some $k > 0$.

Proof of the Virial Theorems and regularity of eigenfunctions

Let $g_1 \in C_0^\infty((-1,1))$ be a real valued function, such that $g_1(0) = 1$, and $g = g_1^2 \in C_0^\infty((-1,1))$, $g(0) = 1$. Choose a real valued function f on $\mathbf{R}$ with the properties that $f(0) = 1$ and $\widehat{f} \in C_0^\infty(\mathbf{R})$ (Fourier transform). Let

$$f_1(x) = \int_{-\infty}^{x} f^2(y)dy,$$

so that $f_1'(x) = f^2(x)$. Note that $\widehat{f_1}$ has compact support, and is smooth except at $s = 0$, where it behaves like s^{-1}; $\widehat{f_1^{(n)}} = (is)^n \widehat{f_1} \in C_0^\infty$, for $n \geq 1$. Let $\alpha, \nu > 0$ be two parameters and define

$$\begin{aligned} g_{1,\nu} &= g_1(\nu N) = \int_{\mathbf{R}} \widehat{g_1}(s) e^{is\nu N} ds, \\ g_\nu &= g_{1,\nu}^2 \\ f_\alpha &= f(\alpha A) = \int_{\mathbf{R}} \widehat{f}(s) e^{is\alpha A} ds, \end{aligned}$$

For $\eta > 0$, define

$$f_{1,\alpha}^\eta = \frac{1}{\alpha} \int_{\mathbf{R}\setminus(-\eta,\eta)} ds \widehat{f_1}(s) e^{is\alpha A} = (f_{1,\alpha}^\eta)^*.$$

$f_{1,\alpha}^\eta$ leaves $\mathcal{D}(\Lambda)$ invariant, and $\|f_{1,\alpha}^\eta\| \leq k/\alpha$, where k is a constant

Suppose ψ is an eigenfunction of L with eigenvalue e. $\psi = (L + i)^{-1}\varphi$, for some $\varphi \in \mathcal{H}$. Let $\{\varphi_n\} \subset \mathcal{D}(\Lambda)$ be a sequence of vectors converging to φ. Then

$$\psi_n := (L + i)^{-1}\varphi_n \to \psi, \quad n \to \infty, \tag{5.158}$$

and, $\psi_n \in \mathcal{D}(\Lambda)$. Assume that $k = 1$. We know that f_α leaves $\mathcal{D}(\Lambda)$ invariant, and g_ν leaves $\mathcal{D}(\Lambda)$ invariant (Λ commutes with N in the strong sense on $\mathcal{D}$). Hence, the regularized eigenfunction

$$\psi_{\alpha,\nu,n} = f_\alpha g_\nu \psi_n$$

satisfies $\psi_{\alpha,\nu,n} \in \mathcal{D}(\Lambda)$, $\psi_{\alpha,\nu,n} \to \psi$, as $\alpha, \nu \to 0$, $n \to \infty$.

We claim

$$\left|\left\langle if_{1,\alpha}^{\eta}(L-e)\right\rangle_{g_\nu \psi_n}\right| \leq k\frac{1}{\alpha}\left(\sqrt{\nu}+o(n)\right), \tag{5.159}$$

where k is some constant independent of η, α, ν, n. This follows from

$$\|(L-e)g_\nu \psi_n\| \leq k\left(\sqrt{\nu}+o(n)\right), \tag{5.160}$$

which is proven as follows.

$$\begin{aligned}
(L-e)g_\nu\psi_n &= g_\nu(L-e)\psi_n && (5.161)\\
&\quad + g_{1,\nu}[L, g_{1,\nu}]\psi_n && (5.162)\\
&\quad + [L, g_{1,\nu}]g_{1,\nu}\psi_n, && (5.163)
\end{aligned}$$

and the RHS of (5.161) is $o(n)$. Both (5.162) and (5.163) are bounded above by $k\sqrt{\nu}$, uniformly in n. The commutator expansion of Theorem gives

$$g_{1,\nu}[L, g_{1,\nu}] = \nu \int_{\mathbf{R}} ds\ \widehat{g_1}(s)e^{is\nu N}\int_0^s ds_1 e^{-is_1\nu N}g_{1,\nu}De^{is_1\nu N}, \tag{5.164}$$

as operators on $\mathcal{D}(\Lambda)$. We use that $g_{1,\nu}$ commutes with $e^{is\nu N}$. From (5.142), $\phi \in \mathcal{D}(\Lambda)$,

$$\begin{aligned}
\|g_{1,\nu}De^{is_1\nu N}\phi\| &= \sup_{\varphi\in\mathcal{D},\varphi\neq 0}\frac{\left|\left\langle\varphi, g_{1,\nu}De^{is_1\nu N}\phi\right\rangle\right|}{\|\varphi\|}\\
\leq \sup_{\varphi\in\mathcal{D},\varphi\neq 0}\frac{\|Dg_{1,\nu}\varphi\|\ \|\phi\|}{\|\varphi\|} &\leq k \sup_{\varphi\in\mathcal{D},\varphi\neq 0}\frac{\|N^{1/2}g_{1,\nu}\varphi\|}{\|\varphi\|}\ \|\phi\| \leq k\frac{1}{\sqrt{\nu}}\|\phi\|,
\end{aligned}$$

and hence,

$$\begin{aligned}
\|g_{1,\nu}[L, g_{1,\nu}]\phi\| &\leq \nu\int_{\mathbf{R}} ds|\widehat{g_1}(s)|\int_0^s ds_1\,\|g_{1,\nu}De^{is_1\nu N}\phi\|\\
&\leq k\sqrt{\nu}\int_{\mathbf{R}} ds\,|s\widehat{g_1}(s)|\ \|\phi\|. && (5.165)
\end{aligned}$$

Similarly for (5.163).This establishes (5.160).

Since $f_{1,\alpha}^{\eta}$ leaves $\mathcal{D}(\Lambda)$ invariant, $[f_{1,\alpha}^{\eta}, L]$ is defined (in the strong sense) on $\mathcal{D}(\Lambda)$, and the commutator theorem gives

$$\begin{aligned}
&[f_{1,\alpha}^{\eta}, L]\\
&= \int_{\mathbf{R}\setminus(-\eta,\eta)} ds\widehat{f_1}(s)e^{is\alpha A}\left(sC_1+\alpha\frac{s^2}{2}C_2\right)\\
&\quad +\alpha^2\int_{\mathbf{R}\setminus(-\eta,\eta)} ds\widehat{f_1}(s)e^{is\alpha A}\int_0^s ds_1\int_0^{s_1} ds_2\int_0^{s_2} ds_3\ e^{-is_3\alpha A}C_3e^{is_3\alpha A}.
\end{aligned} \tag{5.166}$$

For $n \geq 1$,

$$f_1^{(n)}(\alpha A) = \int_{\mathbf{R}} ds (is)^n \widehat{f}_1(s) e^{is\alpha A} = \int_{\mathbf{R}\setminus(-\eta,\eta)} ds (is)^n \widehat{f}_1(s) e^{is\alpha A} - \mathcal{R}_{\eta,n},$$

where

$$\mathcal{R}_{\eta,n} = -\int_{-\eta}^{\eta} ds\ (is)^n \widehat{f}_1(s) e^{is\alpha A}$$

satisfies $\mathcal{R}_{\eta,n} = (\mathcal{R}_{\eta,n})^*$, and $\|\mathcal{R}_{\eta,n}\| \leq k_n \eta$, with a constant k_n that does not depend on α, η. From (5.166)

$$\begin{aligned}
[f_{1,\alpha}^{\eta}, L] &= -i\left(f_1'(\alpha A) + \mathcal{R}_{\eta,1}\right) C_1 - \frac{\alpha}{2}\left(f_1''(\alpha A) + \mathcal{R}_{\eta,2}\right) C_2 \\
&\quad +\alpha^2 \int_{\mathbf{R}\setminus(-\eta,\eta)} ds \widehat{f}_1(s) e^{is\alpha A} \int_0^s ds_1 \int_0^{s_1} ds_2 \int_0^{s_2} ds_3\ e^{-is_3\alpha A} C_3 e^{is_3\alpha A}.
\end{aligned} \tag{5.167}$$

Moreover,

$$\begin{aligned}
-if_\alpha^2 C_1 &= -if_\alpha C_1 f_\alpha \\
&\quad -if_\alpha \int_{\mathbf{R}} ds \widehat{f}(s) e^{is\alpha A} \left(\alpha s C_2 + \alpha^2 \int_0^s ds_1 \int_0^{s_1} ds_2 e^{-is_2\alpha A} C_3 e^{is_2\alpha A}\right) \\
&= -if_\alpha C_1 f_\alpha - \alpha f_\alpha f_\alpha' C_2 \\
&\quad -i\alpha^2 f_\alpha \int_{\mathbf{R}} ds \widehat{f}(s) e^{is\alpha A} \int_0^s ds_1 \int_0^{s_1} ds_2 e^{-is_2\alpha A} C_3 e^{is_2\alpha A},
\end{aligned} \tag{5.168}$$

where $f_\alpha' = f'(\alpha A)$. Since $f_\alpha f_\alpha' = \frac{1}{2}(f^2)'(\alpha A) = \frac{1}{2} f_1''(\alpha A)$, one has from (5.167), (5.168):

$$\begin{aligned}
[f_{1,\alpha}^{\eta}, L] &= -if_\alpha C_1 f_\alpha - \alpha f_1''(\alpha A) C_2 - i\mathcal{R}_{\eta,1} C_1 - \frac{\alpha}{2} \mathcal{R}_{\eta,2} C_2 \\
&\quad +\alpha^2 \int_{\mathbf{R}\setminus(-\eta,\eta)} ds \widehat{f}_1(s) e^{is\alpha A} \int_0^s ds_1 \int_0^{s_1} ds_2 \int_0^{s_2} ds_3\ e^{-is_3\alpha A} C_3 e^{is_3\alpha A} \\
&\quad -i\alpha^2 f_\alpha \int_{\mathbf{R}} ds \widehat{f}(s) e^{is\alpha A} \int_0^s ds_1 \int_0^{s_1} ds_2 e^{-is_2\alpha A} C_3 e^{is_2\alpha A}.
\end{aligned} \tag{5.169}$$

Using (5.144), one obtains

$$\begin{aligned}
\left\langle i[f_{1,\alpha}^{\eta}, L]\right\rangle_{g_\nu\psi_n} &= \langle C_1\rangle_{\psi_{\alpha,\nu,n}} - Re\, i\alpha \left\langle f''(\alpha A) C_2\right\rangle_{g_\nu\psi_n} + Re \left\langle \mathcal{R}_{\eta,1} C_1\right\rangle_{g_\nu\psi_n} \\
&\quad -Re\ i\frac{\alpha}{2} \left\langle \mathcal{R}_{\eta,2} C_2\right\rangle_{g_\nu\psi_n} + \mathcal{O}\frac{\alpha^2}{\sqrt{\nu}}.
\end{aligned} \tag{5.170}$$

Note that

$$\begin{aligned}
&-Re \left\langle i\alpha f''(\alpha A) C_2\right\rangle_{g_\nu\psi_n} = -\frac{\alpha}{2} \left\langle i[f''(\alpha A), C_2]\right\rangle_{g_\nu\psi_n} \\
&= -\frac{\alpha^2}{2} \left\langle \int_{\mathbf{R}} ds\ \widehat{f''}(s) e^{is\alpha A} \int_0^s ds_1\ e^{-is_1\alpha A} C_3 e^{is_1\alpha A} \right\rangle_{g_\nu\psi_n} = \mathcal{O}\frac{\alpha^2}{\sqrt{\nu}},
\end{aligned}$$

where (5.144) has been used again. Similarly,

$$Re\ i\frac{\alpha}{2}\left\langle \mathcal{R}_{\eta,2}C_2\right\rangle_{g_\nu\psi_n} = -i\frac{\alpha}{4}\left\langle [\mathcal{R}_{\eta,2},C_2]\right\rangle_{g_\nu\psi_n} = \mathcal{O}\frac{\alpha^2\eta}{\sqrt{\nu}},$$

and

$$\left\langle \mathcal{R}_{\eta,1}C_1\right\rangle_{g_\nu\psi_n} = \mathcal{O}\frac{\eta}{\nu^p}.$$

(5.170) and (5.159) imply

$$\left|\langle C_1\rangle_{\psi_{\alpha,\nu,n}}\right| \le k\left(\frac{\sqrt{\nu}+o(n)}{\alpha}+\frac{\alpha^2}{\sqrt{\nu}}+\frac{\eta}{\nu^p}\right). \tag{5.171}$$

By taking the limit $n\to\infty$ in (5.171)

$$\left|\langle C_1\rangle_{\psi_{\alpha,\nu}}\right| \le k\left(\frac{\sqrt{\nu}}{\alpha}+\frac{\alpha^2}{\sqrt{\nu}}+\frac{\eta}{\nu^p}\right).$$

For example, choose $\nu=\alpha^3$, $\eta=\alpha^{3p+\delta}$, for any $\delta>0$, then

$$\lim_{\alpha\to 0}\langle C_1\rangle_{\psi_{\alpha,\alpha^3}} = 0.$$

This proves Theorem A3.2. To show Theorem A3.3, it is sufficient to

$$\lim_{\alpha\to 0}\langle \psi_\alpha, i[L,A_0]\psi_\alpha\rangle = 0,$$

where $\psi_\alpha = \psi_{\alpha,\nu}|_{\nu=\alpha^3}$. Moreover,

$$\begin{aligned}|\langle \psi_\alpha, i[L,A_0]\psi_\alpha\rangle| &\le 2\left|\langle (L-e)\psi_\alpha, A_0\psi_\alpha\rangle\right| \\ &\le 2\|P(N\le n_0)(L-e)\psi_\alpha\|\ \|A_0\psi_\alpha\|.\end{aligned}$$

We have

$$P(N\le n_0)(L-e)\psi_{\alpha,\nu} = \lim_{n\to\infty}P(N\le n_0)[L,f_\alpha]g_\nu\psi_n \tag{5.172}$$

$$+\lim_{n\to\infty}P(N\le n_0)f_\alpha[L,g_\nu]\psi_n. \tag{5.173}$$

Note that $\|P(N\le n_0)[L,f_\alpha]g_\nu\psi_n\|\le k_{n_0}\alpha$ and $\|P(N\le n_0)f_\alpha[L,g_\nu]\psi_n\|\le k\sqrt{\nu}$. It follows that $\|P(N\le n_0)(L-e)\psi_\alpha\|\le k_{n_0}\alpha$.

We still need to prove the regularity of the eigenfunctions. Using the inequality $C\ge\mathcal{P}-B$, the continuity of B, and (5.147) one has, for any $\epsilon>0$, an $\alpha_0(\epsilon)$, such that if $\alpha<\alpha_0(\epsilon)$ then

$$\langle\psi_\alpha,\mathcal{P}\psi_\alpha\rangle \le \langle\psi, B\psi\rangle+\epsilon. \tag{5.174}$$

Denote by μ_ϕ be the spectral measure of $\mathcal{P}$ corresponding to some $\phi\in\mathcal{H}$. Then

$$\langle\psi_\alpha,\mathcal{P}\psi_\alpha\rangle = \int_{\mathbf{R}_+} p\,d\mu_{\psi_\alpha}(p) = \lim_{R\to\infty}\int_{\mathbf{R}_+} p\chi(p\le R)\,d\mu_{\psi_\alpha}(p),$$

where $\chi(p \le R)$ is the indicator of $[0, R]$. It follows from (5.174) that

$$\lim_{R\to\infty} \langle \psi_\alpha, \chi(\mathcal{P} \le R)\mathcal{P}\psi_\alpha\rangle = \lim_{R\to\infty} \left\|\chi(\mathcal{P} \le R)\mathcal{P}^{1/2}\psi_\alpha\right\|^2 \le \langle \psi, B\psi\rangle + \epsilon \equiv k.$$

One has $\left\|\chi(\mathcal{P} \le R)\mathcal{P}^{1/2}\psi\right\| \le R^{1/2}\|\psi - \psi_\alpha\| + \sqrt{k}$, and taking $\alpha \to 0$ yields $\|\chi(\mathcal{P} \le R)\mathcal{P}^{1/2}\psi\| \le \sqrt{k}$, uniformly in R, so $\lim_{R\to\infty} \int_0^R p d\mu_\psi(p)$ is finite (by the monotone convergence theorem). Since $\mathcal{D}(\mathcal{P}^{1/2}) = \left\{\psi \,\middle|\, \int_0^\infty p d\mu_\psi(p) < \infty\right\}$, one has $\psi \in \mathcal{D}(\mathcal{P}^{1/2})$, and $\|\mathcal{P}^{1/2}\psi\| \le \langle \psi, B\psi\rangle$. □

5.3.4 Some operator calculus

For the sake of completeness, we very briefly review operator calculus for functions of selfadjoint operators used in the previous sections. For a more detailed review, see for example [HS].

Let $f \in C_0^k(\mathbf{R})$, $k \ge 2$, and define the compactly supported complex measure

$$d\widetilde{f}(z) = -\frac{1}{2\pi}\left(\partial_x + i\partial_y\right)\widetilde{f}(z)dxdy,$$

where $z = x + iy$ and $\widetilde{f}$ is an almost analytic complex extension of f in the sense that

$$\left(\partial_x + i\partial_y\right)\widetilde{f}(z) = 0, \quad z \in \mathbb{R}.$$

Then, for a selfadjoint operator A,

$$f(A) = \int d\widetilde{f}(z)(A - z)^{-1},$$

which is absolutely convergent. Given f, one can construct explicitely an almost analytic extension $\widetilde{f}$ supported in a complex neighbourhood of the support of f, and for $p \le k - 2$,

$$\int \left|d\widetilde{f}(z)\right| |Imz|^{-p-1} \le C\sum_{j=0}^{k} \|f^{(j)}\|_{j-p-1}, \tag{5.175}$$

where $\|f\|_n = \int dx\langle x\rangle^n |f(x)|$, and $\langle x\rangle = (1 + x^2)^{1/2}$. Moreover, the derivatives of $f(A)$ are given by

$$f^{(p)}(A) = p! \int d\widetilde{f}(A)(A - z)^{-p-1}. \tag{5.176}$$

These results extend by a limiting argument to functions f that do not have compact support, as long as the norms in the RHS of (5.175) are finite.

Chapter 6

The C_n paradigm

The results of this chapter are an extension of the analysis in [JP1,2,3] to fermionic reservoirs and to models with *time-dependent* interaction (since we are interested in thermodynamic processes). The analysis presented here is important for later chapters, in particular, to prove an adiabatic theorem for NESS in chapter 8, section 2, and to apply the isothermal theorem to a concrete example in chapter 8, section 3. Moreover, the methods developed here are applied in chapter 9 to study the spectrum of the so called Floquet Liouvillean, which we use to prove convergence to time-periodic states in cyclic thermodynamic processes.

We first study the spectrum of the *standard* Liouvillean using complex deformations (translations) for Model C_n introduced in chapter 4, section 4: a two level system coupled to n free fermionic reservoirs. For the case $n = 1$, and for time-independent interaction, we show that the system possesses the property of RTE in the mixing sense. We then introduce the C-Liouvillean of the coupled system, which is related to non-equilibrium steady states, and we study its spectrum using complex deformation techniques. Finally we establish the existence of the so called deformed time evolution, which we use in chapter 8 to prove adiabatic theorems in NEQSM.

6.1 Complex translations and the spectrum of $\mathcal{L}_g$

We recall the basic properties of complex translations, and how they relate to the problem at hand. We are a bit pedantic in the presentation, so that the material is self-contained as much as possible. A reader who is familiar with the method may opt to skip this section in a first reading.

We work in the Araki-Wyss representation of the fermionic reservoirs for Model C_n (see section 4.4 for a discussion of this model). Assume $(C_n.1)$. For $\theta \in \mathbf{R}$, let $\mathbf{u}_i(\theta)$ be the unitary transformation generating translations in energy for the i^{th} reservoir, $i = 1, \cdots, n$,

$$(\mathbf{u}_i(\theta)f_i)(u_i) = f_i^{(\theta)}(u_i) = f_i(u_i + \theta) , \tag{6.1}$$

and let $U_i(\theta) = d\Gamma(\mathbf{u}_i(\theta))$ the second quantization of $\mathbf{u}_i(\theta)$,

$$U_i(\theta)\varphi(f_{i,\beta})U_i(-\theta) = \varphi(f_{i,\beta}^{(\theta)}) \ , \tag{6.2}$$
$$U_i(\theta)d\Gamma(u_i)U_i(\theta) = d\Gamma(u_i) + N_i\theta \ , \tag{6.3}$$

where N_i is the number operator of the i^{th}-reservoir $\mathcal{R}_i$. Let $N = \sum_i N_i$, the total number of particles, and $U(\theta) = \mathbf{1}^\Sigma \otimes \mathbf{1}^\Sigma \otimes U_1(\theta) \otimes \cdots \otimes U_n(\theta)$. It follows that the deformed *standard* Liouvillean is

$$\mathcal{L}_g(t,\theta) := U(\theta)\mathcal{L}_g(t)U(-\theta) = \mathcal{L}_0 + N\theta + V_g^{tot}(t,\theta) \ , \tag{6.4}$$

where $\mathcal{L}_0 = \mathcal{L}^\Sigma + \sum_i \mathcal{L}^{\mathcal{R}_i}$, $\mathcal{L}^{\mathcal{R}_i} = d\Gamma(u_i), i = 1, \cdots, n$, and

$$\begin{aligned} V_g^{tot}(t,\theta) \ &= \ gV^{tot}(t,\theta) = g\sum_{i=1}^{n}\{\sigma_- \otimes \mathbf{1}^\Sigma \otimes b^*(f_{i,\beta_i}^{(\theta)}(t)) + \sigma_+ \otimes \mathbf{1}^\Sigma \otimes b(f_{i,\beta_i}^{(\theta)}(t)) \\ &- \ i\mathbf{1}^\Sigma \otimes \sigma_- \otimes (-1)^{N_i} b^*(f_{i,\beta_i}^{\#(\theta)}(t)) - i\mathbf{1}^\Sigma \otimes \sigma_+ \otimes (-1)^{N_i} b(f_{i,\beta_i}^{\#(\theta)}(t))\} \ . \end{aligned}$$

Explicitly, $U_i(\theta) = e^{iA_{\mathcal{R}_i}\theta}, i = 1, \cdots, n$, where $A_{\mathcal{R}_i} = d\Gamma(i\partial_{u_i})$, the second quantization of the energy translations in the i^{th} reservoir.

The follwoing lemmas are needed for applying complex deformation techniques.

Lemma 6.1

The following holds for $0 < \delta' < \delta$.

(i) If $f \in H^2(\delta, \mathcal{B})$, the Hardy class of analytic functions as defined in section 4.4, then $f' \in H^2(\delta', \mathcal{B})$, where the prime stands for differentiation with respect to u. Furthermore, the following inequality holds

$$\|f'\|_{H^2(\delta',\mathcal{B})} \leq \frac{1}{\delta - \delta'}\|f\|_{H^2(\delta,\mathcal{B})} \ . \tag{6.5}$$

(ii) If $f \in H^2(\delta, \mathcal{B})$. then the map $I(\delta) \ni \theta \to f^{(\theta)} \in L^2(\mathbf{R}; \mathcal{B})$ is analytic in θ, where the strip $I(\delta)$ has been defined in chapter 4. Moreover, $\frac{df^{(\theta)}}{d\theta} = f'^{(\theta)}$.

(iii) If $\theta_1, \theta_2 \in I(\delta')$, then, for any $f \in H^2(\delta, \mathcal{B})$, one has the following estimate

$$\|f^{(\theta_1)} - f^{(\theta_2)}\|_{L^2(\mathbf{R};\mathcal{B})} \leq \frac{|\theta_1 - \theta_2|}{\delta - \delta'}\|f\|_{H^2(\delta,\mathcal{B})} \ . \tag{6.6}$$

Proof. Since $f \in H^2(\delta, \mathcal{B})$, this implies that $f : I(\delta) \to \mathcal{B}$ is analytic. We will prove the boundedness of f' by looking at its Fourier transform. Denote by $\hat{f} \in L^2(\mathbf{R}; \mathcal{B})$ the Fourier transform of f, then

$$\|f\|_{H^2(\delta,\mathcal{B})} = \sup_{|\eta|<\delta}\int_{-\infty}^{\infty}\|f(u + i\eta)\|_{\mathcal{B}}^2 du = \sup_{|\theta|<\delta}\|e^{\theta r}\hat{f}(r)\|.$$

Therefore,

$$\begin{aligned}
\|f'\|_{H^2(\delta',\mathcal{B})} &= \sup_{|\theta|<\delta'} \|re^{r\theta}\hat{f}\| \\
&\le \sup_{r\in\mathbf{R}} |re^{-(\delta-\delta')|r|}| \sup_{|\theta|<\delta'} \|e^{\theta r+(\delta-\delta')|r|}\hat{f}\| \\
&\le \frac{1}{e(\delta-\delta')} \sup_{|\theta|<\delta} \|e^{|\theta r|}\hat{f}\| \\
&\le \frac{\sqrt{2}}{e}\frac{1}{\delta-\delta'}\|f\|_{H^2(\delta,\mathcal{B})},
\end{aligned}$$

which implies claim (i).

