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**Complex Analysis and Operator Theory**

# Miniatures on Open Quantum Systems

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## Abstract

We present a unified and concise exposition of key topics in the mathematical theory of open quantum systems, developed within the framework of operator algebras. The manuscript consolidates and extends a series of invited articles originally prepared for the Modern Encyclopedia of Mathematical Physics, combining foundational material with modern perspectives on non-equilibrium quantum statistical mechanics. After introducing the C*- and W*-algebraic formulation of quantum mechanics, the paper reviews quantum dynamical systems, KMS states, and Tomita-Takesaki modular theory, as well as CCR and CAR algebras for bosonic and fermionic systems. Particular emphasis is placed on infinite systems, non-equilibrium steady states, entropy production, and linear response theory. The later sections develop a systematic treatment of small systems coupled to reservoirs, open lattice quantum spin systems, culminating in a detailed discussion of competing notions of quantum entropy production. The presentation highlights structural insights, conceptual clarity, and connections between equilibrium and non-equilibrium phenomena, providing a self-contained reference for researchers and graduate students in mathematical physics.


## Contents



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## 1 Introduction

At the turn of the 21st century, there was a revival of C*-algebraic methods in the study of equilibrium and non-equilibrium quantum statistical mechanics, a development to which the authors contributed. This contribution was acknowledged in 2006 through an invitation to take part in the ambitiously conceived *Modern Encyclopedia of Mathematical Physics*. (Fig. 1).

The topics, titles, and length of invited articles were specified by the Editors of the *Encyclopedia*. Our articles were completed in the summer of 2007.

Unfortunately, the *Encyclopedia*'s publication was repeatedly delayed and the project was eventually discontinued, so our articles never appeared in print.

On the occasion of the thematic program *Quantum Mathematics @ Polimi* held at the Politecnico di Milano in Spring 2025, in which the authors took part, we have

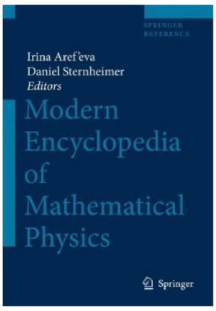


**Fig. 1** The cover of *Encyclopedia* from Springer 2011 web page

decided to consolidate these contributions into a single, unified publication. The articles in Parts I-IV appear largely in their original form, as we have deliberately limited revisions and references to work published after 2007. Parts V–VIII extend and modernize our Encyclopedia article on *Quantum non-equilibrium statistical mechanics*.

The notation is not uniform across sections, and some themes are repeated, as in the original articles. The Parts I-IV correspond to individual articles and are self-contained. Parts V–VIII are interconnected and should be read together.

We hope these concise treatments of important topics in modern mathematical physics will prove useful to readers.

## Part I

### Elements of operator algebras

## 2 The $C^*$-algebra Approach

### 2.1 Why Operator Algebras?

A quantum mechanical description of a system involving only a finite number of particles or degrees of freedom is given by a Hilbert space $\mathscr{H}$ and a Hamiltonian $H$, a selfadjoint operator on $\mathscr{H}$. Such systems will be called finite. States of those systems are described by unit vectors $\psi \in \mathscr{H}$ or more generally statistical mixtures, *i.e., density matrices*. Physical quantities, or observables, are described by all selfadjoint operators on $\mathscr{H}$. Their time evolution is governed by its Hamiltonian. In the Schrödinger picture, the state evolves according to the Schrödinger equation $\mathrm{i}\partial_t \psi_t = H\psi_t$ while observables are time-independent. In the equivalent Heisenberg picture, the state is time-independent and observables evolve according to the Heisenberg equation $\partial_t A_t = \mathrm{i}[H, A_t]$. As a consequence of the tight relation between Hamiltonian and dynamics, the spectrum $\mathrm{sp}(H)$ of $H$ contains a lot of information about the physics of the system.

From a mathematical perspective, constructing $\mathscr{H}$ and $H$ for a given physical system can often be presented as a problem in representation theory. In the case of a non-relativistic system of $N$ point-like particles in Euclidean space $\mathbb{R}^3$, the cor-

respondence between the classical and quantum description is based on *canonical quantization*. This procedure provides a representation of the positions $Q_1, \ldots, Q_{3N}$ and conjugate canonical momenta $P_1, \ldots, P_{3N}$ by selfadjoint operators satisfying the *canonical commutation relations* (CCR)

$$\mathrm{i}[P_i, Q_j] = \delta_{ij}, \quad \mathrm{i}[P_i, P_j] = 0, \quad \mathrm{i}[Q_i, Q_j] = 0. \tag{2.1}$$

If the particles have spin, then $\mathscr{H}$ has to carry $N$ representations of the Lie algebra of $SU(2)$, the quantum mechanical rotation group. If the particles are indistinguishable, then Pauli's principle imposes a definite covariance (as prescribed by the spin-statistics theorem) with respect to the natural action of the symmetric group $S_N$ on $\mathscr{H}$.

It is a deep fact that for finite systems representations of the CCR are unique, up to unitary transformations and mostly irrelevant multiplicities. This is the content of the celebrated *Stone-von Neumann* theorem (see [118] for a review).

When dealing with systems with an infinite number of particles or degrees of freedom – quantum fields or quantum statistical mechanics in the thermodynamic limit – we are faced with a radically different situation. The breakdown of Stone-von Neumann theorem implies the existence of a large number of unitarily inequivalent irreducible representations of the CCR. This phenomenon is not a special feature of CCR. The following example shows that it occurs also for representations of the group $SU(2)$; see [137] for a related discussion.

Consider an infinite chain of quantum spins with $s = 1/2$. To each site $x \in \mathbb{Z}$ we associate observables $\sigma_x^{(1)}, \sigma_x^{(2)}, \sigma_x^{(3)}$, which satisfy the $SU(2)$ commutation relations

$$[\sigma_x^{(j)}, \sigma_y^{(k)}] = 2\mathrm{i}\delta_{xy}\epsilon_{jkl}\sigma_x^{(l)}. \tag{2.2}$$

The Hamiltonian is formally given by $H = J\sum_{x\in\mathbb{Z}} \sigma_x^{(3)}$, so that

$$\mathrm{i}[H, \sigma_x^{(j)}] = -2J\epsilon_{3jk}\sigma_x^{(k)}. \tag{2.3}$$

Set $\mathfrak{h}_x = \mathbb{C}^2$ for any $x \in \mathbb{Z}$. The naive candidate for the Hilbert space of the system is the maximal tensor product of all the spaces $\mathfrak{h}_x$, which we will denote $\otimes_{x\in\mathbb{Z}}\mathfrak{h}_x$. It is defined as the completion of the pre-Hilbert space spanned by vectors of the form $\otimes_{x\in\mathbb{Z}}\varphi_x$, where each $\varphi_x$ is a unit vector in $\mathfrak{h}_x$. The inner product between two such vectors is defined by

$$(\otimes_{x\in\mathbb{Z}}\psi_x \mid \otimes_{x\in\mathbb{Z}}\varphi_x) = \prod_{x\in\mathbb{Z}}(\psi_x \mid \varphi_x), \tag{2.4}$$

whenever the infinite product on the right-hand side of (2.4) is absolutely convergent. Otherwise, the inner product is set to be zero. The space $\otimes_{x\in\mathbb{Z}}\mathfrak{h}_x$ was first considered by von Neumann in [102] (he called it the complete direct product of the family $(\mathfrak{h}_x)_{x\in\mathbb{Z}}$). This space is much too big for most applications. In particular, it is not separable, *i.e.*, it does not have a countable orthonormal basis[1].

[1] Except for recent developments in quantum gravity, most Hilbert spaces of quantum physics are separable.

Let us describe another candidate for the notion of the infinite tensor product, which is more useful in quantum physics. For all $x \in \mathbb{Z}$ fix an orthonormal basis $\{\chi_x^-, \chi_x^+\}$ of $\mathfrak{h}_x$. To each finite subset $X \subset \mathbb{Z}$ associate the vector

$$e_X = \left(\bigotimes_{x\in X} \chi_x^+\right) \bigotimes \left(\bigotimes_{x\in\mathbb{Z}\setminus X} \chi_x^-\right).$$

According to (2.4) one has $(e_X|e_Y) = \delta_{XY}$. Thus, finite linear combinations of the vectors $e_X$ form a pre-Hilbert space. The Hilbert space $\mathscr{H}$ obtained by completion is separable since $\{e_X \mid X \subset \mathbb{Z}, |X| < \infty\}$ is a countable orthonormal basis.

A pair $(\mathfrak{h}, \chi)$, where $\mathfrak{h}$ is a Hilbert space and $\chi \in \mathfrak{h}$ a unit vector, is often called a grounded Hilbert space. The above construction is a special case of the tensor product of grounded Hilbert spaces, namely $\mathscr{H} = \otimes_{x\in\mathbb{Z}}(\mathfrak{h}_x, \chi_x^-)$. The interested reader may consult [35] for the general construction.

Remark that the maximal tensor product $\otimes_{x\in\mathbb{Z}}\mathfrak{h}_x$ naturally splits into the direct sum of sectors, where each sector has the form $\otimes_{x\in\mathbb{Z}}(\mathfrak{h}_x, \chi_x^-)$ for a certain sequence of unit vectors $\chi_x^- \in \mathfrak{h}_x$.

If $J > 0$, then the ground state of the chain has all spins pointing down in the direction 3. If we interpret $\chi_x^\pm$ as the eigenstates of the spin at $x$ in direction 3 with eigenvalue $\pm 1/2$, the vector $e_\emptyset$ clearly describes this ground state. The vector $e_X$ describes a local excitation of the chain, the spins at $x \in X$ pointing up in direction 3. This immediately leads to the following representation of the commutation relations (2.2) on $\mathscr{H}$:

$$\sigma_x^{(1)+} e_X = e_{X\odot x}, \quad \sigma_x^{(2)+} e_X = \mathrm{i} s_X(x) e_{X\odot x}, \quad \sigma_x^{(3)+} e_X = s_X(x) e_X,$$

where

$$X \odot x = \begin{cases} X \setminus \{x\} & \text{if } x \in X, \\ X \cup \{x\} & \text{if } x \notin X, \end{cases} \qquad s_X(x) = \begin{cases} +1 & \text{if } x \in X, \\ -1 & \text{if } x \notin X. \end{cases}$$

We obtain a different representation of the commutation relations (2.2) on the same space $\mathscr{H}$ if we think of $\chi_x^\pm$ as the eigenstates of the spin in direction 3 with eigenvalue $\mp 1/2$, namely

$$\sigma_x^{(1)-} = \sigma_x^{(1)+}, \quad \sigma_x^{(2)-} = -\sigma_x^{(2)+}, \quad \sigma_x^{(3)-} = -\sigma_x^{(3)+}.$$

Note that although $\sigma_x^{(3)+} e_\emptyset = -e_\emptyset$ for all $x \in \mathbb{Z}$, one easily checks that there is no unit vector $\Psi \in \mathscr{H}$ such that $\sigma_x^{(3)-}\Psi = -\Psi$ for all $x \in \mathbb{Z}$. Thus, in the second representation of the system the ground state *does not belong to* $\mathscr{H}$. In particular, there is no unitary operator $U$ on $\mathscr{H}$ such that $U\sigma_x^{(3)-}U^* = \sigma_x^{(3)+}$ – the two representations are inequivalent. Since

$$e_Y = \prod_{x\in X\Delta Y} \sigma_x^{(1)\pm} e_X,$$

the two representations are also irreducible.

Expressing the formal Hamiltonian $H$ in the two representations leads to

$$He_X = J\sum_{x\in X} \pm e_X + J\sum_{x\notin X} \mp e_X = \left(\pm 2J|X| \mp J\sum_{x\in\mathbb{Z}} 1\right) e_X.$$

Discarding a constant – the infinite energy of the state $e_\emptyset$ – we may thus set

$$H_\pm e_X = \pm 2J|X|e_X,$$

which defines two selfadjoint operators on $\mathscr{H}$. The physical meaning of $H_\pm$ is clear: it describes the energy of the system relative to the infinite energy of the state $e_\emptyset$. One easily verifies that

$$\mathrm{i}[H_\pm, \sigma_x^{(j)\pm}] = -2J\epsilon_{3jk}\sigma_x^{(k)\pm},$$

*i.e.*, that the commutation relations (2.3) are satisfied. Note, however, that the spectra of the two Hamiltonians are quite different,

$$\mathrm{sp}(H_\pm) = \pm 2J\mathbb{N}.$$

This is not surprising, since $H_\pm$ measures the energy relative to two distinct reference states: one of them has all spins up while the other has all spins down.

In conclusion, there are many ways to represent the algebraic structure induced by commutation relations (2.2) and (2.3) in a Hilbert space. To select such a representation one needs to specify a reference state. In equilibrium statistical mechanics this fact does not lead to difficulties since it is always possible to define thermodynamic quantities (free energy, pressure, ...) as limits of quantities related to finite systems. The situation is different in non-equilibrium statistical mechanics where dynamics plays a much more important role. To give a mathematically precise sense to non-equilibrium steady states, for example, requires a consideration of infinite systems from the outset; see Section 11.

In the algebraic approach to quantum mechanics the central object is the algebraic structure – in the above example, Relations (2.2) and (2.3). Hilbert spaces and Hamiltonians only appear when this structure gets represented by linear operators. Such representations are induced by the states of the system, usually via the Gelfand-Naimark-Segal construction; see Section 2. States with different physical properties (e.g. different particle or energy density) lead to inequivalent representations and hence the Hamiltonians describing their dynamics may have different spectral properties.

The mathematical framework of algebraic approach to quantum mechanics is the theory of *operator algebras*. *$C^*$-algebras*, *von Neumann algebras*, and *$W^*$-algebras* are the most commonly used types of operator algebras in this context. There is a huge literature devoted to this subject. The reader may consult [45, 46, 89, 128, 133, 135] for mathematical introductions and [33–35, 41, 67, 126, 129] for applications to quantum physics and statistical mechanics.

## 2.2 Examples of $C^*$-algebras

To illustrate the algebraic approach, we consider a few systems for which $C^*$-algebras provide a natural framework. See also Section 6. We shall be only concerned with operator algebras here. We refer to Section 3 for examples of dynamics on these algebras.

### 2.2.1 Lattice spin systems

To describe a *quantum spin system* on an infinite lattice $\Gamma$ (for example, $\Gamma = \mathbb{Z}^d$ with $d \geq 1$), let $\mathfrak{h}$ be the finite dimensional Hilbert space of a single spin, and $\mathfrak{h}_x$ a copy of $\mathfrak{h}$ associated to each $x \in \Gamma$. For finite subsets $\Lambda \subset \Gamma$ we set $\mathfrak{h}_\Lambda \equiv \otimes_{x\in\Lambda}\mathfrak{h}_x$, and define the local $C^*$-algebras as

$$\mathfrak{A}_\Lambda \equiv \mathscr{B}(\mathfrak{h}_\Lambda).$$

If $\Lambda \subset \Lambda'$, the natural isometric injection $A \mapsto A \otimes I_{\mathfrak{h}_{\Lambda'\setminus\Lambda}}$ allows one to identify $\mathfrak{A}_\Lambda$ with a subalgebra of $\mathfrak{A}_{\Lambda'}$. With this identification, we may define

$$\|A\| = \|A\|_{\mathfrak{A}_\Lambda} \text{ if } A \in \mathfrak{A}_\Lambda,$$

unambiguously for all $A \in \mathfrak{A}_{\mathrm{loc}} \equiv \cup_{\Lambda\subset\Gamma}\mathfrak{A}_\Lambda$, the union being over finite subsets of $\Gamma$. This defines a $C^*$-norm on the $*$-algebra $\mathfrak{A}_{\mathrm{loc}}$. Denote by $\mathfrak{A} = \mathfrak{A}(\Gamma, \mathfrak{h})$ the $C^*$-algebra obtained as norm completion of $\mathfrak{A}_{\mathrm{loc}}$. We can identify each local algebra $\mathfrak{A}_\Lambda$ with the corresponding subalgebra of $\mathfrak{A}$, hence

$$\mathfrak{A} = \left(\bigcup_{\Lambda\subset\Gamma} \mathfrak{A}_\Lambda\right)^{\mathrm{cpl}}, \tag{2.5}$$

where each $\mathfrak{A}_\Lambda$ is a full matrix algebra, and cpl denotes the completion. $C^*$-algebras of this type are called *uniformly hyperfinite* (UHF) or *Glimm algebras*.

### 2.2.2 CAR algebras

Let $\mathfrak{h}$ be the Hilbert space of a single *fermion* (typically $\mathfrak{h} = L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$, but other geometries and additional internal degrees of freedom may lead to different single particle Hilbert spaces). A system of such fermions is described by the *second quantization* formalism. Denote by $\Gamma_{\mathrm{a}}(\mathfrak{h})$ the fermionic (or anti-symmetric) *Fock space* over $\mathfrak{h}$. The fermion *creation/annihilation operators* $a^*(f)$, $a(f)$ are bounded operators on $\Gamma_{\mathrm{a}}(\mathfrak{h})$ satisfying the canonical anti-commutation relations (CAR)

$$[a(f), a^*(g)]_+ = (f|g)\mathbb{1}, \quad [a(f), a(g)]_+ = 0, \tag{2.6}$$

for all $f, g \in \mathfrak{h}$. A convenient choice of observables is given by polynomials in $a, a^*$, that is, finite linear combinations of monomials

$$a^\#(f_1)\cdots a^\#(f_n),$$

where each $a^\#$ stands for either $a$ or $a^*$ and the $f_j$ are elements of $\mathfrak{h}$ or more generally of some subspace $\mathfrak{h}_0 \subset \mathfrak{h}$. This set is clearly a unital $*$-algebra. Its norm closure is a $C^*$-subalgebra of $\mathscr{B}(\Gamma_{\mathrm{a}}(\mathfrak{h}))$. It turns out that this algebra is completely characterized by $\mathfrak{h}_0$ and the CAR (2.6).

**Theorem 2.1** *Let $\mathfrak{h}_0$ be a pre-Hilbert space. Up to $*$-isomorphisms, there exists a unique unital $C^*$-algebra $\mathrm{CAR}(\mathfrak{h}_0)$ satisfying the following two properties:*

1. *There exists an anti-linear map $a : \mathfrak{h}_0 \to \mathrm{CAR}(\mathfrak{h}_0)$ such that the CAR (2.6) hold for any $f, g \in \mathfrak{h}_0$.*
2. *The set of monomials $\{a^\#(f_1)\cdots a^\#(f_n) \mid f_1, \ldots, f_n \in \mathfrak{h}_0\}$ is total in the algebra $\mathrm{CAR}(\mathfrak{h}_0)$.*

***Remarks*** **1.** For $f \neq 0$, Equ. (2.6) yields that $a(f) \neq 0$ and that $(a^*(f)a(f))^2 = \|f\|^2 a^*(f)a(f)$. Thus

$$\|a(f)\| = \|f\| \tag{2.7}$$

holds for any $f \in \mathfrak{h}_0$. In particular, the map $a$ is continuous, extends to the completion $\mathfrak{h}$ of $\mathfrak{h}_0$, and $\mathrm{CAR}(\mathfrak{h}) = \mathrm{CAR}(\mathfrak{h}_0)$.

**2.** By condition *(ii)*, the algebra $\mathrm{CAR}(\mathfrak{h})$ is separable if and only if the Hilbert space $\mathfrak{h}$ is.
**3.** An antilinear map $f \mapsto b(f)$ from $\mathfrak{h}$ to $\mathscr{B}(\mathscr{H})$ satisfying (2.6) extends to a faithful representation of $\mathrm{CAR}(\mathfrak{h})$ in the Hilbert space $\mathscr{H}$.

Set $\phi(f) := \frac{1}{2}\big(a^*(f) + a(f)\big)$. A direct consequence of this theorem is the following

**Corollary 2.2** *Let $\mathfrak{h}_1, \mathfrak{h}_2$ be two Hilbert spaces. Assume that $R : \mathfrak{h}_1 \to \mathfrak{h}_2$ is a bounded invertible real linear map such that*

$$\mathrm{Re}(f|g) = \mathrm{Re}(Rf|Rg). \tag{2.8}$$

*Then there exists a unique $*$-isomorphism $\gamma : \mathrm{CAR}(\mathfrak{h}_1) \to \mathrm{CAR}(\mathfrak{h}_2)$ such that*

$$\gamma(\phi(f)) = \phi(Rf).$$

*$\gamma$ is called the Bogoliubov transformation associated to $R$.*
*Equivalently, if we decompose $R$ into its linear and antilinear part*[2]

$$R = P + Q, \quad P := \frac{1}{2}(R - \mathrm{i}R\mathrm{i}), \quad Q := \frac{1}{2}(R + \mathrm{i}R\mathrm{i}), \tag{2.9}$$

*then (2.12) can be written as*

$$\begin{aligned} P^*P + Q^*Q &= \mathbb{1}_{\mathfrak{h}_1}, \quad & PP^* + QQ^* &= \mathbb{1}_{\mathfrak{h}_2}, \\ P^*Q + Q^*P &= 0 \quad , & PQ^* + QP^* &= 0. \end{aligned}$$

[2] Here, i denotes multiplication by the imaginary unit.

*Moreover,*

$$\gamma(a(f)) = a(Pf) + a^*(Qf).$$

$\gamma$ is called the *Bogoliubov isomorphism* induced by $R$. In the special case of a complex linear $R$, when $R = U$ is unitary, $\gamma$ is called the gauge-invariant or particle preserving Bogoliubov transformation.

When dealing with compound Fermi systems the following result is often useful.

**Theorem 2.3** (Exponential law for fermions) *Let $\mathfrak{h}_1, \mathfrak{h}_2$ be two Hilbert spaces. There is a unique unitary operator $U : \Gamma_a(\mathfrak{h}_1 \oplus \mathfrak{h}_2) \to \Gamma_a(\mathfrak{h}_1) \otimes \Gamma_a(\mathfrak{h}_2)$ such that*

$$U\Omega = \Omega \otimes \Omega, \quad Ua(f_1 \oplus f_2)U^* = a(f_1) \otimes \mathbb{1} + (-1)^N \otimes a(f_2),$$

*where $\Omega$ denotes the Fock vacuum vector and $N = \mathrm{d}\Gamma(I)$ the number operator.*

Note that $N \in \mathrm{CAR}(\mathfrak{h}_1)$ if and only if $\mathfrak{h}_1$ is finite dimensional. Thus, $\mathrm{CAR}(\mathfrak{h}_1 \oplus \mathfrak{h}_2)$ is $*$-isomorphic to the $C^*$-tensor product $\mathrm{CAR}(\mathfrak{h}_1) \otimes \mathrm{CAR}(\mathfrak{h}_2)$ if and only if at least one of the spaces $\mathfrak{h}_1, \mathfrak{h}_2$ is finite dimensional.

### 2.2.3 CCR algebras

Systems of *bosons* are described in an analogous way by creation/annihilation operators $a^*(f)$ and $a(f)$ on the bosonic (or symmetric) Fock space $\Gamma_s(\mathfrak{h})$. These operators satisfy the canonical commutation relations

$$[a(f), a^*(g)] = (f|g), \quad [a(f), a(g)] = 0, \tag{2.10}$$

for $f, g \in \mathfrak{h}$. However, dealing with bosonic systems is more delicate since the operators $a^*(f)$ and $a(f)$ are unbounded. This follows readily from the algebraic structure described by the CCR. Indeed, suppose that $a(f)$ is bounded. Then, since $a^*(f)a(f)$ is positive, it follows from the CCR that $\|a(f)a^*(f)\| = \|a^*(f)a(f)\| + \|f\|^2$, which contradicts the fact that $\|a(f)a^*(f)\| = \|a^*(f)a(f)\| = \|a(f)\|^2$.

Thus it is not a priori clear how the CCR should be interpreted without referring to some domain $\mathscr{D} \subset \Gamma_s(\mathfrak{h})$ on which they are supposed to hold. The operator

$$\frac{1}{\sqrt{2}}\big(a^*(f) + a(f)\big)$$

is essentially selfadjoint on the dense subspace $\Gamma_{s,\mathrm{fin}}(\mathfrak{h})$ of finite particle vectors of $\Gamma_s(\mathfrak{h})$. Its selfadjoint closure is called *Segal field operator* and denoted by $\phi(f)$. Segal field operators satisfy the commutation relations $[\phi(f), \phi(g)] = \mathrm{i}\,\mathrm{Im}(f|g)$ which are formally equivalent to (2.10). The unitary operators

$$W(f) = \mathrm{e}^{\mathrm{i}\phi(f)}$$

are called *Weyl operators*. They satisfy the *Weyl relations*

$$W(f)W(g) = \mathrm{e}^{-\mathrm{i}\,\mathrm{Im}(f,g)/2}W(f+g). \tag{2.11}$$

Finite linear combinations of Weyl operators build a $*$-algebra. Its closure is a $C^*$-algebra which is completely characterized by the Weyl relations (2.11).

**Theorem 2.4** *Let $\mathfrak{h}_0$ be a pre-Hilbert space. Up to $*$-isomorphisms, there exists a unique unital $C^*$-algebra $\mathrm{CCR}(\mathfrak{h}_0)$ with the following properties:*

1. *There is a map $f \mapsto W(f)$ from $\mathfrak{h}_0$ to $\mathrm{CCR}(\mathfrak{h}_0)$ such that*

$$W(-f) = W(f)^*, \quad W(0) \neq 0,$$

   *and the Weyl relations (2.11) are satisfied for all $f, g \in \mathfrak{h}_0$.*
2. *The set $\{W(f) \mid f \in \mathfrak{h}_0\}$ is total in $\mathrm{CCR}(\mathfrak{h}_0)$.*

***Remarks*** **1.** It follows from (2.11) and conditions *(i)-(ii)* that $W(0) = \mathbb{1}$ and that $W(f)^* = W(f)^{-1}$, *i.e.*, that $W(f)$ is unitary. Moreover, if $f \neq g$, then $\|W(f) - W(g)\| = 2$.
**2.** Unlike in the CAR-case, if $\mathfrak{h}_0 \neq \mathfrak{h}_1$, then $\mathrm{CCR}(\mathfrak{h}_0) \neq \mathrm{CCR}(\mathfrak{h}_1)$. Moreover, $\mathrm{CCR}(\mathfrak{h}_0)$ is not separable if $\mathfrak{h}_0 \neq \{0\}$.
**3.** A map $f \mapsto W_\pi(f)$ from $\mathfrak{h}_0$ to the unitary operators on $\mathscr{H}$ satisfying the Weyl relations (2.11) extends to a representation $(\mathscr{H}, \pi)$ of $\mathrm{CCR}(\mathfrak{h}_0)$.

Bogoliubov isomorphisms between CCR algebras are defined in a similar way as in the CAR case.

**Corollary 2.5** *Let $\mathfrak{h}_1$, $\mathfrak{h}_2$ be two pre-Hilbert spaces and $R : \mathfrak{h}_1 \to \mathfrak{h}_2$ an invertible real-linear map such that*

$$\mathrm{Im}(Rf|Rg) = \mathrm{Im}(f|g) \tag{2.12}$$

*Then there is a unique $*$-isomorphism $\gamma : \mathrm{CCR}(\mathfrak{h}_1) \to \mathrm{CCR}(\mathfrak{h}_2)$ such that $\gamma(W(f)) = W(Rf)$. $\gamma$ is called the Bogoliubov transformation associated to $R$.*

*Equivalently, if we decompose $R$ into the linear and antilinear part*

$$R = P + Q, \quad P := \frac{1}{2}(R - \mathrm{i}R\mathrm{i}), \quad Q := \frac{1}{2}(R + \mathrm{i}R\mathrm{i}), \tag{2.13}$$

*then (2.12) can be written as*

$$\begin{aligned} P^*P - Q^*Q &= \mathbb{1}_{\mathfrak{h}_1}, \quad & PP^* - QQ^* &= \mathbb{1}_{\mathfrak{h}_2}, \\ P^*Q - Q^*P &= 0, \quad & PQ^* - QP^* &= 0. \end{aligned}$$

*Moreover, (in a representation where we can define creation and annihilation operators, so that we can extend the Bogoliubov isomorphism to affiliated unbounded operators)*

$$\gamma(a(f)) = a(Pf) + a^*(Qf).$$

In the special case of a complex linear $R$, when $R = U$ is unitary, $\gamma$ is called the gauge-invariant or particle preserving Bogoliubov transformation.

An exponential law similar to Theorem 2.3 holds for bosons.