Assume that $|Im\theta| < \delta' < \delta$, then for small enough $\epsilon \in \mathbf{C}$,

$$\begin{aligned}
\|f^{(\theta+\epsilon)} - f^{(\theta)} - \epsilon f'^{(\theta)}\| &= \|e^{i\theta r}(e^{i\theta\epsilon} - 1 - i\epsilon r)\hat{f}\| \\
&\le \sup_{r\in\mathbf{R}} |e^{-Im\theta r-\delta'|r|}(e^{i\epsilon r} - 1 - i\epsilon r)|\|e^{\delta'|r|}\hat{f}\| \\
&\le O(\epsilon)\|f\|_{H^2(\delta,\mathcal{B})},
\end{aligned}$$

as $\epsilon \to 0$. This implies (ii).

It follows from (ii) that

$$\begin{aligned}
\|f^{(\theta_1)} - f^{(\theta_2)}\| &= \|(\theta_1-\theta_2)\int_0^1 (f')^{(\theta_2+t(\theta_1-\theta_2))}dt\| \\
&\le |\theta_1-\theta_2| \sup_{0\le t\le 1} \|(f')^{(\theta_2+t(\theta_1-\theta_2))}\| \\
&\le |\theta_1-\theta_2|\|f'\|_{H^2(\delta',\mathcal{B})} \\
&\le \frac{\theta_1-\theta_2}{\delta-\delta'}\|f\|_{H^2(\delta',\mathcal{B})},
\end{aligned}$$

which is (iii). $\square$

For $\theta \in I(\delta)$, it follows from $(C_n.1)$ and (6.4) that the perturbed standard Liouvillean is well-defined on the domain $\mathcal{D} := \mathcal{D}(N) \cap \mathcal{D}(\mathcal{L}^{\mathcal{R}_1}) \cap \cdots \cap \mathcal{D}(\mathcal{L}^{\mathcal{R}_n})$. As an operator on $\mathcal{D}$, $V_g^{tot}(\theta)$ satisfies $V_g^{tot}(\theta)^* \supset V_{\overline{g}}^{tot}(\overline{\theta})$, and $V_g^{tot}(\theta)$ is closable for each $(g,\theta) \in \mathbf{C} \times I(\delta)$. We will denote the closure of operators by the same symbol.

Lemma 6.2

For $\theta \in \mathbf{C}$, the following hold:

(i) For any $\psi \in \mathcal{D}$, one has

$$\|\mathcal{L}_0(\theta)\psi\|^2 = \|\mathcal{L}_0(Re\theta)\psi\|^2 + |Im\theta|^2\|N\psi\|^2 \,. \tag{6.7}$$

(ii) If $Im\theta \neq 0$, then $\mathcal{L}_0(\theta)$ is a normal operator satisfying

$$\mathcal{L}_0(\theta)^* = \mathcal{L}_0(\overline{\theta}) \ , \tag{6.8}$$

and $\mathcal{D}(\mathcal{L}_0(\theta)) = \mathcal{D}$.

(iii) The spectrum of $\mathcal{L}_0(\theta)$ is

$$\sigma(\mathcal{L}_0(\theta)) = \{n\theta + s : n \in \mathbf{N} \textit{ and } s \in \mathbf{R}\} \cup \sigma(\mathcal{L}^\Sigma) \ . \tag{6.9}$$

Proof. The first claim follows directly by looking at the sector $N = n$, since $\mathcal{L}_0(\theta)$ restricted to this sector is reduced to

$$\mathcal{L}_0^n(\theta) = \mathcal{L}^\Sigma + s_1 + \cdots + s_n + n\theta \ .$$

Since $\mathcal{D} = \{\psi = \{\psi^{(n)}\} : \psi^{(n)} \in \mathcal{D}(\mathcal{L}_0^{(n)}(\theta)) \textit{ and } \sum_n \|\mathcal{L}_0^{(n)}(\theta)\psi^{(n)}\| < \infty\}$, it follows that $\mathcal{L}_0(\theta)$ is a closed normal operator on $\mathcal{D}$. Claims (ii) and (iii) follow from the corresponding statements on $\mathcal{L}_0^{(n)}(\theta)$. $\Box$

Note that $V_g^{tot}(\theta)$ is bounded as a consequence of assumption $(C_n.1)$.

Lemma 6.3

Assume that $(g, \theta) \in \mathbf{C} \times I^-(\delta)$, then

(i) $\mathcal{D}(\mathcal{L}_g(t,\theta)) = \mathcal{D}$ and $\mathcal{L}_g(t,\theta)^* = \mathcal{L}_{\overline{g}}(t,\overline{\theta})$.

(ii) The spectrum of $\mathcal{L}_g(t,\theta)$ satisfies

$$\sigma(\mathcal{L}_g(t,\theta)) \subset \{z \in \mathbf{C} : Imz \leq C(g,\theta)\} \ , \tag{6.10}$$

where

$$C(g,\theta) := \sup_{t\in\mathbf{R}} \{\frac{|Reg|}{\delta - Img}|Im\theta|^{1/2} + |Img||Im\theta|^{-1/2}\} \sum_i \|f_{i,\beta_i}(t)\|_{H^2(\delta,\mathcal{B})}. \tag{6.11}$$

Furthermore, if $Imz > C(g,\theta)$, then

$$\|(\mathcal{L}_g(t,\theta) - z)^{-1}\| \leq \frac{1}{Imz - C(g,\theta)} \ . \tag{6.12}$$

(iii) The map $(g,\theta) \to \mathcal{L}_g(t,\theta)$ from $\mathbf{C} \times I^-(\delta)$ to the set of closed operators on $\mathcal{H}$ is an analytic family in each variable separately; (see [Ka1], chapter V, section 3.2).

Proof. The first claim (i) follows from the fact that $V_g^{tot}(t,\theta)$ is infinitesimally small with respect to $\mathcal{L}_0(\theta)$ for $\theta \in I(\delta)$. To establish the second assertion, let $\hat{C}(t,g,\theta) := \sup Im(\eta(\mathcal{L}_g(t,\theta))$, where $\eta(\mathcal{L}_g(t,\theta))$ is the numerical range of $\mathcal{L}_g(t,\theta)$. We know that $\sigma(\mathcal{L}_g(t,\theta)) \subset \eta(\mathcal{L}_g(t,\theta))$, and that $\|(\mathcal{L}_g(t,\theta)-z)^{-1}\| \leq \frac{1}{dist(z,\eta(\mathcal{L}_g(t,\theta)))}$ for $z \in \mathbf{C}\backslash\eta(\mathcal{L}_g(t,\theta))$ (see [Hu]). One may readily check that $\hat{C}(t,g,\theta) \leq C(g,\theta)$ from Lemma 6.1 and (6.4). This suffices to prove the second claim. Since $\|\mathcal{L}_g(t,\theta+\epsilon) - \mathcal{L}_g(t,\theta) - \epsilon\frac{\partial\mathcal{L}_g(t,\theta)}{\partial\theta}\| = O(\sum_i \|f_{i,\beta_i}^{(\theta+\epsilon)} - f_{i,\beta_i}^{(\theta)} - \epsilon f_{i,\beta_i}^{\prime(\theta)}\|)$, it follows that the map $(g,\theta) \rightarrow \mathcal{L}_g(t,\theta)$ is analytic in θ. Analyticity in g is obvious from definition (6.4).
□

Denote by

$$\Xi(\eta) := \{z \in \mathbf{C} : Imz > \eta\},$$

which is an open half-plane.

Proposition 6.4

Suppose $(C_n.1)$ and $(C_n.2)$. Then there is a constant $g_1 > 0$, independent of $\beta_i \in [\beta_0,\beta_*], i = 1,\cdots,n, 0 < \beta_0 < \beta_* < \infty$ fixed, such that the following hold.

(i) If $|g| < g_1|Im\theta|$, then the spectrum of the operator $\mathcal{L}_g(t,\theta)$ in the half-plane $\Xi(Im\theta + \frac{|g|}{g_1})$ is purely discrete and independent of θ.

(ii) If $|g| < \frac{1}{4}g_1|Im\theta|$, then the spectral projection $P_g(t,\theta)$ associated to the spectrum of $\mathcal{L}_g(t,\theta)$ in the half-plane $\Xi(Im\theta + \frac{|g|}{g_1})$ is analytic in g and satisfies the estimate

$$\|P_g(t,\theta) - P_0\| < \frac{3|g|}{g_1|Im\theta|} \,. \tag{6.13}$$

Proof. The resolvent formula

$$(\mathcal{L}_g(t,\theta)-z)^{-1} = (\mathcal{L}_0(\theta)-z)^{-1}(1+V_g^{tot}(t,\theta)(\mathcal{L}_0(\theta)-z)^{-1})^{-1} \,, \tag{6.14}$$

holds for small g, as long as z belongs to the cone $\{z \in \mathbf{C} : 0 < c_1 < |z| < c_2 Imz\}$, since $V_g^{tot}(t,\theta)$ is infinitesimally small with respect to $\mathcal{L}_0(\theta)$ for $\theta \in I(\delta)$. The strategy of the proof is as follows: We extend the domain of validity of (6.14) by refining the estimate on $V_g^{tot}(t,\theta)(\mathcal{L}_0(\theta)-z)^{-1}$, and then use analytic perturbation theory as developed in [HP].

Note that

$$\|V_g^{tot}(t,\theta)(\mathcal{L}_0(\theta)-z)^{-1}\| \leq g\sum_i \|f_{i,\beta_i}(t)\|_{H^2(\delta,\mathcal{B})}\|(\mathcal{L}_0(\theta)-z)^{-1}\|. \tag{6.15}$$

Since N and $\mathcal{L}_0(\theta)$ are commuting operators, one may apply the spectral theorem to evaluate the norm of $A(z) := V^{tot}(t,\theta)(\mathcal{L}_0(\theta)-z)^{-1}$. On the sector $N = 0$,

$$\|A^{(0)}(z)\| = \|(\mathcal{L}^\Sigma - z)^{-1}\| = \frac{1}{dist(z,\sigma(\mathcal{L}^\Sigma))} \,. \tag{6.16}$$

Without loss of generality, assume that $Im\theta =: -\mu < 0$, ie, $\theta \in I^-(\delta)$. On the sector $N = n > 0$,

$$\|A^{(n)}(z)\} = \| \frac{\sqrt{n+1}}{(\mathcal{L}^\Sigma + s_1 + \cdots + s_n + nRe\theta - Rez) - i(n\mu + Imz)} \| \tag{6.17}$$

$$= \frac{\sqrt{n+1}}{|n\mu + Imz|} \; . \tag{6.18}$$

Since $\|A(z)\| = \sup_{n\geq 0} \|A^{(n)}(z)\|$,

$$\|A(z)\| \leq \begin{cases} \frac{\sqrt{2}}{dist(z,\sigma(\mathcal{L}_0(\theta)))}, -\mu < Imz < 3\mu, \\ \frac{1}{2\sqrt{\mu(Imz-\mu)}}, 3\mu \leq Imz \end{cases} . \tag{6.19}$$

Let

$$g_1 := \sup_t \frac{1}{4\sum_i \|f_{i,\beta_i}(t)\|_{H^2(\delta,\mathcal{B})}} \; , \tag{6.20}$$

and $G(\theta, \epsilon) := \{z \in \mathbf{C} : Imz > Im\theta; dist(z, \sigma(\mathcal{L}_0(\theta)) > \epsilon)\}$. It follows from (6.19) and (6.20) that, for $\epsilon < \mu$,

$$\sup_{z\in G(\theta,\epsilon)} \|V_g^{tot}(t,\theta)(\mathcal{L}_0(\theta) - z)^{-1}\| \leq \frac{|g|}{g_1\epsilon}. \tag{6.21}$$

If $|g| < g_1\epsilon$, the resolvent formula (6.14) holds on $G(\theta, \epsilon)$, and for $N \geq 0$,

$$\sup_{z\in G(\theta,\epsilon)} \|(z - \mathcal{L}_g(t,\theta))^{-1} - \sum_{j=0}^{N-1}(z - \mathcal{L}_0(\theta))^{-1}(V_g^{tot}(t,\theta)(z - \mathcal{L}_0(\theta))^{-1})^j\| \leq \frac{1}{\epsilon}\frac{(\frac{|g|}{g_1\epsilon})^N}{1 - \frac{|g|}{g_1\epsilon}}.$$

For small enough $|g|$, it follows that

$$\Xi(Im\theta)\backslash\sigma(\mathcal{L}^\Sigma) = \bigcup_{\epsilon>0} G(\theta, \epsilon) \subset \rho(\mathcal{L}_g(t,\theta)) \; , \tag{6.22}$$

where $\rho(\mathcal{L}_g(t,\theta))$ is the resolvent set of $\mathcal{L}_g(t,\theta)$. Therefore, the discrete spectrum of $\mathcal{L}_g(t,\theta)$ is stable, and one may apply analytic perturbation theory. We still need to prove the independence of (i) from $\theta \in I^-(\delta)$. Fix $(g_0, \theta_0) \in \mathbf{C} \times I^-(\delta)$ such that $|g_0| < g_1|Im\theta|$. The discrete eigenvalues of $\mathcal{L}_{g_0}(t,\theta)$ are analytic functions with at most algebraic singularities in the neighbourhood of θ_0, since $\mathcal{L}_{g_0}(t,\theta)$ is analytic in θ. Moreover, since $\mathcal{L}_{g_0}(t,\theta_0)$ and $\mathcal{L}_{g_0}(t,\theta)$ are unitarily equivalent if $(\theta - \theta_0) \in \mathbf{R}$, it follows that the discrete spectrum of $\mathcal{L}_{g_0}(t,\theta)$ is independent of θ.

To prove (ii), assume that $2\epsilon < |Im\theta|$ and $|g| < g_1\epsilon$, and let the contour $\gamma = \gamma_+ - \gamma_-$, where $\gamma_\pm := \{z \in \mathbf{C} : Imz = \pm Im\theta/2\}$. At the formal level (for now!), let

$$P_g(t,\theta) := \oint_\gamma \frac{dz}{2\pi i}(z - \mathcal{L}_g(t,\theta))^{-1} \; , \tag{6.23}$$

which is the spectral projection onto the discrete spectrum of $\mathcal{L}_g(t,\theta)$.

Iterating the resolvent identity (6.14), one obtains

$$P_g(t,\theta) = P_0 + \Pi_g^{(1)}(t,\theta) + \Pi_g^{(2)}(t,\theta)\ , \tag{6.24}$$

where

$$P_0 = P_0(\theta)\ , \tag{6.25}$$

$$\Pi_g^{(1)}(t,\theta) = \oint_\gamma \frac{dz}{2\pi i}(\mathcal{L}_0(\theta)-z)^{-1}V_g^{tot}(t,\theta)(\mathcal{L}_0(\theta)-z)^{-1}\ , \tag{6.26}$$

$$\Pi_g^{(2)}(t,\theta) = -\oint_\gamma \frac{dz}{2\pi i}(\mathcal{L}_0(\theta)-z)^{-1}V_g^{tot}(t,\theta)(\mathcal{L}_g(t,\theta)-z)^{-1}V_g^{tot}(t,\theta)(\mathcal{L}_0(\theta)-z)^{-1}\ . \tag{6.27}$$

Applying the spectral theorem (with respect to $\mathcal{L}_0(\theta)$, which is normal),

$$\Pi_g^{(1)}(t,\theta) = -i\int_{-\infty}^{\infty} e^{-\mu|s|}\Theta_s ds\ , \tag{6.28}$$

where

$$\Theta_s := \begin{cases} P_0 e^{i\mathcal{L}_0 s}V_g^{tot}e^{-i\mathcal{L}_0 s},\ s<0 \\ e^{i\mathcal{L}_0 s}V_g^{tot}e^{-i\mathcal{L}_0 s}P_0,\ s>0. \end{cases} \tag{6.29}$$

Since $\|\Theta_s\| \le \frac{|g|}{2\sqrt{2}g_1}$, we have the following estimate

$$\|\Pi_g^{(1)}(t,\theta)\| \le \frac{|g|}{g_1\mu}\ , \tag{6.30}$$

uniformly in $t\in\mathbf{R}$.

We still need to estimate the norm of $\Pi_g^{(2)}$. Consider two vectors $\varphi,\psi\in\mathcal{H}$. By the Cauchy-Schwarz inequality,

$$|\langle\varphi,\Pi_g^{(2)}\psi\rangle| \le \sup_{z\in\gamma}\|V_g^{tot}(t,\theta)(\mathcal{L}_g(t,\theta)-z)^{-1}V_g^{tot}(t,\theta)\|\nu(\varphi)\nu(\psi)\ , \tag{6.31}$$

where $\nu(\cdot) := \{\int_\gamma \frac{d|z|}{2\pi}\|(\mathcal{L}_0(\theta)-z)^{-1}\cdot\|^2\}^{1/2}$. By the spectral theorem,

$$\nu(\varphi) \le \sqrt{2/\mu}\|\varphi\|\ ,$$

and

$$\sup_{z\in\gamma}\|V_g^{tot}(t,\theta)(\mathcal{L}_0(\theta)-z)^{-1}V_g^{tot}(t,\theta)\| \le \frac{2g^2}{g_1^2\mu}\ .$$

Again using the resolvent of the identity and the previous estimates,

$$\sup_{z\in\gamma}\|V_g^{tot}(t,\theta)(\mathcal{L}_g(t,\theta)-z)^{-1}V_g^{tot}(t,\theta)\| \le \frac{2g^2}{g_1^2\mu}(1-\frac{|g|}{g_1\epsilon})^{-1}.$$

Optimizing the latter equation with respect to ϵ gives $\epsilon = \mu/2$, and hence

$$\|\Pi_g^{(2)}(t,\theta)\| \leq \frac{4g^2}{g_1^2\mu^2}(1-\frac{2|g|}{g_1\mu})^{-1} \ , \tag{6.32}$$

uniformly in $t \in \mathbf{R}$.

Estimates (6.30) and (6.32) imply that

$$\|P_g(t,\theta) - P_0\| \leq x(\frac{1+2x}{1-2x}) \ , \tag{6.33}$$

with $x = \frac{|g|}{g_1\mu} < 1/2$, independent of $t \in \mathbf{R}$. □

Proposition 6.4 allows one to apply reduction theory to the discrete spectrum of resonances as developed in [HP,JP1,2,3], and to construct a quasi-Liouvillean acting on $\mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma$ by transforming the reduced Liouvillean $\widetilde{\mathcal{L}_g} := P_g\mathcal{L}_gP_g$ from $Ran(P_g(\theta))$ to $\mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma$.

If $|g| < \frac{g_1\mu}{4}$, estimate (6.33) implies that $\|P_g(t,\theta) - P_0\| < 1$. It follows that the maps

$$P_0 : Ran(P_g(t,\theta)) \to \mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma \ ;$$
$$P_g(t,\theta) : \mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma \to Ran(P_g(t,\theta))$$

are isomorphisms for each fixed t.

Let $T_g(t) := P_0P_g(t,\theta)P_0$, then

$$S_g(t,\theta) := T_g(t)^{-1/2}P_0P_g(t,\theta) : Ran(P_g(t,\theta)) \to \mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma \tag{6.34}$$

has an inverse

$$S_g^{-1}(t,\theta) := P_g(t,\theta)P_0T_g^{-1/2}(t) : \mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma \to Ran(P_g(t,\theta)). \tag{6.35}$$

Let

$$M_g(t) := P_0P_g(t,\theta)\mathcal{L}_g(t,\theta)P_g(t,\theta)P_0 \ , \tag{6.36}$$

and define the *quasi-Liouvillean*

$$\Sigma_g(t) := S_g(t,\theta)P_g(t,\theta)\mathcal{L}_g(t,\theta)P_g(t,\theta)S_g^{-1}(t,\theta) = T_g^{-1/2}(t)M_g(t)T_g^{1/2}(t) \ , \tag{6.37}$$

which is nothing but the mapping of the reduced Liouvillean $\widetilde{\mathcal{L}_g}$ from $Ran(P_g)$ to $\mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma$.[HP,JP1,2,3]

Since $U(\theta)P_0 = P_0U(\theta) = P_0$, $\forall\theta \in \mathbf{C}$, the operators $T_g(t)$ and $M_g(t)$ are independent of θ for $|g| < \frac{g_1\mu}{4}$.

Proposition 6.5

Suppose assumptions (C_n.1) and (C_n.2) hold, and that $|g| < \frac{g_1\mu}{4}$. Then, for each fixed time t, the quasi-Liouvillean $\Sigma_g(t)$ defined in (6.37) depends analytically on g, and has a Taylor expansion of the form

$$\Sigma_g(t) = \mathcal{L}^\Sigma + \sum_{j=1}^{\infty} g^{2j}\Sigma^{(2j)} \; . \tag{6.38}$$

The first non-trivial coefficient in (6.38) is

$$\Sigma^{(2)}(t) = \frac{1}{2}\oint_\gamma \frac{dz}{2\pi i}(K(t,z)(z-\mathcal{L}^\Sigma)^{-1} + (z-\mathcal{L}^\Sigma)^{-1}K(t,z)) \; , \tag{6.39}$$

where $K(t,z) = P_0 V_g^{tot}(t,\theta)(z-\mathcal{L}_0(\theta))^{-1}V_g^{tot}(t,\theta)P_0$.

Proof. Fix the time $t \in \mathbf{R}$. Analyticity of T_g directly follows from the previous proposition and the definition of T_g. Since $\|T_g - 1\| < 1$ for $|g| < \frac{g_1\mu}{4}$, $T_g^{-1/2}$ is also analytic in g. Inserting the Neumann series for the resolvent of $\mathcal{L}_g(t,\theta)$, gives

$$T_g = 1 + \sum_{j=1}^{\infty} g^j T^{(j)} \; , \tag{6.40}$$

with

$$T^{(j)}(t) = \oint_\gamma \frac{dz}{2\pi i}(z-\mathcal{L}^\Sigma)^{-1}P_0V^{tot}(t,\theta)((z-\mathcal{L}_0(\theta))^{-1}V^{tot}(t,\theta))^{j-1}P_0(z-\mathcal{L}^\Sigma)^{-1} \; . \tag{6.41}$$

Similarly,

$$M_g(t) = \mathcal{L}^\Sigma + \sum_{j=1}^{\infty} g^j M^{(j)} \; , \tag{6.42}$$

with

$$M^{(j)}(t) = \oint_\gamma \frac{dz}{2\pi i}z(z-\mathcal{L}^\Sigma)^{-1}P_0V^{tot}(t,\theta)((z-\mathcal{L}_0(\theta))^{-1}V^{tot}(t,\theta))^{j-1}P_0(z-\mathcal{L}^\Sigma)^{-1} \; . \tag{6.43}$$

The odd terms in the above two expansions are zero due to the fact that P_0 projects onto the $N=0$ sector. The first non-trivial coefficient in the Taylor series of Σ_g is

$$\Sigma^{(2)}(t) = M^{(2)}(t) - \frac{1}{2}(T^{(2)}(t)\mathcal{L}^\Sigma + \mathcal{L}^\Sigma T^{(2)}(t)) \tag{6.44}$$

$$= \frac{1}{2}\oint_\gamma \frac{dz}{2\pi i}(K(t,z)(z-\mathcal{L}^\Sigma)^{-1} + (z-\mathcal{L}^\Sigma)^{-1}K(t,z)) \; , \tag{6.45}$$

with $K(t,z) = P_0 V_g^{tot}(t,\theta)(z-\mathcal{L}_0(\theta))^{-1}V_g^{tot}(t,\theta)P_0$. □

Up until now we have assumed that $Im\theta \neq 0$. The following lemma asserts that under certain assumptions, one can take the limit $Im\theta \uparrow 0$ in the resolvent.

Lemma 6.6

Suppose that assumptions (C_n.1) and (C_n.2) hold. Then, for $g \in \mathbf{R}$ and Imz large enough,

$$s - \lim_{Im\theta\uparrow 0} (\mathcal{L}_g(t,\theta) - z)^{-1} = (\mathcal{L}_g(t, Re\theta) - z)^{-1} \ , \tag{6.46}$$

for each fixed time $t \in \mathbf{R}$.

Proof. Without loss of generality, assume that $Re\theta = 0$. Since $(\mathcal{L}_g(t,\theta) - z)^{-1}$ is uniformly bounded as $Im\theta \uparrow 0$ for $g \in \mathbf{R}$ and Imz large enough, it is enough to prove (6.48) on a dense subspace. Let $\mathcal{B}_v := \{\psi \in \mathcal{H} : N\psi < v\}$, the subspace of finite particle vectors and let $\mathcal{D}_v := \{(\mathcal{L}_g(\theta) - z)\psi : \psi \in \mathcal{B}_v\}$. For $\varphi \in D_v$,

$$\begin{aligned}
&[(\mathcal{L}_g(t,\theta) - z)^{-1} - (\mathcal{L}_g(t) - z)^{-1}]\varphi \\
&= (\mathcal{L}_g(t) - z)^{-1}(\mathcal{L}_g(t) - \mathcal{L}_g(t,\theta))(\mathcal{L}_g(t,\theta) - z)^{-1}\varphi \\
&= (\mathcal{L}_g(t) - z)^{-1}(V_g^{tot}(t) - V_g^{tot}(t,\theta) - N\theta)(\mathcal{L}_g(t,\theta) - z)^{-1}\varphi \ .
\end{aligned}$$

Using this and the fact that $\mathcal{D}_v$ is dense in $\mathcal{D} = \mathcal{D}(N) \cap \mathcal{D}(\mathcal{L}_0)$, it follows that

$$\begin{aligned}
&\|[(\mathcal{L}_g(t,\theta) - z)^{-1} - (\mathcal{L}_g(t) - z)^{-1}](N+1)^{-1}\| \\
&\leq \frac{|\theta|}{Imz}(1 + \frac{2\sqrt{2}|g|}{\delta - \mu}\sum_{i=1}^{n} \|f_{i,\beta_i}(t)\|_{H^2(\delta,\mathcal{B})})\|(N+1)(\mathcal{L}_g(t,\theta) - z)^{-1}(N+1)^{-1}\| \ .
\end{aligned}$$

Moreover, since $(N+1)(\mathcal{L}_g(t,\theta) - z)^{-1}(N+1)^{-1}$ is uniformly bounded as $Im\theta \uparrow 0$, it follows that

$$\lim_{Im\theta\uparrow 0} \|[(\mathcal{L}_g(t,\theta) - z)^{-1} - (\mathcal{L}_g(t) - z)^{-1}](N+1)^{-1}\| = 0 \ . \tag{6.47}$$

□

Recall that for model C_n, we set all the chemical potentials equal to $\nu \in \mathbf{R}$. The result can be generalized to arbitrary chemical potentials (see remark after Theorem 6.7).

Theorem 6.7 (Spectrum of the standard Liouvillean of C_n)

Suppose assumptions (C_n.1) and (C_n.2) hold. Then there is a constant g_1 independent of $\beta_i \in [\beta_0, \beta_*], 0 < \beta_0 < \beta_* < \infty, i = 1, \cdots, n$, such that the following holds for $|g| < g_1$ and fixed t.

(i) If there are at least two reservoirs to which the small system is connected with different temperatures (ie, $\exists i, j \in 1, \cdots, n$ such that $\beta_i \neq \beta_j$) *, then the spectrum of $\mathcal{L}_g(t)$ is absolutely continuous for all $t \in \mathbf{R}$. All the eigenvalues of $\mathcal{L}_g$ become resonances in this case.

*(or different chemical potentials $\nu_i \neq \nu_j$; see remark after Theorem 6.7)

(ii) If there is only one reservoir at inverse temperature β and chemical potential ν, then $dim\ Ker\mathcal{L}_g(t) = 1$. In particular, if the coupling of the small system Σ to the reservoir $\mathcal{R}$ is *time-independent*, ie, $V(t) = V$, then the system possesses the property of return to equilibrium. For all states $\rho \in \mathcal{N}$, the set of states normal to the initial state

$$\omega = \omega^{\Sigma} \otimes \omega_{\beta}^{\mathcal{R}},$$

we have

$$\lim_{t\to\infty} \rho(\alpha_g^t(A)) = \omega_{\beta,\nu,g}(A) , \tag{6.48}$$

where $A \in \mathcal{O} = \mathcal{O}^{\Sigma} \otimes \mathcal{O}^{\mathcal{R}}$ and $\omega_{\beta,\nu,g}$ is the (α_g^t, β, ν)-KMS state of the coupled system. The limit is exponentially fast, in the sense that $\exists\gamma(g) > 0$, a set of states $\mathcal{N}_0$ dense in $\mathcal{N}$, and a norm-dense subalgebra $\mathcal{O}_0 \subset \mathcal{O}$, such that for all $\rho \in \mathcal{N}_0$, $A \in \mathcal{O}_0$, and $t > 0$,

$$|\rho(\alpha_g^t(A)) - \omega_{\beta,\nu,g}(A)| \leq C(A, \beta, g)e^{-\gamma(g)t} , \tag{6.49}$$

and $\omega_{\beta,g}$ is analytic in the coupling g.

Proof. The proof relies on the method of complex translations as developed in [JP1,2,3]. Fix $t \in \mathbf{R}$, and choose k such that $0 < k < \min(\frac{\pi}{\beta_1}, \cdots, \frac{\pi}{\beta_n}, \delta)$, where $\beta_i, i = 1, \cdots, n$, are the inverse temperatures of the reservoirs and δ appears in assumption $(C_n.1)$, chapter 4. Recall that

$$\mathcal{L}_g(t, \theta) := U(\theta)\mathcal{L}_g(t)U(-\theta) = \mathcal{L}_0 + N\theta + V_g^{tot}(t, \theta) . \tag{6.50}$$

The function $I^-(k) \otimes \mathbf{C} \ni (\theta, g) \to \mathcal{L}_g(t, \theta)$ with values in the closed operators on $\mathcal{H}$, is an analytic family of type A in each variable separately (see for example [Ka1]). The spectrum of $\mathcal{L}_0(\theta)$ consists of two simple eigenvalues $E_2 = -2$ and $E_3 = 2$, a doubly degenerate eigenvalue at 0, $E_0 = E_1 = 0$, and a sequence of lines $\{inIm\theta + \mathbf{R} : n \in \mathbf{N}^+\}$.

Let $C(\delta, \beta_i) := \sup_{|Imz|<\delta} |1 + e^{-\beta_i(z-\nu)}|^{-1/2}$, which is finite. Then

$$C := \sup_{\theta\in I^-(k)} \|V^{(tot)}(t, \theta)\| \leq 2\sqrt{2} \sum_{i=1}^{n} C(k, \beta_i)\|f_{i,\beta_i}(t)\|_{H^2(k)} < \infty , \tag{6.51}$$

due to $(C_n.1)$. Choose g_1 such that $g_1C < (k-\mu)/4$, where $\mu = |Im\theta|$. Then, for $|g| < g_1$ and $-k < Im\theta < -(k + \mu)/2$, the essential spectrum $\sigma_{ess}(\mathcal{L}_g(t, \theta))$ is contained in the half-plane $\{z \in \mathbf{C} : Imz < -\mu\}$. The location of the discrete spectrum of $\mathcal{L}_g(t, \theta)$ inside the half-plane $\Xi(-\mu)$ can be computed using regular perturbation theory. Taking g_1 small enough, the discrete spectrum of $\mathcal{L}_g(t, \theta)$ consists of four points (resonances) $\{E_k(g)\}_{k=0}^3$, such that $E_0(t, g), E_1(t, g)$ are localized near 0, while $E_2(t, g), E_3(t, g)$ are localized near ∓2 respectively.

From Proposition 6.5, we know that

$$\Sigma^{(2)} = \frac{1}{2}\oint_\gamma \frac{dz}{2\pi i}\{P_0 V^{tot}(t,\theta)(z-\mathcal{L}_0(\theta))^{-1}V^{tot}(t,\theta)P_0(z-\mathcal{L}^\Sigma)^{-1} \tag{6.52}$$

$$+ (z-\mathcal{L}^\Sigma)^{-1}P_0V^{tot}(t,\theta)(z-\mathcal{L}_0(\theta))^{-1}V^{tot}(t,\theta)P_0\}\ . \tag{6.53}$$

We now apply regular perturbation theory to compute the shift of the eigenvalues of $\mathcal{L}_g(\theta)$ to second order in g. Let $P_k, k = 0, \cdots, 3$ be the spectral projection corresponding to the eigenvalues E_k of $\mathcal{L}^\Sigma$ (recall that $E_0 = E_1 = 0, E_2 = -2; E_3 = 2$), and let

$$\Gamma_k^{(2)}(t) := P_k\Sigma^{(2)}(t)P_k\ . \tag{6.54}$$

To compute the shift in $E_3 = 2$, look at $\Gamma_3^{(2)}(t) = P_3\Sigma^{(2)}(t)P_3$. Applying the Cauchy integration formula to (6.53) gives

$$\Gamma_3^{(2)}(t) = \frac{1}{2}\{P_3P_0\sigma_+\otimes \mathbf{1}^\Sigma\otimes b(f_{i,\beta_i}^{(\theta)}(t))(2-\mathcal{L}_0(\theta))^{-1}\sigma_-\otimes\mathbf{1}^\Sigma\otimes b^*(f_{i,\beta_i}^{(\theta)}(t))P_0P_3$$
$$+ P_3P_0\mathbf{1}^\Sigma\otimes\sigma_+\otimes b(f_{i,\beta_i}^{\#(\theta)}(t))(2-\mathcal{L}_0(\theta))^{-1}\mathbf{1}^\Sigma\otimes\sigma_-\otimes b^*(f_{i,\beta_i}^{\#(\theta)}(t))P_0P_3\}\ .$$

Using the fact that

$$\lim_{\epsilon\searrow 0} Re\frac{1}{x-i\epsilon} = \mathcal{PV}\frac{1}{x}\ ,$$
$$\lim_{\epsilon\searrow 0} Im\frac{1}{x-i\epsilon} = i\pi\delta(x)\ ,$$

where $\mathcal{PV}$ stands for the Cauchy principal value, it follows that

$$Re\Gamma_3^{(2)} = \sum_{i=1}^n \mathcal{PV}\int_{\mathbf{R}} du\frac{\|f_{i,\beta_i}(u,t)\|_{\mathcal{B}}^2}{2-u}\ , \tag{6.55}$$

$$Im\Gamma_3^{(2)} = -\pi\sum_{i=1}^n\int_{\mathbf{R}} du\|f_{i,\beta_i}(u,t)\|_{\mathcal{B}}^2\delta(u-2) = -\pi\sum_{i=1}^n\|f_{i,\beta_i}(2,t)\|_{\mathcal{B}}^2\ . \tag{6.56}$$

Similarly,

$$Re\Gamma_2^{(2)} = -\sum_{i=1}^n \mathcal{PV}\int_{\mathbf{R}} du\frac{\|f_{i,\beta_i}(u,t)\|_{\mathcal{B}}^2}{2-u}\ , \tag{6.57}$$

$$Im\Gamma_2^{(2)} = -\pi\sum_{i=1}^n\int du_{\mathbf{R}}\|f_{i,\beta_i}(u,t)\|_{\mathcal{B}}^2\delta(u-2) = -\pi\sum_{i=1}^n\|f_{i,\beta_i}(2,t)\|_{\mathcal{B}}^2\ . \tag{6.58}$$

We need to apply degenerate perturbation theory for the zero eigenvalue of $\mathcal{L}^\Sigma$. Using the definition of $f_{i,\beta_i}, f_{i,\beta_i}^{\#}$ and $\widetilde{f}_i$ given in section 4.4,

$$Re\Gamma_{0,1}^{(2)} = 0\ , \tag{6.59}$$

$$Im\Gamma_{0,1}^{(2)} = -\pi\sum_{i=1}^n\frac{\|\widetilde{f}_i(2,t)\|_{\mathcal{B}}^2}{2\cosh(\beta_i(2-\nu)/2)}\begin{pmatrix} e^{\beta_i(2-\nu)/2} & -1 \\ -1 & e^{-\beta_i(2-\nu)/2}\end{pmatrix}\ . \tag{6.60}$$

Therefore, to second order in the coupling g,

$$E_{2,3}(t,g) = \pm(2+g^2\mathcal{P}V\int_{\mathbf{R}} du\frac{1}{2-u}\sum_{i=1}^{n}\|f_{i,\beta_i}(u,t)\|_{\mathcal{B}}^2) - i\pi g^2\sum_{i=1}^{n}\|f_{i,\beta_i}(2,t)\|_{\mathcal{B}}^2 + O(g^4)\ . \tag{6.61}$$

Note that $ImE_{2,3}(t,g) < 0$. Furthermore,

$$E_{0,1}(t,g) = g^2 a_{0,1}(t) + O(g^4)\ , \tag{6.62}$$

where $a_{0,1}(t)$ are the eigenvalues of the 2×2 matrix

$$-i\pi\sum_{i=1}^{n}\frac{\|\widetilde{f}_i(2,t)\|_{\mathcal{B}}^2}{cosh(\beta_i(2-\nu)/2)}\begin{pmatrix} e^{\beta_i(2-\nu)/2} & -1 \\ -1 & e^{-\beta_i(2-\nu)/2}\end{pmatrix}\ . \tag{6.63}$$

(i) If $\exists\beta_i \neq \beta_j$, for $i,j\in\{1,\cdots,n\}$, it follows from (6.63) that $ImE_{0,1}(t,g) < 0$, and together with Lemma 6.6, it follows that all the eigenvalues of the $\mathcal{L}_g(t)$ are pushed to the lower half-plane, ie, they all become resonances, and the spectrum of $\mathcal{L}_g(t)$ is purely absolutely continuous.

(ii) Suppose there is only one reservoir at inverse temperature β(or equivalently several reservoirs with the same temperature), then $\Omega_V(t)\in Ker\mathcal{L}_g(t)$ (see chapter 3). It follows from (6.63) that $ImE_1(t) = -\pi g^2\|\widetilde{f}(2,t)\|_{\mathcal{B}}^2 + O(g^4) < 0$, while $E_0(t,g) = 0$ with $\psi_\beta = \begin{pmatrix} e^{-\beta(2-\nu)/4} \\ e^{\beta(2-\nu)/4}\end{pmatrix}$ the corresponding eigenvector of $\Sigma_g^{(2)}$ (which is consistent with $Ker\mathcal{L}_g \geq 1$). Together with Lemma 6.6, this implies that 0 is a simple eigenvalue of $\mathcal{L}_g(t)$, and that the spectrum of the Liouvillean away from zero is absolutely continuous, $\sigma(\mathcal{L}_g(t))\backslash\{0\} = \sigma_{ac}(\mathcal{L}_g(t))$.

In particular, if the perturbation is time-independent ($V(t)\equiv V$), the system possesses the property of return to equilibrium in the mixing sense; (see chapter 3), with an explicit rate of convergence to the perturbed equilibrium state $\omega_{\beta,\nu,g}$ as $t\to\infty$.

Let

$$\mathcal{E}\subset\mathcal{F}_-(L^2(\mathbf{R};\mathcal{B}))$$

be the set of entire functions for the group $U(\theta)$, ie, for $\psi\in\mathcal{F}_-(L^2(\mathbf{R};\mathcal{B}))$, $U(\theta)\psi$ has an entire extension. Denote by $\mathcal{C} := \mathcal{H}^\Sigma\otimes\mathcal{H}^\Sigma\otimes\mathcal{E}$, which is dense in $\mathcal{H}$. For $\Phi,\Psi\in\mathcal{C}, g\in\mathbf{R}$, and Imz large enough, the function

$$\theta\to h(\theta) = \langle U(\overline{\theta})\Phi, (\mathcal{L}_g(\theta)-z)^{-1}U(\theta)\Psi\rangle \tag{6.64}$$

is analytic on $I^-(k)$, and continuous on $I^-(k)\cup\mathbf{R}$ due to Lemma 6.6. Hence, the map

$$z\to\langle U(\overline{\theta})\Phi, (\mathcal{L}_g(\theta)-z)^{-1}U(\theta)\Psi\rangle\ , \tag{6.65}$$

provides the meromorphic extension to the half-plane $\Xi(Im\theta + \frac{|g|}{g_1})$. To see the exponential convergence to the perturbed equilibrium state, define

$$f(t) := \langle \Phi, e^{-i\mathcal{L}_g t}\Psi\rangle \ . \tag{6.66}$$

For $Imz > 0$, the transform (Fourier-Laplace)

$$\hat{f}(z) := \int_0^\infty f(t)e^{izt}dt = -i\langle \Phi, (\mathcal{L}_g - z)^{-1}\Psi\rangle \tag{6.67}$$

is well-defined, with inverse

$$f(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \hat{f}(u+i\eta)e^{-i(u+i\eta)t}du \ , \tag{6.68}$$

where $t, \eta > 0$. Rewriting (6.68),

$$f(t) = \frac{1}{2\pi}\oint_\gamma \hat{f}(z)e^{-izt} + \frac{1}{2\pi}\int_{-\infty}^{\infty} \hat{f}(u - i(\mu - \epsilon'))e^{-i(u-i(\mu-\epsilon'))t}du \ , \tag{6.69}$$

where the contour γ is as before, $\mu = |Im\theta|$ and $\mu > \epsilon' > \epsilon$. The first term in (6.69) is

$$\frac{1}{2\pi}\oint_\gamma \hat{f}(z)e^{-izt}dz = \langle U(\overline{\theta})\Phi, S_g^{-1}(\theta)e^{-i\Sigma_g t}S_g(\theta)U(\theta)\Psi\rangle \ , \tag{6.70}$$

which converges to the (α_g^t, β, ν)-KMS state with a life-time $\tau_{\mathcal{R}} = O(g^{-2})$. The second term in (6.69) is of order $O(e^{-(\mu-\epsilon'')})$, for $\mu > \epsilon'' > \epsilon$; (see, for example, Theorem 19.2 in [Rud]).

□

Remark. One may show using a similar computation that if all the temperatures of the reservoirs are equal, but the chemical potential of at least two reservoirs are different, the spectrum of the Liouvillean is absolutely continuous.

The fact that the kernel of the standard Liouvillean is empty if at least two reservoirs have *different* temperatures (or chemical potentials) is consistent with expectation that the property of return to equilibrium does not hold if one starts with asymmetric boundary conditions. This *motivates* the introduction of the so-called C-Liouvillean, which has a non-trivial kernel even when one starts with asymmetric initial conditions, for the study of non-equilibrium steady states (NESS). The C-Liouvillean was introduced for the first time in [JP3].

6.2 NESS and the C-Liouvillean

Consider the Model $C_n, n > 1$, such that the unperturbed initial state of the system is

$$\Omega = \Omega^{\Sigma} \otimes \Omega_{\beta_1} \otimes \cdots \Omega_{\beta_n} \ , \tag{6.71}$$

where, without loss of generality, Ω^{Σ} is the vector in $\mathcal{H}^{\Sigma} \otimes \mathcal{H}^{\Sigma}$ corresponding to the trace state, and Ω_{β_i} the vacuum of $\mathcal{F}_{-}^{\mathcal{R}_i}(L^2(\mathbf{R}; \mathcal{B}))$.[†] Construct the Banach space $C(\mathcal{O}, \Omega)$, which is the vector space $\mathcal{O}\Omega = \{A\Omega : A \in \mathcal{O}\}$ with norm $\|A\Omega\|_{\infty} = \|A\|$. There is a Banach space isomorphism,

$$\mathcal{O} \ni A \to A\Omega \in C(\mathcal{O}, \Omega) \ . \tag{6.72}$$

Under the isomorphism (6.72), the time evolution from time t' to t is mapped to

$$\alpha_g^{t,t'}(A) \to \widetilde{U}_g(t', t) A\Omega \ , \tag{6.73}$$

such that $\widetilde{U}_g(t', t)\Omega = \Omega$. Let L_g be the generator of $\widetilde{U}_g$, such that

$$\partial_t \widetilde{U}_g(t, t') = -iL_g(t)\widetilde{U}_g(t, t') \tag{6.74}$$

$$\widetilde{U}_g(t, t) = 1 \ . \tag{6.75}$$

Differentiating both sides of the equation

$$\alpha_g^{t,t'}(A)\Omega = \widetilde{U}_g(t', t) A\Omega$$

with respect to t and setting $t = t'$ gives

$$\begin{aligned}
[(\mathcal{L}_0 + gV(t))A - A(\mathcal{L}_0 + gV(t))]\Omega &= [(\mathcal{L}_0 + gV(t))A - (V(t)A^*)^*]\Omega \\
&= (\mathcal{L}_0 + gV(t) - gJ\Delta^{1/2}V(t)\Delta^{-1/2}J)A\Omega \\
&\equiv L_g(t)A\Omega \ ,
\end{aligned}$$

where $J = J^{\Sigma} \otimes J^{\mathcal{R}_1} \otimes \cdots \otimes J^{\mathcal{R}_n}$ and $\Delta = \mathbf{1}^{\Sigma} \otimes \Delta^{\mathcal{R}_1} \otimes \cdots \otimes \Delta^{\mathcal{R}_n}$ are the modular conjugation and the modular operator of the Model C_n.

We define the C-Liouvillean to be

$$L_g(t) := \mathcal{L}_0 + gV(t) - gJ\Delta^{1/2}V(t)\Delta^{-1/2}J \ . \tag{6.76}$$

Assumption (C_n.3) on the perturbation is sufficient to show that $L_g(t)$ satisfy the conditions of the Yosida-Hille-Phillips Theorem, and Theorem X.70 in [RS2], and hence $\widetilde{U}_g^t \equiv \widetilde{U}_g(t, 0)$ can be extended to a strongly continuous group on the Banach space $C(\mathcal{O}, \Omega)$.

[†]The results of this section hold for initial states that are normal to Ω.

We will show later in this chapter that when the perturbation is time-independent, the state of the coupled system converges to a non-equilibrium steady state. The NESS is related to the zero energy resonance of the adjoint of the C-Liouvillean. Before doing so, we study the spectrum of $L_g(t)$, which is generally time-dependent. (As an application of the latter, we will prove a novel adiabatic theorem for states close to NESS in chapter 8.)

The results of the previous section regarding complex deformations are directly translated to this case.

6.3 Spectrum of the C-Liouvillean for C_n

We study the spectrum of the (adjoint of the) C-Liouvillean for Model C_n in the time-dependent case using the method of complex deformations as developed earlier in this chapter; (see also [JP1,2,3]). The deformed adjoint of the C-Liouvillean is

$$L_g^*(t,\theta) := U(\theta)L_g^*(t)U(-\theta) = \mathcal{L}_0 + N\theta + g\widetilde{V}^{tot}(t,\theta) \ , \tag{6.77}$$

where $\mathcal{L}_0 = \mathcal{L}^\Sigma + \sum_i \mathcal{L}^{\mathcal{R}_i}$, $\mathcal{L}^{\mathcal{R}_i} = d\Gamma(u_i), i = 1, \cdots, n$, and

$$\begin{aligned}\widetilde{V}^{tot}(t,\theta) \ &= \ \sum_i \{\sigma_+ \otimes \mathbf{1}^\Sigma \otimes b(f_{i,\beta}^{(\theta)}(t)) + \sigma_- \otimes \mathbf{1}^\Sigma \otimes b^*(f_{i,\beta}^{(\theta)}(t)) \\ &- \ i\mathbf{1}^\Sigma \otimes \sigma_+ \otimes (-1)^{N_i} b(e^{-\beta_i(u_i-\nu)/2} f_{i,\beta_i}^{\#(\theta)}(t)) - i\mathbf{1}^\Sigma \otimes \sigma_- \otimes (-1)^{N_i} b^*(e^{\beta_i(u_i-\nu)/2} f_{i,\beta_i}^{\#(\theta)})\} \ .\end{aligned}$$

Let

$$P_g'(t,\theta) := \oint_\gamma \frac{dz}{2\pi i}(z - L_g^*(t,\theta))^{-1} \ , \tag{6.78}$$

where the contour γ as in section 6.1, and $T_g'(t) := P_0 P_g'(t,\theta) P_0$, and

$$S_g'(t,\theta) := (T_g'(t))^{-1/2} P_0 P_g'(t,\theta) : Ran(P_g'(t,\theta)) \to \mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma \tag{6.79}$$

which we will show has an inverse

$$(S_g')^{-1}(t,\theta) := P_g'(t,\theta) P_0 (T_g')^{-1/2}(t) : \mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma \to Ran(P_g'(t,\theta)) \ . \tag{6.80}$$

Moreover, let

$$M_g'(t) := P_0 P_g'(t,\theta) L_g(t,\theta) P_g'(t,\theta) P_0 \ , \tag{6.81}$$

and define the quasi-C-Liouvillean

$$\Sigma_g'(t) := S_g'(t,\theta) P_g'(t,\theta) L_g^*(t,\theta) P_g'(t,\theta)(S_g')^{-1}(t,\theta) = (T_g')^{-1/2}(t) M_g'(t)(T_g')^{1/2}(t) \ , \tag{6.82}$$

which is nothing but the mapping of the reduced C-Liouvillean $\widetilde{L_g} = P_g' L_g P_g'$ from $Ran(P_g')$ to $\mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma$.