**Theorem 2.6** (Exponential law for bosons) *Let $\mathfrak{h}_1$, $\mathfrak{h}_2$ be two Hilbert spaces. There is a unique unitary operator $U : \Gamma_s(\mathfrak{h}_1 \oplus \mathfrak{h}_2) \to \Gamma_s(\mathfrak{h}_1) \otimes \Gamma_s(\mathfrak{h}_2)$ such that*

$$U\Omega = \Omega \otimes \Omega, \quad UW(f_1 \oplus f_2)U^* = W(f_1) \otimes W(f_2),$$

*where $\Omega$ denotes the Fock vacuum vector. Moreover,* $\mathrm{CCR}(\mathfrak{h}_1 \oplus \mathfrak{h}_2)$ *is $*$-isomorphic to the $C^*$-tensor product* $\mathrm{CCR}(\mathfrak{h}_1) \otimes \mathrm{CCR}(\mathfrak{h}_2)$.[3]

In practice the $C^*$-algebra $\mathrm{CCR}(\mathfrak{h}_0)$ of Theorem 2.4 is not very convenient and one often prefers to work with von Neumann algebras when dealing with bosons. Let $(\mathscr{H}, \pi)$ be a representation of $\mathrm{CCR}(\mathfrak{h}_0)$. The von Neumann algebra on $\mathscr{H}$ generated by $\{\pi(A) \mid A \in \mathrm{CCR}(\mathfrak{h}_0)\}$ is given by the *bicommutant*

$$\mathfrak{M}_\pi(\mathfrak{h}_0) = \pi(\mathrm{CCR}(\mathfrak{h}_0))''.$$

It is the enveloping von Neumann algebra of the representation $\pi$, see Section 6 for an example.

### 2.2.4 Quasi-local structure of $\mathfrak{A}(\Gamma, \mathfrak{h})$ and of $\mathrm{CAR}(\mathfrak{h})$

As already mentioned, in most physical applications the single-fermion Hilbert space is $\mathfrak{h} = L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$ or some straightforward variant of it. To each bounded open subset $\Lambda \subset \mathbb{R}^d$ a local Hilbert space $\mathfrak{h}_\Lambda = L^2(\Lambda) \otimes \mathbb{C}^n$. The canonical isometric injections $\mathfrak{h}_\Lambda \hookrightarrow \mathfrak{h}$ yield injections $\mathrm{CAR}(\mathfrak{h}_\Lambda) \hookrightarrow \mathrm{CAR}(\mathfrak{h})$, allowing us to identify the local algebra $\mathrm{CAR}(\mathfrak{h}_\Lambda)$ with a $C^*$-subalgebra of $\mathrm{CAR}(\mathfrak{h})$. It follows immediately from remark 1 that

$$\mathrm{CAR}(\mathfrak{h}) = \left( \bigcup_{\Lambda \subset \mathbb{R}^d} \mathrm{CAR}(\mathfrak{h}_\Lambda) \right)^{\mathrm{cl}},$$

to be compared with Equ. (2.5). Note, however, that while $\Lambda \cap \Lambda' = \emptyset$ implies $[\mathfrak{A}_\Lambda, \mathfrak{A}_{\Lambda'}] = \{0\}$, the CAR algebras of disjoint subsets do not commute. This is of course due to the fact that $a(f)$ and $a(g)$ anticommute. Let $\theta$ be the $*$-automorphism defined by $\theta(a(f)) = -a(f)$ and denote by

$$\mathrm{CAR}_\pm(\mathfrak{h}) = \{A \in \mathrm{CAR}(\mathfrak{h}) \mid \theta(A) = \pm A\},$$

the even and odd parts of $\mathrm{CAR}(\mathfrak{h})$ with respect to $\theta$. Alternatively, these sets are the closed linear spans of monomials of even and odd degree in the $a^\#$. Then one has $\mathrm{CAR}(\mathfrak{h}_\Lambda) = \mathrm{CAR}_+(\mathfrak{h}_\Lambda) \oplus \mathrm{CAR}_-(\mathfrak{h}_\Lambda)$, and one easily checks that

$$[\mathrm{CAR}_\pm(\mathfrak{h}_\Lambda), \mathrm{CAR}_\pm(\mathfrak{h}_{\Lambda'})] = \{0\}, \quad [\mathrm{CAR}_\pm(\mathfrak{h}_\Lambda), \mathrm{CAR}_\mp(\mathfrak{h}_{\Lambda'})]_+ = \{0\}.$$

From a physical point of view, observables localized in disjoint regions of space should be simultaneously measurable. Hence physical observables of a fermionic system

[3] Since CCR algebras are nuclear $C^*$-algebras, their $C^*$-tensor product is unique.

should be elements of the even subalgebra $\mathrm{CAR}_+(\mathfrak{h})$. In fact, the stronger requirement of gauge-invariance further reduces the observable algebra to the subalgebra of $\mathrm{CAR}_+(\mathfrak{h})$ generated by monomials in the $a^\#$ containing the same number of $a$ and $a^*$; see Section 7 for a discussion of this point. In both the UHF-algebra $\mathfrak{A}$ and the CAR-algebra $\mathrm{CAR}(\mathfrak{h})$, the family of local subalgebras define the so-called quasi-local structure. We refer the reader to [34, Section 2.6] for a general discussion.

### 2.3 States and the GNS Construction

Let $\mathscr{O}$ be a $C^*$-algebra. A linear functional $\varphi$ on $\mathscr{O}$ is positive if $\varphi(A^*A) \geq 0$ for all $A \in \mathscr{O}$. A positive linear functional is automatically bounded, *i.e.*, is an element of the dual $\mathscr{O}^\#$. It is called a state if $\|\varphi\| = 1$. If $\mathscr{O}$ has a unit $\mathbb{1}$ then $\|\varphi\| = \varphi(\mathbb{1})$ for any positive linear functional $\varphi$.

A representation of $\mathscr{O}$ on a Hilbert space $\mathscr{H}$ is a $*$-morphism $\pi : \mathscr{O} \to \mathscr{B}(\mathscr{H})$. Given such a representation and a unit vector $\Omega \in \mathscr{H}$, the formula $\varphi(A) = (\Omega|\pi(A)\Omega)$ defines a state on $\mathscr{O}$. The GNS construction shows that any state on $\mathscr{O}$ is of this form.

**Theorem 2.7** *Let $\omega$ be a state on the $C^*$-algebra $\mathscr{O}$. Then there exist a Hilbert space $\mathscr{H}_\omega$, a representation $\pi_\omega$ of $\mathscr{O}$ in $\mathscr{H}_\omega$ and a unit vector $\Omega_\omega \in \mathscr{H}_\omega$ such that*

1. *$\omega(A) = (\Omega_\omega|\pi_\omega(A)\Omega_\omega)$ for all $A \in \mathscr{O}$.*
2. *$\pi_\omega(\mathscr{O})\Omega_\omega$ is dense in $\mathscr{H}_\omega$.*

*The triple $(\mathscr{H}_\omega, \pi_\omega, \Omega_\omega)$ is unique up to unitary equivalence. It is called the GNS representation or the cyclic representation of $\mathscr{O}$ induced by the state $\omega$.*

An important object associated with the GNS representation is the *enveloping von Neumann algebra:* The $\sigma$-weak closure $\mathscr{O}_\omega$ of $\pi_\omega(\mathscr{O})$ in $\mathscr{B}(\mathscr{H}_\omega)$. By von Neumann's *bicommutant theorem*, it is given by the bicommutant

$$\mathscr{O}_\omega = \pi_\omega(\mathscr{O})''.$$

We note that if $\mathscr{O}$ is itself a von Neumann or a $W^*$-algebra and $\omega$ is $\sigma$-weakly continuous (*i.e.*, a *normal state*) then $\pi_\omega$ is $\sigma$-weakly continuous and $\mathscr{O}_\omega = \pi_\omega(\mathscr{O})$.

Two states $\omega, \nu$ on $\mathscr{O}$ are quasi-equivalent if there exists a $*$-isomorphism $\phi : \mathscr{O}_\omega \to \mathscr{O}_\nu$ such that $\pi_\nu = \phi \circ \pi_\omega$.

The folium of a state $\omega$ is the set $\mathscr{N}_\omega$ of all states of the form $\nu(A) = \mathrm{tr}(\rho\pi_\omega(A))$ for some density matrix $\rho$ on $\mathscr{H}_\omega$. A state $\nu \in \mathscr{N}_\omega$ is said to be $\omega$-normal. Thus, $\omega$-normal states on $\mathscr{O}$ are characterized by the fact that they extend to normal states on the enveloping von Neumann algebra $\mathscr{O}_\omega$.

**Theorem 2.8** *The following propositions are equivalent.*

1. *$\mu$ and $\nu$ are quasi-equivalent.*
2. *$\mu$ and $\nu$ have the same folium.*
3. *There exist Hilbert spaces $\mathscr{K}_\mu$ and $\mathscr{K}_\nu$ and a unitary map $V : \mathscr{H}_\mu \otimes \mathscr{K}_\mu \to \mathscr{H}_\nu \otimes \mathscr{K}_\nu$ such that*

$$\pi_\nu \otimes \mathbb{1} = V(\pi_\mu \otimes \mathbb{1})V^*.$$

The reader should consult [34] for a more detailed discussion.

## 3 Quantum Dynamical Systems

In the most common approach to quantum physics, observables are described by bounded operators on a Hilbert space. This formalism is usually sufficient at zero temperature. To describe quantum systems in the thermodynamic limit at positive temperatures, or more generally, at positive densities, it is convenient to use a more sophisticated formalism where observables are described by elements of some operator algebra, see Sections 2 and 6. In this algebraic approach, quantum dynamics in the Heisenberg picture is given by a one-parameter group of automorphisms of the algebra of observables. In analogy with the theory of classical dynamical systems, such a group defines a quantum dynamical system. There are two main versions of the algebraic approach, which differ in the topological properties of the algebra and of the dynamical group: the $C^*$- and the $W^*$-approach.

### 3.1 $C^*$-dynamical Systems

**Definition 3.1** A $C^*$-dynamics on a *$C^*$-algebra* $\mathscr{O}$ is a strongly continuous one-parameter group $\mathbb{R} \ni t \to \tau^t$ of *$*$-automorphisms* of $\mathscr{O}$. A $C^*$-dynamical system is a pair $(\mathscr{O}, \tau)$, where $\mathscr{O}$ is a $C^*$-algebra and $\tau$ a $C^*$-dynamics on $\mathscr{O}$.

The strong continuity of $\tau$ means that the map $t \mapsto \tau^t(A)$ is norm-continuous for any $A \in \mathscr{O}$. From the general theory of *strongly continuous groups* on a Banach space, a $C^*$-dynamics $\tau$ admits a densely defined, closed *infinitesimal generator* $\delta$ such that

$$\delta(A) = \lim_{t \to 0} \frac{\tau^t(A) - A}{t} \tag{3.1}$$

for $A \in \mathrm{Dom}(\delta)$. In particular, if $\mathscr{O}$ has a unit $\mathbb{1}$, then $\mathbb{1} \in \mathrm{Dom}(\delta)$ and $\delta(\mathbb{1}) = 0$. It follows immediately that $\delta$ is a $*$-derivation, *i.e.*, that

1. $\mathrm{Dom}(\delta)$ is a $*$-algebra.
2. $\delta(AB) = \delta(A)B + A\delta(B)$ for all $A, B \in \mathrm{Dom}(\delta)$.
3. $\delta(A^*) = \delta(A)^*$ for all $A \in \mathrm{Dom}(\delta)$.

Generators of $C^*$-dynamics are characterized by the following simple adaptation of the *Hille-Yosida Theorem*, see [34, Section 3.2]).

**Theorem 3.2** *Let $\mathscr{O}$ be a $C^*$-algebra. A norm densely defined and closed operator $\delta$ on $\mathscr{O}$ generates a $C^*$-dynamics if and only if*

1. *$\delta$ is a $*$-derivation.*
2. *$\mathrm{Ran}(\mathrm{Id} + \lambda\delta) = \mathscr{O}$ for all $\lambda \in \mathbb{R}$.*
3. *$\|A + \lambda\delta(A)\| \geq \|A\|$ for all $\lambda \in \mathbb{R}$ and $A \in \mathrm{Dom}(\delta)$.*

***Example 1*** Let $\mathscr{H}$ be a Hilbert space and $H$ a bounded selfadjoint operator on $\mathscr{H}$. Then $\tau^t(A) = \mathrm{e}^{\mathrm{i}tH} A \mathrm{e}^{-\mathrm{i}tH}$ is a $C^*$-dynamics on $\mathscr{B}(\mathscr{H})$. Its generator $\delta(A) = \mathrm{i}[H, A]$ is bounded. Note that boundedness of $H$ is required for the strong continuity of $t \to \tau^t$.

***Example 2*** The following is based on the material of Section 2.2.2. Let $\mathfrak{h}$ be a Hilbert space and $h$ a selfadjoint operator on $\mathfrak{h}$. The group of gauge invariant Bogoliubov automorphisms of the $C^*$-algebra $\mathrm{CAR}(\mathfrak{h})$ defined by $\tau^t(a(f)) = a(\mathrm{e}^{\mathrm{i}th} f)$ is a $C^*$-dynamics. This is a consequence of the strong continuity of the unitary group $t \mapsto \mathrm{e}^{\mathrm{i}th}$ and of the norm continuity of the map $f \mapsto a(f)$ from $\mathfrak{h}$ to $\mathrm{CAR}(\mathfrak{h})$. The $*$-subalgebra generated by $\{a(f) \mid f \in \mathrm{Dom}(h)\}$ is contained in the domain of the generator $\delta$ of $\tau$ and $\delta(a(f)) = a(\mathrm{i}hf)$.

### 3.2 *W**-dynamical Systems

In some cases, such as systems of bosons, the $C^*$-approach is not adequate and one has to use the $W^*$ setting.

**Definition 3.3** Let $\mathfrak{M}$ be a *von Neumann algebra* or a *$W^*$-algebra*. A $W^*$-dynamics on $\mathfrak{M}$ is a $\sigma$-weakly continuous group $\mathbb{R} \ni t \mapsto \tau^t$ of $*$-automorphisms of $\mathfrak{M}$. A $W^*$-dynamical system is a pair $(\mathfrak{M}, \tau)$, where $\mathfrak{M}$ is a von Neumann algebra and $\tau$ a $W^*$-dynamics on $\mathfrak{M}$.

The continuity condition on the group $\tau$ means that, for any $A \in \mathfrak{M}$, the map $t \mapsto \tau^t(A)$ is continuous in the *$\sigma$-weak topology* of $\mathfrak{M}$. The generator $\delta$ of a $W^*$-dynamics $\tau$ on a von Neumann algebra $\mathfrak{M}$ is defined by Equ. (3.1), as in the $C^*$-case, except that the limit is now understood in the $\sigma$-weak topology. It is a $\sigma$-weakly densely defined and closed $*$-derivation on $\mathfrak{M}$ such that $\mathbb{1} \in \mathrm{Dom}(\delta)$ and $\delta(\mathbb{1}) = 0$. Generators of $W^*$-dynamics are characterized by the following analog of Theorem 3.2, see [34, Section 5.2].

**Theorem 3.4** *Let $\mathfrak{M}$ be a von Neumann algebra. A $\sigma$-weakly densely defined and closed operator $\delta$ on $\mathfrak{M}$ generates a $W^*$-dynamics if and only if*

1. *$\delta$ is a $*$-derivation and $\mathbb{1} \in \mathrm{Dom}(\delta)$.*
2. *$\mathrm{Ran}(\mathrm{Id} + \lambda\delta) = \mathfrak{M}$ for all $\lambda \in \mathbb{R}$.*
3. *$\|A + \lambda\delta(A)\| \geq \|A\|$ for all $\lambda \in \mathbb{R}$ and $A \in \mathrm{Dom}(\delta)$.*

***Example 3*** Let $\mathscr{H}$ be a Hilbert space and $H$ a selfadjoint operator on $\mathscr{H}$. Then $\tau^t(A) = \mathrm{e}^{\mathrm{i}tH} A \mathrm{e}^{-\mathrm{i}tH}$ is a $W^*$-dynamics on $\mathscr{B}(\mathscr{H})$.

***Example 4*** The following is based on the material of Section 2.2.3. Let $\mathfrak{h}$ be a Hilbert space and $h$ a selfadjoint operator on $\mathfrak{h}$. Denote by $\mathfrak{h}_0$ a subspace of $\mathfrak{h}$ invariant under the unitary group $\mathrm{e}^{\mathrm{i}th}$. The following formula defines a group of gauge-invariant automorphisms of the $C^*$-algebra $\mathrm{CCR}(\mathfrak{h}_0)$:

$$\tau^t(W(f)) = W(\mathrm{e}^{\mathrm{i}th} f).$$

Except in trivial cases, this group fails to be a $C^*$-dynamics because $\|\tau^t(W(f)) - W(f)\| = 2$ for all $t \in \mathbb{R}$ and $f \in \mathfrak{h}_0$ such that $\mathrm{e}^{\mathrm{i}th} f \neq f$.

Denote by $\mathfrak{M}$ the von Neumann algebra acting on the bosonic Fock space $\Gamma_{\mathrm{s}}(\mathfrak{h})$ and generated by the *Weyl operators* $\{W(f) \mid f \in \mathfrak{h}_0\}$. Then $\tau$ has an extension to $\mathfrak{M}$ given by

$$\tau^t(A) = \mathrm{e}^{\mathrm{i}t\mathrm{d}\Gamma(h)} A \mathrm{e}^{-\mathrm{i}t\mathrm{d}\Gamma(h)}.$$

It defines a $W^*$-dynamics on $\mathfrak{M}$.

### 3.3 Invariant States and Liouvilleans

In this and the following sections we use freely the notation introduced in Section 2.3. We shall say that $(\mathscr{O}, \tau)$ is a *quantum dynamical system* if it is either a $C^*$- or a $W^*$-dynamical system.

**Definition 3.5** Let $(\mathscr{O}, \tau)$ be a quantum dynamical system. A *state* $\omega$ on $\mathscr{O}$ is $\tau$-invariant if $\omega \circ \tau^t = \omega$ holds for all $t \in \mathbb{R}$.

As in the theory of classical dynamical systems, invariant states (and more specifically normal invariant states in the $W^*$-case) play an important role in the analysis of quantum dynamical systems. As an illustration, we explore the *GNS representation* induced by an invariant state.

Let $\omega$ be an invariant state of the quantum dynamical system $(\mathscr{O}, \tau)$ and $(\mathscr{H}_\omega, \pi_\omega, \Omega_\omega)$ the GNS representation of $\mathscr{O}$ induced by $\omega$. The uniqueness of the GNS representation implies that there exists a unique one-parameter group $t \mapsto U_\omega(t)$ of unitary operators on $\mathscr{H}_\omega$ such that

$$\pi_\omega(\tau^t(A)) = U_\omega(t)\pi_\omega(A)U_\omega(t)^*, \quad U_\omega(t)\Omega_\omega = \Omega_\omega,$$

for any $t \in \mathbb{R}$ and $A \in \mathscr{O}$. Assuming $\omega$ to be normal in the $W^*$-case, it is easy to show that the group $U_\omega$ is strongly continuous. Hence, by Stone's theorem, there exists a unique selfadjoint operator $L_\omega$ such that

$$\mathrm{e}^{\mathrm{i}tL_\omega}\pi_\omega(A)\mathrm{e}^{-\mathrm{i}tL_\omega} = \pi_\omega(\tau^t(A)), \quad L_\omega\Omega_\omega = 0.$$

The operator $L_\omega$ is sometimes called the $\omega$-Liouvillean of $(\mathscr{O}, \tau)$. Important information about the dynamics of the system can be deduced from its spectral properties, see Sections 5, 9 and 18.

Next we note that

$$\tilde{\omega}(A) = (\Omega_\omega | A\Omega_\omega), \quad A \in \mathscr{O}_\omega,$$

defines a normal extension of the state $\omega$ to the *enveloping von Neumann algebra* $\mathscr{O}_\omega$: $\omega = \tilde{\omega} \circ \pi_\omega$. Similarly,

$$\tilde{\tau}^t(A) = \mathrm{e}^{\mathrm{i}tL_\omega} A \mathrm{e}^{-\mathrm{i}tL_\omega}$$

defines a $W^*$-dynamics on $\mathscr{O}_\omega$ such that $\tilde{\tau}^t \circ \pi_\omega = \pi_\omega \circ \tau^t$. Thus, the GNS construction maps a $C^*$-dynamical system $(\mathscr{O}, \tau)$ with invariant state $\omega$ into a $W^*$-dynamical system $(\mathscr{O}_\omega, \tilde{\tau})$ with normal invariant state $\tilde{\omega}$.

The above construction can be performed under weaker continuity conditions than the strong/$\sigma$-weak continuity used here; see [111] for a more general definition of quantum dynamical systems.

### 3.4 Perturbation Theory

Let $(\mathscr{O}, \tau)$ be a $C^*$-dynamical system and $V \in \mathscr{O}$ a selfadjoint element. If $\delta$ denotes the generator of $\tau$, then

$$\delta_V = \delta + \mathrm{i}[V, \cdot]$$

is well defined on the domain $\mathrm{Dom}(\delta)$ and generates a perturbed dynamics $\tau_V^t = \mathrm{e}^{t\delta_V}$ on $\mathscr{O}$. One says that $\tau_V$ is a local perturbation of $\tau$. Such local perturbations play an important role in the theory of $C^*$-dynamical systems.

Iterating the integral equation (Duhamel formula)

$$\tau_V^t(A) = \tau^t(A) + \int_0^t \tau^{t-s}(\mathrm{i}[V, \tau_V^s(A)])\,\mathrm{d}s$$

leads to the Araki-Dyson expansion

$$\tau_V^t(A) = \tau^t(A) + \sum_{n=1}^{\infty} \int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \cdots \int_0^{t_{n-1}} \mathrm{d}t_n\, \mathrm{i}[\tau^{t_n}(V), \mathrm{i}[\cdots, \mathrm{i}[\tau^{t_1}(V), \tau^t(A)]\cdots]],$$

which is norm convergent for any $t \in \mathbb{R}$ and $A \in \mathscr{O}$. Another useful representation of the locally perturbed dynamics is given by the interaction picture $\tau_V^t(A) = \Gamma_V^t \tau^t(A) \Gamma_V^{t*}$. The operator $\Gamma_V^t$ is the solution of the Cauchy problem

$$\partial_t \Gamma_V^t = \mathrm{i}\Gamma_V^t \tau^t(V), \quad \Gamma_V^0 = \mathbb{1}.$$

It follows that $\Gamma_V^t \in \mathscr{O}$ is unitary and has the norm convergent Dyson expansion

$$\Gamma_V^t = \mathbb{1} + \sum_{n=1}^{\infty} \mathrm{i}^n \int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \cdots \int_0^{t_{n-1}} \mathrm{d}t_n\, \tau^{t_n}(V) \cdots \tau^{t_1}(V),$$

which satisfies the cocycle relation

$$\Gamma_V^{t+s} = \Gamma_V^t \tau^t(\Gamma_V^s) = \tau_V^t(\Gamma_V^s)\Gamma_V^t.$$

Local perturbations of $W^*$-dynamical systems can be handled in a similar way, replacing the norm topology with the $\sigma$-weak topology and interpreting all integrals in the weak-$*$ sense.

If $\omega$ is an invariant state for the unperturbed dynamical system $(\mathscr{O}, \tau)$ (supposed to be normal in the $W^*$-case) then, in the induced GNS representation and with the notation of the previous subsection, the perturbed dynamics is implemented by the unitary group generated by $L_\omega + Q$ where $Q = \pi_\omega(V)$,

$$\pi_\omega(\tau_V^t(A)) = \mathrm{e}^{\mathrm{i}t(L_\omega + Q)} \pi_\omega(A) \mathrm{e}^{-\mathrm{i}t(L_\omega + Q)}.$$

Note that the perturbed unitary group is related to the cocycle $\Gamma_V$ through the interaction picture formula

$$\mathrm{e}^{\mathrm{i}t(L_\omega+Q)} = \widetilde{\Gamma}_V^t\, \mathrm{e}^{\mathrm{i}tL_\omega},$$
$$\widetilde{\Gamma}_V^t = \pi_\omega(\Gamma_V^t) = \mathbb{1} + \sum_{n=1}^{\infty} \mathrm{i}^n \int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \cdots \int_0^{t_{n-1}} \mathrm{d}t_n\, \tilde{\tau}^{t_n}(Q) \cdots \tilde{\tau}^{t_1}(Q).$$

Consequently, the perturbed dynamics extends to a $W^*$-dynamics

$$\tilde{\tau}_V^t(A) = \mathrm{e}^{\mathrm{i}t(L_\omega+Q)} A \mathrm{e}^{-\mathrm{i}t(L_\omega+Q)} = \widetilde{\Gamma}_V^t \tilde{\tau}^t(A) \widetilde{\Gamma}_V^{t*},$$

on the enveloping von Neumann algebra $\mathscr{O}_\omega$. In the $W^*$-case this formula is the starting point for an extension of perturbation theory to unbounded perturbations. If $Q$ is a selfadjoint operator on $\mathscr{H}_\omega$ affiliated to $\mathscr{O}_\omega = \pi_\omega(\mathscr{O})$ and such that $L_\omega + Q$ is essentially selfadjoint on $\mathrm{Dom}(L_\omega) \cap \mathrm{Dom}(Q)$, then the unitary group $\mathrm{e}^{\mathrm{i}t(L_\omega+Q)}$ defines a $W^*$-dynamics on $\mathscr{O}_\omega$. This extension of perturbation theory has been developed in [48].

Except for its important role in Araki's perturbation theory of KMS-states discussed in Section 4, the operator $L_\omega + Q$ is of little value in the study of dynamical properties of $\tau_V$. This is due to the fact that it is not adapted to the structure of the enveloping von Neumann algebra $\mathscr{O}_\omega$. The standard Liouvillean, introduced in Section 5, corrects this problem.

If $t \mapsto V(t) = V(t)^* \in \mathscr{O}$ is continuous, then equation $\partial_t \tau_V^{s\to t}(A) = \tau_V^{s\to t}(\delta_{V(t)}(A))$ together with the condition $\tau_V^{s\to s} = \mathrm{Id}$ defines a two-parameter family of $*$-automorphisms of $\mathscr{O}$ such that $\tau_V^{s\to t} \circ \tau_V^{t\to r} = \tau_V^{s\to r}$. Perturbation theory can be developed as in the time-independent case starting from the integral equation

$$\tau_V^{s\to t}(A) = \tau^{t-s}(A) + \int_s^t \tau_V^{s\to u}\left(\mathrm{i}[V(u), \tau^{t-u}(A)]\right) \mathrm{d}u.$$

## 4 KMS–States

The KMS condition plays a fundamental role in quantum statistical mechanics where it provides a general abstract definition of equilibrium state. It is also deeply rooted in the mathematical structure of von Neumann algebras, see Section 5. Consequently, there is an enormous literature on the subject and the following section only provides a crude and condensed introduction. We refer the reader to [33, Chapters 5.3+5.4] and [67, Chapter 5] for a more elaborate introduction. We also recommend reading the pioneering article [69].

### 4.1 Motivation and Definition

Consider a quantum system with finite dimensional Hilbert space $\mathscr{H}$ (e.g. an $N$-level atom). Such a system is described by a *$C^*$-dynamical system* $(\mathscr{B}(\mathscr{H}), \tau)$ where

$$\tau^t(A) = \mathrm{e}^{\mathrm{i}tH} A \mathrm{e}^{-\mathrm{i}tH},$$

and $H = H^*$ denotes the Hamiltonian. For any $\beta \in \mathbb{R}$ this system has a unique thermal equilibrium state $\omega_\beta$ at inverse temperature $\beta$ given by the Gibbs-Boltzmann prescription

$$\omega_\beta(A) = \frac{\mathrm{tr}(\mathrm{e}^{-\beta H} A)}{\mathrm{tr}(\mathrm{e}^{-\beta H})}.$$

Note that the equilibrium correlation function

$$F_\beta(A, B; t) = \omega_\beta(A\tau^t(B)) \tag{4.1}$$

is an entire function of $t$. The cyclicity of the trace yields the identity

$$\mathrm{tr}(\mathrm{e}^{-\beta H} A\tau^t(B)) = \mathrm{tr}(\mathrm{e}^{-\beta H} A \mathrm{e}^{\mathrm{i}tH} B \mathrm{e}^{-\mathrm{i}tH}) = \mathrm{tr}(\mathrm{e}^{-\mathrm{i}(t-\mathrm{i}\beta)H} A \mathrm{e}^{\mathrm{i}tH} B).$$

Analytic continuation from $t \in \mathbb{R}$ to $t \in \mathbb{R} + \mathrm{i}\beta$ further gives

$$\mathrm{tr}(\mathrm{e}^{-\beta H} A\tau^{t+\mathrm{i}\beta}(B)) = \mathrm{tr}(\mathrm{e}^{-\mathrm{i}tH} A \mathrm{e}^{\mathrm{i}(t+\mathrm{i}\beta)H} B) = \mathrm{tr}(\mathrm{e}^{-\beta H} \tau^t(B) A),$$

from which we conclude that

$$F_\beta(A, B; t + \mathrm{i}\beta) = \omega_\beta(\tau^t(B)A). \tag{4.2}$$

Relations (4.1) and (4.2) relate the values of the analytic function $F_\beta(A, B; z)$ on the boundary of the strip

$$S_\beta = \{z \in \mathbb{C} \,|\, 0 < \mathrm{Im}(z\,\mathrm{sign}\beta) < |\beta|\}$$

to the state $\omega_\beta$. They are called Kubo-Martin-Schwinger (KMS) boundary conditions. It is a simple exercise in linear algebra to show that the Gibbs state $\omega_\beta$ is the only state on $\mathscr{B}(\mathscr{H})$ satisfying the KMS boundary conditions (4.1) and (4.2) for all $A, B \in \mathscr{B}(\mathscr{H})$. This fact motivates the following general definition.