Theorem 6.8

Suppose (C_n.2) and (C_n.3) (see section 4.4). Then there is a constant $g_1 > 0$ such that the following holds.

(i) Assume that $(g,\theta) \in \mathbf{C} \times I^-(\delta)$, then $\mathcal{D}(L_g^*(t,\theta)) = \mathcal{D}$ and $(L_g^*(t,\theta))^* = L_{\overline{g}}(t,\overline{\theta})$. Moreover, the spectrum of $L_g^*(t,\theta)$ satisfies

$$\sigma(L_g^*(t,\theta)) \subset \{z \in \mathbf{C} : Imz \leq C(g,\theta)\} \ , \tag{6.83}$$

where

$$C(g,\theta) := \sup_{t\in\mathbf{R}} \{2\frac{|Reg|}{\delta - Img}|Im\theta|^{1/2} + |Img||Im\theta|^{-1/2}\} \times \\ \times \sum_i \{\|f_{i,\beta_i}(t)\|_{H^2(\delta,\mathcal{B})} + \|e^{-\beta_i(u_i-\nu)/2} f_{i,\beta_i}(t)\|_{H^2(\delta,\mathcal{B})}\} \ .$$

Furthermore, if $Imz > C(g,\theta)$, then

$$\|(L_g^*(t,\theta) - z)^{-1}\| \leq \frac{1}{Imz - C(g,\theta)} \ , \tag{6.84}$$

and the map $(g,\theta) \to L_g^*(t,\theta)$ from $\mathbf{C} \times I^-(\delta)$ to the set of closed operators on $\mathcal{H}$ is an analytic family in each variable separately.

(ii) If $|g| < g_1|Im\theta|$, then the spectrum of the operator $L_g^*(t,\theta)$ in the half-plane $\Xi(Im\theta + \frac{|g|}{g_1})$ is purely discrete and independent of θ. If $|g| < \frac{1}{4}g_1|Im\theta|$, then the spectral projection $P_g'(t,\theta)$ associated to the spectrum of $L_g^*(t,\theta)$ in the half-plane $\Xi(Im\theta + \frac{|g|}{g_1})$ is analytic in g and satisfies the estimate

$$\|P_g'(t,\theta) - P_0\| < \frac{3|g|}{g_1|Im\theta|} \ . \tag{6.85}$$

(iii) If $|g| < \frac{g_1|Im\theta|}{4}$, then, for each fixed time t, the quasi-C-Liouvillean $\Sigma_g'(t)$ defined in (6.82) depends analytically on g, and has a Taylor expansion of the form

$$\Sigma_g'(t) = \mathcal{L}^\Sigma + \sum_{j=1}^\infty g^{2j}(\Sigma')^{(2j)} \ . \tag{6.86}$$

The first non-trivial coefficient in (6.86) is

$$(\Sigma')^{(2)}(t) = \frac{1}{2}\oint_\gamma \frac{dz}{2\pi i}\{P_0\widetilde{V}^{tot}(\theta,t)(z-\mathcal{L}_0(\theta))^{-1}\widetilde{V}^{tot}(\theta,t)P_0(z-\mathcal{L}^\Sigma)^{-1} + \\ + (z-\mathcal{L}^\Sigma)^{-1}P_0\widetilde{V}^{tot}(\theta,t)(z-\mathcal{L}_0(\theta))^{-1}\widetilde{V}^{tot}(\theta,t)P_0\} \ .$$

(iv) For $g \in \mathbf{R}$ and Imz large enough,

$$s - \lim_{Im\theta\uparrow 0}(L_g^*(t,\theta) - z)^{-1} = (L_g^*(t,Re\theta) - z)^{-1} \ , \tag{6.87}$$

for each fixed time $t \in \mathbf{R}$.

The proof of the claims of Theorem 6.8 are very similar to those in section 6.1: the proof of claim (i) is similar to that of Lemma 6.3, of claim (ii) to Proposition 6.4, of claim (iii) to Proposition 6.5 and of claim (iv) to Lemma 6.6. In order to avoid redundancy, we will not repeat the proofs.

We are interested in the spectrum of the adjoint of the C-Liouvillean in order to prove convergence to NESS and an adiabatic theorem for states close to NESS. Let $k = min(\frac{\pi}{\beta_1}, \cdots, \frac{\pi}{\beta_n}, \delta)$, where δ appears in assumption $(C_n.3)$, and choose $\theta \in I^-(k)$.

Proposition 6.9 (Spectrum of $L_g^*(\theta)$)

Assume $(C_n.2)$ and $(C_n.3)$, choose $\theta \in I^-(k)$ and fix $t \in \mathbf{R}$. Then there exists a constant $g_1 > 0$ independent of t and θ, such that, for $0 < |g| < g_1$, the essential spectrum of $L_g^*(\theta, t)$, $\sigma_{ess}(L_g^*(\theta, t)) \in \mathbf{C}\backslash\Xi(-\mu)$, where $\mu = |Im\theta|$, and the discrete spectrum $\sigma_{disc}(L_g^*(\theta)) \in \Xi(-\mu)$, with all eigenvalues in the lower half-plane *except* for *one* eigenvalue at zero.

Proof. Since we assumed $(C_n.2)$ and $(C_n.3)$, the results of Theorem 6.8 hold. Similar to the proof of Theorem 6.7, the essential spectrum $\sigma(L_g^*(\theta, t)) \in \mathbf{C}\backslash\Xi(-\mu)$ for $|g| < g_1$. The perturbation of the discrete spectrum can be studied by mapping the reduced operator $P_g'(\theta, t)L_g^*(\theta, t)P_g'(\theta, t)$ to the quasi-C-Liouvillean $\Sigma_g'(t)$, defined in (6.76), which acts on $\mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma$, as in Theorem 6.7, section 6.7.

The remaining discussion is very similar to the proof of Theorem 6.7. Let

$$(\Gamma')_k^{(2)}(t) := P_k(\Sigma')^{(2)}(t)P_k \ . \tag{6.88}$$

Applying the Cauchy integration formula to (6.88) gives

$$(\Gamma')_3^{(2)}(t) = \frac{1}{2}\{P_3P_0\sigma_+ \otimes \mathbf{1}^\Sigma \otimes b(f_{i,\beta_i}^{(\theta)}(t))(2 - \mathcal{L}_0(\theta))^{-1}\sigma_- \otimes \mathbf{1}^\Sigma \otimes b^*(f_{i,\beta_i}^{(\theta)}(t))P_0P_3$$
$$+ P_3P_0\mathbf{1}^\Sigma \otimes \sigma_+ \otimes b(e^{-\beta_i(u_i-\nu)/2}f_{i,\beta_i}^{\#(\theta)}(t))(2 - \mathcal{L}_0(\theta))^{-1}\mathbf{1}^\Sigma \otimes \sigma_- \otimes b^*(e^{\beta_i(u_i-\nu)/2}f_{i,\beta_i}^{\#(\theta)}(t))P_0P_3\} \ .$$

It follows that

$$Re(\Gamma')_3^{(2)} = \sum_{i=1}^n \mathcal{PV}\int_{\mathbf{R}} du \frac{\|f_{i,\beta_i}(u,t)\|_{\mathcal{B}}^2}{2-u} \ , \tag{6.89}$$

$$Im(\Gamma')_3^{(2)} = -\pi\sum_{i=1}^n \int_{\mathbf{R}} du \|f_{i,\beta_i}(u,t)\|_{\mathcal{B}}^2 \delta(u-2) = -\pi\sum_{i=1}^n \|f_{i,\beta_i}(2,t)\|_{\mathcal{B}}^2 \ . \tag{6.90}$$

Similarly,

$$Re(\Gamma')_2^{(2)} = -\sum_{i=1}^n \mathcal{PV}\int_{\mathbf{R}} du \frac{\|f_{i,\beta_i}(u,t)\|_{\mathcal{B}}^2}{2-u} \ , \tag{6.91}$$

$$Im(\Gamma')_2^{(2)} = -\pi\sum_{i=1}^n \int du_{\mathbf{R}} \|f_{i,\beta_i}(u,t)\|_{\mathcal{B}}^2 \delta(u-2) = -\pi\sum_{i=1}^n \|f_{i,\beta_i}(2,t)\|_{\mathcal{B}}^2 \ . \tag{6.92}$$

Now apply degenerate perturbation theory for the zero eigenvalue. Using the definition of f_{i,β_i} and $f^{\#}_{i,\beta_i}$ given in section 4.4,

$$Re(\Gamma')^{(2)}_{0,1} = 0 , \tag{6.93}$$

$$Im(\Gamma')^{(2)}_{0,1} = -\pi \sum_{i=1}^{n} \frac{\|\widetilde{f}_i(2,t)\|^2_{\mathcal{B}}}{cosh(\beta_i(2-\nu)/2)} \begin{pmatrix} e^{\beta_i(2-\nu)/2} & -e^{\beta_i(2-\nu)/2} \\ -e^{-\beta_i(2-\nu)/2} & e^{-\beta_i(2-\nu)/2} \end{pmatrix} . \tag{6.94}$$

Therefore, to second order in the coupling g,

$$E'_{2,3}(t,g) = \pm(2+g^2\mathcal{P}V\int_{\mathbf{R}} du \frac{1}{2-u} \sum_{i=1}^{n} \|f_{i,\beta_i}(u,t)\|^2_{\mathcal{B}}) - i\pi g^2 \sum_{i=1}^{n} \|f_{i,\beta_i}(2,t)\|^2_{\mathcal{B}} + O(g^4) , \tag{6.95}$$

while

$$E'_{1,2}(g,t) = g^2 a_{1,2}(t) + O(g^4) , \tag{6.96}$$

where $a_{1,2}(t)$ are the eigenvalues of the matrix

$$-i\pi \sum_{i=1}^{n} \frac{\|\widetilde{f}_i(2,t)\|^2_{\mathcal{B}}}{2\cosh(\beta_i(2-\nu)/2)} \begin{pmatrix} e^{\beta_i(2-\nu)/2} & -e^{\beta_i(2-\nu)/2} \\ -e^{-\beta_i(2-\nu)/2} & e^{-\beta_i(2-\nu)/2} \end{pmatrix} . \tag{6.97}$$

Since Ω is an eigenvector corresponding to the isolated zero eigenvalue of $L_g(\theta,t)$ (by construction, $L_g(t,\theta)\Omega = 0$), then zero is also an isolated eigenvalue of $L^*_g(\theta,t)$. (One way of seeing this is to take the adjoint of the spectral projection of $L_g(\theta,t)$ corresponding to Ω, which is defined using the resolvent and functional calculus.) In fact, $\psi = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ is the eigenvector corresponding to the zero eigenvalue of $(\Sigma'_g)^2(t)$. Hence,

$$E'_0(g,t) = 0 , \tag{6.98}$$

$$E'_1(g,t) = -i\pi g^2 \sum_{i=1}^{n} \|\widetilde{f}_i(2,t)\|^2_{\mathcal{B}} + O(g^4) . \tag{6.99}$$

Moreover, we know from Theorem 6.8, (iv), that $s - \lim_{Im\theta\uparrow 0}(z - L^*_g(\theta,t))^{-1} = (z - L^*_g(Re\theta,t))^{-1}$ for Imz big enough, and hence the claim of this proposition. □

The following corollary says that when the interaction is *time-independent*, $V(t) = V$, the coupled system converges to a non-equilibrium steady-state exponentially fast. *This result has been proven in [JP3], but we mention it for the sake of completeness.* The NESS will correspond to the zero energy resonance of L^*_g. This provides some of the background for stating and proving a novel adiabatic theorem for states close to NESS in chapter 8.

Let D be a positive bounded operator on $\mathcal{H}$ such that $Ran(D)$ is dense in $\mathcal{H}$ and $D\Omega = \Omega$.

Corollary 6.10 (NESS)

Suppose assumptions (C_n.2) and (C_n.3), and that the perturbation $V(t) \equiv V$ is *time-independent*. Then there exists $g_1 > 0$ such that, for $|g| < g_1$ and $a \in \mathcal{D}(D^{-1})$, the following limit exists,

$$\lim_{t\to\infty} \langle \Omega, \alpha_g^t(a)\Omega\rangle = \langle \Omega_g, D^{-1} a\Omega\rangle \ , \tag{6.100}$$

where Ω_g corresponds to the zero-energy resonance of L_g^*, and α_t^g is the perturbed dynamics. This limit is exponentially fast, with relaxation time $\tau_R = O(g^{-2})$.

Proof. Choose $k = \min(\frac{\pi}{\beta_1}, \cdots, \frac{\pi}{\beta_n}, \delta)$, where δ appears in assumption (C_n.3), and let $\theta \in I^-(k)$. We already know the spectrum of $L_g^*(\theta)$ from Proposition 6.9. Let

$$D := \mathbf{1}^\Sigma \otimes \mathbf{1}^\Sigma \otimes e^{-k\widetilde{A}_{\mathcal{R}_1}} \otimes \cdots \otimes e^{-k\widetilde{A}_{\mathcal{R}_n}} \ , \tag{6.101}$$

where $\widetilde{A}_{\mathcal{R}_j} = d\Gamma(\sqrt{p_j^2+1})$, and $p_j = i\partial_{u_j}$ is the generator of energy translations for the $\mathcal{R}_j$ reservoir, $j = 1, \cdots, n$. Moreover, let $\mathbf{h}^{test} = D(e^{k\sqrt{p^2+1}})$, and $\mathcal{O}^{test} = \mathcal{F}_-(\mathbf{h}^{test})$, which is dense in $\mathcal{F}_-(L^2(\mathbf{R};\mathcal{B}))$. For $a \in \mathcal{O}^\Sigma \otimes \mathcal{O}_1^{test} \otimes \cdots \mathcal{O}_n^{test}$,

$$\lim_{t\to\infty} \langle \Omega, \alpha_g^t(a)\Omega\rangle = \lim_{t\to\infty} \langle \Omega, e^{itL_g} a e^{-itL_g}\Omega\rangle \tag{6.102}$$

$$= \lim_{t\to\infty} \langle e^{-itL_g^*}\Omega, a\Omega\rangle \tag{6.103}$$

$$= \lim_{t\to\infty} \langle e^{-itL_g^*(\theta)}\Omega, a(\overline{\theta})\Omega\rangle \tag{6.104}$$

$$= \lim_{t\to\infty} \frac{1}{2\pi i}\langle \int_{-\infty}^{\infty} du(u+i\eta - L_g^*(\theta))^{-1} e^{-i(u+i\eta)t}\Omega, a(\overline{\theta})\Omega\rangle \ , \tag{6.105}$$

for $\eta > 0$. One may decompose the last integral into two parts (as in the proof of Theorem 6.7,(ii)). The first part is

$$\lim_{t\to\infty} \frac{1}{2\pi i}\langle \oint_\gamma dz(z - L_g^*(\theta))^{-1} e^{-izt}\Omega, a(\overline{\theta})\Omega\rangle = \langle \Omega_g, D^{-1}a\Omega\rangle \ , \tag{6.106}$$

where the zero energy resonance is

$$\Omega_g := DU(-\theta)P_g'(\theta)U(\theta)D\Omega = DU(-\theta)P_g'(\theta)\Omega \ . \tag{6.107}$$

The second term converges to zero exponentially fast as $t \to \infty$, since

$$\frac{1}{2\pi i}\langle \int_{-\infty}^{\infty} (u - i(\mu-\epsilon) - L_g^*(\theta))^{-1} e^{-i(u-i(\mu-\epsilon))t}\Omega, a(\overline{\theta})\Omega\rangle = O(e^{-(\mu-\epsilon')t}) \ , \tag{6.108}$$

where $0 < \epsilon' < \epsilon < |Im\theta| = \mu$.

□

6.4 Existence of the *deformed* time evolution

In the following we let

$$A(t) := \mathcal{L}_0 + g\mathbf{V}^{tot}(t) \tag{6.109}$$

where $\mathbf{V}^{tot}(t)$ equals $V(t) - JV(t)J$ or $V(t) - J\Delta^{-1/2}V(t)\Delta^{1/2}J$, ie, $A(t) = \mathcal{L}_g(t)$ or $L_g^*(t)$. We also make the following assumption.

(C_n.7) Assume (C_n.1) if $A(t) = \mathcal{L}_g$, and assume (C_n.3) if $A(t) = L_g^*$. (see section 4.4)

Let $\mathbf{U}(t)$ be the propagator generated by $A(t)$, and which satisfies the initial value problem

$$\partial_t \mathbf{U}(t) = -iA(t)\mathbf{U}(t) \ , \mathbf{U}(t=0) = 1 \ , \tag{6.110}$$

ie, $\mathbf{U}(t) = U_g(t)$ if $A(t) = \mathcal{L}_g(t)$, and $\mathbf{U}(t) = \widetilde{U}_g(t)$ if $A(t) = L_g^*(t)$. (Remark regarding the notation: In the previous section, $\widetilde{U}_g$ was generated by L_g, but it will denote the propagator generated by L_g^* here.)

Choose $\theta \in I^-(\delta)$, where δ appears in assumption (C_n.7), and let $A(t,\theta) := U(\theta)A(t)U(-\theta)$. The *deformed* time evolution is given by the propagator $\mathbf{U}(t,t',\theta)$ which satisfies the initial value problem

$$\partial_t \mathbf{U}(t,t',\theta) = -iA(t,\theta)\mathbf{U}(t,t',\theta) \ , \mathbf{U}(t,t,\theta) = 1 \ . \tag{6.111}$$

The following two Lemmas guarantee the existence of $\mathbf{U}(t,t',\theta)$. Let $\mathcal{E}_i \subset \mathcal{F}_-^{\mathcal{R}_i}(L^2(\mathbf{R};\mathcal{B}))$ the set of entire states for $U_i(\theta)$, $\mathcal{C} = \mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma \otimes (D(\mathcal{L}^{\mathcal{R}_1}) \cap \mathcal{E}_1) \otimes \cdots \otimes (D(\mathcal{L}^{\mathcal{R}_n}) \cap \mathcal{E}_n)$, and

$$C := \sup_{t\in\mathbf{R}} \sup_{\theta \in I^-(\delta)} \|\mathbf{V}^{tot}(t,\theta)\| \ . \tag{6.112}$$

Lemma 6.11

Assume (C_n.7), choose $\theta \in I^-(\delta) \cup \mathbf{R}$ and $|g| < g_1$, and fix $t \in \mathbf{R}$. Then

(i) $A(t,\theta)$ with domain $\mathcal{D}$ generates a contraction semi-group $e^{-i\sigma A(t,\theta)}, \sigma \geq 0$ on $\mathcal{H}$, such that

$$\|(iA(t,\theta) - z)^{-1}\| \leq |Re(z+C)|^{-1} \ , \tag{6.113}$$

for $Rez < 0$.

(ii) The $\mathcal{B}(\mathcal{H})$-valued function $e^{-i\sigma A(t,\theta)}$ is analytic in $\theta \in I^-(\delta)$. For $\theta' \in \mathbf{R}$ and $\theta \in I^-(\delta) \cup \mathbf{R}$,

$$U(\theta')e^{-i\sigma A(t,\theta)}U(-\theta') = e^{-i\sigma A(t,\theta+\theta')} \ . \tag{6.114}$$

Proof. Claim (i) follows from Phillip's Theorem for the perturbation of semigroups (see [Ka1] chapter IX). Analyticity of $e^{-i\sigma A(t,\theta)}$ and (6.114) follow from assumption (C_n.7), the resolvent equation

$$(A(t,\theta)-z)^{-1} = (\mathcal{L}_0(\theta)-z)^{-1}(1+\mathbf{V}^{tot}(t,\theta)(\mathcal{L}_0(\theta)-z)^{-1})^{-1} \ ,$$

$$U(\theta')A(t,\theta)U(-\theta') = A(t,\theta+\theta') \ ,$$

and the fact that

$$e^{-i\sigma A(t,\theta)} = \frac{1}{2\pi i}\int_\Gamma e^{-\sigma z}(iA(t,\theta)-z)^{-1}dz \ ,$$

where Γ is a contour encircling the spectrum of $A(t)$. □

Lemma 6.12

Assume (C_n.7) and let $\theta \in I^-(\delta)\cup\mathbf{R}$, $|g| < g_1$. Then (6.111) generates a unique propagator $\mathbf{U}(t,t',\theta)$ such that the following hold.

(i) $\mathbf{U}(t,t',\theta)\mathbf{U}(t',t'',\theta) = \mathbf{U}(t,t'',\theta)$ for $t \geq t' \geq t''$.

(ii) $\mathbf{U}(t,t',\theta)\mathcal{D} \subset \mathcal{D}$, and for $\psi \in \mathcal{D}$, $\mathbf{U}(t,t',\theta)\psi$ is differentiable in t and t' such that

$$\partial_t \mathbf{U}(t,t',\theta)\psi = -iA(t,\theta)\mathbf{U}(t,t',\theta)\psi \ , \tag{6.115}$$

$$\partial_{t'} \mathbf{U}(t,t',\theta)\psi = i\mathbf{U}(t,t',\theta)A(t',\theta)\psi \ . \tag{6.116}$$

(iii) For $\theta' \in \mathbf{R}$,

$$U(\theta')\mathbf{U}(t,t',\theta)U(-\theta') = \mathbf{U}(t,t',\theta+\theta') \ . \tag{6.117}$$

Moreover, $\mathbf{U}(t,t',\theta)$ is analytic in $\theta \in I^-(\delta)$.

Proof. Claims (i) and (ii) are consequences of Kato's Theorem [Ka2], to which we refer the reader. Without loss of generality, rescale time such that $t = \tau s, s \in [0,1]$, and let $A^n(s\tau,\theta) = A(\tau\frac{k}{n},\theta)$ for $n \in \mathbf{N}^+$ and $s \in [\frac{k}{n},\frac{k+1}{n}], k = 0,\cdots,n-1$. Moreover, define $\mathbf{U}^n(\tau s,\tau s',\theta) = e^{-i\tau(s-s')A^n(\tau\frac{k}{n},\theta)}$ if $\frac{k}{n} \leq s' \leq s \leq \frac{k+1}{n}$, and $\mathbf{U}^n(\tau s,\tau s',\theta) = \mathbf{U}^n(\tau s,\tau s'',\theta)\mathbf{U}^n(\tau s'',\tau s',\theta)$ if $0 \leq s' \leq s'' \leq s \leq 1$. It follows from Lemma 6.11 that, for $\theta' \in \mathbf{R}$,

$$U(\theta')\mathbf{U}^n(\tau s,\tau s',\theta)U(-\theta) = \mathbf{U}^n(\tau s,\tau s',\theta+\theta') \ ,$$

and that $\mathbf{U}^n(\tau s,\tau s',\theta)$ is analytic in $\theta \in I^-(\delta)$, where δ appears in (C_n.7). Claim (iii) follows by taking the $n \to \infty$ limit. □

Chapter 7

Isothermal theorem and (reversible) isothermal processes

In this chapter, we investigate isothermal processes of a finitely extended, driven quantum system Σ in contact with an infinite heat bath $\mathcal{R}$ at inverse temperature β from the point of view of quantum statistical mechanics. A theorem characterizing *reversible* isothermal processes as *quasi-static* processes ("*isothermal theorem*") is described, which is an adiabatic theorem for states close to thermal equilibrium at constant temperature. We also discuss corollaries of this theorem and their physical significance pertaining to the changes of entropy and free energy in reversible isothermal processes and on the 0^{th} law of thermodynamics.

As discussed in chapter 2, the dynamics of a system composed of a small system Σ with a finite dimensional Hilbert space coupled to an infinitely extended dispersive reservoir is generated by a (generally time-dependent) thermal Hamiltonian, or *standard* Liouvillean,

$$\mathcal{L}_g(t) := \mathcal{L}_0(t) + g(t)I \ , \tag{7.1}$$

where

$$\mathcal{L}_0(t) = (\mathbf{1} \otimes \mathbf{1}) \otimes \mathcal{L}_\beta^{\mathcal{R}} + (H_0^{\Sigma}(t) \otimes \mathbf{1}) \otimes \mathbf{1} - (\mathbf{1} \otimes H_0^{\Sigma}(t)) \otimes \mathbf{1} \tag{7.2}$$

is the Liouvillean of the uncoupled system, $\mathcal{L}_\beta^{\mathcal{R}}$ is the Liouvillean of the heat bath, $H_0^{\Sigma}(t)$ is the Hamiltonian of the small system, and where $g(t)I$ is a spatially localized term describing the interactions between $\mathcal{R}$ and Σ, with a time-dependent coupling constant $g(t)$.

We will only consider heat baths with a unique equilibrium $\Omega_\beta^{\mathcal{R}}$ state at each temperature (ie, with no phase coexistence). We have seen in chapters 3 that if $\mathcal{L}_0(t) \equiv \mathcal{L}_0$ and $g(t) \equiv g$ are independent of t, for $t \geq t_*$, "return to equilibrium" holds true if we can prove that $\mathcal{L}_g$ has a simple eigenvalue at 0 and that the spectrum, $\sigma(\mathcal{L}_g)$, of $\mathcal{L}_g$ is purely continuous away from 0. The eigenvector, $\Omega_\beta \equiv \Omega_\beta^{\Sigma \vee \mathcal{R}}$, of $\mathcal{L}_g$ corresponding to the eigenvalue 0 is the thermal equilibrium state of the coupled system $\Sigma \vee \mathcal{R}$ at temperature $(k_B\beta)^{-1}$. Under suitable hypotheses on $\mathcal{R}$ and Σ, we have shown the property of RTE in the mixing case is described by an *exponential* *law* involving a finite *relaxation time*, $\tau_{\mathcal{R}}$; (see chapters 5 and 6 where the property of RTE has been verified for physical models).

If the interacting Liouvillean $\mathcal{L}_g(t)$ of $\Sigma \vee \mathcal{R}$ depends on time t, but with the property that, for all times t, $\mathcal{L}_g(t)$ has a simple eigenvalue at 0 corresponding to an eigenvector $\Omega_\beta(t)$, then $\Omega_\beta(t)$ can be viewed as an *instantaneous equilibrium* (or *reference*) *state*, and $\tau_{\mathcal{R}}(t)$ is called instantaneous relaxation time of $\Sigma \vee \mathcal{R}$. Let τ be the time scale over which $\mathcal{L}_g(t)$ changes appreciably. Assuming that, at some time t_0, the state , $\Psi(t_0)$, of $\Sigma \vee \mathcal{R}$ is given by $\Omega_\beta(t_0)$, it is natural to compare the state $\Psi(t)$ of $\Sigma \vee \mathcal{R}$ at a *later* time t with the instantaneous equilibrium state $\Omega_\beta(t)$ and to estimate the norm of the difference $\Psi(t) - \Omega_\beta(t)$. One would expect that if $\tau \gg \sup_t \tau_{\mathcal{R}}(t)$, then

$$\Psi(t) \simeq \Omega_\beta(t) \ .$$

In this chapter, we prove an adiabatic theorem for states close to thermal equilibrium, which we call "*isothermal theorem*", saying that

$$\Psi(t) \overset{\tau\to\infty}{\to} \Omega_\beta(t) \ , \tag{7.3}$$

for all times $t \geq t_0$. The physical consequences of this theorem have been sketched in chapter 2; e.g., to show that *quasi-static* ($\tau \to \infty$) isothermal processes are *reversible* and that, in the quasi-static limit, a variant of the 0^{th} *law* holds. We propose general definitions of heat flux and of entropy for trajectories of states of $\Sigma \vee \mathcal{R}$ sampled in arbitrary isothermal processes and use the isothermal theorem to relate these definitions to more common ones from equilibrium statistical mechanics.

7.1 An adiabatic theorem

In this section we carefully state and prove an adiabatic theorem, which is a slight improvement of results in [AE,Te] concerning adiabatic theorems for Hamiltonians without spectral gaps. Our simplest result follows from those in [AE,Te] merely by eliminating the superfluous hypothesis of semiboundedness of the generator of time evolution.

Let $\mathcal{H}$ be a separable Hilbert space, and let $\{L(s)\}_{s\in I}$, with $I \subset \mathbf{R}$ a compact interval, be a family of selfadjoint operators on $\mathcal{H}$ with the following properties:

(H7.1) The operators $L(s), s \in I$, are selfadjoint on a common domain, $\mathcal{D}$, of definition dense in $\mathcal{H}$.

(H7.2) The resolvent $R(i,s) := (L(s)-i)^{-1}$ is bounded and differentiable, and $L(s)\dot{R}(i,s)$ is bounded uniformly in $s \in I$, where $(\dot{\ })$ denotes the derivative with respect to s.

Lemma 7.1 (Existence of time evolution). If assumptions (H7.1) and (H7.2) hold then there exist unitary operators $\{U(s,s')|s,s'\in I\}$ with the properties:

For all s, s', s'' in I,

$$U(s,s)=\mathbf{1}\ ,U(s,s')U(s',s'')=U(s,s'')\ ,$$

$U(s,s')$ is strongly continuous in s and s', and

$$i\frac{\partial}{\partial s}U(s,s')\Psi=L(s)U(s,s')\Psi\ , \tag{7.4}$$

for arbitrary $\Psi\in\mathcal{D}$, s, s' in I; (U is called a "*propagator*").

Proof. Note that $A(s):=iL(s)+1$ is a generator of a contraction semigroup, which follows from the fact that $A(s)$ satisfies the conditions of the Yosida-Hille theorem: $(-\infty,0]\in\rho(A(s))$ and $||(\lambda+A(s))^{-1}||\le\frac{1}{\lambda}$ for all $\lambda>0$ and every $s\in I$, where $\rho(A(s))$ is the resolvent of $A(s)$ (see, for example, Theorem X.47 in [RS2]). Furthermore, $0\in\rho(A(s))$, for $s,s'\in I$, $A(s')A(s)^{-1}$ is bounded by the closed graph theorem and (H7.1), and for small $|s-s'|$, $\|(s'-s)A(s')^{-1}A(s)-\mathbf{1}\|=\|\dot{A}^{-1}(s)A(s)\|+o(|s-s'|)$ is bounded due to (H7.2). Hence, by Theorem X.70 in [RS2] (or Theorem 2 in Chp XIV [Yo], section 4), $\widetilde{U}^{\tau}(s,s')$, which satisfies the initial value problem

$$\partial_s\widetilde{U}(s,s')=-\tau A(s)\widetilde{U}(s,s')\ ;\ \widetilde{U}(s,s)=1\ ,$$

exists uniformly in $s,s'\in I$ and $s'<s$. The existence of the unitary evolution $U(s,s')$ follows by noting that $U(s,s')=\widetilde{U}(s,s')e^{(s-s')\tau}$. $\square$

In order to prove an adiabatic theorem, one must require some additional assumptions on the operators $L(s)$.

(H7.3) We assume that $L(s)$ has an eigenvalue $\lambda(s)$, that $\{P(s)\}$ is a family of finite rank projections such that $L(s)P(s)=\lambda(s)P(s)$, $P(s)$ is twice continuously differentiable in s with bounded first and second derivatives, for all $s\in I$, and that $P(s)$ is the spectral projection of $L(s)$ corresponding to the eigenvalue $\lambda(s)$ for almost all $s\in I$.

We consider a quantum system whose time evolution is generated by a family of operators

$$L_\tau(t):=L(\frac{t}{\tau}),\ \frac{t}{\tau}=:s\in I\ , \tag{7.5}$$

where $\{L(s)\}_{s\in I}$ satisfies assumptions (H7.1)-(H7.3). The propagator of the system is denoted by $U_\tau(t,t')$. We define

$$U^{(\tau)}(s,s'):=U_\tau(\tau s,\tau s') \tag{7.6}$$

and note that $U^{(\tau)}(s,s')$ solves the equation

$$i\frac{\partial}{\partial s}U^{(\tau)}(s,s')\Psi=\tau L(s)U^{(\tau)}(s,s')\Psi\ ,\Psi\in\mathcal{D}\ , \tag{7.7}$$

and $U^{(\tau)}(s,s) = 1$.

Next, we define

$$L_a(s) := L(s) + \frac{i}{\tau}[\dot{P}(s), P(s)] \tag{7.8}$$

and the corresponding propagator, $U_a^{(\tau)}(s,s')$, which solves the equation

$$i\frac{\partial}{\partial s}U_a^{(\tau)}(s,s')\Psi = \tau L_a(s)U_a^{(\tau)}(s,s')\Psi,\ \Psi \in \mathcal{D}\ , \tag{7.9}$$

and $U_a^{(\tau)}(s,s) = 1$. The propagator $U_a^{(\tau)}$ describes what one calls the *adiabatic time evolution*. (Note that the operators $L_a(s), s \in I$, satisfy (H7.1) and (H7.2), since, by (H7.3), $\frac{i}{\tau}[\dot{P}(s), P(s)]$ are bounded, selfadjoint operators with bounded derivative in s.)

Theorem 7.2 (Adiabatic Theorem).

If assumptions (H7.1)-(H7.3) hold then

(i) $U_a^{(\tau)}(s',s)P(s)U_a^{(\tau)}(s,s') = P(s')$ (*intertwining property*) ,

f*or arbitrary* s, s' in I, *and*

(ii) $\lim_{\tau\to\infty}\sup_{s,s'\in I}||U^{(\tau)}(s,s') - U_a^{(\tau)}(s,s')|| = 0$.

Proof. The proof essentially follows that of [Te].

(i) Equality trivially holds when $s = s'$. Moreover, the derivative of the LHS with respect to s is zero

$$\begin{aligned}
&\partial_s[U_a^{(\tau)}(s',s)P(s)U_a^{(\tau)}(s,s')]\\
&= \dot{U}_a^{(\tau)}(s',s)P(s)U_a^{(\tau)}(s,s') + U_a^{(\tau)}(s',s)\dot{P}(s)U_a^{(\tau)}(s,s') + U_a^{(\tau)}(s',s)P(s)\dot{U}_a^{(\tau)}(s,s')\\
&= -U_a^{(\tau)}(s',s)[\dot{P}(s)P(s) + P(s)\dot{P}(s)]U_a^{(\tau)}(s,s') + U_a^{(\tau)}(s',s)\dot{P}(s)U_a^{(\tau)}(s,s')\\
&= 0\ ,
\end{aligned}$$

using equations (7.7) and (7.9), assumption (H7.3) and the fact that $P(s)\dot{P}(s) + \dot{P}(s)P = \dot{P}(s)$ (the latter follows from differentiating $P^2(s) = P(s)$).

(ii) We will use Cook's argument and an extension of Kato's commutator equation for cases when there is no spectral gap.

Consider $\psi \in \mathcal{D}$. Using the *Duhamel* formula,

$$\begin{aligned}
(U^{(\tau)}(s,s') - U_a^{(\tau)}(s,s'))\psi &= -\int_{s'}^{s} du\partial_u(U^{(\tau)}(s,u)U_a^{(\tau)}(u,s'))\psi\\
&= -\int_{s'}^{s} duU^{(\tau)}(s,u)[\dot{P}(u), P(u)]U_a^{(\tau)}(u,s')\psi\ .
\end{aligned}$$

Since $\mathcal{D}$ is dense in $\mathcal{H}$, it follows that

$$||U^{(\tau)}(s,s') - U_a^{(\tau)}(s,s')|| = ||\int_{s'}^{s} du U^{(\tau)}(s,u)[\dot{P}(u), P(u)]U_a^{(\tau)}(u,s')|| \ .$$

Now, using the commutator equation

$$[\dot{P}(u), P(u)] = [L(u), X_\epsilon(u)] + i\epsilon X_\epsilon(u) \ ,$$

where $X_\epsilon(u) = R(\lambda(u) - i\epsilon, u)\dot{P}(u)P(u) + P(u)\dot{P}(u)R(\lambda(u) + i\epsilon, u)$, one can write the integrand as a total derivative plus a remainder. One may check that the commutator equation is satisfied by direct substitution.

We claim that there is a constant $C < \infty$ such that, for small enough ϵ,

$$\begin{aligned}
&(a)||X_\epsilon(u)|| < \frac{C}{\epsilon} \ , \\
&(b)||\dot{X}_\epsilon(u)|| < \frac{C}{\epsilon^2} \ , \\
&(c)\lim_{\epsilon\to 0} \epsilon^{1/2}||X_\epsilon(u)|| = 0 \ .
\end{aligned}$$

Inequality (a) is a direct consequence of assumptions (H7.1) and (H7.3),

$$\begin{aligned}
||R(\lambda(u) - i\epsilon, u)\dot{P}(u)P(u)|| &\leq ||R(\lambda(u) - i\epsilon, u)||||\dot{P}(u)P(u)|| \\
&< \frac{C}{\epsilon} \ .
\end{aligned}$$

To prove inequality (b), note that, using the resolution of the identity,

$$\begin{aligned}
&\dot{R}(\lambda(u) - i\epsilon, u) = -R(\lambda(u) - i\epsilon, u)(\dot{L}(u) - \dot{\lambda}(u))R(\lambda(u) - i\epsilon, u) \\
&= -R(i,u)(L(s) - i - \lambda(u) + \lambda(u) - i\epsilon + i\epsilon)\times \\
&\quad \times R(\lambda(u) - i\epsilon, u)(\dot{L}(u) - \dot{\lambda}(u))R(\lambda(u) - i\epsilon, u) \\
&= -R(i,u)(\dot{L}(u) - \dot{\lambda}(u))R(\lambda(u) - i\epsilon, u) - \\
&\quad - (\lambda(u) - i\epsilon - i)R(i,u)R(\lambda(u) - i\epsilon, u)(\dot{L}(u) - \dot{\lambda}(u))R(\lambda(u) - i\epsilon, u) \ ,
\end{aligned}$$

and that $\lambda(u) = \frac{Tr(L(u)P(u))}{Tr(P(u))}$ is continuously differentiable since $P(u)$ and $L(u)$ are differentiable.

Inequality (b) now follows from assumptions (H7.1)-(H7.3) for small enough ϵ.

In order to prove (c), consider $\psi \in \mathcal{D}$, and let $\varphi(u) := \dot{P}(u)P(u)\psi$. Since $P(u)\dot{P}(u)P(u) = 0$, it follows that

$$P(u)\varphi(u) = P(u)(1 - P(u))\dot{P}(u)P(u)\psi = 0 \ .$$

Now, using the spectral theorem,

$$\begin{aligned}\lim_{\epsilon^{1/2}\to 0} ||\epsilon^{1/2}X_\epsilon(u)\psi||^2 &= \lim_{\epsilon\to 0} 2\epsilon\langle R(\lambda(u)-i\epsilon,u)\varphi(u), R(\lambda(u)-i\epsilon,u)\varphi(u)\rangle \\ &= \lim_{\epsilon\to 0} 2\epsilon\langle \varphi(u), R(\lambda(u)+i\epsilon,u)R(\lambda(u)-i\epsilon,u)\varphi(u)\rangle \\ &= \lim_{\epsilon\to 0} 2\int_{\sigma(L(u))} d\mu_{\varphi(u)}(\eta)\frac{\epsilon}{(\eta-\lambda(u))^2+\epsilon^2} \\ &= 2\mu_{\varphi(u)}(\lambda(u)) = 0\ ,\end{aligned}$$

since $\varphi(u)\in Ker\{P(s)\}$.

Furthermore, using (7.7) and (7.9),

$$\|\int_{s'}^{s} duU^{(\tau)}(s,u)[L(u),X_\epsilon(u)]U_a^{(\tau)}(u,s')\| \le \frac{1}{\tau}\sup_s\{(2\|\dot{P}(s)P(s)\|+1)\|X_\epsilon(s)\|+\|\dot{X}_\epsilon(s)\|\}\ . \tag{7.10}$$

From (H7.3), equation (7.1), and estimates $(a)-(c)$,(7.10), it follows that

$$\|U^\tau(s,s')-U_a^\tau(s,s')\| < \frac{A}{\tau\epsilon}+\frac{B}{\tau\epsilon^2}+\epsilon^{1/2}C(\epsilon)\ , \tag{7.11}$$

where $A,B<\infty$ are constants independent of ϵ, and $\lim_{\epsilon\to 0}C(\epsilon)=0$. The second claim in the Theorem follows if we choose ϵ such that $\epsilon\to 0$ and $\tau\epsilon^2\to\infty$ as $\tau\to\infty$. $\square$

Remarks.

(1) We note that $U^{(\tau)}(s',s)=U^{(\tau)}(s,s')^*$.

(2) With more precise knowledge about the nature of the spectrum of $\{L(s)\}$, one can obtain information about the speed of convergence in (ii), as $\tau\to\infty$; see chapter 8.

(3) *Adiabatic Theorem for Resonances.* This result resembles the adiabatic theorem described above, but eigenstates of $L(s)$ are replaced by resonance states, and one must require the adiabatic time scale τ to be small as compared to the life time, $\tau_{res}(s)$, of a resonance of $L(s)$, uniformly in $s\in I$. (For shape resonances, the techniques in [FP] are useful; see [A-SF1].)

7.2 The isothermal theorem

In this section, we turn to the study of isothermal processes of "small" driven quantum systems, Σ, in diathermal contact with a heat bath, $\mathcal{R}$, at a fixed temperature $(k\beta)^{-1}$.

Let $\mathcal{L}_g^\tau(t) := \mathcal{L}_g(\frac{t}{\tau})$ denote the Liouvillian of the coupled system $\Sigma\vee\mathcal{R}$, where $\{\mathcal{L}_g(s)\}_{s\in I}$ is as in eqs.(7.1) and (7.2) of section 7.1 and satisfies assumptions (H7.1) and (H7.2) of section 7.2. The interval

$$I_\tau = \{t \mid \frac{t}{\tau} \in I \subset \mathbf{R}\}$$

is the time interval during which an isothermal process of $\Sigma \vee \mathcal{R}$ is studied.

We assume that Σ is driven "slowly", i.e., that τ is large as compared to the relaxation time $\tau_{\mathcal{R}} = \max_{s\in I} \tau_{\mathcal{R}}(s)$ of $\Sigma \vee \mathcal{R}$.

Assumption (H7.3) of section 7.2 is supplemented with the following more specific assumption.

(H7.4) For all $s \in I \equiv [s_0, s_1]$, the operator $\mathcal{L}_g(s)$ has a *single, simple eigenvalue* $\lambda(s) = 0$, the spectrum, $\sigma(\mathcal{L}_g(s))\backslash\{0\}$, of $\mathcal{L}_g(s)$ being *purely continuous* away from 0. It is also assumed that, for $s \le s_0$, $\mathcal{L}_g(s) \equiv \mathcal{L}_g$ is independent of s and has spectral properties sufficient to prove return to equilibrium, as discussed in chapters 5 and 6.

Let $\Omega_\beta(s) \in \mathcal{H}$ denote the eigenvector of $\mathcal{L}_g(s)$ corresponding to the eigenvalue 0, for $s \le s_1$. Then $\Omega_\beta(\frac{t}{\tau})$ is the *instantaneous equilibrium state* of $\Sigma \vee \mathcal{R}$ at time t. Let

$$P_g(s) = |\Omega_\beta(s)\rangle\langle\Omega_\beta(s)| \tag{7.12}$$

denote the orthogonal projection onto $\Omega_\beta(s)$; $P_g(s)$ is assumed to satisfy (H7.3).

Let $\Psi(t)$ be the "true" state of $\Sigma \vee \mathcal{R}$ at time t; in particular

$$\Psi(t) = U_\tau(t,t')\Psi(t') ,$$

where $U_\tau(t,t')$ is the propagator corresponding to $\{L_\tau(t)\}$; see eqs.(7.5)-(7.7), section 7.2. By the property of return to equilibrium and assumption (H7.4),

$$\Psi(t) = \Omega_\beta \ , t \le \tau s_0 , \tag{7.13}$$

for an arbitrary initial condition $\Psi(-\infty) \in \mathcal{H}$ at $t = -\infty$.

We set

$$\Psi^{(\tau)}(s) = \Psi(\tau s) , \tag{7.14}$$

and note that,

$$\Psi^{(\tau)}(s) = U^{(\tau)}(s, s_0)\Omega_\beta , \tag{7.15}$$

for $s \in I$.

Theorem 7.3 (Isothermal Theorem). Suppose that $\mathcal{L}_g(s)$ and $P_g(s)$ satisfy assumptions (H7.1)-(H7.4). Then

$$\lim_{\tau\to\infty} \sup_{s\in I} ||\Psi^{(\tau)}(s) - \Omega_\beta(s)|| = 0 .$$

Proof. This follows readily from equations (7)-(9), (12) and (15), and the Adiabatic Theorem (Theorem 7.2) of Sect.7.2. □

Remarks

(1) We define the expectation values (states)

$$\omega_t^{\beta}(a) := \langle \Omega_\beta(\frac{t}{\tau}), a\Omega_\beta(\frac{t}{\tau})\rangle \tag{7.16}$$

and

$$\rho_t(a) := \langle \Psi(t), a\Psi(t)\rangle \ , \tag{7.17}$$

where a is an arbitrary bounded operator on $\mathcal{H} = \mathcal{H}^{\Sigma\vee\mathcal{R}}$. Then the isothermal theorem says that

$$\rho_t(a) = \omega_t^{\beta}(a) + \epsilon_t^{(\tau)}(a) \ , \tag{7.18}$$

where

$$\lim_{\tau\to\infty} \frac{|\epsilon_t^{(\tau)}(a)|}{||a||} = 0 \ , \tag{7.19}$$

for all times $t \in I_\tau$.

(2) In chapter 8, we show that if the complex spectral deformation techniques, as developed in chapter 6, are applicable to the analysis of the coupled system $\Sigma \vee \mathcal{R}$ then

$$|\epsilon_t^{(\tau)}(a)| \leq \mathcal{O}(\tau^{-1})||a|| \ ; \tag{7.20}$$

.

(3) All the assumptions (H7.1)-(H7.4), are admissible for the classes of systems for which RTE has been established, such as a *quantum dot* interacting with electrons in a metal or a spin impurity interacting with magnons in a magnet; see chapters 5 and 6. For example, suppose that, for a system which is at equilibrium at $s = 0$, the perturbation Hamiltonian $V(s)$ is such that

(a) $\sup_{s\in I} ||V(s) - V(0)|| < \infty$,

(b) $\dot{V}(s)$ and $\ddot{V}(s)$ are bounded ,

(c) $V(s)$ is such that the system possesses the property of RTE at each fixed $s \in I$,

then all the assumptions are satisfied.

(i) Assumption (H7.1) trivially follows from (a), since the perturbation is bounded.

(ii) Assumption (H7.2) follows from (a) and (b) and the resolvent equation

$$(\mathcal{L}_g - i)^{-1} = (\mathcal{L}_0 - i)^{-1}(1 + gI(\mathcal{L}_0 - i)^{-1})^{-1} \ .$$

(iii) Assumptions (H7.3) and (H7.4) follow from (b), (c), (7.12) and the Dyson expansion of the instantaneous equilibrium state when the perturbation has finite norm (see chapter 3).

7.3 (Reversible) isothermal processes

In this section, we study general isothermal processes and use the so called isothermal theorem to characterize *reversible* isothermal processes.

It will be convenient to view the heat bath $\mathcal{R}$ as the *thermodynamic limit* of an increasing family of quantum systems confined to compact subsets of physical space, as discussed in [Ru1,BR] and in chapter 3. The pure states of a quantum mechanical system confined to a bounded region of physical space are unit rays in a separable Hilbert space, while its mixed states are described by density matrices, which are positive trace-class operators with unit trace. Before passing to the thermodynamic limit of the heat bath, the dynamics of the coupled system, $\Sigma \vee \mathcal{R}$, is generated by a family of time-dependent Hamiltonians

$$H(t) \equiv H^{\Sigma \vee \mathcal{R}}(t) := H^{\Sigma}(t) + H^{\mathcal{R}} \ , \tag{7.21}$$

where

$$H^{\Sigma}(t) = H_0^{\Sigma}(t) + g(t)W \ , \tag{7.22}$$

$H_0^{\Sigma}(t)$ is as in section 7.1, and W is the interaction Hamiltonian (as opposed to the interaction Liouvillian, $I = ad_W$, introduced in section 7.1).

Let $\mathsf{P}(t)$ denote the density matrix describing the state of the coupled system, $\Sigma \vee \mathcal{R}$, at time t, (*before* the thermodynamic limit for $\mathcal{R}$ is taken). Then $\mathsf{P}(t)$ satisfies the Liouville equation

$$\dot{\mathsf{P}}(t) = -i[H(t), \mathsf{P}(t)] \ . \tag{7.23}$$

The instantaneous equilibrium-, or reference state of the coupled system is given, in the *canonical* ensemble, by the density matrix

$$\mathsf{P}^{\beta}(t) = Z^{\beta}(t)^{-1} e^{-\beta H(t)} \ , \tag{7.24}$$

where

$$Z^{\beta}(t) = Tr(e^{-\beta H(t)}) \tag{7.25}$$

is the partition function, and Tr denotes the trace. We assume that the thermodynamic limits

$$\rho_t(\cdot) = TD \lim_{\mathcal{R}} Tr(\mathsf{P}(t)(\cdot)) \tag{7.26}$$

$$\omega_t^{\beta}(\cdot) = TD \lim_{\mathcal{R}} Tr(\mathsf{P}^{\beta}(t)(\cdot)) \tag{7.27}$$

exist on a suitable kinematical algebra of operators describing $\Sigma \vee \mathcal{R}$.