**Definition 4.1** Let $(\mathscr{O}, \tau)$ be a $C^*$- or $W^*$-dynamical system. A state $\omega$ on $\mathscr{O}$, assumed to be normal in the $W^*$-case, is $(\tau, \beta)$-KMS for some $\beta \in \mathbb{R}$ if the following holds: for any $A, B \in \mathscr{O}$ there exists a function $z \mapsto F_\beta(A, B; z)$ analytic in the strip $S_\beta$, continuous on its closure, and satisfying the Kubo-Martin-Schwinger conditions (4.1)–(4.2) on its boundary.

***Remarks*** **1.** KMS states for negative temperatures rarely have a physical meaning. However, for historical reasons, they are widely used in the mathematical literature. For example, any modular state on a von Neumann algebra is a KMS state at inverse temperature $\beta = -1$ for its modular group, see Section 5.
**2.** In the special case $\beta = 0$ the KMS conditions degenerate to $\omega(AB) = \omega(BA)$. In mathematics such states are called *tracial*. Physicists sometimes refer to these infinite-temperature equilibrium states as *stochastic*.
**3.** If $\omega$ is $(\tau, \beta)$-KMS, then it is also $(\tau^{\gamma t}, \beta/\gamma)$-KMS. Note however that there is no simple connection between KMS states at different temperatures for the same dynamics $\tau^t$.
**4.** If $\omega$ is a $\beta$-KMS state for the $C^*$-dynamical system $(\mathscr{O}, \tau)$, then its normal extension $\tilde{\omega}$ to the enveloping von Neumann algebra $\mathscr{O}_\omega$ is a $\beta$-KMS state for the induced $W^*$-dynamical system $(\mathscr{O}_\omega, \tilde{\tau})$ defined in Section 3.2.

### 4.2 Characterizations

Let $(\mathscr{O}, \tau)$ be a $C^*$- or $W^*$-dynamical system. An element $A \in \mathscr{O}$ is called $\tau$-analytic if the function $t \mapsto \tau^t(A)$ extends to an entire function on $\mathbb{C}$. The set $\mathscr{O}_\tau$ of $\tau$-analytic elements is a dense $*$-subalgebra of $\mathscr{O}$ in the appropriate topology (uniform topology in the $C^*$-case, $\sigma$-weak topology in the $W^*$-case). If $\omega$ is a $(\tau, \beta)$-KMS state and $A, B \in \mathscr{O}_\tau$, then the function $F_\beta(A, B; \cdot)$ of Definition 4.1 is given by $F_\beta(A, B; z) = \omega(A\tau^z(B))$. In particular one has $\omega(A\tau^{i\beta}(B)) = \omega(BA)$. The following theorem shows that this property characterizes KMS states.

**Theorem 4.2** *Let $(\mathscr{O}, \tau)$ be a $C^*$- or $W^*$-dynamical system. A state $\omega$ on $\mathscr{O}$, assumed to be normal in the $W^*$-case, is a $(\tau, \beta)$-KMS state for some $\beta \in \mathbb{R}$ if and only if the following holds. There exists a dense, $\tau$-invariant $*$-subalgebra $\mathscr{M} \subset \mathscr{O}$ of $\tau$-analytic elements such that $\omega(A\tau^{i\beta}(B)) = \omega(BA)$ for all $A, B \in \mathscr{M}$.*

A fundamental property of KMS states – namely the invariance under time evolution – is a simple corollary of Theorem 4.2.

**Theorem 4.3** *If $\omega$ is a $(\tau, \beta)$-KMS state then it is $\tau$-invariant, i.e., $\omega \circ \tau^t = \omega$ holds for all $t \in \mathbb{R}$.*

Remarkably, Definition 4.1 which involves global properties of the dynamics $\tau$ can be rephrased in terms of its infinitesimal generator. To formulate this result let us set

$$s(x, y) = \begin{cases} x(\log x - \log y) & x, y > 0, \\ 0 & x = 0, y \geq 0, \\ +\infty & x > 0, y = 0. \end{cases}$$

**Theorem 4.4** (Araki [12]) *Let $(\mathscr{O}, \tau)$ be a $C^*$-dynamical system and denote by $\delta$ the infinitesimal generator of $\tau$. A state $\omega$ is $(\tau, \beta)$-KMS if and only if it is $\tau$-invariant and satisfies the so-called differential $\beta$-KMS condition*

$$-\mathrm{i}\beta\omega(A^*\delta(A)) \geq s(\omega(A^*A), \omega(AA^*)) \tag{4.3}$$

*for all* $A \in \mathrm{Dom}(\delta)$.

KMS states satisfy various correlation inequalities of the type (4.3), and some of them completely characterize them, see [33, 59]. They play an important role in proving other characterizations of KMS states: Araki's *Gibbs condition* (a quantum substitute for the DLR equation) and the variational principle for lattice spin systems [33, Chapter 6.2] and lattice fermions [4]; see also Section 20.

### 4.3 Perturbation Theory

As thermodynamic equilibrium states, KMS states enjoy several stability properties. Here we discuss only one of them: structural stability with respect to local perturbations of the dynamics. For additional information, the reader may consult [33, Section 5.4].

Let $(\mathscr{O}, \tau)$ be a $C^*$- or $W^*$-dynamical system and $\omega$ a $(\tau, \beta)$-KMS state. Consider the local perturbation $\tau_V$ of $\tau$ by a selfadjoint element $V \in \mathscr{O}$. In the GNS representation $(\mathscr{H}_\omega, \pi_\omega, \Omega_\omega)$ the perturbed dynamics is unitarily implemented by

$$\pi_\omega(\tau_V^t(A)) = \mathrm{e}^{\mathrm{i}t(L_\omega+Q)}\pi_\omega(A)\mathrm{e}^{-\mathrm{i}t(L_\omega+Q)},$$

where $L_\omega$ is the $\omega$-Liouvillean and $Q = \pi_\omega(V)$.

**Theorem 4.5** (Araki [9]) *The cyclic vector* $\Omega_\omega$ *belongs to the domain of* $\mathrm{e}^{-\beta(L_\omega+Q)/2}$ *and*

$$\omega^V(A) = (\Psi_V|\pi_\omega(A)\Psi_V), \qquad \Psi_V = \frac{\mathrm{e}^{-\beta(L_\omega+Q)/2}\Omega_\omega}{\|\mathrm{e}^{-\beta(L_\omega+Q)/2}\Omega_\omega\|},$$

*is a* $(\tau_V, \beta)$*-KMS state. The GNS representation of* $\mathscr{O}$ *induced by* $\omega^V$ *is* $(\mathscr{H}_\omega, \pi_\omega, \Psi_V)$. *Moreover, the map* $\omega \mapsto \omega^V$ *is a bijection between the set of* $(\tau, \beta)$*-KMS states and the set of* $(\tau_V, \beta)$*-KMS states.*

In the $W^*$-case, Araki's theorem extends to perturbed dynamics generated by unbounded perturbations $Q$ affiliated to $\pi_\omega(\mathscr{O})$, see [48].

## 5 Tomita–Takesaki Theory

### 5.1 Modular States

Let $\mathfrak{M}$ be a *von Neumann algebra* acting on a Hilbert space $\mathscr{H}$. Its *commutant*

$$\mathfrak{M}' = \{A \in \mathscr{B}(\mathscr{H}) \mid AB = BA \text{ for all } B \in \mathfrak{M}\}$$

is also a von Neumann algebra. Von Neumann's *bicommutant theorem* states that $\mathfrak{M}'' = \mathfrak{M}$.

**Definition 5.1** A vector $\Psi \in \mathscr{H}$ is cyclic for $\mathfrak{M}$ if the subspace $\mathfrak{M}\Psi$ is dense in $\mathscr{H}$. It is separating for $\mathfrak{M}$ if $A\Psi = 0$ for some $A \in \mathfrak{M}$ implies $A = 0$. It is modular if it is both cyclic and separating for $\mathfrak{M}$.

A vector $\Psi \in \mathscr{H}$ is separating for $\mathfrak{M}$ if and only if the corresponding normal state $\omega_\Psi(A) = (\Psi|A\Psi)$ is faithful.

The support $s_\omega$ of a *normal state* $\omega$ on $\mathfrak{M}$ is the smallest orthogonal projection $P \in \mathfrak{M}$ such that $\omega(P) = 1$. It follows that $\omega(A^*A) = 0$ if and only if $As_\omega = 0$. In particular, $\omega$ is faithful if and only if $s_\omega = \mathbb{1}$.

**Lemma 5.2** *The support of the vector state $\omega_\Psi$ is the orthogonal projection on the closure of $\mathfrak{M}'\Psi$. Consequently, a vector $\Psi \in \mathscr{H}$ is separating for $\mathfrak{M}$ if and only if it is cyclic for $\mathfrak{M}'$.*

***Remark*** Since $\mathfrak{M}'' = \mathfrak{M}$, it follows that $\Psi$ is cyclic for $\mathfrak{M}$ if and only if it is separating for $\mathfrak{M}'$.

Let $\mathscr{O}$ be a $C^*$-algebra and $\omega$ a state on $\mathscr{O}$. Denote by $(\mathscr{H}_\omega, \pi_\omega, \Omega_\omega)$ the GNS representation of $\mathscr{O}$ induced by $\omega$.

**Definition 5.3** The state $\omega$ is modular if the vector $\Omega_\omega$ is modular for the enveloping von Neumann algebra $\mathscr{O}_\omega = \pi_\omega(\mathscr{O})''$.

We warn the reader that this definition of a modular state is more general than the one we will adopt in Section 19.

Note that the state $\omega$ is modular if and only if the vector state induced by $\Omega_\omega$ is faithful on $\mathscr{O}_\omega$. This does not imply, nor is it implied by the faithfulness of $\omega$. However, if $\mathscr{O}$ is a von Neumann algebra, then a faithful normal state $\omega$ is modular.

The following result links modular theory with the theory of KMS states. It is often useful in applications to statistical mechanics.

**Theorem 5.4** *Let $(\mathscr{O}, \tau)$ be a $C^*$- or $W^*$-dynamical system. Then every $(\tau, \beta)$-KMS state for $\beta \in \mathbb{R}$ is modular.*

### 5.2 Modular Structure

Let $\Psi$ be a modular vector for $\mathfrak{M}$. Since $\Psi$ is separating for $\mathfrak{M}$, the map

$$A\Psi \mapsto A^*\Psi,$$

defines an anti-linear involution $S_0$ of $\mathfrak{M}\Psi$. Inspection of the graph of $S_0$ and the fact that $\Psi$ is cyclic for $\mathfrak{M}'$ show that $S_0$ is closable and that its closure $S$ is involutive. Since $\Psi$ is cyclic for $\mathfrak{M}$, $S$ is densely defined and hence has a densely defined adjoint $S^* = S_0^*$. Define the selfadjoint operator $\Delta = S^*S$ and write the polar decomposition of $S$ as $S = J\Delta^{1/2}$. Since $S$ is injective and has dense range $J$ is anti-unitary. From $\mathbb{1} = S^2 = J\Delta^{1/2}J\Delta^{1/2}$ we conclude that $J\Delta^{1/2} = \Delta^{-1/2}J^*$. It follows that $J^2\Delta^{1/2} = J\Delta^{-1/2}J^*$ and the uniqueness of the polar decomposition yields $J^2 = \mathbb{1}$, *i.e.*, $J = J^*$.

**Definition 5.5** The positive selfadjoint operator $\Delta$ is the modular operator and the anti-unitary involution $J$ the modular conjugation of the pair $(\mathfrak{M}, \Psi)$.

The fundamental algebraic properties of the modular operator and conjugation are the content of Tomita-Takesaki's theorem:

**Theorem 5.6** *Let $\Psi$ be a modular vector for a von Neumann algebra $\mathfrak{M}$. If $\Delta$ and $J$ are the corresponding modular operator and modular conjugation, then the following hold:*

1. $J\mathfrak{M}J = \mathfrak{M}'$.
2. *For any $t \in \mathbb{R}$ one has $\Delta^{\mathrm{i}t}\mathfrak{M}\Delta^{-\mathrm{i}t} = \mathfrak{M}$.*

Since $S$ is an unbounded operator, the proof of this theorem is technically involved. It was first published in [134]; a more concise exposition can be found in [34]. For a technically simpler proof see [114].

**Definition 5.7** The group of $*$-automorphisms of $\mathfrak{M}$ defined by $\sigma^t(A) = \Delta^{\mathrm{i}t}A\Delta^{-\mathrm{i}t}$ is the modular group of the pair $(\mathfrak{M}, \Psi)$.

More generally, if $\omega$ is a faithful normal state on the von Neumann algebra $\mathfrak{M}$ and $\Delta$ the modular operator of $(\mathfrak{M}, \Omega_\omega)$ then $\sigma^t_\omega(A) = \pi_\omega^{-1}(\Delta^{\mathrm{i}t}\pi_\omega(A)\Delta^{-\mathrm{i}t})$ is the modular group of $\omega$.

The main property of the modular group is the following result due to Takesaki which can be seen as a reverse of Theorem 5.4.

**Theorem 5.8** *Let $\omega$ be a faithful normal state on the von Neumann algebra $\mathfrak{M}$. Then $\omega$ is a KMS state for the modular group $\sigma_\omega$ at inverse temperature $\beta = -1$. Moreover, the modular group is the only dynamics on $\mathfrak{M}$ for which $\omega$ has this property.*

The modular conjugation allows us to construct another central object of modular theory.

**Definition 5.9** The natural cone associated to the pair $(\mathfrak{M}, \Psi)$ is the closed subset of $\mathscr{H}$ defined by

$$\mathscr{H}_+ = \{AJAJ\Psi \mid A \in \mathfrak{M}\}^{\mathrm{cl}}.$$

The most important properties of the natural cone are the following.

**Theorem 5.10** *The natural cone $\mathscr{H}_+$ is self-dual, i.e.,*

$$\mathscr{H}_+ = \widehat{\mathscr{H}_+} := \{\Omega \in \mathscr{H} \mid (\Phi \mid \Omega) \geq 0 \text{ for all } \Phi \in \mathscr{H}_+\}.$$

*In particular, $\mathscr{H}_+$ is convex. Moreover, the following hold:*

1. $J\Phi = \Phi$ *for all* $\Phi \in \mathscr{H}_+$.
2. $AJA\mathscr{H}_+ \subset \mathscr{H}_+$ *for all* $A \in \mathfrak{M}$.
3. $JAJ = A^*$ *for all* $A \in \mathfrak{M} \cap \mathfrak{M}'$.

### 5.3 Standard Representation

**Definition 5.11** A quadruple $(\mathscr{H}, \pi, J, \mathscr{H}_+)$ is a standard representation of the $W^*$-algebra $\mathfrak{M}$ if $\pi : \mathfrak{M} \to \mathscr{B}(\mathscr{H})$ is a representation of $\mathfrak{M}$, $J$ an antiunitary involution on $\mathscr{H}$ and $\mathscr{H}_+$ a self-dual cone in $\mathscr{H}$ satisfying the following conditions:

1. $J\pi(\mathfrak{M})J = \pi(\mathfrak{M})'$;
2. $J\pi(A)J = \pi(A)^*$ for all $A \in \mathfrak{M} \cap \mathfrak{M}'$;
3. $J\Psi = \Psi$ for all $\Psi \in \mathscr{H}_+$;
4. $\pi(A)J\pi(A)\mathscr{H}_+ \subset \mathscr{H}_+$ for all $A \in \mathfrak{M}$.

One of the key results in the theory of $W^*$-algebras is the following.

**Theorem 5.12** *Any $W^*$-algebra $\mathfrak{M}$ has a faithful standard representation. Moreover, this representation is unique, up to unitary equivalence.*

If the von Neumann algebra $\mathfrak{M}$ is such that any family of mutually orthogonal projections is at most countably infinite, then it has a faithful normal state $\omega$, and it follows from Theorem 5.10 that the corresponding GNS representation is standard. This applies, in particular, to many von Neumann algebras arising in physical applications. See [34, Proposition 2.5.6], and [133] for the general case.

The standard representation has two properties which are of crucial importance in the study of quantum dynamical systems. The first one concerns normal states.

**Theorem 5.13** *Let $(\mathscr{H}, \pi, J, \mathscr{H}_+)$ be a standard representation of $\mathfrak{M}$. Any normal state $\omega$ on $\mathfrak{M}$ has a unique vector representative $\Phi_\omega \in \mathscr{H}_+$ such that $\omega(A) = (\Phi_\omega|\pi(A)\Phi_\omega)$. Moreover,*

$$\|\Phi_\omega - \Phi_\nu\| \leq \|\omega - \nu\| \leq \|\Phi_\omega - \Phi_\nu\| \, \|\Phi_\omega + \Phi_\nu\|$$

*holds for all normal states $\omega, \nu$. Thus, there is a homeomorphic correspondence between normal states and unit vectors of $\mathscr{H}_+$. Finally, $(\pi(\mathfrak{M})\Phi_\omega)^{\mathrm{cl}} = J\left(\pi(\mathfrak{M})'\Phi_\omega\right)^{\mathrm{cl}}$, and in particular*

$$\omega \text{ is faithful} \Leftrightarrow \Phi_\omega \text{ is separating for } \pi(\mathfrak{M}) \Leftrightarrow \Phi_\omega \text{ is cyclic for } \pi(\mathfrak{M}).$$

The second property concerns the unitary implementation of $*$-automorphisms of $\mathfrak{M}$ in a standard representation $(\mathscr{H}, \pi, J, \mathscr{H}_+)$. Denote by $\mathrm{Aut}(\mathfrak{M})$ the topological group of $*$-automorphisms of $\mathfrak{M}$ with the topology of pointwise $\sigma$-weak convergence. Let $\mathscr{U}$ be the set of unitaries of $\mathscr{H}$ satisfying $U\pi(\mathfrak{M})U^* = \pi(\mathfrak{M})$ and $U\mathscr{H}_+ \subset \mathscr{H}_+$. Equipped with the strong operator topology, $\mathscr{U}$ is a topological group and $\tau_U(A) = \pi^{-1}(U\pi(A)U^*)$ defines a continuous morphism $\mathscr{U} \to \mathrm{Aut}(\mathfrak{M})$.

**Theorem 5.14** *The map $U \mapsto \tau_U$ is a topological isomorphism. Moreover, for any $U \in \mathscr{U}$ and any normal state $\omega$ on $\mathfrak{M}$, one has*

1. $JUJ = U$.
2. $U\pi(\mathfrak{M})'U^* = \pi(\mathfrak{M})'$.

3. $U^*\Phi_\omega = \Phi_{\omega\circ\tau_U}$.

In particular, if $(\mathfrak{M}, \tau)$ is a $W^*$-dynamical system, then there exists a unique self-adjoint operator $L$ on $\mathscr{H}$ such that $\pi(\tau^t(A)) = \mathrm{e}^{\mathrm{i}tL}\pi(A)\mathrm{e}^{-\mathrm{i}tL}$ and $\mathrm{e}^{\mathrm{i}tL}\mathscr{H}_+ \subset \mathscr{H}_+$.

**Definition 5.15** The generator $L$ is called the standard Liouvillean of the dynamical system $(\mathfrak{M}, \tau)$.

The standard Liouvillean is uniquely defined up to unitary equivalence. If $\omega$ is a modular $\tau$-invariant state, then the induced GNS representation is standard, and the $\omega$-Liouvillean of Section 3.3 coincides with the standard Liouvillean. This is in particular the case if $\omega$ is a KMS state for $\tau$.

Spectral properties of the standard Liouvillean are intimately related to those of the corresponding dynamical system. As an illustration, the following result is a direct consequence of Theorem 5.13; see Section 9 for additional information.

**Theorem 5.16** *Let $L$ be the standard Liouvillean of a $W^*$-dynamical system $(\mathfrak{M}, \tau)$.*

1. *$L$ has no eigenvalues if and only if there is no normal $\tau$-invariant state on $\mathfrak{M}$.*
2. *$\mathrm{Ker}(L)$ is one-dimensional if and only if there is a unique normal $\tau$-invariant state $\omega$ on $\mathfrak{M}$. In this case $\Phi_\omega$ is the unique unit vector in $\mathrm{Ker}(L) \cap \mathscr{H}_+$.*

### 5.4 The Finite Dimensional Case

It is instructive to work out the standard representation of a finite dimensional von Neumann algebra $\mathfrak{M} \subset \mathscr{B}(\mathbb{C}^N)$. This case is particularly simple since $\mathscr{B}(\mathbb{C}^N)$ is itself a Hilbert space for the inner product $(X|Y) = \mathrm{tr}(X^*Y)$. One has $\mathscr{B}(\mathbb{C}^N) = \mathfrak{M} \oplus \mathfrak{M}^\perp$ and the predual $\mathfrak{M}_*$ can be identified with $\mathfrak{M}$. Since any $A \in \mathfrak{M}$ can be written as a linear combination of 4 non-negative elements of $\mathfrak{M}$, it is easy to see that there exists a basis $\rho_1, \ldots, \rho_n$ of $\mathfrak{M}$ such that $\rho_j \geq 0$ and $\mathrm{tr}\ \rho_j = 1$. It follows that

$$\omega = \frac{1}{n}\sum_{j=1}^{n} \rho_j$$

defines a faithful state on $\mathfrak{M}$. Consider $\mathscr{H} = \mathfrak{M}$ as a Hilbert space (a subspace of $\mathscr{B}(\mathbb{C}^N)$). Then $\Omega = \omega^{1/2}$ is a unit vector in $\mathscr{H}$. Moreover, the map $\pi : \mathfrak{M} \to \mathscr{B}(\mathscr{H})$ defined by $\pi(A)X = AX$ is a $*$-morphism such that $\omega(A) = (\Omega|\pi(A)\Omega)$. Denote by $P$ the orthogonal projection on $(\mathrm{Ker}\ \omega)^\perp$. Clearly $P \in \mathfrak{M}$ and, since $\rho_j \geq 0$, one has $\mathrm{Ker}\ \omega \subset \cap_j \mathrm{Ker}\ \rho_j$ and $\mathrm{Ker}\ \omega \subset \mathrm{Ker}\ A$ for all $A \in \mathfrak{M}$. It follows that $\mathrm{Ran}\ A \subset \mathrm{Ran}\ P$ and hence $A = PA$ for all $A \in \mathfrak{M}$. Since the last identity is equivalent to $A^* = A^*P$, we conclude that $A = AP = PA = PAP$ for all $A \in \mathfrak{M}$, *i.e.*, that $P$ is the unit of $\mathfrak{M}$. Since there exists $T \in \mathfrak{M}$ such that $T\omega^{1/2} = P$ we can write $\pi(XT)\Omega = X$ and conclude that $\pi(\mathfrak{M})\Omega = \mathscr{H}$. We have shown that $(\mathscr{H}, \pi, \Omega)$ is the GNS representation of $\mathfrak{M}$ induced by $\omega$. Note that since $\omega$ is a normal faithful state, this representation is itself faithful.

The formulas $JX = X^*$ and $\Delta^{1/2}X = \omega^{1/2}XT$ define an anti-unitary involution and a positive selfadjoint operator on $\mathscr{H}$ such that

$$J\Delta^{1/2}\pi(A)\Omega = \pi(A)^*\Omega.$$

Thus, $J$ and $\Delta$ are the modular conjugation and the modular operator of the pair $(\pi(\mathfrak{M}), \Omega)$.

Elements of the natural cone are given by $\pi(A)J\pi(A)\Omega = A\omega^{1/2}A^*$, from which we can conclude that

$$\mathscr{H}_+ = \{A \in \mathfrak{M} \mid A \geq 0\},$$

and one easily checks the validity of Theorem 5.10.

Let $C$ be an element of $\pi(\mathfrak{M})'$. For all $A \in \mathfrak{M}$ and $X \in \mathscr{H}$ one has

$$C(AX) = C(\pi(A)X) = \pi(A)(C(X)) = AC(X).$$

Setting $X = P$, the unit of $\mathfrak{M}$, and $B = C(P) \in \mathfrak{M}$, we get $C(A) = AB$. We conclude that $\pi(\mathfrak{M})'$ consists of the linear maps $X \mapsto XB$ with $B \in \mathfrak{M}$. Thus, $J\pi(\mathfrak{M})J = \pi(\mathfrak{M})'$ and we have obtained the standard representation of the finite dimensional von Neumann algebra $\mathfrak{M}$.

Any normal state $\nu$ on $\mathfrak{M}$ is given by $\nu(A) = \mathrm{tr}(\rho A)$ for a density matrix $\rho \in \mathfrak{M}$. It follows that $\nu \mapsto \Phi_\nu = \rho^{1/2} \in \mathscr{H}_+$ is the homeomorphism described in Theorem 5.13.

## Part II

### CCR and CAR algebras

## 6 Free Bose and Fermi Gases – The Algebraic Approach

We will describe the algebraic approach to free Bose and Fermi gases, which allows us to discuss these systems in the thermodynamic limit at a positive temperature, or more generally, at a positive density. We will use the terminology of Section 2.

First we will follow the $W^*$-approach, working in a concrete Hilbert space. More precisely, we will describe Araki-Woods representations of the CCR and Araki-Wyss representations of the CAR, often used to describe free Bose and Fermi gases at a positive density. Then we will describe the $C^*$-algebraic approach to Bose and Fermi gases, which has a number of conceptual advantages. Unfortunately, as we shall see, the $C^*$-algebraic approach is somewhat problematic in the bosonic case.

For an in-depth treatment of the material of this chapter, see [44].

### 6.1 Araki-Woods and Araki-Wyss Operators

We fix a nonnegative function $\xi \mapsto \gamma(\xi)$ and define

$$\rho(\xi) := (\gamma(\xi)^{-1} \mp 1)^{-1}, \tag{6.1}$$

where the minus sign corresponds to the bosonic case and the plus sign to the fermionic case. The function $\gamma$, or equivalently, $\rho$ will parametrize a certain class of representations of the *canonical commutation relations* (CCR) and *canonical anticommutation relations* (CAR). As we shall see, $\rho(\xi)$ has the physical interpretation of the density of the mode $\xi$.

We consider the bosonic/fermionic Fock space $\Gamma_{\mathrm{s/a}}\big(L^2(\Xi) \oplus L^2(\Xi)\big)$, in which the one-particle space has been "doubled" to account for both "excitations", corresponding to the "left space", as well as "holes", corresponding to the "right space". The creation/annihilation operators corresponding to the left/right space are distinguished by the subscript $\mathrm{l/r}$. The subscript $\mathrm{s/a}$ indicates that we consider the bosonic/fermionic Fock space.

Define

$$\begin{aligned} a^*_{\gamma,\mathrm{l}}(\xi) &:= (1 \pm \rho(\xi))^{\frac{1}{2}} a^*_{\mathrm{l}}(\xi) + \rho(\xi)^{\frac{1}{2}} a_{\mathrm{r}}(\xi), \\ a_{\gamma,\mathrm{l}}(\xi) &:= (1 \pm \rho(\xi))^{\frac{1}{2}} a_{\mathrm{l}}(\xi) + \rho(\xi)^{\frac{1}{2}} a^*_{\mathrm{r}}(\xi), \end{aligned} \tag{6.2}$$

where the plus corresponds to the bosonic case and minus to the fermionic case. In the bosonic case, (6.2) are called the (left) *Araki-Woods creation/annihilation operators*. They satisfy the usual CCR. In the fermionic case, (6.2) are called the (left) *Araki-Wyss creation/annihilation operators*. They satisfy the usual CAR.

Let $\Omega$ denote the vacuum vector for $\Gamma_{\mathrm{s/a}}\big(L^2(\Xi) \oplus L^2(\Xi)\big)$. Then $(\Omega \mid \cdot\, \Omega)$ is an example of a *quasifree state*. Its 2-point function is

$$(\Omega \mid a^*_{\gamma,\mathrm{l}}(\xi) a_{\gamma,\mathrm{l}}(\xi')\Omega) = \delta(\xi, \xi')\rho(\xi),$$

where $\delta(\xi, \xi')$ denotes the delta function. This justifies the name "the density of the mode $\xi$" for $\rho(\xi)$; see [16, 33, 41].