The equilibrium state and partition function of a finitely extended heat bath are given by

$$\begin{aligned} \mathsf{P}_{\mathcal{R}}^{\beta} &= (Z_{\mathcal{R}}^{\beta})^{-1} e^{-\beta H^{\mathcal{R}}} \ , & (7.28) \\ Z_{\mathcal{R}}^{\beta} &= Tr(e^{-\beta H^{\mathcal{R}}}) \ , & (7.29) \end{aligned}$$

respectively.

Next, we introduce *thermodynamic potentials* for the small system Σ: The *internal energy* of Σ in the "true" state, ρ_t, of $\Sigma \vee \mathcal{R}$ at time t is defined by

$$U^{\Sigma}(t) := \rho_t(H^{\Sigma}(t)) \tag{7.30}$$

and the *entropy* of Σ in the state ρ_t at time t by

$$S^{\Sigma}(t) := -k\; TD \lim_{\mathcal{R}} Tr(\mathsf{P}(t)[ln\mathsf{P}(t) - ln\mathsf{P}^{\beta}_{\mathcal{R}}]) \; . \tag{7.31}$$

Note that we here define $S^{\Sigma}(t)$ as a *relative* entropy (with the aim of subtracting the divergent contribution of the heat bath to the *total* entropy). It follows from a general inequality for traces that*

$$S^{\Sigma}(t) \leq 0 \; . \tag{7.36}$$

The *free energy* of Σ in an *instantaneous equilibrium state*, ω^{β}_t, of $\Sigma \vee \mathcal{R}$ is defined by

$$F^{\Sigma}(t) := -kT\; TD \lim_{\mathcal{R}} ln(\frac{Z^{\beta}(t)}{Z^{\beta}_{\mathcal{R}}}) \; . \tag{7.37}$$

Lemma. Consider f a real convex function on $\mathbf{R}$, and A and B selfadjoint operators on a Hilbert space $\mathcal{H}$ with discrete spectrum such that $f(A)$ and $f(B)$ are trace-class. Then

$$Tr(f(B) - f(A)) \geq Tr(f'(A)(B-A)) \; .$$

If f is strictly convex, equality holds only when $A = B$.

Proof. Let $\{\psi_j\}_{j=0}^{\infty}$ be an eigenbasis of B, such that $B\psi_j = b_j\psi_j$. Moreover, for $\psi \in \mathcal{H}$, let $c_j := \langle \psi_j, \psi\rangle$. Then

$$\langle \psi, f(B)\psi\rangle = \sum_j |c_j|^2 f(b_j) \tag{7.32}$$

$$\geq f(\sum_j |c_j|^2 b_j) = f(\langle \psi, B\psi\rangle) \; , \tag{7.33}$$

where we have used the convexity of f in the last line. Convexity of f also gives

$$f(\langle \psi, B\psi\rangle) \geq f(\langle \psi, A\psi\rangle) + f'(\langle \psi, A\psi\rangle)\langle \psi, (B-A)\psi\rangle \; . \tag{7.34}$$

When ψ is an eigenvector of A, the RHS of the above inequality becomes

$$\langle \psi, [f(A) + f'(A)(B-A)]\psi\rangle \; . \tag{7.35}$$

Summing over an eigenbasis of A gives

$$Tr(f(B) - f(A)) \geq Tr(f'(A)(B-A)) \; .$$

In particular, for $f(x) = x\log(x)$ and $A \geq 0, B > 0$, we have

$$Tr(A\log A - A\log B) \geq Tr(A - B).$$

Next, we define quantities associated not with states but with the *thermodynamic process* carried out by $\Sigma \vee \mathcal{R}$: the *heat flux* into Σ and the *work rate*, or *power*, of Σ. Let δ denote the so called inexact differential. Then

$$\frac{\delta Q^{\Sigma}}{dt}(t) := TD\lim_{\mathcal{R}} -\frac{d}{dt}Tr(\mathsf{P}(t)H^{\mathcal{R}}) \ , \tag{7.38}$$

and

$$\frac{\delta A^{\Sigma}}{dt}(t) := \rho_t(\dot{H}^{\Sigma}(t)) \ . \tag{7.39}$$

We are now prepared to summarize our main results on isothermal processes. The first two results are general and concern the first law of thermodynamics and the relationship between the rate of change of entropy and the heat flux into Σ. The remaining three results are corollaries pertaining to free energy and changes of entropy in reversible isothermal processes, i.e., processes in which states are sampled at equilibrium, and on the zeroth law of thermodynamics.

(1) From definitions (7.28), (7.32) and (7.33) and the Liouville equation (7.21) it follows that

$$\dot{U}^{\Sigma}(t) = \frac{\delta Q^{\Sigma}}{dt}(t) + \frac{\delta A^{\Sigma}}{dt}(t) \ , \tag{7.40}$$

which is the *first law of thermodynamics.*

(2) Note that, by the unitarity of time evolution and the cyclic invariance of the trace,

$$\frac{d}{dt}Tr(\mathsf{P}(t)ln\mathsf{P}(t)) = 0 \ ,$$

and

$$\frac{d}{dt}Tr(\mathsf{P}(t)lnZ^{\beta}_{\mathcal{R}}) = \frac{d}{dt}lnZ^{\beta}_{\mathcal{R}} = 0 \ .$$

Together with definitions (7.26), (7.29) and (7.32), this implies that

$$\dot{S}^{\Sigma}(t) = \frac{1}{T}\frac{\delta Q^{\Sigma}}{dt}(t) \ , \tag{7.41}$$

for *arbitrary* isothermal processes at temperature $T = (k\beta)^{-1}$.

(3) Next, we consider an isothermal process of $\Sigma \vee \mathcal{R}$ during a finite time interval $I_\tau = [\tau s_0, \tau s_1]$, with s_0 and s_1 fixed. The initial state $\rho_{\tau s_0}$ of $\Sigma \vee \mathcal{R}$ is assumed to be an equilibrium state $\omega^{\beta}_{\tau s_0}$ of the Liouvillian $L_\tau(\tau s_0) = L(s_0)$. We are interested in the properties of such a process when τ becomes large, i.e., when the process is *quasi-static.*

Result. Quasi-static isothermal processes are *reversible* (in the sense that all intermediate states ρ_t of $\Sigma \vee \mathcal{R}$, $t \in I_\tau$, converge in norm to *instantaneous equilibrium states* ω^{β}_{t}, as $\tau \to \infty$).

This result is an immediate consequence of the isothermal theorem. It means that, for all practical purposes, an isothermal process with time scale τ is reversible if $\tau \gg \tau_{\mathcal{R}} = \max_{s\in I} \tau_{\mathcal{R}}(s)$.

(4) For reversible isothermal processes, the usual *equilibrium definitions* of internal energy and entropy of the small system Σ can be used:

$$U^{\Sigma}_{rev}(t) := \omega^{\beta}_{t}(H^{\Sigma}(t)) \ , \tag{7.42}$$

$$S^{\Sigma}_{rev}(t) := -k \ TD \lim_{\mathcal{R}} Tr(\mathsf{P}^{\beta}(t)[ln\mathsf{P}^{\beta}(t) - ln\mathsf{P}^{\mathcal{R}}]) = \frac{1}{T}(U^{\Sigma}_{rev}(t) - F^{\Sigma}(t)) \ , \tag{7.43}$$

where the free energy $F^{\Sigma}(t)$ has been defined in (7.31), and the second equation in (7.37) follows from (7.22), (7.26), (7.31) and (7.36). Eqs.(7.37) and (7.31) then imply that

$$\dot{S}^{\Sigma}_{rev}(t) = \frac{1}{T}(\frac{d}{dt}\omega^{\beta}_{t}(H^{\Sigma}(t)) - \omega^{\beta}_{t}(\dot{H}^{\Sigma}(t))) \ .$$

Recalling (7.34) and (7.35), and applying the isothermal theorem, we find that

$$\dot{S}^{\Sigma}(t) \to \dot{S}^{\Sigma}_{rev}(t) \ , \tag{7.44}$$

$$\frac{\delta A^{\Sigma}}{dt}(t) \to \dot{F}^{\Sigma}(t) \ , \tag{7.45}$$

as $\tau \to \infty$.

(5) We conclude this chapter by considering a quasi-static isothermal process of $\Sigma \vee \mathcal{R}$ with $H^{\Sigma}(s) \to H^{\Sigma}_{0}$, $g(s) \to 0$, as $s \nearrow s_1$, i.e., the interactions between $\mathcal{R}$ and Σ are switched off at the end of the process. Then the isothermal theorem implies that

$$\lim_{\tau\to\infty} \lim_{s\nearrow s_1} \rho_{\tau s} = \omega^{\beta}_{\Sigma} \otimes \omega^{\beta}_{\mathcal{R}} \ , \tag{7.46}$$

where $\omega^{\beta}_{\mathcal{R}}(\cdot) = TD \lim_{\mathcal{R}} (Z^{\beta}_{\mathcal{R}})^{-1} Tr(e^{-\beta H^{\mathcal{R}}} \cdot)$, see (7.26), and

$$\omega^{\beta}_{\Sigma}(\cdot) = (Z^{\beta}_{\Sigma})^{-1} Tr(e^{-\beta H^{\Sigma}_{0}} \cdot) \tag{7.47}$$

is the Gibbs state of the small system Σ at the temperature $(k\beta)^{-1}$ of the heat bath, *independently* of the properties of the diathermal contact (i.e., of the interaction Hamiltonian W), assuming that (H7.1)-(H7.4) hold for $s < s_1$.

This result is part of the zeroth law of thermodynamics, as discussed in chapter 2.

Chapter 8

Adiabatic theorems in nonequilibrium quantum statistical mechanics

In this chapter, we prove a novel adiabatic theorem which is general enough to handle generators of time evolution that are not necessarily normal or bounded. We discuss two applications of this theorem in non-equilibrium quantum statistical mechanics: an adiabatic theorem for states close to non-equilibrium steady states, and an isothermal theorem with an *explicit* rate of convergence to the instantaneous equilibrium state in the *quasi-static* limit.

8.1 A general adiabatic theorem for (non-)normal and (un)bounded generators of time evolution

Consider a family of closed operators $\{A(t)\}, t \in \mathbf{R}$ acting on a Hilbert space $\mathcal{H}$. We make the following assumptions on $A(t)$ in order to prove the existence of a time evolution and to prove an adiabatic theorem. *All* of these assumptions will be verified in the applications we consider later in this chapter.

(H8.1) $A(t)$ is a generator of a contraction semi-group for all $t \in \mathbf{R}$.

(H8.2) $A(t)$ have a common dense domain $\mathcal{D} \in \mathcal{H}$ for all $t \in \mathbf{R}$.

(H8.3) For $z \in \rho(A(t))$, the resolvent set of $A(t)$, let $R(z,t) := (z - A(t))^{-1}$. Assume that $R(-1,t)$ is bounded and differentiable as a bounded operator on $\mathcal{H}$, and that $A(t)\dot{R}(-1,t)$ is bounded, where the $(\dot{})$ stands for differentiation with respect to t. Moreover, assume that for every $\epsilon > 0$, $-\epsilon \in \rho(A(t))$.

Let $U(t)$ be the propagator that satisfies

$$\partial_t U(t)\psi = -A(t)U(t)\psi \, , U(t=0) = 1 \, , \ \psi \in \mathcal{D} \, , \tag{8.1}$$

for $t \geq 0$.

Lemma 8.1

Suppose that assumptions (H8.1)-(H8.3) hold. Then the propagator $U(t)$ satisfying (8.1) exists and is unique, and $\|U(t)\psi\| \leq \|\psi\|$.

Proof. For $t, t' \in \mathbf{R}$, $A(t')A(t)^{-1}$ is bounded by the closed graph theorem and (H8.2) (see [RS2]). Moreover, for small $|t-t'|$, $||(t'-t)A(t')^{-1}A(t)-\mathbf{1}|| = ||\dot{A}^{-1}(t)A(t)||+ o(|t-t'|)$, which is bounded due to (H8.3).By Theorem X.70 in [RS2] (or Theorem 2 in Chp XIV [Yo], section 4), this implies, together with (H8.1), that $U(t)$ exists and is unique. Furthermore, choose $\epsilon > 0$ and let $\widetilde{U}(t)$ be the propagator generated by $A(t) + \epsilon$. Then from (H8.3), $0 \in \rho(A(t) + \epsilon)$, and hence by Theorem X.70 in [RS2], $\widetilde{U}(t)$ is a contraction semigroup for $t > 0$. In particular, $\|\widetilde{U}(t)\psi\| \leq 1$ (for $\|\psi\| = 1$). We also have $\|U(t)\| = e^{\epsilon t}\|\widetilde{U}(t)\|$. Taking the limit $\epsilon \to 0$ gives $\|U(t)\psi\| \leq 1$. □

Assume that $A(t) \equiv A(0)$ for $t \leq 0$, and that it is perturbed *slowly* over a time τ such that $A^{(\tau)}(t) \equiv A(s)$, where $s := \frac{t}{\tau} \in [0, 1]$ is the reduced time. The following two assumptions are needed to prove an adiabatic theorem.

(H8.4) The eigenvalue $\lambda(s) \in \sigma(A(s))$ is isolated and simple, such that

$$dist(\lambda(s), \sigma(A(s))\backslash\{\lambda(s)\}) > \delta,$$

where $\delta > 0$ is a constant independent of $s \in [0, 1]$, and $\lambda(s)$ is continuously differentiable in $s \in [0, 1]$.

(H8.5) The projection onto $\lambda(s)$,

$$P_\lambda(s) := \frac{1}{2\pi i} \oint_{\gamma_\lambda(s)} R(z, s) dz \ , \tag{8.2}$$

where $\gamma_\lambda(s)$ is a contour enclosing $\lambda(s)$ only, is twice differentiable as a bounded operator.

Note that, since $\lambda(s)$ is simple, the resolvent of $A(s)$ in a neighborhood $\mathcal{N}$ of $\lambda(s)$ contained in a ball $\mathbf{B}(\lambda(s), r)$ centered at $\lambda(s)$ with radius $r < \delta$ is

$$R(z, s) = \frac{P_\lambda(s)}{z - \lambda(s)} + R_{analytic}(z, s) \ , \tag{8.3}$$

where $R_{analytic}(z, s)$ is analytic in $\mathcal{N}$. We list some useful properties of the resolvent and the spectral projection $P_\lambda(s)$.

(i) It follows by direct application of the contour integration formula that

$$(P_\lambda(s))^2 = P_\lambda(s) \ , \tag{8.4}$$

and hence

$$P_\lambda(s)\dot{P}_\lambda(s)P_\lambda(s) = 0 \ . \tag{8.5}$$

(ii)
$$A(s)P_\lambda(s) = P_\lambda(s)A(s) = \lambda(s)P_\lambda(s)\ . \tag{8.6}$$

Proof.
$$\begin{aligned}
A(s)P_\lambda(s) &= \frac{1}{2\pi i}\oint_{\gamma_\lambda(s)} (A(s)-z+z)(z-A(s))^{-1}dz \\
&= \frac{1}{2\pi i}\{-\oint_{\gamma_\lambda(s)} dz + \oint_{\gamma_\lambda(s)} (\frac{zP_\lambda(s)}{z-\lambda(s)} + zR_{analytic})dz\} \\
&= \lambda(s)P_\lambda(s)\ ,
\end{aligned}$$

and similarly, $P_\lambda(s)A(s) = \lambda(s)P_\lambda(s)$.

(iii) It follows from (8.3) and (H8.4) that, for $\eta \in \mathbf{C}$ and $\frac{\delta}{2} \leq |\eta| < \delta$, there exists a constant $C < \infty$, independent of η, such that
$$\|R(\lambda(s)+\eta, s)\| < C\ , \tag{8.7}$$
uniformly in $s \in [0,1]$. Moreover, since $(\lambda(s)+\eta) \in \rho(A(s))$, it follows by the spectral mapping theorem (see for example [Yo], Chp. VIII, section 7) and (H8.3) that $R(\lambda(s)+\eta, s)$ is twice differentiable as a bounded operator.*

We now discuss our general adiabatic theorem. Let $U_\tau(s,s')$ be the propagator satisfying
$$\partial_s U_\tau(s,s') = -\tau A(s)U_\tau(s,s')\ , U_\tau(s,s) = 1\ , \tag{8.8}$$
for $s \geq s'$. Moreover, define the generator of the *adiabatic time evolution*,
$$A_a(s) := A(s) - \frac{1}{\tau}[\dot{P}_\lambda(s), P_\lambda(s)]\ , \tag{8.9}$$
with the corresponding propagator $U_a(s,s')$ which satisfies
$$\partial_s U_a(s,s') = -\tau A_a(s)U_a(s,s')\ ; U_a(s,s) = 1\ , \tag{8.10}$$
for $s \geq s'$.

By Lemma 8.1 and (H8.1)-(H8.3) and (H8.5), both propagators $U_\tau(s,s')$ and $U_a(s,s')$ exist and are unique, and $\|U_\tau(s,s')\|, \|U_a(s,s')\| < C$ for $s \geq s'$, where C is a finite constant independent of $s, s' \in [0,1]$.

We are in a position to state our adiabatic theorem.

Theorem 8.2 (A general adiabatic theorem)

Assume (H8.1)-(H8.5). Then the following holds.

*This follows from the fact that, for $z, \omega \in \rho(A)$,
$$(z-A)^{-1} = (1+(z-\omega)(\omega-A)^{-1})^{-1}(\omega-A)^{-1}.$$

(i)
$$P_\lambda(s)U_a(s,0) = U_a(s,0)P_\lambda(0) \ , \tag{8.11}$$
for $s \geq 0$ (the intertwining property).

(ii) $\sup_{s\in[0,1]} \|U_\tau(s,0) - U_a(s,0)\| = O(\tau^{-1})$ as $\tau \to \infty$.

Proof.

(i) Equality holds trivially for $s = 0$, since $U_a(s,s) = 1$. Let
$$h(s,s') := U_a(s,s')P_\lambda(s')U_a(s',0) \ , \tag{8.12}$$
for $0 \leq s' \leq s$, and
$$g(s) := U_a(s,0)P_\lambda(0) \ , \tag{8.13}$$
for $0 \leq s$.

Using (8.6), (8.10) , the definition of $A_a(s)$ and the fact that $\dot{P}_\lambda(s)P_\lambda(s) + P_\lambda(s)\dot{P}_\lambda(s) = \dot{P}_\lambda(s)$, it follows that
$$\begin{aligned}\partial_{s'}h(s,s') &= \partial_{s'}(U_a(s,s')P_\lambda(s')U_a(s',0)) \\ &= \tau U_a(s,s')\{A_a(s')P_\lambda(s') - P_\lambda(s')A_a(s')\}U_a(s',0) + U_a(s,s')\dot{P}_\lambda(s')U_a(s',0) \\ &= U_a(s,s')\{-\dot{P}_\lambda(s')P_\lambda(s') - P_\lambda(s')\dot{P}_\lambda(s') + \dot{P}_\lambda(s')\}U_a(s',0) \\ &= 0 \ .\end{aligned}$$

Note also that $\partial_{s'}g(s) = 0$ and $h(s,s'=0) = g(s)$. Furthermore,
$$\partial_s h(s,s') = -\tau A_a h(s,s') \ , \tag{8.14}$$
$$\partial_s g(s) = -\tau A_a g(s) \ , \tag{8.15}$$
$$h(s=0,s'=0) = g(s=0) \ . \tag{8.16}$$

Together with assumptions (H8.1)-(H8.3) and (H8.5), it follows that
$$h(s,s') = g(s) \ .$$

In particular, when $s' = s$,
$$P_\lambda(s)U_a(s,0) = U_a(s,0)P_\lambda(0) \ . \tag{8.17}$$

(ii) Consider $\psi \in \mathcal{D}$, where the dense domain $\mathcal{D}$ appears in assumption (H8.2). We are interested in estimating the norm of the difference $(U_\tau(s) - U_a(s))\psi$ as $\tau \to \infty$. Using (8.8), (8.10) and the Duhamel formula,
$$(U_\tau(s,0) - U_a(s,0))\psi = -\int_0^s ds'\partial_{s'}(U_\tau(s,s')U_a(s',0))\psi \tag{8.18}$$
$$= \int_0^s ds'(U_\tau(s,s')[\dot{P}_\lambda(s'),P_\lambda(s')]U_a(s',0))\psi \ . \tag{8.19}$$

Let

$$X(s) := \frac{1}{2\pi i}\oint_{\gamma_\lambda(s)} dz R(z,s)\dot{P}_\lambda(s)R(z,s) \ , \tag{8.20}$$

where $\gamma_\lambda(s)$ is a contour of radius $\delta/2$ centered at $\lambda(s)$, and where δ appears in (H8.4). Then

$$\begin{aligned}
[X(s), A(s)] &= \frac{1}{2\pi i}\oint_{\gamma_\lambda(s)} dz[z - A(s), X(s)] &(8.21)\\
&= \dot{P}_\lambda(s)P_\lambda(s) - P_\lambda(s)\dot{P}_\lambda(s) = [\dot{P}_\lambda(s), P_\lambda(s)] \ . &(8.22)
\end{aligned}$$

Assumptions (H8.3),(H8.4) and the spectral mapping theorem imply that, for $z \in \gamma_\lambda(s) \subset \rho(A(s)), R(z,s)$ is differentiable as a bounded operator. Together with (H8.5), this implies that,

$$\begin{aligned}
\|X(s)\| &< C_1 \ , &(8.23)\\
\|\dot{X}(s)\| &< C_2 \ , &(8.24)
\end{aligned}$$

where C_1 and C_2 are finite constants independent of $s \in [0,1]$. Moreover,

$$U_\tau(s,s')[X(s'), A(s')]U_a(s',0) = \frac{1}{\tau}\{-\partial_{s'}U_\tau(s,s')X(s')U_a(s',0)$$
$$+ U_\tau(s,s')(X(s')[\dot{P}_\lambda(s'), P_\lambda(s')])U_a(s',0) + U_\tau(s,s')\dot{X}(s')U_a(s',0)\} \ .$$

Together with (8.22), one may write the integrand in (8.18) as a total derivative plus a remainder term. Using the fact that $\mathcal{D}$ is dense in $\mathcal{H}$ and (H8.5),

$$\|U_\tau(s,0) - U_a(s,0)\| \le \frac{1}{\tau}[C_1\|X(s)\| + C_2\|\dot{X}(s)\|] \ , \tag{8.25}$$

where $C_i, i = 1,2$ are finite constants independent of $s \in [0,1]$.
Together with (8.23) and (8.24), this implies

$$\|U_\tau(s,0) - U_a(s,0)\| \le \frac{C}{\tau} \ , \tag{8.26}$$

as $\tau \to \infty$, where $C < \infty$ is independent of $s \in [0,1]$. □

Remarks.

(1) One may improve the results of Theorem 8.2 (also to cover the case of eigenvalue crossing) by making further smoothness assumptions on $A(s)$ and applying methods developed, for example in [J,Ne].

(2) An application of Theorem 8.2 other than in NEQSM is an adiabatic theorem for quantum resonances.[A-SF1]

8.2 Application 1: an adiabatic theorem for non-equilibrium steady states (NESS)

In this section, we consider again the C_n paradigm of a two level system coupled to n fermionic reservoirs (see chapter 4, section 4). It is important to note that the result can be generalized to bosonic reservoirs, but the analysis will be technically more cumbersome since the interaction in the bosonic case is unbounded.

Together with assumptions (C_n.2), we assume (C_n.4), ie, that $V^\tau(t) = V(s)$, where $s \in [0,1]$ is the rescaled time with sufficient smoothness properties to apply Theorem 8.2. From Proposition 6.9, we know the spectrum of the deformed adjoint of the C-Liouvillean $L_g^*(t,\theta) = U(\theta)L_g^*(t)U(-\theta)$ for $\theta \in I^-(k) = \{z \in \mathbf{C} : -k < Imz < 0\}$, where $k = \min(\frac{\pi}{\beta_1}, \cdots, \frac{\pi}{\beta_n}, \delta)$, and δ appears in assumption (C_n.5). Let γ_0 be a contour only enclosing the zero eigenvalue of $L_g^*(s,\theta)$, for all $s \in [0,1]$, and

$$P_g'(\theta, s) := \oint_{\gamma_0} \frac{dz}{2\pi i}(z - L_g^*(s,\theta))^{-1}, \tag{8.27}$$

the spectral projection onto the state corresponding to the zero eigenvalue of $L_g^*(s,\theta)$, and let D be the positive operator as defined in Corollary 6.10, section 6.3 (ie, $RanD$ dense in $\mathcal{H}$ and $D\Omega = \Omega$)

$$D := \mathbf{1}^\Sigma \otimes \mathbf{1}^\Sigma \otimes e^{-k\widetilde{A}_{\mathcal{R}_1}} \otimes \cdots \otimes e^{-k\widetilde{A}_{\mathcal{R}_n}} , \tag{8.28}$$

where $\widetilde{A}_{\mathcal{R}_j} = d\Gamma(\sqrt{p_j^2+1})$, and $p_j = i\partial_{u_j}$ is the generator of energy translations for the $\mathcal{R}_j$ reservoir, $j = 1, \cdots, n$.

Let $\mathbf{h}^{test} = D(e^{k\sqrt{p^2+1}})$, and $\mathcal{O}^{test} = \mathcal{F}_-(\mathbf{h}^{test})$, which is dense in $\mathcal{F}_-(L^2(\mathbf{R};\mathcal{B}))$, and define

$$\mathcal{C} := \mathcal{O}^\Sigma \otimes \mathcal{O}^{\mathcal{R}_1,test} \otimes \cdots \otimes \mathcal{O}^{\mathcal{R}_n,test} , \tag{8.29}$$

which is dense in $\mathcal{O}$. We will make the following additional assumption.

(H8.6) The perturbation of the Hamiltonian $V(s) \in \mathcal{C}$ for $s \in [0,1]$.

In order to characterize the quasi-static evolution of nonequilibrium steady states, we introduce the new notion of *instantaneous* NESS. Define the *instantaneous* NESS vector to be

$$\Omega_g(s) := DU(-\theta)P_g'(s,\theta)U(\theta)D\Omega . \tag{8.30}$$

It is important to note that introducing the operator D is needed so that one can remove the complex deformation.

We have the following Theorem, which effectively says that if a system, which is initially in a NESS, is perturbed slowly over a time scale $\tau \gg \tau_R$, where τ_R is some generic time scale ($\tau_R = \max_{s\in[0,1]} \tau_{R(s)}$, where $\tau_{R(s)}$ is the relaxation time to a NESS, see Corollary 6.10), then the real state of the system is infinitesimally close to the *instantaneous* NESS, and the difference of the two states is bounded form above by a term of order $O(\tau^{-1})$.

Theorem 8.3 (Adiabatic Theorem for NESS)
Suppose $(C_n.2)$, $(C_n.4)$, as specified in section 4.4, and (H8.6). Then there exists $g_1 > 0$, independent of $s \in [0,1]$, such that, for $a \in \mathcal{C}, s \in [0,1]$, and $|g| < g_1$, the following estimate holds

$$\sup_{s\in[0,1]} |\langle \Omega_g(0), D^{-1}\alpha_g^{\tau s}(a)\Omega\rangle - \langle \Omega_g(s), D^{-1}a\Omega\rangle| = O(\tau^{-1}) \ , \tag{8.31}$$

as $\tau \to \infty$.

Proof. The proof is reduced to mainly showing that the assumptions of Theorem 8.2 are satisfied. Choose $\theta \in I^-(k)$. It follows from assumption $(C_n.4)$ and Lemmas 6.11 and 6.12 in chapter 6, section 3, that the deformed C-Liouvillean $L_g^*(s,\theta)$ with common dense domain $\mathcal{D} = \mathcal{D}(\mathcal{L}_0) \cap \mathcal{D}(D^{-1}) \subset C(\mathcal{O}, \Omega)$ generates the propagator $\widetilde{U}_g^{(\tau)}(s,s',\theta), s' \leq s$ which satisfied the initial value problem

$$\partial_s \widetilde{U}_g^{(\tau)}(s,s',\theta) = -i\tau L_g^*(s,\theta)\widetilde{U}_g^{(\tau)}(s,s',\theta) \ , \text{ for } s' \leq s; \widetilde{U}^{(\tau)}(s,s,\theta) = 1. \tag{8.32}$$

This implies that (H8.1) and (H8.2) are satisfied. Furthermore, (H8.3) follows from the second resolvent identity

$$(L_g^*(s,\theta) - z)^{-1} = (\mathcal{L}_0(\theta) - z)^{-1}(1 + g\widetilde{V}^{tot}(s,\theta)(\mathcal{L}_0(\theta) - z)^{-1})^{-1} \ , \tag{8.33}$$

where $\widetilde{V}^{tot}$ has been defined in section 6.3, and assumption $(C_n.4)$. The results of Proposition 6.9 (section 6.3) follow from $(C_n.2)$ and $(C_n.4)$, and hence we know that zero is an isolated simple eigenvalue of $L_g^*(s,\theta)$ such that $dist(0, \sigma(L_g^*(s,\theta))\backslash\{0\}) > \delta$, where $\delta > 0$ is a constant independent of $s \in [0,1]$. This implies that assumption (H8.4) holds. Again using the resolvent equation (8.33) and assumption $(C_n.4)$, $P_g'(s,\theta)$ defined in (8.27) is twice differentiable as a bounded operator for all $s \in [0,1]$, which imply (H8.5). Since (H8.1)-(H8.5) are satisfied, the result of Theorem 8.2 holds.

$$P_g'(s,\theta)\widetilde{U}_a^{(\tau)}(s,0,\theta) = \widetilde{U}_a^{(\tau)}(s,0,\theta)P_g'(0,\theta) \ , \tag{8.34}$$

and

$$\sup_{s\in[0,1]} \|\widetilde{U}_g^{(\tau)}(s,0,\theta) - \widetilde{U}_a^{(\tau)}(s,0,\theta)\| = O(\tau^{-1}) \ , \tag{8.35}$$

as $\tau \to \infty$, where $\widetilde{U}_a^{(\tau)}(s,s',\theta)$ is the propagator of the *deformed* adiabatic evolution satisfying

$$\partial_s \widetilde{U}_a^{(\tau)}(s,\theta) = -i\tau L_a^*(s,\theta)\widetilde{U}_a^{(\tau)}(s,s',\theta) \text{ for } s' \leq s \ ; \widetilde{U}_a^{(\tau)}(s,s,\theta) = 1 \ , \tag{8.36}$$

and

$$L_a^*(s,\theta) = L_g^*(s,\theta) + \frac{i}{\tau}[\dot{P}_g'(s,\theta), P_g'(s,\theta)] \ . \tag{8.37}$$

(Here, the $\dot{()}$ stands for differentiation with respect to s.)

For h the single particle Hamiltonian of the free fermions (see section 4.4),e^{iht} leaves $D(e^{k\sqrt{p^2+1}})$ invariant. Therefore, for $a \in \mathcal{C}$, $\alpha_0^t(a) \in \mathcal{C}$, where α_0^t corresponds to the free time evolution. Moreover, together with assumption (H8.6) and the boundedness of V, this implies (using a Dyson series expansion) that $\alpha_g^{\tau s}(a) \in \mathcal{C} = \mathcal{D}(D^{-1})$.

Now, applying the time evolution on $C(\mathcal{O}, \Omega)$, and remembering that $D\Omega = \Omega$, $U(\theta)\Omega = \Omega$, the fact that $U(\theta)$ and D commute, and the definition of the instantaneous NESS,

$$\langle \Omega_g(0), D^{-1}\alpha_g^{(\tau s)}(a)\Omega\rangle = \langle \widetilde{U}_g^{(\tau)}(s,0,\theta)P_g'(0,\theta)\Omega, a(\overline{\theta})\Omega\rangle \ . \tag{8.38}$$

Using the results of Theorem 8.2, it follows that

$$\begin{aligned}
&\langle \widetilde{U}_g^{(\tau)}(s,0,\theta)P_g'(0,\theta)\Omega, a(\overline{\theta})\Omega\rangle \\
&= \langle \widetilde{U}_a^{(\tau)}(s,0,\theta)P_g'(0,\theta)\Omega, a(\overline{\theta})\Omega\rangle + O(\tau^{-1}) \\
&= \langle P_g'(s,\theta)\widetilde{U}_a^{(\tau)}(s,0,\theta)\Omega, a(\overline{\theta})\Omega\rangle + O(\tau^{-1}) \\
&= \langle P_g'(s,\theta)\widetilde{U}_g^{(\tau)}(s,0,\theta)\Omega, a(\overline{\theta})\Omega\rangle + O(\tau^{-1}) \ .
\end{aligned}$$

The fact that $(\widetilde{U}_g^{(\tau)}(s,0,\theta))^*\Omega = \Omega$ implies that

$$\begin{aligned}
DP_g'(s,\theta)\widetilde{U}_g^{(\tau)}(s,0,\theta) &= |\Omega_g(s,\theta)\rangle\langle\Omega|\widetilde{U}^{(\tau)}(s,0,\theta) \\
&= |\Omega_g(s,\theta)\rangle\langle(\widetilde{U}^{(\tau)}(s,0,\theta))^*\Omega| \\
&= |\Omega_g(s,\theta)\rangle\langle\Omega| = DP_g'(s,\theta) \ .
\end{aligned}$$

It follows that

$$\langle \Omega_g(0), D^{-1}\alpha_g^{(\tau s)}(a)\Omega\rangle = \langle \Omega_g(s), D^{-1}a\Omega\rangle + O(\tau^{-1}) \ ,$$

for large τ. $\square$

Remark.

A weaker adiabatic theorem for states close to NESS using scattering theory can be proven using the approach developed in [Ru2,3] and extending the adiabatic theorem in [NT]. However, this theorem relies on the rather strong assumption of asymptotic abelianness. For further details about adiabatic theorems in NEQSM, see [A-S].

8.3 Application 2: a concrete example of the isothermal theorem

As a second application of Theorem 8.2, we consider in this section a concrete example of an isothermal process for model C_n (see section 4.4), and calculate an explicit rate of convergence ($O(\tau^{-1})$) between the instantaneous equilibrium state and real state of the system in the quasi-static limit $\tau \to \infty$; (see chapter 7 for our notation and the relevant definitions).

Theorem 8.4 (Isothermal Theorem revisited) Suppose (C_n.2), (C_n.5), as specified in section 4.4, and (H8.6). Then there exists a constant $g_1 > 0$ such that, for $a \in \mathcal{D}(D^{-1})$ and $|g| < g_1$, the following estimate holds

$$|\rho_{\tau s}(a) - \omega^{\beta}_{\tau s}(a)| = O(\tau^{-1}) \ , \tag{8.39}$$

as $\tau \to \infty$, where $\rho_{\tau s}$ is the real state of the system at time $t = \tau s$, and $\omega^{\beta}_{\tau s}$ is the instantaneous equilibrium state defined in chapter 7.

Proof. Choose $\theta \in I^-(k)$. It follows from assumption (C_n.5) and Lemmas 6.11 and 6.12 in section 6.3 that the deformed Liouvillean $\mathcal{L}_g(s,\theta)$ with common dense domain $\mathcal{D} = \mathcal{D}(\mathcal{L}_0) \cap \mathcal{D}(D^{-1}) \subset C(\mathcal{O},\Omega)$ generates the propagator $U^{(\tau)}_g(s,s',\theta)$ which satisfied the initial value problem

$$\partial_s U^{(\tau)}_g(s,s',\theta) = -i\tau \mathcal{L}_g(s,\theta) U^{(\tau)}_g(s,s',\theta) \ ; U^{(\tau)}(s,s,\theta) = 1, \tag{8.40}$$

which implies (H8.1) and (H8.2). Moreover (H8.3) follows from the second resolvent identity

$$(\mathcal{L}_g(s,\theta) - z)^{-1} = (\mathcal{L}_0(\theta) - z)^{-1}(1 + gV^{tot}(s,\theta)(\mathcal{L}_0(\theta) - z)^{-1})^{-1} \ , \tag{8.41}$$

and assumption (C_n.5). The results of Theorem 6.7 follow from (C_n.2) and (C_n.5), and hence we know that zero is an isolated simple eigenvalue of $\mathcal{L}_g(s,\theta)$ such that $dist(0, \sigma(\mathcal{L}_g(s,\theta)) \backslash \{0\}) > \delta'$, where $\delta' > 0$ is a constant independent of $s \in [0,1]$. This implies assumption (H8.4). Using the resolvent equation (8.41) and assumption (C_n.5), $P_g(s,\theta) := \frac{1}{2\pi i} \oint_{\gamma_0} dz (z - \mathcal{L}_g(s,\theta))^{-1}$ is twice differentiable as a bounded operator for all $s \in [0,1]$, which implies (H8.5). Since (H8.1)-(H8.5) are satisfied, the result of Theorem 8.2 holds.

$$P_g(s,\theta) U^{(\tau)}_a(s,0,\theta) = U^{(\tau)}_a(s,0,\theta) P_g(0,\theta) \ ; \tag{8.42}$$

$$\sup_{s\in[0,1]} \|U^{(\tau)}_g(s,0,\theta) - U^{(\tau)}_a(s,0,\theta)\| = O(\tau^{-1}) \ , \tag{8.43}$$

as $\tau \to \infty$, where $U^{(\tau)}_a(s,s',\theta)$ is the propagator which satisfies

$$\partial_s U^{(\tau)}_a(s,s',\theta) = -i\tau \mathcal{L}_a(s,\theta) U^{(\tau)}_a(s,s',\theta) \ \text{for} s' \leq s \ ; U^{(\tau)}_a(s,s,\theta) = 1 \ , \tag{8.44}$$

and

$$\mathcal{L}_a(s,\theta) = \mathcal{L}_g(s,\theta) + \frac{i}{\tau}[\dot{P}_g(s,\theta), P_g(s,\theta)]\ . \tag{8.45}$$

Assumption (H8.6) implies that, for $a \in \mathcal{C}$, $\alpha_g^{\tau s}(a) \in \mathcal{C}$.

Using the fact that $U(\pm\theta)|\Omega\rangle = |\Omega\rangle$ and the results of Theorem 8.2, it follows that

$$\begin{aligned}
U(\theta)U_g^{(\tau)}(s,0)|\Omega\rangle &= U_g^{(\tau)}(s,0,\theta)P_g(0,\theta)|\Omega\rangle \\
&= U_a^{(\tau)}(s,0,\theta)P_g(0,\theta)|\Omega\rangle + O(\tau^{-1}) \\
&= P_g(s,\theta)U_a(s,0,\theta)|\Omega\rangle + O(\tau^{-1}) \\
&= P_g(s,\theta)U_g(s,0,\theta)|\Omega\rangle + O(\tau^{-1})\ .
\end{aligned}$$

We know that $P_g(s,\theta)U_g(s,0,\theta)|\Omega\rangle = c|\Omega(s,\theta)\rangle$, where $\Omega(s,\theta)$ is the vector corrsponding to the instantaneous equilibrium state and $c \in \mathbf{C}$. Since

$$\begin{aligned}
\langle P_g(s,\overline{\theta})U_g^{(\tau)}(s,0,\overline{\theta})\Omega, P_g(s,\theta)U_g^{(\tau)}(s,0,\theta)\Omega\rangle &= \langle U_g^{(\tau)}(s,0)\Omega, U_g^{(\tau)}(s,0)\Omega\rangle + O(\tau^{-1}) \\
&= 1 + O(\tau^{-1})\ ,
\end{aligned}$$

and

$$\langle \Omega(s,\overline{\theta}), \Omega(s,\theta)\rangle = 1\ ,$$

it follows that c is a phase up to an error of order $O(\tau^{-1})$. Therefore,

$$\rho_{\tau s}(a) = \langle \Omega, U_g^{(\tau)}(0,s)aU^{(\tau)}(s,0)\Omega\rangle = \langle \Omega(s), a\Omega(s)\rangle + O(\tau^{-1})\ . \tag{8.46}$$

Note that unlike in the proof of Theorem 8.3, zero is an *eigenvalue* of the undeformed Liouvillean $\mathcal{L}_g(s)$, which is selfadjoint, and hence $P_g(s)$ is well-defined as a spectral projection by the spectral theorem. □

Chapter 9

Cyclic thermodynamic processes and Floquet theory

In this chapter, we study cyclic thermodynamic processes of a small quantum system coupled to n fermionic reservoirs by extending Floquet theory for quantum mechanical systems that are driven by periodic forcing. We introduce a new operator, which we call the Floquet Liouvillean, and we show that under certain assumptions, the time-periodic state to which the coupled system converges is related to the zero-energy resonance of the adjoint of the Floquet Liouvillean. We study the spectrum of the Floquet operator using complex deformation techniques, as developed in chapter 6; (see also [JP1,2,3]). Although technically more complicated, since the perturbation will be unbounded , the analysis is in principle applicable to the case when the reservoirs are bosonic. On the mathematical side, it is interesting to extend the strong spectral methods developed in [BFS] based on operator theoretic renormalization group or the positive commutator method developed in [M1, M2, FM1](see also chapter 5) to study the spectrum of the Floquet operator.

One result that follows from our analysis is that one can compute entropy production per cycle and the degree of efficiency η to arbitrary orders in the weak coupling (see remark after Theorem 9.3).

We again consider the same paradigm: Model C_n of a two level system coupled to n-fermionic reservoirs that are not necessarily at the same temperature. Together with assumptions (C_n.2) and (C_n.3), chapter 4, section 4, we assume (C_n.6), which pertains to the periodicity of the perturbation, $V(t+\tau_*) = V(t), \tau_* < \infty$.

Assume further that the initial state of the system is

$$\Omega = \Omega^{\Sigma} \otimes \Omega^{\mathcal{R}_1} \otimes \cdots \otimes \Omega^{\mathcal{R}_n} ,$$

where $\Omega^{\mathcal{R}_i}, i = 1, \cdots , n$ are the KMS-states of the uncoupled reservoirs, and, without loss of generality, Ω^{Σ} is the vector in $\mathcal{H}^{\Sigma} \otimes \mathcal{H}^{\Sigma}$ corresponding to the trace state on Σ. The C-Liouvillean of the coupled system $L_g(t)$, which has been introduced in chapter 6, generates the dynamics on the Banach space $C(\mathcal{O}, \Omega)$. It is obviously time-periodic with period τ_* if assumption (C_n.6) holds. By construction,

$$L_g(t)\Omega = 0 \ .$$

Now denote by $\widetilde{U}_g(t,t')$ the propagator generated by $L_g^*(t)$ (note the change in notation), which satisfies the initial value problem

$$\partial_t \widetilde{U}_g(t,t') = -iL_g^*(t)\widetilde{U}_g(t,t') \ ; \widetilde{U}_g(t,t) = 1 \ .$$

The existence of $\widetilde{U}_g$ follows from assumption (C_n.3), section 4.4, and the Yosida-Hille-Phillips Theorem, as discussed in chapter 6, section 4.

9.1 The *Floquet Liouvillean*

Introduce the *Floquet Liouvillean*

$$K_g^* := -i\partial_t + L_g(t)^* \ , \tag{9.1}$$

acting on $\widetilde{\mathcal{H}} = L^2([0,\tau_*]) \otimes \mathcal{H}$, where the GNS Hilbert space $\mathcal{H}$ for Model C_n has been defined in section 4.4, with periodic boundary conditions in t. Note that under the previous assumptions, K_g^* is a closable operator (since the perturbation is bounded), and we denote its closure by the same symbol.

Let $\omega := \frac{2\pi}{\tau^*}$. By Fourier transformation, $\widetilde{\mathcal{H}}$ is isomorphic to $\bigcup_{n\in\mathbf{Z}} \langle e^{in\omega t}\rangle \otimes \mathcal{H} = \bigcup_{n\in\mathbf{Z}} \mathbf{h}^{(n)} \otimes \mathcal{H}$.

According to Floquet theory of quantum mechanical systems driven by periodic perturbation [Ho,Ya1,Ya2], the semi-group generated by K_g^* is given by

$$(e^{-i\sigma K_g^*} f)(t) = \widetilde{U}_g(t, t-\sigma)(f)(t-\sigma) \ , \tag{9.2}$$

where $f \in \widetilde{\mathcal{H}}$ and $\sigma \in \mathbf{R}$. Relation (9.2) can be seen by differentiating both sides with respect to σ and setting $\sigma = 0$ (see [Ho]). (Alternatively, use the Trotter product formula.[RS1]) Note that if

$$K_g^*\phi(t) = \lambda\phi(t) \ , \tag{9.3}$$

for $\phi(t) \in \widetilde{\mathcal{H}}$ and $\lambda \in \mathbf{C}$, then $\phi(t)$ satisfies

$$\widetilde{U}_g(t,0)\phi(0) = e^{-i\lambda t}\phi(t) \ . \tag{9.4}$$

Conversely, if

$$\widetilde{U}_g(\tau_*,0)\phi(0) = e^{-i\lambda\tau_*}\phi_0 \ , \tag{9.5}$$

then

$$\phi(t) = e^{i\lambda t}\widetilde{U}_g(t,0)\phi_0 \tag{9.6}$$

is an eigenfunction of K_g^* with eigenvalue λ.

Before proving the convergence to a time-periodic state of the coupled system, we first study the spectrum of the adjoint of the Floquet Liouvillean.

9.2 Spectrum of K_g^*

We study the spectrum of K_g^* using complex deformation techniques developed in chapter 6. This is why we only sketch the main steps of the proofs.

Let $k = min(\frac{\pi}{\beta_1}, \cdots, \frac{\pi}{\beta_n}, \delta)$, where δ appears in assumption $(C_n.3)$. For $\theta \in I^-(k)$, let

$$K_g^*(\theta) := U(\theta) K_g^* U(-\theta) \tag{9.7}$$
$$= -i\partial_t + L_g^*(\theta, t) \ , \tag{9.8}$$

where $L_g^*(\theta, t)$ is given in section 6.3 by

$$L_g^*(t, \theta) := U(\theta) L_g^*(t) U(-\theta) = \mathcal{L}_0 + N\theta + g\widetilde{V}^{tot}(t, \theta) \ , \tag{9.9}$$

$\mathcal{L}_0 = \mathcal{L}^\Sigma + \sum_i \mathcal{L}^{\mathcal{R}_i}$, $\mathcal{L}^{\mathcal{R}_i} = d\Gamma(u_i), i = 1, \cdots, n$, and

$$\widetilde{V}^{tot}(t, \theta) = \sum_i \{\sigma_+ \otimes \mathbf{1}^\Sigma \otimes b(f_{i,\beta_i}^{(\theta)}(t)) + \sigma_- \otimes \mathbf{1}^\Sigma \otimes b^*(f_{i,\beta_i}^{(\theta)}(t))$$
$$- i\mathbf{1}^\Sigma \otimes \sigma_+ \otimes (-1)^{N_i}(b(e^{-\beta_i(u_i-\nu)/2} f_{i,\beta_i}^{\#(\theta)}(t)) - i\mathbf{1}^\Sigma \otimes \sigma_- \otimes (-1)^{N_i} b^*(e^{\beta_i(u_i-\nu)/2} f_{i,\beta_i}^{\#(\theta)}(t))\} \ .$$

For $n \in \mathbf{Z}$, let

$$\widetilde{P}_{g,(n)}(\theta) := \oint_{\gamma_n} \frac{dz}{2\pi i}(z - K_g^*(\theta))^{-1} \ , \tag{9.10}$$

such that γ_n is a contour that encloses only the eigenvalues $E_j^{(n)}(g) = n\omega + E_j'(g), j = 0, \cdots, 3, n \in \mathbf{Z}$, where $E_j'(g), j = 0, \cdots, 3$ are the eigenvalues of $L_g^*(\theta)$ (see section 6.3). Moreover, let $\widetilde{T}_{g,(n)} := \widetilde{P}_{0,(n)} \widetilde{P}_{g,(n)}(\theta) \widetilde{P}_{0,(n)}$, then we will show that the isomorphism

$$\widetilde{S}_{g,(n)}(\theta) := \widetilde{T}_{g,(n)}^{-1/2} \widetilde{P}_{0,(n)} \widetilde{P}_{g,(n)}(\theta) : Ran(\widetilde{P}_{g,(n)}(\theta)) \to \mathbf{h}^{(n)} \otimes \mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma \tag{9.11}$$

has an inverse

$$\widetilde{S}_{g,(n)}^{-1}(\theta) := \widetilde{P}_{g,(n)}(\theta) \widetilde{P}_{0,(n)} \widetilde{T}_{g,(n)}^{-1/2}(t) : \mathbf{h}^{(n)} \otimes \mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma \to Ran(\widetilde{P}_{g,(n)}(\theta)). \tag{9.12}$$

Let

$$\widetilde{M}_{g,(n)}(t) := \widetilde{P}_{0,(n)} \widetilde{P}_{g,(n)}(\theta) K_g^*(\theta) \widetilde{P}_{g,(n)}(\theta) \widetilde{P}_{0,(n)} \ , \tag{9.13}$$

and define the quasi-Floquet Liouvillean by

$$\widetilde{\Sigma}_{g,(n)} := \widetilde{S}_{g,(n)}(\theta) \widetilde{P}_{g,(n)}(\theta) K_g^*(\theta) \widetilde{P}_{g,(n)}(\theta) \widetilde{S}_{g,(n)}^{-1}(\theta) = \widetilde{T}_{g,(n)}^{-1/2} \widetilde{M}_{g,(n)} \widetilde{T}_{g,(n)}^{1/2} \ , \tag{9.14}$$

which is nothing but the mapping of the reduced Floquet Liouvillean $\widetilde{K}_{g(n)}$ from $Ran(\widetilde{P}_{g(n)})$ to $\mathbf{h}^{(n)} \otimes \mathcal{H}^\Sigma \otimes \mathcal{H}^\Sigma$.