### 6.2 The Commutant of the Algebra of the Bose/Fermi Gas

Let $\mathfrak{M}^{\mathrm{AW}}_{\gamma,\mathrm{l}}$ be the $W^*$-algebra in $\mathscr{B}(\Gamma_{\mathrm{s/a}}(L^2(\Xi) \oplus L^2(\Xi)))$ generated by smeared-out bosonic/fermionic operators introduced in the previous section (in the bosonic case in addition we need to take bounded functions of these operators). Note that $\mathfrak{M}^{\mathrm{AW}}_{\gamma,\mathrm{l}}$ can be a rather nontrivial $W^*$-algebra – typically it is of *type III*.

For nonzero $\rho$ the state $(\Omega \mid \cdot\, \Omega)$ on the algebra $\mathfrak{M}^{\mathrm{AW}}_{\gamma,\mathrm{l}}$ is faithful. Therefore, we can apply *Tomita-Takesaki theory*, see Section 5, obtaining in particular the so-called modular conjugation $J_{\mathrm{s/a}}$, which is an antiunitary operator on $\Gamma_{\mathrm{s/a}}(L^2(\Xi \oplus \Xi))$

satisfying

$$J_{\mathrm{s/a}}^2 = \mathbb{1}, \qquad J_{\mathrm{s/a}}\Omega = \Omega, \qquad J_{\mathrm{s/a}}\mathfrak{M}_{\gamma,\mathrm{l}}^{\mathrm{AW}} J_{\mathrm{s/a}} = \left(\mathfrak{M}_{\gamma,\mathrm{l}}^{\mathrm{AW}}\right)',$$

where $\left(\mathfrak{M}_{\gamma,\mathrm{l}}^{\mathrm{AW}}\right)'$ denotes the commutant of $\mathfrak{M}_{\gamma,\mathrm{l}}^{\mathrm{AW}}$. Let $\epsilon$ be the antiunitary operator on $L^2(\Xi) \oplus L^2(\Xi)$ defined by

$$\epsilon(f_1, f_2) := (\bar{f}_2, \bar{f}_1).$$

Then, in the bosonic case, $J_{\mathrm{s}} = \Gamma(\epsilon)$. In the fermionic case, $J_{\mathrm{a}} = \Gamma(\epsilon)(-1)^{N(N-1)/2}$. Here $\Gamma(\epsilon)$ denotes the second quantization of the operator $\epsilon$ and $N$ is the number operator.

Later on we will need the Araki-Woods/Araki-Wyss creation and annihilation operators transformed by $J_{\mathrm{s/a}}$ (which will be called the "right" operators, as opposed to the "left" operators introduced above). The right Araki-Woods creation/annihilation operators are given by

$$a_{\gamma,\mathrm{r}}^*(\xi) := J_{\mathrm{s}} a_{\gamma,\mathrm{l}}^*(\xi) J_{\mathrm{s}} = \rho(\xi)^{\frac{1}{2}} a_{\mathrm{l}}^*(\xi) + (1+\rho(\xi))^{\frac{1}{2}} a_{\mathrm{r}}(\xi),$$

$$a_{\gamma,\mathrm{r}}(\xi) := J_{\mathrm{s}} a_{\gamma,\mathrm{l}}(\xi) J_{\mathrm{s}} = \rho(\xi)^{\frac{1}{2}} a_{\mathrm{l}}(\xi) + (1+\rho(\xi))^{\frac{1}{2}} a_{\mathrm{r}}^*(\xi).$$

The right Araki-Wyss creation/annihilation operators are given by

$$a_{\gamma,\mathrm{r}}^*(\xi) := J_{\mathrm{a}} a_{\gamma,\mathrm{l}}^*(\xi) J_{\mathrm{a}} = \rho(\xi)^{\frac{1}{2}} a_{\mathrm{l}}^*(\xi)(-1)^N - (1-\rho(\xi))^{\frac{1}{2}} a_{\mathrm{r}}(\xi)(-1)^N,$$

$$a_{\gamma,\mathrm{r}}(\xi) := J_{\mathrm{a}} a_{\gamma,\mathrm{l}}(\xi) J_{\mathrm{a}} = -\rho(\xi)^{\frac{1}{2}} a_{\mathrm{l}}(\xi)(-1)^N + (1-\rho(\xi))^{\frac{1}{2}} a_{\mathrm{r}}^*(\xi)(-1)^N.$$

Note that the left and the right operators commute with one another.

### 6.3 Quasi-free Dynamics

Consider Bose or Fermi gas with the 1-particle space $L^2(\Xi)$ and the 1-particle excitation spectrum $\omega(\xi)$. One usually assumes that $\omega$ is positive.

At zero temperature, the Hilbert space of the system is $\Gamma_{\mathrm{s/a}}(L^2(\Xi))$, and its Hamiltonian is

$$H = \int \omega(\xi) a^*(\xi) a(\xi) \mathrm{d}\xi.$$

Although an advanced algebraic language in this case is not necessary, it is often convenient to introduce the $W^*$-dynamical system $\left(\mathscr{B}(\Gamma_{\mathrm{s/a}}(L^2(\Xi))), \mathrm{e}^{\mathrm{i}tH} \cdot \mathrm{e}^{-\mathrm{i}tH}\right)$. Clearly,

$$\mathrm{e}^{\mathrm{i}tH} a^*(\xi) \mathrm{e}^{-\mathrm{i}tH} = \mathrm{e}^{\mathrm{i}t\omega(\xi)} a^*(\xi), \qquad \mathrm{e}^{\mathrm{i}tH} a(\xi) \mathrm{e}^{-\mathrm{i}tH} = \mathrm{e}^{-\mathrm{i}t\omega(\xi)} a(\xi). \tag{6.3}$$

We now consider the Bose/Fermi gas at a positive density described by $\gamma$. Its observables are elements of $\mathfrak{M}_{\gamma,\mathrm{l}}^{\mathrm{AW}}$. Its dynamics is given by $\tau_t(A) = \mathrm{e}^{\mathrm{i}tL} A \mathrm{e}^{-\mathrm{i}tL}$,

where the *Liouvillean* $L$ is given by

$$L := \int \omega(\xi) a_{\mathrm{l}}^*(\xi) a_{\mathrm{l}}(\xi) \mathrm{d}\xi - \int \omega(\xi) a_{\mathrm{r}}^*(\xi) a_{\mathrm{r}}(\xi) \mathrm{d}\xi,$$

see Section 2. Note that

$$\tau_t(a_{\gamma,\mathrm{l}}^*(\xi)) = \mathrm{e}^{\mathrm{i}t\omega(\xi)} a_{\gamma,\mathrm{l}}^*(\xi), \qquad \tau_t(a_{\gamma,\mathrm{l}}(\xi)) = \mathrm{e}^{-\mathrm{i}t\omega(\xi)} a_{\gamma,\mathrm{l}}(\xi),$$

and so the dynamics $\tau^t$ acts on left creation/annihilation operators in the same way as the zero-temperature dynamics in (6.3). However

$$\tau_t(a_{\gamma,\mathrm{r}}^*(\xi)) = \mathrm{e}^{-\mathrm{i}t\omega(\xi)} a_{\gamma,\mathrm{r}}^*(\xi), \qquad \tau_t(a_{\gamma,\mathrm{r}}(\xi)) = \mathrm{e}^{\mathrm{i}t\omega(\xi)} a_{\gamma,\mathrm{r}}(\xi),$$

indicates that the "particles" created by $a_{\gamma,\mathrm{r}}^*(\xi)$ behave like a "hole". We emphasize that the $W^*$-dynamical systems $\left(\mathfrak{M}_{\gamma,\mathrm{l}}^{\mathrm{AW}}, \tau\right)$ for distinct $\gamma$ are often non-equivalent.

The state $(\Omega \mid \cdot\, \Omega)$ is $\beta$-KMS for the dynamics $\tau$ iff $\gamma(\xi) = \mathrm{e}^{-\beta\omega(\xi)}$. In the bosonic case the density is then given by the *Planck law*: $\rho(\xi) = (\mathrm{e}^{\beta\omega(\xi)} - 1)^{-1}$. In the fermionic case we obtain the *Fermi-Dirac law*: $\rho(\xi) = (\mathrm{e}^{\beta\omega(\xi)} + 1)^{-1}$.

### 6.4 $C^*$-algebraic Approach to the CAR

The CAR algebra over $L^2(\Xi)$, sometimes denoted $\mathrm{CAR}(L^2(\Xi))$, is defined as the $C^*$-algebra generated by the elements $\{a(f)\ f \in L^2(\Xi)\}$ satisfying

$$[a(f_1), a(f_2)]_+ = 0, \qquad [a(f_1), a^*(f_2)]_+ = 2\,\mathrm{Re}(f_1|f_2)\mathbb{1}.$$

One can show that for an infinite dimensional separable space $L^2(\Xi)$ this algebra is isomorphic to the uniformly hyperfinite algebra $\mathrm{UHF}(2^\infty)$. In the case of a finite dimension, this algebra coincides with the complex Clifford algebra. $a(f)$ and $a^*(f)$ are called (abstract) annihilation and creation operators of $f$.

If $\mathrm{e}^{\mathrm{i}t\omega}$ is a unitary group on $L^2(\Xi)$, then $\tau_t(a(f)) := a(\mathrm{e}^{ti\omega} f)$ extends to a unique $C^*$-dynamics on $\mathrm{CAR}(L^2(\Xi))$. Such dynamics are often called gauge-invariant quasi-free dynamics.

Let $\rho, \gamma$ be as in (6.1). Then there exists a unique state $\psi_\gamma$ on $\mathrm{CAR}(L^2(\Xi))$ such that

$$\psi_\gamma\left(a^*(f_1)\cdots a^*(f_n)a(g_m)\cdots a(g_1)\right) = \begin{cases} \displaystyle\sum_{\sigma\in S_n}\prod_{j=1}^{n} \mathrm{sign}(\sigma) \int \bar{f}_j(\xi)\rho(\xi) g_{\sigma(j)}(\xi)\mathrm{d}\xi, & \text{if } n = m; \\ 0 & \text{otherwise,} \end{cases}$$

where $S_n$ denotes the set of permutations of $\{1, \ldots, n\}$ and $\mathrm{sign}(\sigma)$ is the signature of $\sigma \in S_n$.

Let $a^*_{\gamma,1}(\xi)$, $a_{\gamma,1}(\xi)$ be the Araki-Wyss representation of the CAR. Then

$$\pi_\gamma(a(f)) := \int a_{\gamma,1}(\xi)\bar{f}(\xi)\mathrm{d}\xi$$

extends uniquely to a representation of $\mathrm{CAR}(L^2(\Xi))$ in $\Gamma_{\mathrm{a}}(L^2(\Xi) \oplus L^2(\Xi))$, which is a GNS representation generated by the state $\psi_\gamma$.

### 6.5 $C^*$-algebraic Approach to the CCR

In the bosonic case, several algebras could be referred to as $\mathrm{CCR}(L^2(\Xi))$. The choice made by most authors is the $C^*$-algebra generated by $\{W(f) \mid f \in L^2(\Xi)\}$ satisfying the relations

$$W(f)^* = W(-f), \qquad W(f_1)W(f_2) = \mathrm{e}^{-\frac{\mathrm{i}}{2}\mathrm{Im}(f_1|f_2)}W(f_1 + f_2).$$

We will denote it $\mathrm{CCR}(L^2(\Xi))$. $W(f)$'s are called Weyl operators, and this algebra is sometimes called the Weyl CCR algebra. An important result about this algebra was obtained by J. Slawny [33]. This is the reason for another name for $\mathrm{CCR}(L^2(\Xi))$, the Slawny CCR algebra.

If $\mathrm{e}^{\mathrm{i}t\omega}$ is a unitary group on $L^2(\Xi)$, then $\tau_t(W(f)) := W(\mathrm{e}^{\mathrm{i}t\omega}f)$ extends to a unique 1-parameter group of $*$-automorphisms of $\mathrm{CCR}(L^2(\Xi))$, often called a gauge-invariant quasi-free dynamics. Note that $t \mapsto \tau_t$ is not continuous, hence it is not a $C^*$-dynamics. This is a signature of the difficulties the $C^*$-algebraic approach encounters in the CCR case.

Let $\rho, \gamma$ be as in (6.1). Then

$$\psi_\gamma(W(f)) := \exp\left(-\frac{1}{4}\int |f(\xi)|^2\rho(\xi)\mathrm{d}\xi\right)$$

extends by linearity to a state on $\mathrm{CCR}(L^2(\Xi))$.

Let $a^*_{\gamma,1}(\xi)$, $a_{\gamma,1}(\xi)$ be the Araki-Woods creation/annihilation operators. Then

$$\pi_\gamma(W(f)) := \exp\left(\frac{\mathrm{i}}{\sqrt{2}}\int \left(f(\xi)a^*_{\gamma,1}(\xi) + \bar{f}(\xi)a_{\gamma,1}(\xi)\right)\mathrm{d}\xi\right)$$

extends to a representation of $\mathrm{CCR}(L^2(\Xi))$ in $\Gamma_{\mathrm{s}}(L^2(\Xi) \oplus L^2(\Xi))$, which is a GNS representation induced by the state $\psi_\gamma$.

## 7 Araki-Wyss Representation

### 7.1 Non-interacting Fermions

A system of non-interacting fermions is specified by a one-particle Hilbert space $\mathfrak{h}$ and a one-particle Hamiltonian $h$, a selfadjoint operator on $\mathfrak{h}$. Within the *$C^*$-algebraic approach*, observables of this system are elements of the $C^*$-algebra of *Canonical Anticommutation Relations* $\mathrm{CAR}(\mathfrak{h})$. Their time evolution is given by the group of *Bogoliubov automorphisms*

$$\tau^t(a(f)) = a(\mathrm{e}^{\mathrm{i}th} f)$$

associated to $h$. Thus, the dynamics of the system is described by the $C^*$-dynamical system $(\mathrm{CAR}(\mathfrak{h}), \tau)$. Taking gauge-invariance into account, we should in fact restrict the algebra to its gauge-invariant part $\mathrm{CAR}_0(\mathfrak{h})$, see Section 8.1. It is often more convenient to retain the full CAR algebra and consider only gauge-invariant states.

### 7.2 Gauge-invariant Quasi-free States

In the *Fock representation* the dynamical group $\tau$ as well as the gauge group $\vartheta$ are unitarily implemented by the second quantized Hamiltonian $H = \mathrm{d}\Gamma(h)$ and the number operator $N = \mathrm{d}\Gamma(\mathbb{1})$,

$$\pi_F(\tau^t(A)) = \mathrm{e}^{\mathrm{i}tH}\pi_F(A)\mathrm{e}^{-\mathrm{i}tH}, \qquad \pi_F(\vartheta^\varphi(A)) = \mathrm{e}^{\mathrm{i}\varphi N}\pi_F(A)\mathrm{e}^{-\mathrm{i}\varphi N}.$$

The Hamiltonian $h$ of a single fermion confined in a finite volume $\Lambda \subset \mathbb{R}^d$ typically has purely discrete spectrum and $\mathrm{e}^{-\beta h}$ is trace class for any $\beta > 0$. Using the identity

$$\det(\mathbb{1} + A) = \mathrm{tr}(\Gamma(A)), \tag{7.1}$$

we conclude that $\mathrm{tr}(\mathrm{e}^{-\beta(H-\mu N)}) = \det(\mathbb{1} + \mathrm{e}^{-\beta(h-\mu)})$ for any $\beta > 0$ and $\mu \in \mathbb{R}$. Hence $\mathrm{e}^{-\beta(H-\mu N)}$ is also trace class and the Gibbs grand canonical ensemble at inverse temperature $\beta$ and chemical potential $\mu$ is a gauge-invariant *Fock state* with density matrix

$$\rho_{\beta\mu} = \frac{\mathrm{e}^{-\beta(H-\mu N)}}{\mathrm{tr}(\mathrm{e}^{-\beta(H-\mu N)})}.$$

It is the unique *$\beta$-KMS state* on $\mathrm{CAR}(\mathfrak{h})$ for the dynamics $t \mapsto \tau^t \circ \vartheta^{-\mu t}$. Using again identity (7.1), a simple calculation shows that the *characteristic function* of this state (see Section 8.2) is given by

$$E_{\beta\mu}(u) = \det(\mathbb{1} + (u - \mathbb{1}) f_{\beta\mu}(h)), \tag{7.2}$$

where

$$f_{\beta\mu}(\varepsilon) = \frac{1}{\mathbb{1} + \mathrm{e}^{\beta(\varepsilon-\mu)}}$$

is the Fermi-Dirac distribution function.

Since $u - \mathbb{1}$ is finite rank, the characteristic function (7.2) still makes sense in the infinite volume limit, despite the fact that the Boltzmann weight $\mathrm{e}^{-\beta(H-\mu N)}$ is no longer trace class in this limit. One can show directly that (7.2) is the characteristic function of the unique $\beta$-KMS state for the group $t \mapsto \tau^t \circ \vartheta^{-\mu t}$. Its restriction to the gauge-invariant sub-algebra $\mathrm{CAR}_0(\mathfrak{h})$ is therefore a $(\tau, \beta)$-KMS state.

More generally, one has the following result.

**Theorem 7.1** *Let $T$ be a selfadjoint operator on the Hilbert space $\mathfrak{h}$ satisfying $0 \leq T \leq \mathbb{1}$. Then*

$$E(u) = \det(\mathbb{1} + (u - \mathbb{1})T)$$

*is the characteristic function of a gauge-invariant state $\omega_T$ on $\mathrm{CAR}(\mathfrak{h})$. $\omega_T$ is called the gauge-invariant quasi-free state generated by $T$. Equivalent ways to characterize this state are:*

1. *For all $f_1, \ldots, f_n \in \mathfrak{h}$ and $g_1, \ldots, g_m \in \mathfrak{h}$ one has*

$$\omega_T(a^*(f_1) \cdots a^*(f_n) a(g_m) \cdots a(g_1)) = \delta_{nm} \det\{(g_i | T f_j)\}.$$

2. *For $f \in \mathfrak{h}$ set $\varphi(f) = 2^{-1/2}(a(f) + a^*(f))$. The Wick theorem*

$$\omega_T(\varphi(f_1) \cdots \varphi(f_{2n+1})) = 0,$$

$$\omega_T(\varphi(f_1) \cdots \varphi(f_{2n})) = \sum_{\pi \in \mathscr{P}_n} \mathrm{sign}(\pi) \prod_{j=1}^{n} \omega_T\left(\varphi(f_{\pi(2j-1)}) \varphi(f_{\pi(2j)})\right),$$

*holds. In the last expression, the sum runs over the set $\mathscr{P}_n$ of pairings, i.e., permutations $\pi$ of $\{1, \ldots, 2n\}$ such that $\pi(2j-1) < \pi(2j)$ and $\pi(2j-1) < \pi(2j+1)$. Moreover, $\mathrm{sign}(\pi)$ denotes the signature of $\pi \in \mathscr{P}_n$.*

The state $\omega_T$ also has an information-theoretic characterization: it has maximal entropy among all the gauge-invariant states $\nu$ such that $\nu(a^*(f)a(g)) = (g|Tf)$ in the following sense. For a finite dimensional subspace $\mathfrak{k} \subset \mathfrak{h}$ define the entropy

$$S(\nu|\mathfrak{k}) = -\mathrm{tr}(\rho \log \rho)$$

where $\rho$ is the density matrix of the restriction of $\nu$ to the finite dimensional algebra $\mathrm{CAR}(\mathfrak{k})$. Then

$$S(\omega_T|\mathfrak{k}) = \max_{\nu \in E_T} S(\nu|\mathfrak{k}),$$

where $E_T$ denotes the set of gauge-invariant states $\nu$ such that $\nu(a^*(f)a(g)) = (g|Tf)$. This follows from a simple adaptation of the proof of [94, Proposition 1a].

We refer the reader to [8, 33] for more information on quasi-free states on $\mathrm{CAR}(\mathfrak{h})$.

### 7.3 Araki-Wyss Representation

Let $\omega_T$ be the gauge-invariant quasi-free state on $\mathrm{CAR}(\mathfrak{h})$ generated by $T$. The associated GNS representation, which we denote by $(\mathscr{H}_T, \pi_T, \Omega_T)$, was first constructed by Araki and Wyss in [17]. It can be described as follows:

1. $\mathscr{H}_T = \Gamma_{\rm a}(\mathfrak{h}_1 \oplus \mathfrak{h}_2) \subset \Gamma_{\rm a}(\mathfrak{h} \oplus \mathfrak{h})$ where $\mathfrak{h}_1 = (\mathrm{Ran}(\mathbb{1} - T))^{\rm cl}$ and $\mathfrak{h}_2 = (\mathrm{Ran}\, T)^{\rm cl}$.
2. $\Omega_T = \Omega$, the Fock vacuum vector.
3. The $*$-morphism $\pi_T$ is given by

$$\pi_T(a(f)) = a\left(\sqrt{\mathbb{1} - T}\, f \oplus 0\right) + a^*\left(0 \oplus \overline{\sqrt{T}\, f}\right),$$

where $\overline{\cdot}$ denotes an arbitrary complex conjugation on $\mathfrak{h}$.

Using the *exponential law for fermions* $U : \Gamma_{\rm a}(\mathfrak{h}_1 \oplus \mathfrak{h}_2) \to \Gamma_{\rm a}(\mathfrak{h}_1) \otimes \Gamma_{\rm a}(\mathfrak{h}_2)$, an equivalent representation with cyclic vector $U\Omega_T = \Omega \otimes \Omega$ is obtained. It is explicitly given by

$$U\pi_T(a(f))U^* = a\left(\sqrt{\mathbb{1} - T}\, f\right) \otimes \mathbb{1} + \Theta \otimes a^*\left(\overline{\sqrt{T}\, f}\right),$$

where $\Theta = \Gamma(-\mathbb{1}) = (-1)^N$. In the limiting cases $T = 0$ and $T = \mathbb{1}$, which correspond to the *vacuum state* **vac** and to the *filled Fermi sea* **full**, the Araki-Wyss representation degenerates to the Fock and anti-Fock representations $\pi_F$ and $\pi_{AF}$.

The reader should consult [8, 41] for an introduction to quasi-free representations of CAR($\mathfrak{h}$).

### 7.4 Enveloping von Neumann Algebra

The following theorem summarizes some interesting features of the *enveloping von Neumann algebra*

$$\mathfrak{M}_T = \pi_T(\mathrm{CAR}(\mathfrak{h}))''$$

of a gauge-invariant quasi-free state $\omega_T$.

**Theorem 7.2** *1. $\omega_T$ is primary, i.e., its enveloping von Neumann algebra is a factor. $\mathfrak{M}_T$ is of type*

*I if either $\mathfrak{h}$ is finite dimensional or $\mathfrak{h}$ is infinite dimensional and $T = 0$ or $T = \mathbb{1}$.*
*II if $\mathfrak{h}$ is infinite dimensional and $T = \mathbb{1}/2$.*
*III$_\lambda$ if $\mathfrak{h}$ is infinite dimensional and $T = (\mathbb{1} + \lambda^{\pm 1})^{-1}$ for some $\lambda \in ]0, 1[$.*
*III$_1$ if the continuous spectrum of $T$ is not empty.*

*2. $\omega_T$ is modular, i.e., the cyclic vector $\Omega_T$ is separating for $\mathfrak{M}_T$, if and only if* $\mathrm{Ker}\, T = \mathrm{Ker}(\mathbb{1} - T) = \{0\}$.
*3. $\omega_T$ and $\omega_S$ are quasi-equivalent if and only if the operators $T^{1/2} - S^{1/2}$ and $(\mathbb{1} - T)^{1/2} - (\mathbb{1} - S)^{1/2}$ are Hilbert-Schmidt.*

If $\mathrm{Ker}\ T = \mathrm{Ker}(\mathbb{1} - T) = \{0\}$, then *modular theory* applies to $\mathfrak{M}_T$, see Section 5. On $\mathscr{H}_T$ there exist an anti-unitary involution $J$ (the modular conjugation) and a positive operator $\Delta$ (the modular operator) such that

$$J\Delta^{1/2}A\Omega_T = A^*\Omega_T$$

for all $A \in \mathfrak{M}_T$. These operators are explicitly given by

$$J = (-1)^{N(N-1)/2}\Gamma(j), \quad \Delta = \Gamma(\mathrm{e}^{s} \oplus \mathrm{e}^{-\overline{s}}),$$

where $j : f \oplus g \mapsto \overline{g \oplus f}$ and $s = \log T(\mathbb{1} - T)^{-1}$.

## 8 Fock and Non-Fock States on CAR-algebras

In the formalism of *second quantization* a system of fermions is described by *creation and annihilation operators* $a^*(f)$, $a(f)$ on the antisymmetric *Fock space* $\Gamma_{\mathrm{a}}(\mathfrak{h})$ over the one-particle Hilbert space $\mathfrak{h}$. For systems confined in a finite volume, this Hilbert space description is sufficient and states of finite positive density can be represented by *density matrices* acting on $\Gamma_{\mathrm{a}}(\mathfrak{h})$. The situation changes when one takes the thermodynamic (infinite volume) limit. In this case, there is no density matrix in Fock space describing a positive density state of an infinitely extended fermionic system. A more sophisticated description is therefore required, see Section 2.

### 8.1 Gauge Invariant States on CAR($\mathfrak{h}$)

Global $U(1)$*-gauge symmetry* is a fundamental property of quantum mechanics. Its implementation on $\mathrm{CAR}(\mathfrak{h})$ is given by the gauge group $\mathbb{R} \ni \varphi \mapsto \vartheta^{\varphi}$, the group of *Bogoliubov automorphisms* defined by

$$\vartheta^{\varphi}(a^*(f)) = a^*(\mathrm{e}^{\mathrm{i}\varphi} f) = \mathrm{e}^{\mathrm{i}\varphi} a^*(f), \quad \vartheta^{\varphi}(a(f)) = a(\mathrm{e}^{\mathrm{i}\varphi} f) = \mathrm{e}^{-\mathrm{i}\varphi} a(f).$$

As a Banach space, $\mathrm{CAR}(\mathfrak{h})$ has a direct sum decomposition into charge sectors

$$\mathrm{CAR}(\mathfrak{h}) = \bigoplus_{n\in\mathbb{Z}} \mathrm{CAR}_n(\mathfrak{h}),$$

where $\mathrm{CAR}_n(\mathfrak{h})$ is the closed linear span of monomials of the form

$$a^*(f_1)\cdots a^*(f_j)a(g_k)\cdots a(g_1)$$

with $j - k = n$. In terms of the gauge-group, one has

$$\mathrm{CAR}_n(\mathfrak{h}) = \{A \in \mathrm{CAR}(\mathfrak{h}) \mid \vartheta^{\varphi}(A) = \mathrm{e}^{\mathrm{i}n\varphi} A\}.$$

If $A \in \mathrm{CAR}_n(\mathfrak{h})$ and $B \in \mathrm{CAR}_m(\mathfrak{h})$, then $AB \in \mathrm{CAR}_{n+m}(\mathfrak{h})$ and $A^* \in \mathrm{CAR}_{-n}(\mathfrak{h})$. In particular, the zero charge sector $\mathrm{CAR}_0(\mathfrak{h})$ is a $C^*$-subalgebra generated by $\mathbb{1}$ and elements of the form $a^*(f)a(g)$. Physical observables of a fermionic system are gauge invariant and hence elements of $\mathrm{CAR}_0(\mathfrak{h})$.

A state $\omega$ on $\mathrm{CAR}(\mathfrak{h})$ is gauge-invariant if $\omega \circ \vartheta^{\varphi} = \omega$ for all $\varphi \in \mathbb{R}$. A state $\omega_0$ on $\mathrm{CAR}_0(\mathfrak{h})$ has a unique extension to a gauge-invariant state $\omega$ on $\mathrm{CAR}(\mathfrak{h})$ given by

$$\omega\left(\bigoplus_n A_n\right) = \omega_0(A_0).$$

Thus, a gauge-invariant state on $\mathrm{CAR}(\mathfrak{h})$ is completely determined by its restriction to the gauge-invariant sub-algebra $\mathrm{CAR}_0(\mathfrak{h})$. When dealing with fermionic systems, it is often convenient to work on the full algebra $\mathrm{CAR}(\mathfrak{h})$ and restrict the gauge-invariant states.

### 8.2 Characteristic Functions

Denote by $\mathscr{U}$ the group of unitaries $u$ on $\mathfrak{h}$ such that $u - \mathbb{1}$ is finite-rank. For each $u \in \mathscr{U}$ there exist a finite-rank selfadjoint operator $k$ such that

$$k = \sum_{j=1}^{n} \kappa_j f_j(f_j|\,\cdot\,), \quad u = \mathrm{e}^{\mathrm{i}k}. \tag{8.1}$$

Moreover, the unitary

$$U(u) = \mathrm{e}^{\mathrm{i}\sum_j \kappa_j a^*(f_j)a(f_j)} \in \mathrm{CAR}(\mathfrak{h}),$$

only depends on $u$, not on the particular choice of the representation (8.1). The Araki-Wyss characteristic function of a gauge-invariant state $\omega$ on $\mathrm{CAR}(\mathfrak{h})$ is defined as

$$\begin{aligned} E : \mathscr{U} &\to \quad \mathbb{C} \\ u &\mapsto \omega(U(u)). \end{aligned}$$

It satisfies

1. For any $u_1, \dots, u_N \in \mathscr{U}$ and $z_1, \dots, z_N \in \mathbb{C}$,

$$\sum_{j,k=1}^{N} E(u_j^* u_k)\bar{z}_j z_k \geq 0.$$

2. For any $u, v \in \mathscr{U}$, $f \in \mathfrak{h}$ and $\lambda \in \mathbb{R}$

$$\frac{E(u\mathrm{e}^{\mathrm{i}\lambda(f|\,\cdot\,)f}v) - E(uv)}{\mathrm{e}^{\mathrm{i}\lambda\|f\|^2} - 1},$$

is independent of $\lambda$.

Reciprocally, any function $E : \mathscr{U} \to \mathbb{C}$ satisfying the above two conditions is the characteristic function of a unique gauge-invariant state $\omega$ on $\mathrm{CAR}(\mathfrak{h})$, see [17].

### 8.3 Vacuum State and Fock Representation

The vacuum state $\mathbf{vac}(\cdot)$ on $\mathrm{CAR}(\mathfrak{h})$ describes the system in absence of any fermion. If $\{e_i \mid i \in I\}$ denotes an arbitrary orthonormal basis of $\mathfrak{h}$, then $n_i = a^*(e_i)a(e_i)$ is the number of fermions in the state $e_i$, and we have $\mathbf{vac}(\prod_{i\in J} n_i) = 0$ for any finite $J \subset I$ (note that $[n_i, n_j] = 0$). It follows immediately that the characteristic function of the vacuum state is $E_{\mathbf{vac}}(u) = 1$.

The GNS representation associated to the vacuum state is the Fock representation $(\mathscr{H}_F, \pi_F, \Omega_F)$ where $\mathscr{H}_F = \Gamma_{\mathrm{a}}(\mathfrak{h})$ is the fermionic Fock space over $\mathfrak{h}$, $\pi_F(a(f)) = a_F(f)$ is the annihilation operator on $\Gamma_{\mathrm{a}}(\mathfrak{h})$, and $\Omega_F$ is the Fock vacuum vector. For $f_i, g_j \in \mathfrak{h}$ one has

$$\begin{aligned}&\mathbf{vac}(a(g_1)\cdots a(g_m)a^*(f_n)\cdots a^*(f_1))\\ &= (a_F^*(g_m)\cdots a_F^*(g_1)\Omega_F | a_F^*(f_n)\cdots a_F^*(f_1)\Omega_F) = \delta_{nm}\det\left\{(g_i|f_j)\right\}.\end{aligned}$$

Special features of the Fock representation are:

1. $\pi_F(\mathrm{CAR}(\mathfrak{h}))$ is irreducible, *i.e.*, any bounded operator on $\Gamma_{\mathrm{a}}(\mathfrak{h})$ commuting with all $a_{\mathrm{F}}^{\#}(f)$ is a multiple of the identity. Equivalently, the enveloping von Neumann algebra $\pi_F(\mathrm{CAR}(\mathfrak{h}))''$ is the $C^*$-algebra of all bounded operators on $\Gamma_{\mathrm{a}}(\mathfrak{h})$.
2. The second quantization $\Gamma(U)$ of a unitary operator $U$ on $\mathfrak{h}$ provides a unitary implementation of the associated Bogoliubov automorphism $\gamma(a(f)) = a(Uf)$,

$$\pi_F(\gamma(a(f))) = \Gamma(U)\pi_F(a(f))\Gamma(U)^*.$$

In particular, the gauge group $\vartheta^t$ is implemented by a strongly continuous unitary group whose generator $N = \mathrm{d}\Gamma(\mathbb{1})$ is the number operator.

A Fock state on $\mathrm{CAR}(\mathfrak{h})$ is a state $\omega$ which is normal with respect to the vacuum state $\mathbf{vac}$. Such a state is therefore defined by $\omega(A) = \mathrm{tr}(\rho\pi_F(A))$ where $\rho$ is a density matrix on $\Gamma_{\mathrm{a}}(\mathfrak{h})$. The GNS representation of a Fock state $\omega$ is a direct sum of Fock representations, *i.e.*, there exists a Hilbert space $\mathscr{K}$ such that $\mathscr{H}_\omega = \mathscr{H}_F \otimes \mathscr{K}$ and $\pi_\omega(A) = \pi_F(A) \otimes \mathbb{1}$. Typical examples of Fock states are finite volume, grand-canonical Gibbs ensembles

$$\rho = \frac{\mathrm{e}^{-\beta(H_\Lambda - \mu N_\Lambda)}}{\mathrm{tr}(\mathrm{e}^{-\beta(H_\Lambda - \mu N_\Lambda)})},$$

for Fermi gases with stable interactions, see [33]. Thermodynamic limits of such states yield non-Fock states with finite density. It is usually impossible to describe explicitly the GNS representations of these infinite volume *KMS states*. Notable exceptions are the ideal Fermi gases which lead to the *Araki-Wyss* representations.

Since there exists a selfadjoint (and hence densely defined) number operator $N = \mathrm{d}\Gamma(\mathbb{1})$ on the Fock space $\mathscr{H}_F$, Fock states describe systems with a finite number of fermions. A number operator can be tentatively defined in the GNS representation of any state $\omega$ as follows. For any finite $J \subset I$ denote by $n_J$ the quadratic form associated to the operator $\sum_{i\in J}\pi_\omega(n_i)$. For $\Psi \in \mathscr{H}_\omega$ set $n_\omega(\Psi) = \sup_J n_J(\Psi)$. It

can be shown that $n_\omega$ is a closed, non-negative quadratic form on the domain $D_\omega = \{\Psi \in \mathscr{H}_\omega \,|\, n_\omega(\Psi) < \infty\}$. If this domain is dense, then $n_\omega$ is the quadratic form of a selfadjoint number operator $N_\omega$, and the state $\omega$ is a Fock state, see [33, Section 5.2.3] for details.

### 8.4 Anti-Fock Representation

A state $\mathbf{full}(\,\cdot\,)$ describing a completely filled Fermi sea must satisfy, for any orthonormal basis $\{e_i \,|\, i \in I\}$ and any finite $J \subset I$, $\mathbf{full}(\prod_{i\in J}(1-n_i)) = 0$. It can be obtained using the particle-hole duality. Denote by $\bar{\cdot}$ an arbitrary complex conjugation on $\mathfrak{h}$ and define the $*$-automorphism $\alpha$ by $\alpha(a(f)) = a^*(\bar{f})$. Since $1-n_i = a(e_i)a^*(e_i) = \alpha(a^*(\bar{e}_i)a(\bar{e}_i))$, we can set $\mathbf{full} = \mathbf{vac} \circ \alpha$. It follows that

$$\mathbf{vac}(a(\bar{f}_1)\cdots a(\bar{f}_n)a^*(\bar{g}_m)\cdots a^*(\bar{g}_1)) = \delta_{nm}\det\left\{(g_i|f_j)\right\}.$$

For $u \in \mathscr{U}$ one has

$$\alpha(U(u)) = \det(u)U(\bar{u}),$$

and so the characteristic function of the filled Fermi sea is $E_{\mathbf{full}}(u) = \det(u)$. The corresponding GNS representation is the anti-Fock representation $(\mathscr{H}_F, \pi_{AF}, \Omega_F)$ where $\pi_{AF} = \pi_F \circ \alpha$.

If $\mathfrak{h}$ is finite dimensional, then the states **vac** and **full** are mutually normal, and the Fock and anti-Fock representations are equivalent. By fixing an orthonormal basis $\{e_1, \ldots, e_n\}$ and setting $a_J = \prod_{i\in J} a(e_i)$, the unitary operator defined by $UA_J^*\Omega_F = A_{I\setminus J}^*\Omega_F$ intertwines $\pi_F$ and $\pi_{AF}$. If $\mathfrak{h}$ is infinite dimensional these two representations are inequivalent and **full** is not a Fock state.

### 8.5 Jordan-Wigner Representation

The equivalence of the Fock and anti-Fock representations of CAR algebras over finite dimensional spaces is a consequence of a more general fact which we discuss briefly in this last section. We refer the reader to [41] for a more detailed discussion.

If $\mathfrak{h}$ is finite dimensional, then $\mathrm{CAR}(\mathfrak{h})$ is $*$-isomorphic to the full matrix algebra $\mathrm{Mat}(2^{\dim\mathfrak{h}})$. An explicit representation is provided by the Jordan-Wigner transformation described below. Since it maps fermions into quantum spins, this transformation is useful in many applications to statistical mechanics.

Let $\{e_1, \ldots, e_n\}$ be an orthonormal basis of $\mathfrak{h}$ and denote by $\sigma^{(1)}$, $\sigma^{(2)}$, $\sigma^{(3)}$ the usual Pauli matrices. On the $n$-fold tensor product $\mathscr{H} = \mathbb{C}^2 \otimes \cdots \otimes \mathbb{C}^2 \simeq \mathbb{C}^{2^n}$ define

$$\sigma_k^{(\alpha)} = \mathbb{1} \otimes \cdots \otimes \sigma^{(\alpha)} \cdots \otimes \mathbb{1},$$

where $\sigma^{(\alpha)}$ acts on the $k$-th copy of $\mathbb{C}^2$. Clearly, this operators generate the full matrix algebra $\mathscr{B}(\mathscr{H}) \simeq \mathrm{Mat}(2^n)$. One easily checks that the operators

$$a_k = \sigma_1^{(3)}\cdots\sigma_{k-1}^{(3)}(\sigma_k^{(1)} - \mathrm{i}\sigma_k^{(2)})/2,$$

satisfy $[a_k, a_l]_+ = 0$ and $[a_k, a_l^*]_+ = \delta_{k,l}$. The Jordan-Wigner representation of CAR($\mathfrak{h}$) is defined by

$$a_{\mathrm{JW}}\left(\sum_k z_k e_k\right) = \sum_k \bar{z}_k a_k.$$

The inversion formulas

$$\sigma_k^{(3)} = 2a_k^* a_k - \mathbb{1}, \quad \sigma_k^{(1)} = \sigma_1^{(3)} \cdots \sigma_{k-1}^{(3)}(a_k + a_k^*), \quad \sigma_k^{(2)} = \mathrm{i}\sigma_1^{(3)} \cdots \sigma_{k-1}^{(3)}(a_k - a_k^*),$$

show that CAR($\mathfrak{h}$) is isomorphic to Mat($2^n$). For fermionic systems, the Jordan–Wigner representation plays the same distinguished role as the Schrödinger representation in the CCR context: when $\dim \mathfrak{h} < \infty$, all irreducible representations of CAR($\mathfrak{h}$) are unitarily equivalent to it.

## Part III

### Non-equilibrium systems

# 9 Quantum Koopmanism

The Koopman-von Neumann spectral approach to ergodic theory is a powerful tool in the study of statistical properties of dynamical systems. Its extension to quantum dynamical systems – the spectral theory of Liouvilleans – is at the center of many recent results in quantum statistical mechanics, see Section 11 and [29, 47, 55, 84].

Let $(\mathscr{O}, \tau)$ be a *$C^*$- or $W^*$-dynamical system* equipped with a $\tau$-invariant state $\omega$, assumed to be normal in the $W^*$-case. By the *GNS-representation* $(\mathscr{H}_\omega, \pi_\omega, \Omega_\omega)$, *to the triple* $(\mathscr{O}, \tau, \omega)$ *we associate* $(\mathscr{O}_\omega, \tilde{\tau}, \tilde{\omega})$, a $W^*$-dynamical system on the *enveloping von Neumann algebra* $\mathscr{O}_\omega = \pi_\omega(\mathscr{O})''$ with a normal invariant state $\tilde{\omega}(A) = (\Omega_\omega | A\Omega_\omega)$. The $W^*$-dynamics $\tilde{\tau}$ is given by

$$\tilde{\tau}^t(A) = \mathrm{e}^{\mathrm{i}tL_\omega} A \mathrm{e}^{-\mathrm{i}tL_\omega},$$

where $L_\omega$ is the $\omega$-Liouvillean, see Section 3.3.

We shall say that $(\pi_\omega, \mathscr{O}_\omega, \mathscr{H}_\omega, L_\omega, \Omega_\omega)$ is the normal form of $(\mathscr{O}, \tau, \omega)$.

## 9.1 Ergodic Properties of Quantum Dynamical Systems

Let $\mathfrak{M}$ be a *von Neumann algebra* acting on a Hilbert space $\mathscr{H}$. The support $s_\omega$ of a *normal state* $\omega$ on $\mathfrak{M}$ is the smallest orthogonal projection $P \in \mathfrak{M}$ such that $\omega(P) = 1$. A normal state $\omega$ is faithful if and only if $s_\omega = \mathbb{1}$. It is easy to see that the support of the state $\omega(A) = (\Omega | A\Omega)$ is the orthogonal projection on the closure of the subspace $\mathfrak{M}'\Omega$.

**Notation.** We write $\nu \ll \omega$ whenever $\nu$ is a *$\omega$-normal* state such that $s_\nu \leq s_\omega$.

***Remark*** If $\mathfrak{M}$ is Abelian, then any $\omega$-normal state $\nu$ satisfies $\nu \ll \omega$. This explains why the support condition is absent in the classical ergodic theory (the reader may

consult [111] for a detailed discussion of this point). In most applications to statistical mechanics, $\omega$ is faithful, and any $\omega$-normal state $\nu$ satisfies $\nu \ll \omega$.

**Definition 9.1** Let $(\mathfrak{M}, \tau)$ be a $W^*$-dynamical system and $\omega$ a normal $\tau$-invariant state.

1. $(\mathfrak{M}, \tau, \omega)$ is ergodic if

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \omega(As_\omega \tau^t(B))\, \mathrm{d}t = \omega(A)\omega(B),$$

   holds for any $A, B \in \mathfrak{M}$.
2. $(\mathfrak{M}, \tau, \omega)$ is weakly mixing if

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \left|\omega(As_\omega \tau^t(B)) - \omega(A)\omega(B)\right| \mathrm{d}t = 0,$$

   holds for all $A, B \in \mathfrak{M}$.
3. $(\mathfrak{M}, \tau, \omega)$ is mixing or returns to equilibrium if

$$\lim_{t\to\infty} \omega(As_\omega \tau^t(B)) = \omega(A)\omega(B),$$

   for any $A, B \in \mathfrak{M}$
4. If $\omega$ is an invariant state of the $C^*$-dynamical system $(\mathscr{O}, \tau)$, we say that $(\mathscr{O}, \tau, \omega)$ is ergodic (resp. mixing, weakly mixing) if $(\mathscr{O}_\omega, \tilde{\tau}, \tilde{\omega})$ is ergodic (resp. mixing, weakly mixing).

Clearly, we have the implication (3)⇒(2)⇒ (1).

***Remark*** Ergodicity (1) is equivalent to the statement that

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \nu(\tau^t(A))\, \mathrm{d}t = \omega(A),$$

holds for all $A \in \mathfrak{M}$ and all states $\nu \ll \omega$. The mixing property (3) is equivalent to the statement that

$$\lim_{t\to\infty} \nu(\tau^t(A)) = \omega(A),$$

holds for all $A \in \mathfrak{M}$ and all states $\nu \ll \omega$, see [84, 117].

### 9.2 Spectral Characterization of Ergodic Properties

We refer to [111] for proofs of the results in this section.

The following theorem is the quantum version of the well-known Koopman-von Neumann spectral characterizations, [1, 88, 101].

**Theorem 9.2** *Let $(\mathscr{O}, \tau)$ be a $C^*$- or $W^*$-dynamical system equipped with a $\tau$-invariant state $\omega$, assumed to be normal in the $W^*$-case. Denote by $(\pi_\omega, \mathscr{O}_\omega, \mathscr{H}_\omega, L_\omega, \Omega_\omega)$ its normal form, and by $\mathscr{K}_\omega$ the closure of $\pi_\omega(\mathscr{O})'\Omega_\omega$.*

1. *The subspace $\mathscr{K}_\omega$ reduces the operator $L_\omega$. Denote by $\mathfrak{L}_\omega$ the restriction $L_\omega\big|_{\mathscr{K}_\omega}$.*
2. *$(\mathscr{O}, \tau, \omega)$ is ergodic if and only if* $\mathrm{Ker}(\mathfrak{L}_\omega)$ *is one-dimensional.*
3. *$(\mathscr{O}, \tau, \omega)$ is weakly mixing if and only if* 0 *is the only eigenvalue of $\mathfrak{L}_\omega$ and* $\mathrm{Ker}(\mathfrak{L}_\omega)$ *is one dimensional.*
4. *$(\mathscr{O}, \tau, \omega)$ is mixing if and only if*

$$\mathrm{w}-\lim_{t\to\infty} \mathrm{e}^{\mathrm{i}t\mathfrak{L}_\omega} = \Omega_\omega(\Omega_\omega|\,\cdot\,).$$

5. *If the spectrum of $\mathfrak{L}_\omega$ on $\{\Omega_\omega\}^\perp$ is purely absolutely continuous, then $(\mathscr{O}, \tau, \omega)$ is mixing.*

Note that $\mathscr{K}_\omega$ is the range of the support of $\tilde{\omega}$, that is, $\mathscr{K}_\omega = \pi_{\tilde{\omega}}\mathscr{H}_\omega$. Thus, if $\tilde{\omega}$ is faithful, then $\mathfrak{L}_\omega = L_\omega$.

Like the classical Koopman operator, the reduced Liouvillean $\mathfrak{L}_\omega$ of an ergodic quantum dynamical system exhibits several special spectral properties.

**Theorem 9.3** *Assume, in addition to the hypotheses of the previous theorem, that $(\mathscr{O}, \tau, \omega)$ is ergodic. Then the following hold:*

1. *The point spectrum of $\mathfrak{L}_\omega$ is a subgroup $\Sigma$ of the additive group $\mathbb{R}$.*
2. *The eigenvalues of $\mathfrak{L}_\omega$ are simple.*
3. *The spectrum of $\mathfrak{L}_\omega$ is invariant under translations in $\Sigma$, that is,* $\mathrm{spec}(\mathfrak{L}_\omega) + \Sigma = \mathrm{spec}(\mathfrak{L}_\omega)$.
4. *If $\Psi$ is a normalized eigenvector of $\mathfrak{L}_\omega$, then $(\Psi|\pi_\omega(A)\Psi) = \omega(A)$ for all $A \in \mathscr{O}$.*
5. *If $\omega$ is a $(\tau, \beta)$-KMS state then $\Sigma = \{0\}$ and the system is weakly mixing.*

## 10 Nonequilibrium Steady States

Equilibrium states lie at the heart of equilibrium statistical mechanics. Much of the success of this theory stems from the fact that these states can be constructed and characterized without explicit reference to the underlying dynamics. This is remarkable, given that the very notion of an equilibrium state–and the traditional justification of the theory following Boltzmann–ultimately relies on the dynamics.

Nonequilibrium statistical mechanics has a fundamentally different status. It is conceptually and technically more demanding, since a detailed understanding of the dynamics is required even to capture the most elementary nonequilibrium properties of a system. Among the vast manifold of nonequilibrium states, the simplest are the steady states that arise when the system is subjected to weak, stationary external forces. Such forcing may be implemented by an external field or by maintaining a gradient of intensive thermodynamic parameters across the system–for instance, a constant temperature drop. Despite significant progress in recent years, a coherent and comprehensive theory of steady states remains out of reach, if such a theory exists at all.

### 10.1 Phenomenological Theory and Linear Response

To appreciate recent rigorous results in the field, a basic knowledge of nonequilibrium thermodynamics is required. This section is a condensed introduction to the phenomenological theory of nonequilibrium steady states (NESS). The interested reader should consult [64] or [36] for detailed expositions.

Consider bringing into contact two systems $\mathscr{S}_1$, $\mathscr{S}_2$, each of which is in thermal equilibrium. Denote by

$$S_\alpha(A_{\alpha 1}, A_{\alpha 2}, \ldots)$$

the entropy of $\mathscr{S}_\alpha$ as a function of its extensive thermodynamic parameters. The combined system $\mathscr{S}_1+\mathscr{S}_2$, being otherwise isolated, has the values of $A_j = A_{1j}+A_{2j}$ fixed, and the entropy of the joint system is given by $S = \sum_\alpha S_\alpha(A_{\alpha 1}, A_{\alpha 2}, \ldots)$. The conditions for joint thermal equilibrium are thus

$$X_j = \frac{\partial S}{\partial A_{1j}} = \frac{\partial S_1}{\partial A_{1j}} - \frac{\partial S_2}{\partial A_{2j}} = I_{1j} - I_{2j} = 0,$$

where $I_{\alpha j}$ denotes the intensive thermodynamic parameter conjugate to $A_{\alpha j}$. If the combined system is not in thermal equilibrium, then the $X_j \neq 0$ act as thermodynamic forces. Their effect is to generate fluxes of the extensive quantities; these fluxes are given by

$$\Phi_j = \frac{\mathrm{d}A_{1j}}{\mathrm{d}t}.$$

The rate of entropy production is then

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \sum_j \frac{\partial S}{\partial A_{1j}} \frac{\mathrm{d}A_{1j}}{\mathrm{d}t} = \sum_j X_j \Phi_j. \tag{10.1}$$

Near equilibrium, the forces $X_j$ are weak, and the first-order perturbation theory in these forces – also called linear response theory – becomes a good approximation. Writing the fluxes as

$$\Phi_j = \sum_k L_{kj} X_k + \text{higher order terms} \tag{10.2}$$

defines the *kinetic* or *transport coefficients* $L_{kj}$. The matrix $L = (L_{kj})$ is called the *Onsager matrix*. It depends only on the intensive parameters $I_{1j}$. One of the most basic problems of nonequilibrium statistical mechanics is the calculation of Onsager's matrix starting from a microscopic description of the system.

In linear response theory the entropy production rate becomes

$$\frac{\mathrm{d}S}{\mathrm{d}t} \simeq \sum_k L_{kj} X_k X_j.$$

The second law of thermodynamics implies that the symmetric part of $L$ is positive. Moreover, if the systems are time-reversal invariant, then the Onsager reciprocity relations

$$L_{kj} = L_{jk},$$

hold, *i.e.*, the matrix $L$ is symmetric. If the systems are not time reversal invariant, these relations have to be appropriately modified. For example, if an external magnetic field $B$ is applied, then the matrix $L$ depends parametrically on $B$, and the Onsager-Casimir relations

$$L_{kj}(B) = L_{jk}(-B),$$

hold.

***Remarks*** **1.** Applying the above discussion to small volume elements of a macroscopic body, it is possible to obtain a phenomenological description of the local structure of a nonequilibrium state under the so-called local thermodynamic equilibrium (LTE) hypothesis. The reader should consult the above mentioned references for details.
**2.** Some variational characterizations of NESS have been proposed, most notably the principle of minimal entropy production. However, the status of such principles is still controversial, and their validity seems to be only approximate and limited to some special systems. See [100] for more information on this topic.

### 10.2 Microscopic Theory

A microscopic theory of NESS must be based on the asymptotic analysis of the dynamics which describes the evolution of the system. A non-isolated system is driven out of equilibrium by forces exerted upon it by its environment. Under appropriate conditions the system eventually settles in a steady state. Denote by $\langle \cdot \rangle_0$ the initial state, in the sense of statistical mechanics, of the system and its environment. If $t \mapsto \langle \cdot \rangle_t$ denotes the evolution of this state, then the limit

$$\langle \cdot \rangle_+ = \lim_{t\to\infty} \langle \cdot \rangle_t,$$

or more generally

$$\langle \cdot \rangle_+ = \lim_{t\to\infty} \frac{1}{t} \int_0^t \langle \cdot \rangle_s \, \mathrm{d}s,$$

defines a stationary state.

On physical grounds, one expects more – namely, that the limiting state $\langle \cdot \rangle_+$ is insensitive to local perturbations of the initial state $\langle \cdot \rangle_0$. To elaborate this essential point, let us consider a smooth dynamical system on a compact phase space $X \subset \mathbb{R}^n$. A physically natural statistics of the configurations of the system is provided by the normalized Lebesgue measure $\mathrm{d}x$ on $X$: initial configurations sampled according to $\mathrm{d}x$ can be considered typical. This choice is independent of the dynamics, and any distribution $\rho(x)\mathrm{d}x$ with strictly positive density $\rho$ would serve the same purpose. Accordingly, we expect that all these initial states lead to the same limiting state $\langle \cdot \rangle_+$. For systems with infinitely many degrees of freedom, no analogue of Lebesgue

measure exists, so a reference state is required to sample initial configurations. The purpose of this state is to specify the thermodynamic state of the system. Suppose, for example, that the system is driven out of equilibrium by several infinite reservoirs. Specifying an equilibrium state (a Gibbs measure or a KMS state) for each reservoir sets the temperature and other relevant thermodynamic parameters of each reservoir. States with different thermodynamic parameters are mutually singular and will lead to different NESS. Local perturbations of these equilibrium states will relax to equilibrium under the reservoir dynamics. Therefore, as in the finite dimensional case, we expect the limiting state $\langle \cdot \rangle_+$ to be insensitive to such local perturbations. In the language of *$C^*$-dynamical systems*, the NESS should only depend on the *folium* of the initial state.

The minimal goal of a microscopic theory of NESS is a mathematical derivation of the main results of linear response theory: Onsager reciprocity relations and fluctuation-dissipation relations (e.g. the Green-Kubo formula for the kinetic coefficients $L_{kj}$); see Section 13. A more ambitious program is to explore the largely unknown domain of far from equilibrium steady-state thermodynamics. Setting aside the obvious distinction between classical and quantum systems, recent progress in these directions can be grouped into two categories, depending on the chosen description of the microscopic dynamics: Hamiltonian or Markovian. The Hamiltonian description is, of course, the more fundamental, as microscopic dynamics is inherently Hamiltonian. However, the facts that

- various routes (scaling limits, coarse graining, restriction to specific degrees of freedom, etc…) lead from Hamiltonian dynamics to Markov processes;
- Hamiltonian dynamics is much more difficult to control than Markovian evolution;

explain why most of the available results belong to the second category. In fact, the Markovian time evolution was already at the heart of the pioneering works of Onsager and his followers, see [64].

A large body of works have been devoted to the study of interacting particle systems, see [28, 87]. We do not consider such models here, and instead focus on a small mechanical system $\mathscr{S}$ with finitely many degrees of freedom, driven out of equilibrium by external forcing.

In the framework of classical mechanics, two approaches are possible. In what we will call *the canonical approach*, the system $\mathscr{S}$ interacts with infinitely extended reservoirs $\mathscr{R}_1, \mathscr{R}_2$ …Apart from its physical appeal, the advantage of the canonical approach is that it allows for a Hamiltonian description of the coupled system $\mathscr{S} + \mathscr{R}_1 + \cdots$. A mathematical disadvantage is the necessity to deal with infinitely many degrees of freedom. As a result, only very simple reservoirs (e.g., ideal gases or free fields) are considered. These simple systems also act as almost ideal reservoirs in the sense that, at least in the dimension larger than two, the local properties of their internal state do not change too much as a result of the coupling to the system. Moreover, it is possible to design the coupling of these reservoirs to the system in such a way that the dynamics of $\mathscr{S}$ becomes essentially Markovian, see [52]. This is a significant feature, one that is seldom realized in other approaches. We refer to [115] for an introduction to recent results in the canonical approach to classical NESS.

It is important to realize that, in the canonical approach, the reservoirs serve two complementary purposes. First, they have a chaotic internal dynamics. The forces they exert on the system $\mathscr{S}$ act as a source of randomness. Under the action of these forces, the dynamics of $\mathscr{S}$ becomes itself chaotic. Second, the dynamics of the reservoir is dissipative: Any local perturbation gets carried away to spatial infinity. This allows the system $\mathscr{S}$ to relax from large fluctuations in its internal state by transferring energy, momentum, …to the reservoirs.