Proposition 9.1

Suppose $(C_n.2)$,$(C_n.3)$ and $(C_n.6)$ (see section 4.4). Then there is a constant $g_1 > 0$ such that the following holds.

(i) Assume that $(g,\theta) \in \mathbf{C} \times I^-(\delta)$, then $\mathcal{D}(K_g^*(\theta)) = \mathcal{D}$, $(K_g^*(\theta))^* = K_{\overline{g}}(\overline{\theta})$ and the spectrum of $K_g(\theta)$ satisfies

$$\sigma(K_g^*(\theta)) \subset \{z \in \mathbf{C} : Imz \leq C(g,\theta)\} \ , \tag{9.15}$$

where

$$C(g,\theta) := \sup_{t\in\mathbf{R}}\{2\frac{|Reg|}{\delta - Img}|Im\theta|^{1/2} + |Img||Im\theta|^{-1/2}\}\times$$
$$\times \sum_i \{\|f_{i,\beta_i}(t)\|_{H^2(\delta,\mathcal{B})} + \|e^{-\beta_i(u_i-\nu)/2}f_{i,\beta_i}(t)\|_{H^2(\delta,\mathcal{B})}\}.$$

Furthermore, if $Imz > C(g,\theta)$, then

$$\|(K_g^*(\theta) - z)^{-1}\| \leq \frac{1}{Imz - C(g,\theta)} \ , \tag{9.16}$$

and the map $(g,\theta) \to K_g^*(\theta)$ from $\mathbf{C} \times I^-(\delta)$ to the set of closed operators on $\widetilde{\mathcal{H}}$ is an analytic family (of type A) in each variable separately.

(ii) If $|g| < g_1|Im\theta|$, then the spectrum of the operator $K_g^*(\theta)$ in the half-plane $\Xi(Im\theta + \frac{|g|}{g_1})$ is purely discrete and independent of θ. If $|g| < \frac{1}{4}g_1|Im\theta|$, then the spectral projections $\widetilde{P}_{g,(n)}(\theta), n \in \mathbf{Z}$ associated to the spectrum of $K_g^*(\theta)$ in the half-plane $\Xi(Im\theta + \frac{|g|}{g_1}) := \{z \in \mathbf{C} : Imz > Im\theta + \frac{|g|}{g_1}\}$ are analytic in g and satisfy the estimate

$$\|\widetilde{P}_{g,(n)}(\theta) - \widetilde{P}_{0,(n)}\| < \frac{3|g|}{g_1|Im\theta|} \ . \tag{9.17}$$

(iii) If $|g| < \frac{g_1|Im\theta|}{4}$, then the quasi-Floquet Liouvillean $\widetilde{\Sigma}_{g,(n)}$ defined in (9.14) depends analytically on g, and has a Taylor expansion

$$\widetilde{\Sigma}_{g,(n)} = K_{(n)}^{\Sigma} + \sum_{j=1}^{\infty} g^{2j}\widetilde{\Sigma}_{(n)}^{(2j)} \tag{9.18}$$

where

$$K_{(n)}^{\Sigma} := n\omega + \mathcal{L}^{\Sigma} \ , n \in \mathbf{Z}. \tag{9.19}$$

The first non-trivial coefficient in (9.18) is

$$\widetilde{\Sigma}_{(n)}^{(2)} = \frac{1}{2}\oint_\gamma \frac{dz}{2\pi i}(\xi_{(n)}(z)(z - K_{(n)}^{\Sigma})^{-1} + (z - K_{(n)}^{\Sigma})^{-1}\xi_{(n)}(z)) \ ,$$

where $\xi_{(n)}(z) = \widetilde{P}_{0,(n)}\widetilde{V}^{tot}(\theta)(z - K_0(\theta))^{-1}\widetilde{V}^{tot}(\theta)\widetilde{P}_{0,(n)}$.

(iv) For $g \in \mathbf{R}$ and Imz large enough,

$$s - \lim_{Im\theta\uparrow 0}(K_g^*(\theta) - z)^{-1} = (K_g^*(Re\theta) - z)^{-1} \,. \tag{9.20}$$

Proof. To evade redundancy, we refer to chapter 6 for details of the proof, since they are very similar to the ones detailed there (with K_g^* instead of $\mathcal{L}_g$). The proof of (i) is similar to that of Lemma 6.3, and the proof of claim (ii) is similar to that of Proposition 6.4, and (iii) to Proposition 6.5. Since $\widetilde{T}_{g,(n)}$ is analytic and $\|\widetilde{T}_{g,(n)} - 1\| < 1$ for $|g| < \frac{g_1\mu}{4}$, $\widetilde{T}_{g,(n)}^{-1/2}$ is also analytic in g. Inserting the Neumann series for the resolvent of $K_g^*(\theta)$,

$$\widetilde{T}_{g,(n)} = 1 + \sum_{j=1}^{\infty} g^j \widetilde{T}_{(n)}^{(j)} \,, \tag{9.21}$$

with

$$\widetilde{T}_{(n)}^{(j)} = \oint_\gamma \frac{dz}{2\pi i}(z - K_{(n)}^{\Sigma})^{-1}\widetilde{P}_{0,(n)}\widetilde{V}^{tot}(\theta)((z - K_0(\theta))^{-1}\widetilde{V}^{tot}(\theta))^{j-1}\widetilde{P}_{0,(n)}(z - K_{(n)}^{\Sigma})^{-1} \,. \tag{9.22}$$

Similarly,

$$\widetilde{M}_{g,(n)} = K_{(n)}^{\Sigma} + \sum_{j=1}^{\infty} g^j \widetilde{M}_{(n)}^{(j)} \,, \tag{9.23}$$

with

$$\widetilde{M}_{(n)}^{(j)} = \oint_\gamma \frac{dz}{2\pi i} z(z - K_{(n)}^{\Sigma})^{-1}\widetilde{P}_0\widetilde{V}^{tot}(\theta)((z - K_0(\theta))^{-1}\widetilde{V}^{tot}(\theta))^{j-1}\widetilde{P}_{0,(n)}(z - K_{(n)}^{\Sigma})^{-1} \,. \tag{9.24}$$

The odd terms in the above two expansions are zero due to the fact that $\widetilde{P}_{0,(n)}$ projects onto the $N = 0$ sector. The first non-trivial coefficient in the Taylor series of $\Sigma_{g,(n)}$ is

$$\widetilde{\Sigma}_{(n)}^{(2)} = \widetilde{M}_{(n)}^{(2)} - \frac{1}{2}(\widetilde{T}_{(n)}^{(2)} K_{(n)}^{\Sigma} + K_{(n)}^{\Sigma}\widetilde{T}_{(n)}^{(2)}) \tag{9.25}$$

$$= \frac{1}{2}\oint_\gamma \frac{dz}{2\pi i}(\xi_{(n)}(z)(z - K_{(n)}^{\Sigma})^{-1} + (z - K_{(n)}^{\Sigma})^{-1}\xi_{(n)}(z)) \,. \tag{9.26}$$

The proof of (iv) is similar to Lemma 6.6, section 6.1. □

Let $\widetilde{P}_j^{(n)}$ be the spectral projections onto $E_j^{(n)} = n\omega + E_j, E_j \in \sigma(\mathcal{L}^{\Sigma}), j = 0, \cdots, 3, n \in \mathbf{Z}$.

Proposition 9.2 (Spectrum of $K_g^*(\theta)$)

Assume $(C_n.2)$,$(C_n.3)$ and $(C_n.6)$ (see section 4.4), and choose $\theta \in I^-(k)$. Then there exists a constant $g_1 > 0$ independent of t and θ, such that, for $|g| < g_1$, the essential spectrum of $K_g^*(\theta)$, $\sigma_{ess}(K_g^*(\theta)) \in \mathbf{C}\backslash\Xi(Im\theta)$, and the discrete spectrum $\sigma_{disc}(K_g^*(\theta)) \in \Xi(Im\theta) \cap \{z \in \mathbf{C} : Imz \leq 0\}$, with at least countably infinite eigenvalues on the real line, $\{\omega n : \ n \in \mathbf{Z}\}$.

Proof. When the coupling $g = 0$, $\sigma_{pp}(\mathcal{L}_0) = \{-2, 0, 2\}$, with double degeneracy at 0, and $\sigma_c(\mathcal{L}_0) = \mathbf{R}$. By Fourier transformation, $L^2([0, \tau_*]) \otimes \mathcal{H}$ is isomorphic to $\bigcup_{n=-\infty}^{\infty} \langle e^{in\omega t} \rangle \otimes \mathcal{H}$, where $\omega = \frac{2\pi}{\tau_*}$. It follows that

$$\sigma_{pp}(K_0) = \{E_j^{(n)} = E_j + n\omega : E_j \in \sigma(\mathcal{L}^\Sigma), j = 0, \cdots, 3; n \in \mathbf{Z}\} \ . \qquad (9.27)$$

From Proposition 9.1, (i), the map

$$(I^-(k), \mathbf{C}) \ni (\theta, g) \rightarrow K_g^*(\theta)$$

with values in the set of closed operators on $L^2([0, \tau_*]) \otimes \mathcal{H}$ is an analytic family in each variable separately. Let

$$C(\beta_i, k) := \sup_{|Imz| < k} \frac{1}{\sqrt{|1 + e^{-\beta_i(z-\nu)}|}}, i = 1, \cdots, n \ , \qquad (9.28)$$

which is finite, and let

$$\widetilde{C} := \sup_t \sup_{\theta \in I^-(k)} \|\widetilde{V}^{tot}(\theta, t)\| \ , \qquad (9.29)$$

which is also finite due to assumption $(C_n.4)$ and the estimate

$$\begin{aligned} \widetilde{C} \leq \sqrt{2} \sum_{i=1}^{n} C(\beta_i, k) \{ \|f_{i,\beta_i}\|_{H^2(k)} + \\ + \|e^{-\beta_i(u_i-\nu)/2} f_{i,\beta_i}\|_{H^2(k)}\} < \infty \ . \end{aligned}$$

The remaining part of the proof is similar to the proof of Theorem 6.7, section 6.1. The essential spectrum of $K_0^*(\theta)$ are lines $\{z \in \mathbf{C} : Imz = inIm\theta, n \in \mathbf{N}^+\}$, while $\sigma_{disc}(K_0(\theta)) = \sigma(K^\Sigma)$.

Choose $g_1 > 0$ such that $g_1\widetilde{C} < (k - \mu)/4$, where $\mu = |Im\theta|$ and $\widetilde{C}$ is defined in (9.29). Then, for $|g| < g_1$ and $-k < Im\theta < -(k + \mu)/2$, the essential spectrum $\sigma_{ess}(K_g(\theta))$ is contained in the half-plane $\{z \in \mathbf{C} : Imz < -\mu\}$. The location of the discrete spectrum of $K_g(\theta)$ inside the half-plane $\Xi(-\mu)$ can be computed using regular perturbation theory (see Proposition 9.1).

We know that

$$\widetilde{\Sigma}^{(2)}_{(n)} = \frac{1}{2}\oint_\gamma \frac{dz}{2\pi i}\{\widetilde{P}_{0,(n)}\widetilde{V}^{tot}(\theta)(z-K_0(\theta))^{-1}\widetilde{V}^{tot}(\theta)\widetilde{P}_{0,(n)}(z-K^{\Sigma}_{(n)})^{-1}$$
$$+ (z-K^{\Sigma}_{(n)})\widetilde{P}_{0,(n)}\widetilde{V}^{tot}(\theta)(z-K_0(\theta))^{-1}\widetilde{V}^{tot}(\theta)\widetilde{P}_{0,(n)}\} \ .$$

Let

$$\widetilde{\Gamma}^{n(2)}_j := \widetilde{P}^{(n)}_j \widetilde{\Sigma}^{(2)}_{(n)} \widetilde{P}^{(n)}_j \ , \tag{9.30}$$

where $\widetilde{P}^{(n)}_j, j = 0, \cdots, 3, n \in \mathbf{Z}$ are the spectral projections onto $E^{(n)}_j = n\omega + E_j$, the eigenvalues of K^{Σ}.

Applying the Cauchy integration formula to the expression of $\widetilde{\Gamma}^{n(2)}_j$ (as in the proof of Proposition 6.9, section 6.3) gives

$$E^{(n)}_{2,3}(g) = n\omega \pm (2+g^2\mathcal{P}V\int_{\mathbf{R}} du \frac{1}{2-u}\sum_{i=1}^{n}\|\widetilde{f}_i(u,t)\|^2_{\mathcal{B}}) - i\pi g^2\sum_{i=1}^{n}\|\widetilde{f}_i(2,t)\|^2_{\mathcal{B}} + O(g^4) \ , \tag{9.31}$$

where $\mathcal{P}V$ stands for the Cauchy prinicipal value, and $n \in \mathbf{Z}$. Note that $ImE^{(n)}_{2,3}(g) < 0, n \in \mathbf{Z}$. Furthermore,

$$E^{(n)}_{0,1}(t,g) = n\omega + g^2 a_{0,1}(t) + O(g^4) \ , \tag{9.32}$$

where $a_{0,1}(t)$ are the eigenvalues of the 2×2 matrix

$$-i\pi\sum_{i=1}^{n}\frac{\|\widetilde{f}_i(2,t)\|^2_{\mathcal{B}}}{2\cosh\beta_i(2-\nu)/2}\begin{pmatrix} e^{\beta_i(2-\nu)/2} & -e^{\beta_i(2-\nu)/2} \\ -e^{-\beta_i(2-\nu)/2} & e^{-\beta_i(2-\nu)/2}\end{pmatrix} \ . \tag{9.33}$$

By construction, $K_g e^{in\omega t}\Omega = n\omega e^{in\omega t}\Omega$ and $U(\theta)e^{in\omega t}\Omega = e^{in\omega t}\Omega$, so $n\omega, n \in \mathbf{Z}$ are also isolated eigenvalues of $K^*_g(\theta)$. In this case, this can be seen by defining the spectral projection to the real isolated eigenvalues of $K_g(\theta)$ using the resolvent, and taking the adjoint to define the corresponding spectral projections for the real isolated eigenvalues of $K^*_g(\theta)$.

In fact, $\psi = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ is the eigenvector corresponding to zero eigenvalue of $\widetilde{\Sigma}^2_{g,(n)}$. Hence,

$$E^{(n)}_0 = n\omega \ , \tag{9.34}$$

$$E^{(n)}_1 = n\omega - i\pi g^2\sum_{i=1}^{n}\|\widetilde{f}_i(2)\|^2_{\mathcal{B}} + O(g^4) \ . \tag{9.35}$$

Note that $ImE^{(n)}_j < 0, j = 1, 2, 3$ and $n \in \mathbf{Z}$. Moreover, we know from Proposition 9.1, (iv), that $s - \lim_{Im\theta\uparrow 0}(z-K^*_g(\theta))^{-1} = (z-K^*_g(Re\theta))^{-1}$ for Imz big enough, and hence the claim of this theorem. □

9.3 Convergence to time-periodic states

The following theorem claims that under suitable sufficient assumptions, the real state of the system converges to a time-periodic state with the same period of the perturbation τ_*.

Let $\mathbf{h}^{test} = D(e^{k\sqrt{p^2+1}})$, and $\mathcal{O}^{test} = \mathcal{F}_-(\mathbf{h}^{test})$, which is dense in $\mathcal{F}_-(L^2(\mathbf{R};\mathcal{B}))$, and define

$$\mathcal{C} := \mathcal{O}^{\Sigma} \otimes \mathcal{O}^{\mathcal{R}_1,test} \otimes \cdots \otimes \mathcal{O}^{\mathcal{R}_n,test} , \tag{9.36}$$

which is dense in $\mathcal{O}$.

We make the following additional assumption.

(H9.1) The perturbation of the Hamiltonian $V(t) \in \mathcal{C}$ for $t \in \mathbf{R}$.

Theorem 9.3 (Convergence to time-periodic states)

Assume $(C_n.2)$,$(C_n.3)$, $(C_n.6)$ and (H9.1), and let D be a positive operator on $\mathcal{H}$ such that $RanD$ is dense in $\mathcal{H}$ and $D\Omega = \Omega$. Assume further that $a \in \mathcal{C}$. Then there is a constant $g_1 > 0$, such that, for $|g| < g_1$, the following holds

$$\lim_{n\to\infty} \langle \Omega, \alpha_g^{n\tau_*+t}(a)\Omega\rangle = \langle \widetilde{\Omega}_g(0), D^{-1}\alpha_g^t(a)\Omega\rangle , \tag{9.37}$$

where $\widetilde{\Omega}_g$ corresponds to the zero-energy resonance of the adjoint of the Floquet Liouvillean, K_g^*.

Proof. Choose k as in Proposition 9.2, and let

$$D := \mathbf{1}^{\Sigma} \otimes e^{-k\sqrt{A_{\mathcal{R}_1}^2+1}} \otimes \cdots \otimes e^{-k\sqrt{A_{\mathcal{R}_n}^2+1}} , \tag{9.38}$$

where $A_{\mathcal{R}_i} = d\Gamma(i\partial_{u_i}), i = 1, \cdots, n$ is the second quantization of the generator of energy translations for the i^{th} reservoir. The operator D is positive such that $RanD$ is dense in $\mathcal{H}$ and $D\Omega = \Omega$. It follows from assumption (H9.1) and the fact that $a \in \mathcal{C}$ that $\alpha_g^t(a) \in \mathcal{D}(D^{-1})$ (as discussed in the proof of Theorem 8.3, section 8.2).

The remainder of the proof relies on the result of Proposition 9.2 and equation (9.2). It follows from (9.2) and the time periodicity of $f \in \widetilde{\mathcal{H}}$ that

$$(e^{-iK_g^* n\tau_*}\mathbf{1} \otimes \Omega)(0) = \widetilde{U}_g(n\tau_*, 0)(\mathbf{1} \otimes \Omega)(0) = \widetilde{U}_g(n\tau_*, 0)\Omega . \tag{9.39}$$

Let $\mathbf{1} \otimes \Omega =: \overline{\Omega} \in \widetilde{\mathcal{H}}$, and $\overline{D} := \mathbf{1} \otimes D$.

Without loss of generality, we assume $\frac{2\pi}{\tau_*} \neq 2$; however, if $\frac{2\pi}{\tau_*} = 2$, the state of the system typically oscillates between two resonance states until it finally converges to a time-periodic state; see remark 1. Using the dynamics on $C(\mathcal{O},\Omega)$, (9.39), and knowledge of $\sigma(K_g^*(\theta))$, it follows that

$$\lim_{n\to\infty}\langle\Omega,\alpha_g^{n\tau_*+t}(a)\Omega\rangle \tag{9.40}$$

$$= \lim_{n\to\infty}\langle\widetilde{U}_g(n\tau_*,0)\Omega,\alpha_g^t(a)\Omega\rangle \tag{9.41}$$

$$= \lim_{n\to\infty}\langle(e^{-iK_g^* n\tau_*}\overline{\Omega})(0),\alpha_g^t(s)\Omega\rangle \tag{9.42}$$

$$= \lim_{n\to\infty}\langle(\overline{D}U(-\theta)e^{-iK_g^*(\theta)n\tau_*}U(\theta)\overline{D\Omega})(0),D^{-1}\alpha_g^t(a)\Omega\rangle \tag{9.43}$$

$$= \lim_{n\to\infty}\langle(\overline{D}U(-\theta)\int_{-\infty}^{\infty}du(u+i\eta-K_g^*(\theta))^{-1}e^{-i(u+i\eta)n\tau_*}$$

$$\overline{\Omega})(0),D^{-1}\alpha_g^t(a)\Omega\rangle \tag{9.44}$$

$$= \lim_{n\to\infty}\langle(\overline{D}U(-\theta)\oint_\gamma dz(z-K_g^*(\theta))^{-1}e^{-izn\tau_*}\overline{\Omega})(0),D^{-1}\alpha_g^t(a)\Omega\rangle+$$

$$+\lim_{n\to\infty}\langle(\overline{D}U(-\theta)\int_{-\infty}^{\infty}du(u+i(\mu-\epsilon)-K_g^*(\theta))^{-1}e^{-i(u+i(\mu-\epsilon))n\tau_*}\overline{\Omega})(0),$$

$$D^{-1}\alpha_g^t(a)\Omega\rangle, \tag{9.45}$$

where $\eta>0$ and $0<\epsilon<\mu$.

Using the results of Propositions 9.1 and 9.2, the first term in the last equation converges to the time-periodic expression,

$$\lim_{n\to\infty}\langle(\overline{D}U(-\theta)\oint_\gamma dz(z-K_g^*(\theta))^{-1}e^{-izn_*}\overline{\Omega})(0),D^{-1}\alpha_g^t(a)\Omega\rangle \tag{9.46}$$

$$=\sum_{k\in\mathbf{Z}}\lim_{n\to\infty}\langle(\overline{D}U(-\theta)\widetilde{S}_{g,(k)}^{-1}(\theta)e^{-i\widetilde{\Sigma}_{g,(k)}(\theta)n\tau_*}\widetilde{S}_{g,(k)}(\theta)\overline{\Omega})(0),D^{-1}\alpha_g^t(a)\Omega\rangle \tag{9.47}$$

$$=\sum_{k\in\mathbf{Z}}\langle(\overline{D}\widetilde{P}_{g,(k)}(\theta)\overline{\Omega})(0),\alpha_g^t(a)\Omega\rangle \tag{9.48}$$

Let

$$\widetilde{\Omega}_{g,(k)} := \overline{D}\widetilde{P}_{g,(k)}(\theta)(e^{ik\omega t}\otimes\Omega)\ , \tag{9.49}$$

then

$$\overline{D}\widetilde{P}_{g,(k)}\overline{D} = \{(e^{ik\omega t}\otimes\Omega),\cdot\}\widetilde{\Omega}_{g,(k)}\ , \tag{9.50}$$

where $\{\cdot,\cdot\}$ denotes the scalar product on $\widetilde{H}$. Therefore,

$$\overline{D}\widetilde{P}_{g,(k)}(\theta)\overline{\Omega} = \{e^{ik\omega t}\otimes\Omega,\mathbf{1}\otimes\Omega\}\widetilde{\Omega}_{g,(k)} \tag{9.51}$$

$$= \widetilde{\Omega}_{g,(0)}\ , \tag{9.52}$$

and hence

$$\sum_{k\in\mathbf{Z}}\langle(\overline{D}\widetilde{P}_{g,(k)}\overline{\Omega})(0),D^{-1}\alpha_g^t(a)\Omega\rangle = \langle(\widetilde{\Omega}_{g,(0)})(0),D^{-1}\alpha_g^t(a)\Omega\rangle\ ,$$

where $\widetilde{\Omega}_{g,(0)}$ is the zero-energy resonance of the Floquet Liouvillean. The second term (9.45) converges exponentially fast to zero since

$$\langle (\overline{D}U(-\theta) \int_{-\infty}^{\infty} du(u+i(\mu-\epsilon)-K_g^*(\theta))^{-1} e^{-i(u+i(\mu-\epsilon))n\tau_*} \overline{\Omega})(0), D^{-1}\alpha_g^t(a)\Omega\rangle = O(e^{-(\mu-\epsilon')n\tau_*}) , \tag{9.54}$$

where $0 < \epsilon' < \epsilon < \mu$. □

Remarks.

(1) When $\frac{2\pi}{\tau_*} = 2$, the system exhibits the phenomena of resonance: The state of the system oscillates between two resonances until it finally converges to the time periodic state corresponding to $\widetilde{\Omega}_g$.[A-SF2] (This can be verified by a second order time-dependent perturbation theory calculation; (see also [Ya2]).

(2) Note that

$$\langle (\widetilde{\Omega}_{g,(0)})(0), D^{-1}\alpha_g^t(a)\Omega\rangle = \langle (\widetilde{\Omega}_{g,(k)})(0), D^{-1}\alpha_g^t(a)e^{ik\omega t}\Omega\rangle ,$$

where $\widetilde{\Omega}_{g,(k)}$ is the state corresponding to the $k\omega$-energy resonance of the adjoint of the Floquet Liouvillean.

(3) For small enough coupling g, it follows from Proposition 9.1,(ii) that $\widetilde{P}_g(\theta)$ is analytic in g. This is of especially *practical* importance, since in principle one can expand $\widetilde{\Omega}_g$ in a Taylor series to arbitrary order in g, and compute the entropy production per cycle. In particular, when there are only two reservoirs, one may explicitly compute the degree of efficiency η and compare it to η^{rev} (see chapter 2). Further details will appear in [A-SF2].

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