In *the microcanonical approach* the same effects of the environment on the motion of the system are obtained in a different way. Fluctuations of the system $\mathscr{S}$ are generated by a non-conservative external force. Under the action of this force the system would constantly heat-up. To avoid this effect and allow the system to settle in a stationary state, a dissipative force is added – a so-called thermostat. A popular example is the Gaussian thermostat which keeps the energy (or the kinetic energy) of $\mathscr{S}$ constant. The advantage of the microcanonical approach is that it leads to a dynamical system on a finite dimensional compact manifold (a surface of constant energy of $\mathscr{S}$). In particular, numerical experiments are much easier to perform on such a system than on the infinite dimensional systems obtained in the canonical approach. This fact has recently led to the numerical discovery of an unexpected fluctuation relation in far from equilibrium NESS [51]. This relation has been turned into a mathematical statement by combining the microcanonical approach with an axiomatic setup – the so called *chaotic hypothesis* [61]. We refer to [50, 127] for detailed introductions to this approach. A proof of the fluctuation relation for the canonical NESS of an anharmonic chain of oscillators has also been obtained in [120]. More recently the fluctuation relation has been observed in real experiments in various systems of very different nature, confirming its apparent universality.

Equivalence of the equilibrium ensembles (microcanonical, canonical, grand-canonical,…) is a cornerstone of equilibrium statistical mechanics. It is conjectured that a similar equivalence holds for NESS. In the thermodynamic limit, *i.e.*, as the size of $\mathscr{S}$ becomes large, one expects that the statistical properties of macroscopic observables in a NESS do not depend on the construction of the NESS. Microcanonical NESS with different kinds of thermostats, as well as canonical NESS with different kinds of reservoirs, should yield the same statistics. To our knowledge the only available result in this direction is [121].

Due to the intrinsic Hamiltonian nature of quantum mechanics the canonical approach is the only way to define and study the NESS of a quantum system (at least within a purely quantum description). We refer to Section 11 for a detailed discussion of quantum NESS.

## 11 NESS in Quantum Statistical Mechanics

In this section we describe the construction of canonical non-equilibrium steady states (NESS) for a small quantum system $\mathscr{S}$ coupled to several extended reservoirs $\mathscr{R}_1,\ldots,\mathscr{R}_M$; see Section 10. We shall work in the framework of $C^*$-*dynamical systems*, and denote by $\mathscr{O}_0$ the $C^*$-algebra of $\mathscr{S}$, which we assume to be finite dimensional. Each reservoir $\mathscr{R}_j$ is described by a $C^*$-algebra $\mathscr{O}_j$. For simplicity, we assume

that the algebra of the joint system $\mathscr{S} + \mathscr{R}_1 + \cdots + \mathscr{R}_M$ is the *$C^*$-tensor product* $\mathscr{O} = \mathscr{O}_{\mathscr{S}} \otimes \mathscr{O}_{\mathscr{R}} = \otimes_{0\le a\le M}\mathscr{O}_a$. The following is easily adapted to more general cases, e.g., fermionic algebras.

For $0 \le a \le M$, let $(\mathscr{O}_a, \tau_a)$ be the $C^*$-dynamical system describing the isolated subsystem $a$. The dynamics of the decoupled joint system is $\tau = \otimes_{0\le a\le M}\tau_a$. The dynamics $\tau_V$ of the coupled joint system is a local perturbation of $\tau$ induced by

$$V = \sum_{1\le j\le M} V_j, \quad V_j = V_j^* \in \mathscr{O}_0 \otimes \mathscr{O}_j,$$

where $V_j$ is the interaction between $\mathscr{S}$ and $\mathscr{R}_j$, see Section 3.

**Definition 11.1** Let $\omega$ be a state on $\mathscr{O}$. We say that $\omega_+$ is a NESS of $\tau_V$ associated to the reference state $\omega$ if there exists a net $t_\alpha \to \infty$ such that

$$\omega_+(A) = \lim_\alpha \frac{1}{t_\alpha}\int_0^{t_\alpha} \omega\circ\tau_V^t(A)\,\mathrm{d}t,$$

for all $A \in \mathscr{O}$. We denote by $\Sigma_+(\tau_V, \omega)$ the set of these NESS.

If the algebra $\mathscr{O}$ is separable, the net can be replaced by a sequence.
A few remarks are in order:

1. By definition, the elements of $\Sigma_+(\tau_V, \omega)$ are $\tau_V$-invariant states on $\mathscr{O}$. Moreover, if $\omega$ is such a state, then $\Sigma_+(\tau_V, \omega) = \{\omega\}$.
2. The limit $\omega_+$ may turn out to be a KMS state for $\tau_V$. This occurs trivially if $\omega$ is such a state, but is also expected when $\omega$ is (normal relative to) a KMS state for the decoupled dynamics $\tau$. This is *return to equilibrium*, see Definition 9.1(3). In this case $\omega_+$, will be $\omega$-normal. Consequently, in this special case the terminology NESS may be misleading, as the state actually corresponds to an equilibrium situation. In genuine nonequilibrium cases $\omega_+$ is expected to be singular with respect to $\omega$.
3. Entropy production plays a central role in nonequilibrium statistical mechanics. We refer to Section 12 for a discussion of related properties of NESS. Let us simply mention here that NESS have a non-negative entropy production rate.
4. Since the set of all states on $\mathscr{O}$ is weak-$*$ compact, $\Sigma_+(\tau_V, \omega)$ is nonempty.
5. If the perturbation $V$ is time-dependent, then natural nonequilibrium states (NNES) are defined in a similar way as limit points

$$\omega_+^t(A) = \lim_\alpha \frac{1}{t_\alpha}\int_{-t_\alpha}^{t} \omega\circ\tau_V^{s\to t}(A)\,\mathrm{d}s.$$

They satisfy $\omega_+^t\circ\tau_V^{t\to r} = \omega_+^r$, see [122].

As stressed in Section 10, a NESS should be insensitive to local perturbations of the initial state $\omega$. The following result shows that this is indeed the case under a rather weak ergodic hypothesis (see also [80]).

**Theorem 11.2** ([14]) *Assume that $\omega$ is a factor state on $\mathscr{O}$ and that, for any $\omega$-normal state $\eta$,*

$$\lim_{t\to\infty}\frac{1}{t}\int_0^t \eta([\tau_V^s(A),\,B])\,\mathrm{d}s = 0$$

*holds for all $A$, $B$ in a dense subset of $\mathscr{O}$ (weak asymptotic Abelianness in mean). Then $\Sigma_+(\tau_V,\eta) = \Sigma_+(\tau_V,\omega)$ holds for all $\omega$-normal states $\eta$.*

In typical applications the reference state $\omega$ is specified by the requirement that its restrictions to the subalgebras $\mathscr{O}_a$ are $\beta_a$-*KMS states*[4] for the corresponding dynamics $\tau_a$. This means that $\omega$ is a KMS state at inverse temperature $-1$ for the dynamics $\sigma_\omega^t = \otimes_a \tau_a^{-\beta_a t}$. In particular, $\omega$ is *modular* and $\sigma_\omega$ is its modular group, see Section 5. The group $\sigma_\omega$ plays an important and somewhat unexpected role in the mathematical theory of linear response, see Section 13.

Accordingly, we shall assume in the remaining part of this paragraph that $\omega$ is modular, and we denote by $(\mathscr{H}_\omega, \pi_\omega, \Omega_\omega)$ the corresponding *GNS representation* of $\mathscr{O}$. The *enveloping von Neumann algebra* $\pi_\omega(\mathscr{O})''$ is in *standard form*, and we denote by $J$ the *modular conjugation*. If $L$ is the *standard Liouvillean* of $\tau$, then $L_V = L + \pi_\omega(V) + J\pi_\omega(V)J$ is the standard Liouvillean of $\tau_V$. The spectral analysis of $L_V$ yields interesting information on the structure of $\Sigma_+(\tau_V,\omega)$, see [14].

**Theorem 11.3** *Assume that the state $\omega$ is modular.*

1. *If* Ker $L_V = \{0\}$*, then there is no $\omega$-normal $\tau_V$-invariant state. In particular, any NESS in $\Sigma_+(\tau_V,\omega)$ is purely $\omega$-singular.*
2. *If the assumptions of Theorem 11.2 hold and if* Ker $L_V \neq \{0\}$*, then* Ker $L_V$ *is one-dimensional and there exists a unique $\omega$-normal $\tau_V$-invariant state $\omega_V$. Moreover, $\Sigma_+(\tau_V,\omega) = \{\omega_V\}$.*

As already mentioned, case *(i)* in the above theorem is the expected behavior out of equilibrium while case *(ii)* describes a typical equilibrium situation.

To our knowledge, there are two approaches to the construction of NESS which we now describe.

### 11.1 The Scattering Approach

The first approach was proposed by Ruelle in [122] and relies on the scattering theory of $C^*$-dynamical systems, see [116]. We also refer to [56, 78] for related works.

The scattering approach assumes the existence of the strong limit

$$\alpha_V = \mathrm{s}-\lim_{t\to\infty}\tau^{-t}\circ\tau_V^t. \tag{11.1}$$

This limit defines an isometric $*$-endomorphism of $\mathscr{O}$ such that $\alpha_V\circ\tau_V^t = \tau^t\circ\alpha_V$, often called Møller morphism. $\alpha_V$ is injective but its range $\mathscr{O}_+$, a $\tau$-invariant $C^*$-subalgebra of $\mathscr{O}$, can be strictly smaller than $\mathscr{O}$. One immediately obtains

[4] chemical potentials can also be prescribed by an appropriate definition of $\tau$

**Proposition 11.4** *Assume that the Møller morphism* (11.1) *exists and that* $\omega$ *is* $\tau$*-invariant. Then, for all* $A \in \mathscr{O}$*,*

$$\lim_{t\to\infty} \omega \circ \tau_V^t(A) = \omega_+(A),$$

*where* $\omega_+ = \omega \circ \alpha_V$*. In particular, one has* $\Sigma_+(\tau_V, \omega) = \{\omega_+\}$*.*

If the previous proposition applies, then $\alpha_V$ provides an isomorphism between the the coupled dynamical system $(\mathscr{O}, \tau_V, \omega_+)$ and the decoupled one $(\mathscr{O}_+, \tau|_{\mathscr{O}_+}, \omega|_{\mathscr{O}_+})$. Ergodic properties of the latter are therefore inherited by the former. The following proposition is a simple consequence of this fact, see [14].

**Proposition 11.5** *Assume that the assumptions of Proposition 11.4 hold.*

1. *If* $\omega|_{\mathscr{O}_+}$ *is ergodic for* $\tau|_{\mathscr{O}_+}$*, then* $\Sigma_+(\tau_V, \eta) = \{\omega_+\}$ *for any* $\omega$*-normal state* $\eta$*.*
2. *If* $\omega|_{\mathscr{O}_+}$ *is mixing for* $\tau|_{\mathscr{O}_+}$*, then*

$$\lim_{t\to\infty} \eta \circ \tau_V^t(A) = \omega_+(A)$$

*holds for all* $A \in \mathscr{O}$ *and any* $\omega$*-normal state* $\eta$*.*

For a finite system coupled to infinite reservoirs, we expect that $\mathscr{O}_+ = \mathscr{O}_{\mathscr{R}}$, and that the coupled system out of equilibrium inherits the ergodic properties of the reservoirs.

At present the only known technique to study $C^*$-scattering is the basic Cook's method, which requires rather restrictive assumptions. We refer to [15, 56, 78, 122] for more details and examples. The Hilbert-space techniques, which we will describe in the next subsection, are often a more flexible alternative.

### 11.2 The Liouvillean Approach

This alternative to the scattering approach has been proposed in [81], where the NESS of a $N$-level quantum system coupled to ideal Fermi reservoirs is constructed. For this kind of systems it has not yet been possible to obtain the propagation estimates needed to construct the Møller morphism. In fact it is not clear that the scattering approach applies in this case.

In the Liouvillean approach, NESS are related to resonances of a new kind of generator of the dynamics in the GNS representation called the $C$-Liouvillean. The main advantage of this method is that the required analysis can be performed in a Hilbert space setting. The technical difficulties are related to the fact that the $C$-Liouvillean is not selfadjoint on the GNS Hilbert space. Here we describe only the strategy and refer the reader to [81] for details of the implementation.

We assume that $\omega$ is modular and work directly in the GNS representation $(\mathscr{H}_\omega, \pi_\omega, \Omega_\omega)$, identifying $\mathscr{O}$ with $\pi_\omega(\mathscr{O})$. Recall that $\sigma_\omega$ is the modular group of $\omega$, $J$ is the modular conjugation, and $L$, $L_V$ are the standard Liouvilleans of $\tau$, $\tau_V$. Denote by $\Delta_\omega$ the *modular operator*.

**Definition 11.6** If $t \mapsto \sigma_\omega^t(V)$ is analytic in the strip $\{z \in \mathbb{C} \mid |\operatorname{Im} z| < 1/2\}$ and bounded continuous in its closure then the $C$-Liouvillean of $\tau_V$ is the closed operator defined on the domain of $L$ by

$$K_V = L + V - J\sigma_\omega^{-\mathrm{i}/2}(V)J.$$

Since $J\sigma_\omega^{-\mathrm{i}/2}(V)J \in \pi_\omega(\mathscr{O})'$, one easily checks that $\mathrm{e}^{\mathrm{i}tK_V}A\mathrm{e}^{-\mathrm{i}tK_V} = \tau_V^t(A)$. Moreover, since $L\Omega_\omega = 0$, it follows from modular theory that

$$K_V\Omega_\omega = V\Omega_\omega - J\Delta_\omega^{1/2}V\Delta_\omega^{-1/2}J\Omega_\omega = V\Omega_\omega - J\Delta_\omega^{1/2}V\Omega_\omega = (V - V^*)\Omega_\omega = 0.$$

Hence $\omega \circ \tau_V^t(A) = (\Omega_\omega|\mathrm{e}^{\mathrm{i}tK_V}A\Omega_\omega) = (\mathrm{e}^{-\mathrm{i}tK_V^*}\Omega_\omega|A\Omega_\omega)$ where $K_V^* = L + V - J\sigma_\omega^{\mathrm{i}/2}(V)J$.

Suppose that there exists a triplet of rigged Hilbert spaces $\mathscr{K} \subset \mathscr{H}_\omega \subset \mathscr{K}'$ and a dense subalgebra $\tilde{\mathscr{O}} \subset \mathscr{O}$ such that $\tilde{\mathscr{O}}\Omega_\omega \subset \mathscr{K}$ and

$$\mathrm{w}^*\text{–}\lim_{t\to\infty} \frac{1}{t}\int_0^t \mathrm{e}^{-\mathrm{i}sK_V^*}\Omega_\omega \,\mathrm{d}s = \Psi \in \mathscr{K}'$$

holds in $\mathscr{K}'$. Then the functional $\tilde{\mathscr{O}} \ni A \mapsto (\Psi|A\Omega_\omega)$ extends by continuity to a state $\omega_+$ on $\mathscr{O}$ and we can conclude that $\Sigma_+(\tau_V, \omega) = \{\omega_+\}$. Note that if $\Psi \in \mathscr{H}_\omega$ then $\omega_+$ is $\omega$-normal. Thus, we expect that $\Psi \notin \mathscr{H}_\omega$ in genuine nonequilibrium situations. Under appropriate conditions, one can show that $\Psi$ is a zero-resonance vector of $K_V^*$, *i.e.*, that there exists an extension of $K_V^*$ to $\mathscr{K}'$ for which $\Psi$ is a zero eigenvector. In [81], and more recently in [99], spectral deformation techniques have been used to gain perturbative control on the resonances of $K_V^*$. This yields a convergent expansion for the NESS $\omega_+$ in powers of the coupling $V$ which, to lowest order, coincide with the weak coupling (van Hove) limit studied in [130]. It also gives the convergence $\nu \circ \tau_V^t(A) \to \omega_+(A)$ for all $\omega$-normal states $\nu$ and all $A \in \mathscr{O}$ with a precise estimates on the exponential rate of convergence for dense sets of such $\nu$ and $A$.

## 12 Entropy Production

Entropy, as defined by Clausius, is the cornerstone of equilibrium thermodynamics. Its statistical interpretation by Boltzmann is the key to our microscopic understanding of equilibrium.

A notion of entropy production (rate) has emerged from recent developments in classical and quantum statistical mechanics of nonequilibrium steady states. Taking this notion seriously, it does not seem possible to define the entropy of a nonequilibrium steady state [125]. As argued in [60], if such an entropy exists, then it is most likely to take the value $-\infty$, because a system in such a state loses entropy at a constant rate.

The purpose of this section is to introduce the notion of entropy production for nonequilibrium steady states of a small quantum system in contact with thermal

reservoirs. Throughout, we shall freely use the concepts and notation introduced in Section 11.

### 12.1 Relative Entropy

The relative entropy of two density matrices $\rho$ and $\rho'$ is defined, in analogy with the relative entropy of two probability measures, by

$$\mathrm{Ent}(\rho'|\rho) = \mathrm{tr}(\rho'(\log\rho - \log\rho')).$$

It has been generalized by Araki to arbitrary states on a von Neumann algebra [10, 11]. To describe the general definition, we need to introduce the notion of relative modular operator.

Let $\mathfrak{M}$ be a von Neumann algebra acting on a Hilbert space $\mathscr{H}$ and let $\Psi, \Phi \in \mathscr{H}$ be two unit vectors. Denote by $s_\Psi$ the support of the state $\psi(A) = (\Psi|A\Psi)$, *i.e.*, the orthogonal projection on the closure of $\mathfrak{M}'\Psi$ (see Section 5). Denote by $s'_\Psi$ the support of the state on $\mathfrak{M}'$ defined by $\psi'(B) = (\Psi|B\Psi)$, $B \in \mathfrak{M}'$, which coincides with the orthogonal projection onto the closure of $\mathfrak{M}\Psi$. Since $A, B \in \mathfrak{M}$ and $A\Psi = B\Psi$ imply $As_\Psi = Bs_\Psi$, formula

$$A\Psi \mapsto s_\Psi A^*\Phi$$

defines a closable antilinear operator on $\mathfrak{M}\Psi$, which is a dense subspace of $s'_\Psi\mathscr{H}$. The operator has values in $s_\Psi\mathscr{H}$. Denote by $S_{\Phi|\Psi}$ its closure. The selfadjoint operator $\Delta_{\Phi|\Psi} = S^*_{\Phi|\Psi}S_{\Phi|\Psi}$ is called the relative modular operator of the pair $(\Phi, \Psi)$.

**Definition 12.1** Let $\omega$ be a *modular state* on the $C^*$-algebra $\mathscr{O}$. Denote by $(\mathscr{H}, \pi, \Psi_\omega)$ the induced *GNS representation* and by $\mathscr{H}_+$ its *natural cone*. For any $\omega$*-normal* state $\nu$ on $\mathscr{O}$, let $\Psi_\nu$ be its unique vector representative in $\mathscr{H}_+$ (see Theorem 5.13). The entropy of a state $\nu$ relative to $\omega$ is defined by

$$\mathrm{Ent}(\nu|\omega) = \begin{cases} (\Psi_\nu|\log\Delta_{\Psi_\omega|\Psi_\nu}\Psi_\nu), & \text{if } \nu \text{ is } \omega\text{-normal,} \\ -\infty & \text{otherwise.} \end{cases}$$

***Remarks*** **1.** We have restricted the above definition to modular $\omega$ for simplicity. To obtain a completely general definition, it suffices to pass to a *standard representation* of the *enveloping von Neumann algebra* $\mathscr{O}_\omega$ if $s_\nu \le s_\omega$, and to set $\mathrm{Ent}(\nu|\omega) = -\infty$ otherwise.

**2.** We use the notation $\mathrm{Ent}(\,\cdot\,|\,\cdot\,)$ of [33, 108] which differs by sign and by the ordering of the arguments from the original notation in [10, 11].

The most important properties of relative entropy for our purposes are

1. $\mathrm{Ent}(\nu|\omega) \le 0$, with equality if and only if $\nu = \omega$.
2. For any $C \in \mathbb{R}$ the set of states $\{\nu \mid \mathrm{Ent}(\nu|\omega) \ge C\}$ is a weak-$*$ compact subset of the *folium* $\mathscr{N}_\omega$.
3. $\mathrm{Ent}(\nu\circ\tau|\omega\circ\tau) = \mathrm{Ent}(\nu|\omega)$ for any $\tau \in \mathrm{Aut}(\mathfrak{M})$.

The reader should consult [108] for a more exhaustive list and a detailed discussion.

### 12.2 The Entropy Balance Equation

The change in relative entropy due to the action of an inner $*$-automorphism is given by the following result.

**Theorem 12.2** ([82]) *Let $\omega$ be a modular state on the $C^*$-algebra $\mathscr{O}$. Denote by $\delta_\omega$ the infinitesimal generator of its* modular group *on the enveloping algebra of $\mathscr{O}$. For any unitary $U \in \mathscr{O}$, set $\tau_U(A) = U^*AU$. Then*

$$\mathrm{Ent}(\nu \circ \tau_U|\omega) = \mathrm{Ent}(\nu|\omega) - \mathrm{i}\,\nu\left(U^*\delta_\omega(U)\right)$$

*for any state $\nu$ on $\mathscr{O}$ and any unitary $U \in \mathrm{Dom}(\delta_\omega)$.*

Using Property (iii) of the relative entropy, a direct application of this theorem to *local perturbations* of quantum dynamical systems (see Section 3.4) yields

**Corollary 12.3** *Let $(\mathscr{O}, \tau)$ be a $C^*$- or $W^*$-dynamical system equipped with a modular invariant state $\omega$. Denote by $\delta_\omega$ the generator of the modular group of $\omega$. For any local perturbation $\tau_V$ induced by $V = V^* \in \mathrm{Dom}(\delta_\omega)$ one has*

$$\mathrm{Ent}(\nu \circ \tau_V^t|\omega) = \mathrm{Ent}(\nu|\omega) - \int_0^t \nu \circ \tau_V^s(\delta_\omega(V))\,\mathrm{d}s. \tag{12.1}$$

***Remark*** In the case of a time-dependent local perturbation $V(t)$ such that $t \mapsto V(t)$ and $t \mapsto \delta_\omega(V(t))$ are continuous in the natural topology of $\mathscr{O}$, Theorem 12.2 yields

$$\mathrm{Ent}(\nu \circ \tau_V^{s\to t}|\omega) = \mathrm{Ent}(\nu|\omega) - \int_s^t \nu \circ \tau_V^{s\to u}(\delta_\omega(V(u)))\,\mathrm{d}s.$$

To our knowledge, this formula was first obtained in [105] for a $(\tau, \beta)$-KMS state $\omega$. In this special case $\delta_\omega = -\beta\delta$ where $\delta$ is the infinitesimal generator of $\tau$.

Assume that $\omega_+ \in \Sigma_+(\tau_V, \omega)$, *i.e.*, that $\omega_+$ is an NESS of the perturbed dynamics (see Section 11). Then there exists a net $t_\alpha \to \infty$ such that

$$\omega_+(A) = \lim_\alpha \frac{1}{t_\alpha}\int_0^{t_\alpha} \omega \circ \tau_V^s(A)\,\mathrm{d}s.$$

The entropy balance formula (12.1) and Property (i) of the relative entropy yield

$$0 \le -\lim_\alpha \frac{\mathrm{Ent}(\omega \circ \tau_V^{t_\alpha}|\omega)}{t_\alpha} = \omega_+(\delta_\omega(V)),$$

from which, given the following definition, the next proposition follows.

**Definition 12.4** 1. We define the entropy production observable of the local perturbation $V$ relative to the reference state $\omega$ by $\sigma(\omega, V) = \delta_\omega(V)$.

2. The entropy production rate of a NESS $\omega_+ \in \Sigma_+(\tau_V, \omega)$ is $\mathrm{Ep}(\omega_+) = \omega_+(\sigma(\omega, V))$.

**Proposition 12.5** *The entropy production rate of a NESS is non-negative.*

For quantum spin systems, our definition formally agrees with Ruelle's proposal [123, 124]. It is also closely related to the definition of entropy production used in [130].

### 12.3 Thermodynamic Interpretation

Let us consider the case of a small system $\mathscr{S}$, with a finite dimensional algebra $\mathscr{O}_0$, coupled to several infinitely extended reservoirs $\mathscr{R}_1, \dots, \mathscr{R}_M$. We freely the notation of Section 11.

Denote by $\delta_a$ the generator of $\tau_a^t = \tau^t|_{\mathscr{O}_a}$ for $0 \le a \le M$. Since $\mathscr{O}_0$ is finite dimensional, one has $\delta_0 = \mathrm{i}[H_{\mathscr{S}}, \cdot\,]$ for some Hamiltonian $H_{\mathscr{S}}$. Observables describing the energy fluxes out of the reservoirs can be obtained in the following way. The total energy of the system is the sum of the energy of each reservoir, of the energy $H_{\mathscr{S}}$ of the small system, and of the interaction energy $V$. Since the total energy is conserved, the rate at which the energy of the reservoirs decreases under the coupled dynamics is

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\tau_V^t(H_{\mathscr{S}} + V) &= \tau_V^t\left(\sum_{1\le j\le M}\delta_j(H_{\mathscr{S}} + V) + \mathrm{i}[H_{\mathscr{S}} + V, H_{\mathscr{S}} + V]\right)\\ &= \tau_V^t\left(\sum_{1\le j\le M}\delta_j(V)\right).\end{aligned}$$

Noting that $\delta_j(V) = \delta_j(V_j) \in \mathscr{O}_0 \otimes \mathscr{O}_j$, we can identify $\Phi_j = \delta_j(V)$ with the energy flux out of reservoir $\mathscr{R}_j$.

Suppose now that each reservoir $\mathscr{R}_j$ is initially at thermal equilibrium at inverse temperature $\beta_j$, the system $\mathscr{S}$ being in an arbitrary $\tau_0$-invariant faithful state. From the observation in the paragraph following Theorem 11.2, we conclude that the generator of the modular group of the initial state $\omega$ takes the form

$$\delta_\omega = -\sum_{1\le j\le M}\beta_j\delta_j + \mathrm{i}[K, \cdot\,],$$

for some $K \in \mathscr{O}_0$ such that $\delta_a(K) = 0$ for $0 \le a \le M$. It follows that the entropy production observable is

$$\sigma(\omega, V) = -\sum_{1\le j\le M}\beta_j\delta_j(V) + \mathrm{i}[K, V] = -\sum_{1\le j\le M}\beta_j\Phi_j - \delta_V(K),$$

where $\delta_V = \sum_a \delta_a + \mathrm{i}[V, \cdot\,]$ is the generator of $\tau_V$. It is important to realize that the second term in the right-hand side of this identity is a total derivative. Consequently,

its contribution to entropy production remains uniformly bounded in time

$$\int_0^t \tau_V^s(\sigma(\omega, V))\,\mathrm{d}s = -\sum_{1\le j\le M} \beta_j \int_0^t \tau_V^s(\Phi_j)\,\mathrm{d}s + \left(\tau_V^t(K) - K\right).$$

In particular, since $\omega_+ \in \Sigma_+(\tau_V, \omega)$ is $\tau_V$-invariant, this boundary term does not contribute to the entropy production rate of the NESS, and we can write

$$\mathrm{Ep}(\omega_+) = -\sum_{1\le j\le M} \beta_j\, \omega_+(\Phi_j),$$

which is the familiar phenomenological expression (10.1). A similar interpretation is possible in the case of time-dependent perturbations, see [105].

For classical, thermostated systems used in the construction of microcanonical NESS, entropy production is usually defined as the local rate of phase space contraction $\alpha$ (see [60]). If $\phi^t$ denotes the phase space flow and $\mu$ the reference measure (typically Lebesgue's measure), then

$$\mu_t(f) = \mu(f \circ \phi^t) = \mu(f\, \mathrm{e}^{\int_0^t \alpha\circ\phi^{-s}\,\mathrm{d}s}).$$

A simple calculation shows that, if $\nu$ is absolutely continuous with respect to $\mu$, then

$$\mathrm{Ent}(\nu_t|\mu) = \mathrm{Ent}(\nu|\mu) - \int_0^t \nu(\alpha\circ\phi^s)\,\mathrm{d}s.$$

Comparison with (12.1) shows perfect agreement with Definition 12.4 (see [110] for a completely parallel treatment of the classical and quantum cases).

### 12.4 Strict Positivity of Entropy Production

We have seen that $\mathrm{Ep}(\omega_+) \ge 0$ for a NESS $\omega_+$. One expects more, namely $\mathrm{Ep}(\omega_+) > 0$. Strict positivity of entropy production is a delicate dynamical problem. It is related to the singularity of the NESS with respect to the reference state, as indicated by the following result.

**Theorem 12.6** ([80]) *If $\omega_+ \in \Sigma_+(\tau_V, \omega)$ is $\omega$-normal, then $\mathrm{Ep}(\omega_+) = 0$. Moreover, if*

$$\sup_{t>0} \left| \int_0^t \left\{\omega\circ\tau_V^s(\sigma(\omega, V)) - \omega_+(\sigma(\omega, V))\right\} \mathrm{d}s \right| < \infty,$$

*then $\mathrm{Ep}(\omega_+) = 0$ implies that $\omega_+$ is $\omega$-normal.*

Strict positivity of entropy production has been proved in a number of models. We refer to the original articles [13, 56, 81, 130]. The strict positivity of entropy production for generic perturbations has been studied in [83].

## 13 Linear Response Theory

Linear response theory is a special instance of first-order perturbation theory. Its purpose is to describe the response of mechanical system to external forces in the regime of weak forcing. Of particular interest is the response of systems that are driven out of some dynamical equilibrium by non-conservative mechanical forces or thermal forces, such as temperature or density gradients. This article is a short introduction to some mathematical results in quantum mechanical linear response theory. We refer to [90] for an introduction to the physical aspects of the subject.

### 13.1 Finite Time Linear Response

The first problem of linear response theory is the determination of the response of the system to the action of driving forces over a finite interval of time. We shall consider separately the simple case of mechanical forcing and the more delicate thermal drives.

The unperturbed system is a *$C^*$- or $W^*$-dynamical system* $(\mathscr{O}, \tau)$ equipped with a *modular* invariant state $\omega$. We denote by $\delta$ the generator of the dynamics $\tau$, by $\sigma$ the modular group of $\omega$, and by $\zeta$ the generator of $\sigma$. $\mathscr{O}_{\rm self}$ further denotes the set of selfadjoint elements of $\mathscr{O}$. We note that the important role of the modular structure in linear response theory was already apparent in [104].

Since $\omega$ is $(\sigma, -1)$-*KMS*, for any $A, B \in \mathscr{O}$ there exists a function $z \mapsto F(A, B; z)$ which is analytic in the strip $\{z \in \mathbb{C} \mid -1 < \operatorname{Im} z < 0\}$, bounded and continuous on its closure, and such that $F(A, B; \theta) = \omega(A\sigma^\theta(B))$ and $F(A, B; \theta - \mathrm{i}) = \omega(\sigma^\theta(B)A)$ for $\theta \in \mathbb{R}$. With a slight abuse of the notation, we denote $F(A, B; z)$ by either $\omega(A\sigma^z(B))$ or $\omega(\sigma^{-z}(A)B)$ for $-1 \leq \operatorname{Im} z \leq 0$. In particular, the canonical correlation of $A, B \in \mathscr{O}$ is defined by

$$\langle A|B\rangle_\omega = \int_0^1 \omega(A\sigma_\omega^{-\mathrm{i}\theta}(B))\,\mathrm{d}\theta = \int_0^1 F(A, B; -\mathrm{i}\theta)\,\mathrm{d}\theta.$$

One easily checks that it defines an inner product on the real vector space $\mathscr{O}_{\rm self}$, see [104].

#### 13.1.1 Mechanical drive

Let $\tau_V^{s\to t}$ be the dynamics on $\mathscr{O}$ generated by $\delta + \mathrm{i}[V(t), \cdot\,]$, *i.e.*, the solution of

$$\begin{aligned}\partial_t \tau_V^{s\to t}(A) &= \tau_V^{s\to t}(\delta(A) + \mathrm{i}[V(t), A]),\\ \partial_s \tau_V^{s\to t}(A) &= \delta(\tau_V^{s\to t}(A)) + \mathrm{i}[V(s), \tau_V^{s\to t}(A)],\end{aligned}$$

which satisfies $\tau_V^{t\to t}(A) = A$. Suppose that $t \mapsto V(t)$ belongs to $C(\mathbb{R}, \mathscr{O}_{\rm self})$.

Standard time-dependent perturbation theory yields (see Section 3)

$$\tau_V^{s\to t}(A) = \tau^{t-s}(A) + \int_s^t \mathrm{i}[\tau^{u-s}(V(u)), \tau^{t-u}(A)]\,\mathrm{d}u + \text{higher order terms}.$$

Using the invariance of $\omega$ under $\tau$ and the identity $\omega \circ \tau^{u-s} = \omega$, the first-order term can be rewritten as

$$(\Delta\omega)^{s\to t}(A) = \int_s^t \omega\big(\mathrm{i}[V(u), \tau^{t-u}(A)]\big)\, \mathrm{d}u,$$

which motivates the definition of the response function $\mathscr{K}$:

$$(\Delta\omega)^{s\to t} = \int_s^t \mathscr{K}(t-u)V(u)\, \mathrm{d}u.$$

The operator-valued response function $\mathscr{K}(u) : \mathscr{O} \to \mathscr{O}^{\#}$, where $\mathscr{O}^{\#}$ denotes the dual of $\mathscr{O}$, is defined by

$$(\mathscr{K}(u)V)(A) = \omega(\mathrm{i}[V, \tau^u(A)]), \tag{13.1}$$

for $u \geq 0$; $\mathscr{K}(u) = 0$ for $u < 0$ (causality).

Note that if $\omega$ is *mixing* for $(\mathscr{O}, \tau)$, then $\lim_{t\to\infty}(\Delta\omega)^{s\to t}(X) = 0$ for any $V \in C(\mathbb{R}, \mathscr{O}_{\mathrm{self}})$ of compact support and any $X \in \mathscr{O}$, *i.e.*, the system recovers from infinitesimal localized perturbations. We refer to [139] for further connections between the mixing property and linear response theory.

For $V \in \mathrm{Dom}(\zeta)$, the KMS property implies that Equ. (13.1) can be rewritten as

$$(\mathscr{K}(u)V)(A) = \langle \tau^u(A) | \zeta(V) \rangle_\omega.$$

Here $\zeta$ denotes the generator of the modular group of $\omega$. This is a typical fluctuation-dissipation relation: the response function $\mathscr{K}$ on the left-hand side describes dissipation, while the correlation function on the right-hand side measures fluctuations.

For later reference, let us consider the special case where $\omega$ is $(\tau, \beta)$-KMS and $V(t) = -\sum_j X_j(t) A_j$. Here the operators $A_j \in \mathscr{O}_{\mathrm{self}} \cap \mathrm{Dom}(\delta)$ describe the coupling of the system to external fields, and the functions $X_j$ are the time-dependent field strengths. One has $\zeta = -\beta\delta$ and the observable $\Phi_j = \delta(A_j)$ describes the flux conjugate to $A_j$. The linear response is given by the finite time Green-Kubo formula

$$(\Delta\omega)^{s\to t}(A) = \sum_j \beta \int_s^t \langle \tau^{t-u}(A) | \Phi_j \rangle_\omega \, X_j(u)\, \mathrm{d}u. \tag{13.2}$$

### 13.1.2 Thermal drive

To discuss thermal forcing, we need more structure. We consider the setting of Section 11: a small system $\mathscr{S}$, described by $(\mathscr{O}_0, \tau_0)$, coupled to infinite reservoirs $\mathscr{R}_1, \ldots, \mathscr{R}_M$ described by $(\mathscr{O}_j, \tau_j)$, $1 \leq j \leq M$. The algebra factorizes accordingly $\mathscr{O} = \otimes_{0\leq a\leq M} \mathscr{O}_a$, and the dynamics of the decoupled system is $\tau_{\mathrm{dec}} = \otimes_{0\leq a\leq M} \tau_a = \mathrm{e}^{t\delta_{\mathrm{dec}}}$. We denote by $\delta_a$ the generator of $\tau_a$ so that $\delta_{\mathrm{dec}} = \sum_a \delta_a$.

The dynamics $\tau$ of the coupled system is defined as the local perturbation of $\tau_{\rm dec}$ by the coupling $V = \sum_{1\le j\le M} V_j$, where $V_j \in \mathscr{O}_0 \otimes \mathscr{O}_j$. Its generator is $\delta = \delta_{\rm dec} + {\rm i}[V, \cdot\,]$.

For simplicity, we shall only consider the case where the fiducial state $\omega$ is $(\tau, \beta)$-KMS, so that the generator of its modular group is $\zeta = -\beta\delta$. We study small departures from this state resulting from imposed temperature gradients. Our discussion can easily be generalized to include other thermodynamic forces, such as inhomogeneous electro-chemical potentials.

To start, we assume the following.

**(H1)** There exists a unique $(\tau_0, \beta)$-KMS state $\omega$. For all sufficiently small $X = (X_1, \dots, X_M) \in \mathbb{R}^M$, there exist unique states $\omega_{j,X_j}$, for $1 \le j \le M$, such that $\omega_{j,X_j}$ is $(\tau_j, \beta - X_j)$-KMS.

We set $\omega_{{\rm dec},X} := \omega_0 \otimes \bigotimes_{1\le j\le M} \omega_{j,X_j}$.

In such a state each reservoir $\mathscr{R}_j$ is in equilibrium at inverse temperature $\beta_j = \beta - X_j$. The $X_j$'s are the thermodynamic forces which drive the system out of equilibrium, see Section 11. The conjugate fluxes are the energy currents $\Phi_j = \delta_j(V)$, see Section 12. To ensure that they are well-defined, we assume

**(H2)** $V \in {\rm Dom}(\delta_j)$ for $1 \le j \le M$.

It follows from Araki's perturbation theory, Theorem 4.4, that $\omega^{(0)}_{X=0}$ (which is the unique $(\tau_{\rm dec}, \beta)$-KMS state) and $\omega$ are mutually normal. We note, however, that since $\omega^{(0)}_{X=0} \neq \omega$, expanding $\omega^{(0)}_X \circ \tau^t(A) - \omega(A)$ around $X = 0$ generates a spurious zeroth-order term. To avoid this problem, we shall construct a family of states $\omega_X$ which, on the one hand, has the same thermodynamic properties as $\omega^{(0)}_X$, and on the other hand satisfies $\omega_{X=0} = \omega$.

By definition, the modular group of $\omega^{(0)}_X$ is generated by $-\beta\delta_{\rm dec} + \sum_{1\le j\le M} X_j\delta_j$. Denote by $\sigma_X$ the group of $*$-automorphisms generated by

$$\zeta_X = -\beta\delta_{\rm dec} + \sum_{1\le j\le M} X_j\delta_j - {\rm i}\beta[V, \cdot\,] = \zeta + \sum_{j=1}^{M} X_j\delta_j.$$

Araki's perturbation theory implies that there exists a unique $(\sigma_X, -1)$-KMS state $\omega_X$ such that $\omega^{(0)}_X$ and $\omega_X$ are mutually normal. Thus, these two states have the same thermodynamic properties, and since $\zeta_{X=0} = \zeta$, one also has $\omega_{X=0} = \omega$.

We say that $A \in \mathscr{O}$ is centered if $\omega_X(A) = 0$ for all sufficiently small $X \in \mathbb{R}^n$.

**Theorem 13.1** ([75]) *Under the Hypothesis* **(H1)** *and* **(H2)**, *the function* $X \mapsto \omega_X \circ \tau^t(A)$ *is differentiable at* $X = 0$ *for any centered observable* $A \in \mathscr{O}$, *and the finite time Green-Kubo formula*

$$\partial_{X_j}\omega_X \circ \tau^t(A)|_{X=0} = \int_0^t \langle \tau^s(A)|\Phi_j\rangle_\omega \, {\rm d}s, \tag{13.3}$$

*holds.*

***Remarks*** **1.** Formula (13.3) is limited to centered observables because, at the current level of generality, we do not have control of $\omega_X(A)$ as $X \to 0$. If $A \in \mathscr{O}$ is such that $X \mapsto \omega_X(A)$ is differentiable at $X = 0$, then the above formula still holds after addition of the static contribution $\partial_{X_k}\omega_X(A)|_{X=0}$ to its right-hand side. We note, however, that for infinite systems the states $\omega_X$ for distinct values of $X$ are usually mutually singular. The differentiability of $\omega_X(A)$ is therefore a delicate question, and is not expected to hold for general observables $A$.
**2.** One can prove that the energy fluxes $\Phi_j$, and more generally the fluxes conjugate to intensive thermodynamic parameters, are centered. We refer to [75] for more details.

### 13.2 The Long Time Problem

The hard problem of linear response theory concerns the validity of the linear response formulas derived in the previous section in the long-time limit. This issue has been widely discussed in the physics literature. The most famous objection to the validity of linear response was raised by van Kampen in [86]. His argument is based on the fact that the microscopic dynamics of a large system with many degrees of freedom is strongly chaotic. He argued that the time scale over which a perturbative calculation remains valid may be very short, and concluded that finite-time linear response may therefore be physically irrelevant on macroscopic time scales. Discussions of van Kampen's objection can be found in [90], and the interested reader may also consult [93].

A mathematical idealization reduces the long time problem to the interchange of two limits: the zero forcing limit involved in the derivation of the finite time linear response formulas and the infinite time limit. To illustrate this point, let us continue the discussion of Section 13.1.2 which led to formula (13.3), under the following assumption:

**(H3)** For all sufficiently small $X \in \mathbb{R}^M$ there exists a NESS $\omega_{X+}$, see Section 11, such that,

$$\lim_{t\to\infty} \omega_X \circ \tau^t(A) = \omega_{X+}(A) \tag{13.4}$$

for any $A \in \mathscr{O}$.

We note that under normal circumstances one expects more, namely that

$$\lim_{t\to\infty} \eta \circ \tau^t(A) = \omega_{X+}(A)$$

holds for any $A \in \mathscr{O}$ and any $\omega_X$-normal (or equivalently $\omega_X^{(0)}$-normal) state $\eta$.

We shall say that an observable $A \in \mathscr{O}$ is regular if the function $X \mapsto \omega_{X+}(A)$ is differentiable at $X = 0$ and

$$\partial_{X_k}\omega_{X+}(A)|_{X=0} = \lim_{t\to\infty} \partial_{X_k}\omega_X \circ \tau^t(A)|_{X=0}.$$

If $A$ is a regular centered observable, then Equ. (13.4) and Formula (13.3) yield the Green-Kubo formula

$$\partial_{X_j}\omega_{X+}(A)|_{X=0} = \int_0^\infty \langle \tau^s(A)|\Phi_j\rangle_\omega \, \mathrm{d}s. \tag{13.5}$$

In particular, if the fluxes $\Phi_k$ are regular, then the transport coefficients (recall Section 10), defined by

$$\omega_{X+}(\Phi_k) = \sum_{1\le j\le M} L_{jk}X_j + \mathrm{o}(X),$$

are given by the formula

$$L_{jk} = \int_0^\infty \langle \tau^s(\Phi_k)|\Phi_j\rangle_\omega \, \mathrm{d}s.$$

To justify the exchange of limits for a sufficiently large set of centered observables $A \in \mathscr{O}$, and in particular for the flux observables, is a delicate problem requiring a fairly good control on the dynamics of the system. This was recently achieved for two classes of systems: $N$-levels systems coupled to free Fermi reservoirs in [77] and locally interacting Fermi gases in [78]. In the first case the NESS was previously constructed in [81] using the Liouvillean approach, see Section 11. In the second case, the NESS is obtained following Ruelle's scattering approach. In both cases, the interchange of limits is validated via the following simple consequence of Vitali's theorem.

**Proposition 13.2** *Suppose that* **(H1)** *and* **(H3)** *hold and let $A \in \mathscr{O}$. Assume that for some $\epsilon > 0$ and any $t \ge 0$, the function $X \mapsto \omega_X \circ \tau^t(A)$ has an analytic extension to the open polydisk $D_\epsilon = \{X \in \mathbb{C}^M \mid \max_j |X_j| < \epsilon\}$. If*

$$\sup_{X\in D_\epsilon, t\ge 0} |\omega_X \circ \tau^t(A)| < \infty$$

*holds, then $A$ is regular.*

It is evident, though sometimes overlooked, that the long-time problem cannot be solved merely by proving that a finite-time linear response formula remains meaningful in the long-time limit. Suppose, for example, that the system $(\mathscr{O}, \tau)$ is $L^1$-asymptotically Abelian, namely that

$$\int_0^\infty \|[A, \tau^t(B)]\| \, \mathrm{d}t < \infty, \tag{13.6}$$

holds for a dense set of $A, B$ in $\mathscr{O}$. It follows that the linear response to the perturbation $V(t) = -\sum_j X_j(t)A_j$ such that $x = \sum_j \sup_t |X_j(t)| < \infty$,

$$(\Delta\omega)^t(A) = \lim_{s\to-\infty}(\Delta\omega)^{s\to t}(A) = \sum_j \int_0^\infty \omega(\mathrm{i}[A_j, \tau^u(A)])X_j(t-u)\,\mathrm{d}u, \tag{13.7}$$

where the integrals are absolutely convergent.[5] This, however, does not mean that (i) the natural nonequilibrium state

$$\omega_t^V(A) = \lim_{s\to-\infty} \omega \circ \tau_V^{s\to t}(A)$$

exists, and (ii) that

$$\omega_t^V(A) - \omega(A) = (\Delta\omega)^t(A) + \mathrm{o}(X).$$

In fact both (i) and (ii) require a precise control of the perturbed dynamics $\tau_V$ whereas Equ. (13.7) only involves the unperturbed $\tau$. If (i) and (ii) hold, and if $\omega$ is $(\tau, \beta)$-KMS, then, by Equ. (13.2), the infinite time Green-Kubo formula

$$(\Delta\omega)^t(A) = \sum_j \beta \int_0^\infty \langle \tau^s(A)|\Phi_j\rangle_\omega \, X_j(t-s)\,\mathrm{d}s,$$

holds.

### 13.3 Time-Reversal Invariance and Onsager Reciprocity Relations

A time-reversal of $(\mathscr{O}, \tau)$ is an involutive antilinear $*$-automorphism $\Theta$ of $\mathscr{O}$ such that $\tau^t \circ \Theta = \Theta \circ \tau^{-t}$ for any $t \in \mathbb{R}$. A state $\nu$ on $\mathscr{O}$ is time-reversal invariant if $\nu \circ \Theta(A) = \nu(A^*)$ for all $A \in \mathscr{O}$. An observable $A \in \mathscr{O}_{\mathrm{self}}$ is even/odd under time-reversal if $\Theta(A) = \pm A$.

The following proposition is a simple consequence of the KMS condition, see [75].

**Proposition 13.3** *Assume that $(\mathscr{O}, \tau)$ is equipped with a time-reversal $\Theta$. Let $\omega$ be a time-reversal invariant, mixing, $(\tau, \beta)$-KMS state. If $A, B \in \mathscr{O}_{\mathrm{self}}$ are both even or odd under time-reversal, then*

$$\int_0^t \langle \tau^s(A)|B\rangle_\omega \,\mathrm{d}s = \frac{1}{2}\int_{-t}^t \omega(A\tau^s(B))\,\mathrm{d}s + \mathrm{o}(1)$$

*in the limit $t \to \infty$.*

***Remark*** If $\omega$ is the unique $(\tau, \beta)$-KMS state, then it is automatically time-reversal invariant.

To apply this proposition to the Green-Kubo formula (13.5) we assume:

**(H4)** $(\mathscr{O}, \tau)$ is equipped with a time-reversal $\Theta$ and $\omega$ is a time-reversal invariant, mixing $(\tau, \beta)$-KMS state. Moreover, the couplings $V_j$ are even under time-reversal.

[5] We assume that (13.6) holds for $A_j$'s and $A$.

**Corollary 13.4** *Under Hypothesis* **(H1)**, **(H2)**, **(H3)** *and* **(H4)**, *the Green-Kubo formula* (13.5) *can be written as*

$$\partial_{X_j}\omega_{X+}(A)|_{X=0} = \frac{1}{2}\int_{-\infty}^{\infty}\omega(A\tau^s(\Phi_j))\,\mathrm{d}s$$

*for regular, centered observables* $A \in \mathscr{O}_{\mathrm{self}}$ *that are odd under time-reversal. In particular, if the fluxes* $\Phi_k$ *are regular, then the transport coefficients are given by*

$$L_{jk} = \frac{1}{2}\int_{-\infty}^{\infty}\omega(\Phi_k\tau^s(\Phi_j))\,\mathrm{d}s. \tag{13.8}$$

If $\omega$ is a mixing $(\tau,\beta)$-KMS state, then the stability condition

$$\lim_{T\to\infty}\int_{-T}^{T}\omega([A,\tau^t(B)])\,\mathrm{d}t = 0$$

holds for any $A, B \in \mathscr{O}$, see [33, Section 5.4.2]. An important consequence of this fact and Equ. (13.8) is

**Corollary 13.5** *Under the assumptions of Corollary 13.4 the transport coefficients satisfy the Onsager reciprocity relations*

$$L_{jk} = L_{kj}.$$

## Part IV

### Small systems coupled to reservoirs

## 14 Coupling to Reservoirs

In this article we introduce classes of models used to describe a (typically small) quantum system interacting with a large external system, often called a "reservoir" or a "heat bath".

A typical small system that we have in mind is a "quantum dot" – an atom or a molecule. We will often restrict ourselves to finitely many eigenstates of such a "quantum dot". Mathematically, it is described by a Hilbert space $\mathscr{K}$, often assumed to be finite dimensional.

We will assume that the reservoir is as simple as possible – in practice it means that it is a *free Bose or Fermi gas.*

We will refrain from presenting detailed physical examples of systems considered in our article – they are easy to provide. We will only describe their general mathematical structure.

### 14.1 Models of a Small Quantum System Coupled to a Reservoir

In the bosonic case we consider the Hilbert space $\mathscr{K}\otimes\Gamma_s(L^2(\Xi))$, where $L^2(\Xi)$ describes the 1-particle space and $\Gamma_s(L^2(\Xi))$ is the corresponding *bosonic Fock space*. $a^*(\xi)$, $a(\xi)$ will denote the *creation/annihilation operators* satisfying the usual commutation relations. They are, strictly speaking, operator-valued distrubitions, which become (unbounded) operators when smeared with appropriate test functions.

A typical Hamiltonian describing the interaction of a small system with a bosonic reservoir has the form

$$H = K\otimes\mathbb{1} + \mathbb{1}\otimes\int \omega(\xi)a^*(\xi)a(\xi)\mathrm{d}\xi + \int v(\xi)\otimes a^*(\xi)\mathrm{d}\xi + \int v(\xi)^*\otimes a(\xi)\mathrm{d}\xi. \tag{14.1}$$

Here $\omega$ is the 1-particle excitation spectrum, $K$ is the Hamiltonian of the small system, and the function $\xi \mapsto v(\xi)$ describes the coupling of the bosons with the small system.

One of the most popular choices is $\mathscr{K} = \mathbb{C}^2$, $K = \sigma_3$, $v(\xi) = \sigma_1 f(\xi)$ for some function $f$, where $\sigma_3$, $\sigma_1$ are the usual *Pauli matrices*. With this choice, $H$ is called the *spin-boson Hamiltonian*.

One often adds a perturbation to $H$ quadratic in the creation/annihilation operators. Adding higher powers may make the definition of $H$ as a selfadjoint operator problematic.

Motivated by [57], we shall call *Pauli-Fierz operators* the operators of the form (14.1); see e.g. [47], Note, however, that this terminology is not universally accepted. Other names found in the literature to denote (14.1) or similar classes of operators include the generalized spin-boson Hamiltonian, the *Nelson Hamiltonian*, the *Fröhlich Hamiltonian*, and the *polaron Hamiltonian*.

A natural example of an operator similar to $H$ (with quadratic terms in the perturbation) is the Hamiltonian of non-relativistic *QED*, which some authors also call the Pauli-Fierz Hamiltonian [131]. This usage differs slightly from the meaning above. The QED in the *dipole approximation* is also of the form (14.1) (without quadratic terms in the perturbation). In this case the bosonic reservoir describes *photons*, $\omega(\xi) = |\xi|$ and $L^2(\Xi)$ is the space of divergence-free vector fields on $\mathbb{R}^3$. Hence one can take $\Xi = \mathbb{R}\times\{1,2\}$, where $\{1,2\}$ labels two photon polarizations.

Operators of the form (14.1) are also used to describe interaction of a small system with lattice vibrations of a crystal lattice; in this case the bosonic reservoir consists of *phonons*.

If the reservoir is fermionic, then the Hilbert space of the composite system is $\mathscr{K}\otimes\Gamma_a(L^2(\Xi))$, where $\Gamma_a(L^2(\Xi))$ is the corresponding *fermionic Fock space* over the 1-particle space $L^2(\Xi)$. We denote the fermionic creation/annihilation operators by $a^*(\xi)$, $a(\xi)$ as well.

A typical Hamiltonian describing a small system interacting with a fermionic reservoir considered in the literature has the form

$$H := K\otimes\mathbb{1} + \mathbb{1}\otimes\int \omega(\xi)a^*(\xi)a(\xi)\mathrm{d}\xi$$
$$+\lambda\sum_{n,m}\int v_{n,m}(\xi_1,\dots,\xi_n,\xi'_m,\dots,\xi'_1)\otimes a^*(\xi_1)\cdots a^*(\xi_n)a(\xi'_m)\cdots$$
$$a(\xi'_1)\mathrm{d}\xi_1\cdots\mathrm{d}\xi_n\mathrm{d}\xi'_m\cdots\mathrm{d}\xi'_1.$$

In physically motivated models the interaction typically contains only terms with $n+m$ even.

A typical example of fermionic reservoir is metal containing conductance electrons.

Often one assumes that the small system is also described by a bosonic or fermionic Fock space and all the terms in the Hamiltonian are quadratic. In this case $\mathrm{e}^{\mathrm{i}tH}$ can be described in terms of the corresponding 1-particle dynamics, which greatly simplifies analysis.

## 15 Coupling to Reservoirs of a Positive Density

Consider a small quantum system interacting with a bosonic or fermionic reservoir of the form described in Section 14. Its Hilbert space is[6] $\mathscr{K}\otimes\Gamma_{\mathrm{s/a}}(L^2(\Xi))$, and its Hamiltonian in the bosonic case has the form

$$H := K\otimes\mathbb{1} + \mathbb{1}\otimes\int \omega(\xi)a^*(\xi)a(\xi)\mathrm{d}\xi + \int v(\xi)\otimes a^*(\xi)\mathrm{d}\xi + \int v(\xi)^*\otimes a(\xi)\mathrm{d}\xi. \tag{15.1}$$

In the fermionic case

$$H := K\otimes\mathbb{1} + \mathbb{1}\otimes\int \omega(\xi)a^*(\xi)a(\xi)\mathrm{d}\xi$$
$$+\sum_{n,m}\int v_{n,m}(\xi_1,\dots,\xi_n,\xi'_m,\dots,\xi'_1)\otimes a^*(\xi_1)\cdots a^*(\xi_n)a(\xi'_m) \tag{15.2}$$
$$\cdots a(\xi'_1)\mathrm{d}\xi_1\cdots\mathrm{d}\xi_n\mathrm{d}\xi'_m\cdots\mathrm{d}\xi'_1,$$

where in physically motivated models the interaction contains only terms with $n+m$ even.

If the function $\omega(\xi)$ is positive, we say that the reservoir is at zero temperature (or at zero density). We will explain how to modify the Hamiltonians (15.1) and (15.2) when the reservoir is at a positive temperature, or, more generally, at a positive density.

We shall adopt the $W^*$-algebraic framework here (although, at least in the fermionic case, one could also use the $C^*$-algebraic framework).

[6] The subscript s/a refers to the bosonic/fermionic Fock space.

### 15.1 The Semi-Standard Representation

We will use the formalism of Araki-Woods representations of the CCR and Araki-Wyss representations of the CAR described in more detail in Section 6. Fixing a nonnegative function $\xi \mapsto \gamma(\xi)$, let us define

$$\rho(\xi) := (\gamma(\xi)^{-1} \mp 1)^{-1},$$

where the minus sign corresponds to the bosonic case and the plus sign to the fermionic case. We consider the bosonic/fermionic Fock space $\Gamma_{\mathrm{s/a}}\left(L^2(\Xi) \oplus L^2(\Xi)\right)$. Consider the "left creation/annihilation operators corresponding to $\gamma$", $a^*_{\gamma,\mathrm{l}}(\xi)$, $a_{\gamma,\mathrm{l}}(\xi)$.

The algebra of observables of the coupled system is defined as the $W^*$-algebra $\mathfrak{M}_\gamma \subset \mathscr{B}(\mathscr{K} \otimes \Gamma_{\mathrm{s/a}}(L^2(\Xi) \oplus L^2(\Xi))$ generated by the operators of the small system $\mathscr{B}(\mathscr{K}) \otimes 1$ and by the reservoir creation/annihilation operators $a^*_{\gamma,\mathrm{l}}(\xi)$, $a_{\gamma,\mathrm{l}}(\xi)$. On $\mathscr{K} \otimes \Gamma_{\mathrm{s}}(L^2(\Xi) \oplus L^2(\Xi))$ we define the operator

$$\begin{aligned} L^{\mathrm{semi}}_\gamma := K \otimes \mathbb{1} + \mathbb{1} \otimes \int \omega(\xi) \left(a^*_{\mathrm{l}}(\xi) a_{\mathrm{l}}(\xi) - a^*_{\mathrm{r}}(\xi) a_{\mathrm{r}}(\xi)\right) \mathrm{d}\xi \\ + \int \left(v(\xi) \otimes a^*_{\gamma,\mathrm{l}}(\xi) + v(\xi)^* \otimes a_{\gamma,\mathrm{l}}(\xi)\right) \mathrm{d}\xi, \end{aligned} \tag{15.3}$$

which is the analog of (15.1) for general $\gamma$. On $\mathscr{K} \otimes \Gamma_{\mathrm{a}}(L^2(\Xi) \oplus L^2(\Xi))$ we define

$$\begin{aligned} L^{\mathrm{semi}}_\gamma := K \otimes \mathbb{1} + \mathbb{1} \otimes \int \omega(\xi) \left(a^*_{\mathrm{l}}(\xi) a_{\mathrm{l}}(\xi) - a^*_{\mathrm{r}}(\xi) a_{\mathrm{r}}(\xi)\right) \mathrm{d}\xi \\ + \sum_{n,m} \int v_{n,m}(\xi_1, \ldots, \xi_n, \xi_1, \ldots, \xi'_m) \otimes a^*_{\gamma,\mathrm{l}}(\xi_1) \cdots a^*_{\gamma,\mathrm{l}}(\xi_n) a_{\gamma,\mathrm{l}}(\xi'_m) \\ \cdots a_{\gamma,\mathrm{l}}(\xi'_1) \mathrm{d}\xi_1 \cdots \mathrm{d}\xi_n \mathrm{d}\xi'_m \cdots \mathrm{d}\xi'_1, \end{aligned} \tag{15.4}$$

which is the analog of (15.2) for general $\gamma$. $L^{\mathrm{semi}}_\gamma$ is sometimes called the semi-Liouvillean. Let

$$\tau_{\gamma,t}(A) := \mathrm{e}^{\mathrm{i}tL^{\mathrm{semi}}_\gamma} A \mathrm{e}^{-\mathrm{i}tL^{\mathrm{semi}}_\gamma}.$$

It is easy to show that $\tau_{\gamma,t}$ preserves the algebra $\mathfrak{M}_\gamma$, and we obtain a $W^*$-dynamical system $(\mathfrak{M}_\gamma, \tau_\gamma)$.

The special case $\gamma = 0$ corresponds to the zero temperature state of the reservoir. In this case, the $W^*$-dynamical system $(\mathfrak{M}_\gamma, \tau_\gamma)$ is equivalent to the system

$$\left(\mathscr{B}(\mathscr{K} \otimes \Gamma_{\mathrm{s/a}}(L^2(\Xi))), \mathrm{e}^{\mathrm{i}tH}(\,\cdot\,)\mathrm{e}^{-\mathrm{i}tH}\right).$$

If $\gamma(\xi) = \mathrm{e}^{-\beta\omega(\xi)}$, then we say that the reservoir is thermal. In this case, the state $\psi$ on the algebra $\mathfrak{M}_\gamma$ defined by

$$\psi(A\otimes B) = \frac{\mathrm{tr}\left(A\mathrm{e}^{-\beta K}\right)}{\mathrm{tr}\left(\mathrm{e}^{-\beta K}\right)}(\Omega|B\Omega), \qquad A \in \mathscr{B}(\mathscr{K}), \quad B \in \mathscr{B}(\Gamma_{\mathrm{s/a}}(L^2(\Xi)\oplus L^2(\Xi))),$$

is $\beta$-*KMS* for the dynamics $\tau$ with no interaction term.

### 15.2 The Standard Representation

Recall from Section 2 that every $W^*$ algebra has a distinguished representation called the *standard representation*. In such a representation every $W^*$-dynamics has a distinguished unitary implementation generated by a selfadjoint operator called the *Liouvillean*.

The standard representation of $\mathfrak{M}$ acts as

$$\pi : \mathfrak{M}_\gamma \to \mathscr{B}\left(\mathscr{K}\otimes\bar{\mathscr{K}}\otimes\Gamma_{\mathrm{s/a}}(L^2(\Xi)\oplus L^2(\Xi))\right),$$

where an element of $\mathfrak{M}_\gamma$ is tensor multiplied by the identity on $\bar{\mathscr{K}}$ (the complex conjugate of $\mathscr{K}$). The Liouvillean corresponding to (15.3) is the selfadjoint operator on $\mathscr{K}\otimes\bar{\mathscr{K}}\otimes\Gamma_{\mathrm{s}}(L^2(\Xi)\oplus L^2(\Xi))$ defined by

$$\begin{aligned} L_\gamma :=& K\otimes\mathbb{1}\otimes\mathbb{1} - \mathbb{1}\otimes\overline{K}\otimes\mathbb{1} + \mathbb{1}\otimes\mathbb{1}\otimes\int\omega(\xi)\left(a_{\mathrm{l}}^*(\xi)a_{\mathrm{l}}(\xi) - a_{\mathrm{r}}^*(\xi)a_{\mathrm{r}}(\xi)\right)\mathrm{d}\xi \\ &+ \int\left(v(\xi)\otimes\mathbb{1}\otimes a_{\gamma,\mathrm{l}}^*(\xi) + v(\xi)^*\otimes\mathbb{1}\otimes a_{\gamma,\mathrm{r}}(\xi)\right)\mathrm{d}\xi \\ &- \int\left(\mathbb{1}\otimes\bar{v}(\xi)\otimes a_{\gamma,\mathrm{l}}^*(\xi) + \mathbb{1}\otimes\bar{v}(\xi)^*\otimes a_{\gamma,\mathrm{r}}(\xi)\right)\mathrm{d}\xi. \end{aligned} \tag{15.5}$$

The Liouvillean corresponding to (15.4) is the selfadjoint operator on $\mathscr{K}\otimes\overline{\mathscr{K}}\otimes\Gamma_{\mathrm{a}}(L^2(\Xi)\oplus L^2(\Xi))$ defined by

$$\begin{aligned} L_\gamma :=& K\otimes\mathbb{1}\otimes\mathbb{1} - \mathbb{1}\otimes\overline{K}\otimes\mathbb{1} + \mathbb{1}\otimes\mathbb{1}\otimes\int\omega(\xi)\left(a_{\mathrm{l}}^*(\xi)a_{\mathrm{l}}(\xi) - a_{\mathrm{r}}^*(\xi)a_{\mathrm{r}}(\xi)\right)\mathrm{d}\xi \\ &+ \sum_{n,m}\int v_{n,m}(\xi_1,\dots,\xi_n,\xi_1,\dots,\xi'_m)\otimes\mathbb{1}\otimes a_{\gamma,\mathrm{l}}^*(\xi_1)\cdots a_{\gamma,\mathrm{l}}^*(\xi_n)a_{\gamma,\mathrm{l}}(\xi'_m) \\ &\cdots a_{\gamma,\mathrm{l}}(\xi'_1)\mathrm{d}\xi_1\cdots\mathrm{d}\xi_n\mathrm{d}\xi'_m\cdots\mathrm{d}\xi'_1 \\ &- \sum_{n,m}\int\mathbb{1}\otimes\bar{v}_{n,m}(\xi_1,\dots,\xi_n,\xi_1,\dots,\xi'_m)\otimes a_{\gamma,\mathrm{r}}^*(\xi_1)\cdots a_{\gamma,\mathrm{r}}^*(\xi_n)a_{\gamma,\mathrm{r}}(\xi'_m) \\ &\cdots a_{\gamma,\mathrm{r}}(\xi'_1)\mathrm{d}\xi_1\cdots\mathrm{d}\xi_n\mathrm{d}\xi'_m\cdots\mathrm{d}\xi'_1. \end{aligned} \tag{15.6}$$

Above we used the "right creation/annihilation operators corresponding to $\gamma$", denoted by $a_{\gamma,\mathrm{r}}^*(\xi)$, $a_{\gamma,\mathrm{r}}(\xi)$ and described in Section 6.

Note that the Liouvillean $L_\gamma$ and the semi-Liouvillean $L_\gamma^{\rm semi}$ describe the same dynamics, but in different representations. This is expressed by

$$\pi\left(\mathrm{e}^{\mathrm{i}tL_\gamma^{\rm semi}}A\mathrm{e}^{-\mathrm{i}tL_\gamma^{\rm semi}}\right)=\mathrm{e}^{\mathrm{i}tL_\gamma}\pi(A)\mathrm{e}^{-\mathrm{i}tL_\gamma},\qquad A\in\mathfrak{M}_\gamma.$$

Note also that the operators (15.3), (15.5), as well as (15.4), (15.6), are special cases of operators of the form (15.1) and (15.2), where we allow the 1-particle excitation spectrum to have negative values.

### 15.3 Composite Reservoirs

Sometimes one considers two (or more) reservoirs, $\mathscr{R}_1$ and $\mathscr{R}_2$, interacting with a single small system. This can be taken into account by assuming that $\Xi$ is the union of two disjoint sets $\Xi_1$ and $\Xi_2$ describing the 1-particle spaces of $\mathscr{R}_1$ and $\mathscr{R}_2$. Then the composite reservoir is the tensor product of the reservoir $\mathscr{R}_1$ and the reservoir $\mathscr{R}_2$, since, using the *exponential property of Fock spaces*, we have the natural identification

$$\Gamma_{\rm s/a}(L^2(\Xi_1\cup\Xi_2))\simeq\Gamma_{\rm s/a}(L^2(\Xi_1)\oplus L^2(\Xi_2))\simeq\Gamma_{\rm s/a}(L^2(\Xi_1))\otimes\Gamma_{\rm s/a}(L^2(\Xi_2)).$$

Physically, an especially important case arises when the reservoirs $\mathscr{R}_1$ and $\mathscr{R}_2$ are thermal but correspond to two distinct inverse temperatures.

## 16 Completely Positive Markov Semigroups

Let $\mathscr{B}(\mathscr{K})$ denote the algebra of bounded operators on a Hilbert space $\mathscr{K}$, which we interpret as the algebra of observables of the small quantum system. We say that a transformation $\Lambda$ on $\mathscr{B}(\mathscr{K})$ is positive if the image of a positive operator is positive. We say that $\Lambda$ is *completely positive* if its extension to $n\times n$ matrices with entries in $\mathscr{B}(\mathscr{K})$ is positive for any $n$. We say it is Markov if it preserves the identity operator.

One can also consider the transformation $\Lambda_\#$ acting on $\mathscr{B}^1(\mathscr{K})$ – the trace class operators on $\mathscr{K}$ – defined by

$$\mathrm{tr}\,(\rho\Lambda(A))=\mathrm{tr}\,(\Lambda_\#(\rho)A)\,,\quad A\in\mathscr{B}(\mathscr{K}),\quad \rho\in\mathscr{B}^1(\mathscr{K}),$$

so that $\Lambda$ is the adjoint of $\Lambda_\#$. Clearly, $\Lambda$ is Markov iff $\Lambda_\#$ preserves the trace (in this case $\Lambda_\#$ preserves the set of *density matrices*).

Both $\Lambda$ and $\Lambda_\#$ can be used to describe dynamics of a quantum system. One says that $\Lambda$ describes it in the *Heisenberg picture* and $\Lambda_\#$ in the *Schrödinger picture*.

Let $t\mapsto\mathrm{e}^{tM}$ be a completely positive Markov semigroup on $\mathscr{B}(\mathscr{K})$. It is well-known that $M$ can be written in the so-called *Lindblad form*:

$$M(A)=\mathrm{i}[\Upsilon,A]-\frac{1}{2}\sum_{i=1}^n[W_i^*W_i,A]_+ +\sum_{i=1}^n W_i^*AW_i,\tag{16.1}$$

where $\Upsilon$ is a selfadjoint operator and $W_i$, $i = 1, \dots, n$ is a family of operators, see, e.g., [3]. We also have the corresponding semigroup in the Schrödinger picture $\mathrm{e}^{tM_\#}$. Its generator has the form

$$M_\#(\rho) = -\mathrm{i}[\Upsilon, \rho] - \frac{1}{2}\sum_{i=1}^{n}[W_i^* W_i, \rho]_+ + \sum_{i=1}^{n} W_i \rho W_i^*.$$

Completely positive Markov semigroups are often used in physics as approximate dynamics of a system weakly interacting with environment; Section 16.2.

### 16.1 Detailed Balance Condition

We say that a density matrix $\rho$ is invariant under $\mathrm{e}^{tM}$ iff $\mathrm{e}^{tM_\#}\rho = \rho$ for any $t > 0$, or equivalently, $M_\#(\rho) = 0$. It is easy to see that for a finite dimensional $\mathscr{K}$ such an invariant density matrix always exists.

In the literature there exist a number of definitions of the Detailed Balance Condition for quantum systems that slightly differ from one another. One of them goes as follows. Let $\rho$ be a nondegenerate density matrix. Introduce the following inner product on the operators on $\mathscr{K}$:

$$(A|B)_\rho := \mathrm{tr}\left(\rho^{\frac{1}{2}} A^* \rho^{\frac{1}{2}} B\right). \tag{16.2}$$

Let $\mathrm{e}^{tM}$ be a completely positive Markov semigroup. We will say that $M$ satisfies the *Detailed Balance Condition* for $\rho$ iff $\rho$ is invariant under $\mathrm{e}^{tM}$ and there exists a selfadjoint operator $\Upsilon$ such that $M - \mathrm{i}[\Upsilon, \cdot\,]$ is selfadjoint for the inner product (16.2).

In another version of the Detailed Balance Condition one uses the inner product

$$\mathrm{tr}(\rho A^* B) \tag{16.3}$$

instead of (16.2), see [42, 130] and references therein.

### 16.2 Weak Coupling Limit for the Reduced Dynamics

Consider a quantum Hamiltonian

$$H_\lambda := K \otimes \mathbb{1} + \mathbb{1} \otimes \int \omega(\xi) a^*(\xi) a(\xi) \mathrm{d}\xi + \lambda \int v(\xi) \otimes a^*(\xi) \mathrm{d}\xi + \lambda \int v(\xi)^* \otimes a(\xi) \mathrm{d}\xi \tag{16.4}$$

on a Hilbert space $\mathscr{K} \otimes \Gamma_{\mathrm{s}}(L^2(\Xi))$. One could consider also fermionic reservoirs, see Section 14 for a discussion of the notation and motivation.

Suppose that we are interested in the measurements performed only at the small system. Such measurements are described by $A \otimes \mathbb{1}$, where $A \in \mathscr{B}(\mathscr{K})$.

Let $\Omega$ denote the vacuum vector. We assume that the initial state of the reservoir is given by the state $(\Omega \mid \cdot\, \Omega)$, and the state of the small system is given by a density matrix $\rho \in \mathscr{B}^1(\mathscr{K})$. Then the expectation value of the measurement of the observable

$A\otimes\mathbb{1}$ at time $t$ is equal to

$$\mathrm{tr}\big(\rho\otimes|\Omega)(\Omega|\big)\big(\mathrm{e}^{\mathrm{i}tH_\lambda}(A\otimes\mathbb{1})\mathrm{e}^{-\mathrm{i}tH_\lambda}\big).$$

These expectation values can be encoded in the following family of completely positive Markov maps:

$$\mathscr{B}(\mathscr{K})\ni A\mapsto I_{\mathscr{K}}^*\mathrm{e}^{\mathrm{i}tH_\lambda}(A\otimes\mathbb{1})\mathrm{e}^{-\mathrm{i}tH_\lambda}I_{\mathscr{K}}\in\mathscr{B}(\mathscr{K}),$$

where $I_{\mathscr{K}}$ denotes the isometric embedding of $\mathscr{K}$ into $\mathscr{K}\otimes\Omega$. The following remarkable fact can be proven.

**Theorem 16.1** *Assume some relatively mild conditions on the interaction. Then there exists a completely positive Markov semigroup* $\mathrm{e}^{tM}$ *on* $\mathscr{B}(\mathscr{K})$ *such that*

$$\mathrm{e}^{tM}(A)=\lim_{\lambda\to0}\mathrm{e}^{-\mathrm{i}\frac{t}{\lambda^2}K}I_{\mathscr{K}}^*\mathrm{e}^{\mathrm{i}\frac{t}{\lambda^2}H_\lambda}(A\otimes1)\mathrm{e}^{-\mathrm{i}\frac{t}{\lambda^2}H_\lambda}I_{\mathscr{K}}\mathrm{e}^{\mathrm{i}\frac{t}{\lambda^2}K}. \tag{16.5}$$

*The semigroup* $\mathrm{e}^{tM}$ *commutes with the free dynamics of the small system* $\mathrm{e}^{\mathrm{i}tK}\cdot\mathrm{e}^{-\mathrm{i}tK}$. *If the reservoir is at the inverse temperature* $\beta$ *(see Section 15), then* $M$ *satisfies the Detailed Balance Condition for* $\mathrm{e}^{-\beta K}/\mathrm{tr}\,\mathrm{e}^{-\beta K}$ *(the Gibbs state of the small system), both in the sense of* (16.2) *and* (16.3).

The above theorem is due to E. B. Davies. It indicates that for small $\lambda$ one can approximate the dynamics reduced to the small system with a completely positive Markov semigroup.

The limit considered in (16.5) goes under the name of the *weak coupling limit* or *van Hove limit*. The latter name is unfortunately ambiguous – it is used in statistical physics with a different meaning.

See [130] for use of Davies generator in context of non-equilibrium open quantum systems.

### 16.3 Quantum Langevin Dynamics

Suppose that $\mathrm{e}^{tM}$ is a completely positive Markov semigroup on $\mathscr{B}(\mathscr{K})$ with the generator $M$ written in the Lindblad form (16.1). Introduce the Hilbert space $\mathscr{Z}=\mathscr{K}\otimes\Gamma_{\mathrm{s}}(\mathbb{C}^n\otimes L^2(\mathbb{R}))$ and the operator

$$Z:=\Upsilon\otimes\mathbb{1}+\sum_{j=1}^n\mathbb{1}\otimes\int\xi a_j^*(\xi)a_j(\xi)\mathrm{d}\xi+\sum_{j=1}^n\int\Big(W_j\otimes a_j^*(\xi)+W_j^*\otimes a_j(\xi)\Big)\,\mathrm{d}\xi. \tag{16.6}$$

Strictly speaking, (16.6) is only a formal expression whose precise meaning as a selfadjoint operator on $\mathscr{Z}$ can be given using an appropriate regularization and a limiting procedure. Then one can show that

$$I_{\mathscr{K}}^*\mathrm{e}^{\mathrm{i}tZ}(A\otimes1)\mathrm{e}^{-\mathrm{i}tZ}I_{\mathscr{K}}=\mathrm{e}^{tM}(A), \tag{16.7}$$

$$I_{\mathscr{K}}^{*}\mathrm{e}^{\mathrm{i}tZ}I_{\mathscr{K}} = \mathrm{e}^{\mathrm{i}t\Gamma}, \tag{16.8}$$

where $\Gamma = \Upsilon + \frac{\mathrm{i}}{2}\sum_{j=1}^{n} W_j^* W_j$ and where $I_{\mathscr{K}}$ denotes the isometric embedding of $\mathscr{K}$ onto $\mathscr{K} \otimes \Omega \subset \mathscr{Z}$.

Relation (16.8) means that $\mathrm{e}^{\mathrm{i}tZ}$ is a *unitary dilation* of the semigroup $\mathrm{e}^{\mathrm{i}t\Gamma}$. More interestingly, (16.7) means that the Heisenberg dynamics given by $\mathrm{e}^{\mathrm{i}tZ}$ reduced to the small system coincides with $\mathrm{e}^{tM}$.

The unitary dynamics generated by $Z$ is called a *quantum Langevin dynamics* or quantum stochastic dynamics for the semigroup $\mathrm{e}^{tM}$. Its construction was first given by Hudson and Parthasarathy. They used a quantum version of the so-called *stochastic calculus*; see [53] and references therein.

There exist versions of the weak coupling limit not just for the reduced dynamics, but also for the dynamics of the full system. They say that in an appropriate version of the weak coupling limit, but without reducing the dynamics to the small system, the dynamics generated by a Hamiltonian of the form (16.4) converges to a quantum Langevin dynamics. First results of this type, under the name of the stochastic limit, are due to Accardi, Frigerio and Lu; there exists also a somewhat different approach under the name of extended weak coupling limit; see [40] and references therein.

## 17 Scattering Theory for a Small System Interacting with Quantum Fields

The aim of scattering theory is to describe a complicated dynamics by a simpler one. In its most basic form, applicable for example to one- and two-body Schrödinger Hamiltonians, one starts from a pair of dynamics: the "full" one $\mathrm{e}^{-\mathrm{i}tH}$ and the "free" one $\mathrm{e}^{-\mathrm{i}tH_0}$. One then defines *wave operators* and *scattering operators*. See [119, 142].

Scattering theory for small quantum systems interacting with quantum fields uses a different formalism. One starts from a "full" dynamics $\mathrm{e}^{-\mathrm{i}tH}$ and then seeks to describe its asymptotic behavior in terms of a simpler dynamics, which must be constructed.

A typical example of a Hamiltonian for which one can try to develop scattering theory is

$$H := K\otimes 1 + 1 \otimes \int \omega(\xi)a^*(\xi)a(\xi)\mathrm{d}\xi + \int v(\xi)\otimes a^*(\xi)\mathrm{d}\xi + \int v(\xi)^*\otimes a(\xi)\mathrm{d}\xi \tag{17.1}$$

on $\mathscr{B}(\mathscr{K})\otimes\Gamma_{\mathrm{s}}(L^2(\mathbb{R}^d))$. (One could consider also similar fermionic systems). We stress that the free dynamics is not given a priori given. In particular, the dynamics generated by the first two terms of the right hand side of (17.1) should not be viewed as the free dynamics in the sense of scattering theory. Therefore one needs a different formalism.

Let us describe a version of scattering theory for the Hamiltonian $H$ given by (17.1), which is adapted to the case when the small system is well localized in space (confined). In our presentation we follow mostly [43]. Note that this formalism of scattering theory is quite different from that used in the case of e.g. Schrödinger operators – it is much closer to the *LSZ formalism* or the *Haag-Ruelle theory* used in quantum field theory.

We first construct the so-called *incoming/outgoing* creation/annihilation operators. In the fermionic case they are given as

$$\int f(\xi)a^{\pm *}(\xi)\mathrm{d}\xi := \mathrm{s}-\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH}\int \mathrm{e}^{-\mathrm{i}t\omega(\xi)}f(\xi)a^{*}(\xi)\mathrm{d}\xi\ \mathrm{e}^{-\mathrm{i}tH}, \tag{17.2}$$

$$\int \bar{f}(\xi)a^{\pm}(\xi)\mathrm{d}\xi := \mathrm{s}-\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH}\int \mathrm{e}^{\mathrm{i}t\omega(\xi)}\bar{f}(\xi)a(\xi)\mathrm{d}\xi\ \mathrm{e}^{-\mathrm{i}tH}, \tag{17.3}$$

where $\mathrm{s}-\lim$ denotes the *strong limit*. In the bosonic case the definition is similar except that we need to take bounded functions of (17.2) and (17.3).

The incoming/outgoing creation/annihilation operators exist under quite weak assumptions and their existence can be usually proven by a version of the *Cook method*. They satisfy the usual commutation/anticommutation relations.

To proceed further one introduces the space of asymptotic Fock vacua $\mathscr{K}^{\pm}$, consisting of vectors annihilated by the asymptotic annihilation operators $a^{\pm}(\xi)$. One can show that bound states of $H$ belong to both $\mathscr{K}^{\pm}$. Then one introduces *wave operators* $W^{\pm}$ – isometric operators from the asymptotic space $\mathscr{K}^{\pm}\otimes\Gamma_{\mathrm{s/a}}(L^2(\Xi))$ into the physical space $\mathscr{K}\otimes\Gamma_{\mathrm{s/a}}(L^2(\Xi))$, defined by the relations

$$W^{\pm}a(\xi) = a^{\pm}(\xi)W^{\pm},\ \ W^{\pm}a^{*}(\xi) = a^{\pm *}(\xi)W^{\pm},\ \ W^{\pm}\Psi\otimes\Omega = \Psi,\ \ \Psi\in\mathscr{K}^{\pm}.$$

($\Omega$, as usual, denotes the vacuum vector). Finally, one introduces the *scattering operator* $S = W^{+*}W^{-}$, which can be used to compute scattering cross-sections.

Here is an example of a rigorous result about scattering theory in the above formalism, see [43] and references therein:

**Theorem 17.1** *Assume that the 1-particle excitation spectrum is positive and has a mass gap, e.g.* $\omega(\xi) = \sqrt{m^2+\xi^2}$, $m > 0$ *(and some additional minor technical assumptions). Then*

1. *the wave operators* $W^{\pm}$ *are unitary;*
2. *the spaces of asymptotic vacua* $\mathscr{K}^{\pm}$ *coincide with the space spanned by eigenvectors of* $H$.

If the above formalism is applicable and Theorem 17.1 holds, then we have a clear physical picture of the dynamics $\mathrm{e}^{\mathrm{i}tH}$ for large times: all vectors can be understood as linear combinations of bound states of $H$ accompanied by "asymptotic bosons" whose 1-particle excitation spectrum coincides with that of "free bosons". Note that Theorem 17.1 can be viewed as the analog of *asymptotic completeness* from scattering theory of $N$-particle Schrödinger operators.

Scattering in the absence of the energy gap in the excitation spectrum remains poorly understood. Even less understood is scattering theory for Hamiltonians similar to (17.1) with a translation symmetry [54].

## 18 Spectral Analysis of Small Quantum Systems Interacting with a Reservoir

In Quantum Optics one often uses various approximate Hamiltonians to describe interaction of photons with nonrelativistic matter. Here is an example:

$$H := (p - \alpha^{3/2} A(\alpha x))^2 - \frac{z}{4\pi |x|} + \sum_{\epsilon} \int |\xi| a_\epsilon^*(\xi) a_\epsilon(\xi) \mathrm{d}\xi \tag{18.1}$$

$H$ acts on $L^2(\mathbb{R}^3) \otimes \Gamma_{\mathrm{s}}(L^2(\mathbb{R}^3 \times \{1, 2\})$. It describes a single electron in the potential of a nucleus interacting with photons through the minimal coupling. Note that $p$ is the momentum operator, $\epsilon$ describes two polarizations of the photon, $\alpha$ is the fine structure constant, $z$ is the charge of the "nucleus", and $A$ is the quantized electromagnetic potential defined with the help of appropriately cut-off photonic creation and annihilation operators $a_\epsilon^*(\xi)$, $a_\epsilon(\xi)$.

Various Hamiltonians similar to (18.1) are used in the literature. For instance, one can argue that the term quadratic in electromagnetic potentials can be eliminated with the help of the so-called Pauli-Fierz transformation [47]. This leads to the following class of Hamiltonians, which we will consider in this section:

$$H := K \otimes \mathbb{1} + \mathbb{1} \otimes \int \omega(\xi) a^*(\xi) a(\xi) \mathrm{d}\xi + \lambda \int v(\xi) \otimes a^*(\xi) \mathrm{d}\xi + \lambda \int v(\xi)^* \otimes a(\xi) \mathrm{d}\xi \tag{18.2}$$

$H$ acts on $\mathscr{B}(\mathscr{K}) \otimes \Gamma_{\mathrm{s}}(L^2(\mathbb{R}^d))$, where we will assume that $\mathscr{K}$ is finite-dimensional. $\Gamma_{\mathrm{s}}(L^2(\mathbb{R}^d))$ denotes the bosonic Fock space over $L^2(\mathbb{R}^d)$. Hamiltonians of this form go under various names: generalized spin-boson Hamiltonians, Pauli-Fierz Hamiltonians, etc.

One can also consider small systems interacting with fermionic reservoirs, see Section 14. Similar mathematical methods work for them.

### 18.1 Absolute Continuity of Spectrum

It is easy to analyze the spectrum of the operators (18.2) for $\lambda = 0$. In typical situations the spectrum is absolutely continuous apart from some point spectrum coming from the eigenvalues of $K$. The non-trivial case $\lambda \neq 0$ is much more difficult to study.

There are a number of results saying that for nonzero $\lambda$ most of the spectrum of $H$ is absolutely continuous as well. Two basic methods are used to prove this: the *analytic deformation method* and the *method of positive commutators*, often also called the *Mourre method*. Both methods were originally discovered in the context of *N-body Schrödinger operators*, but they can be adapted to the operators considered in this article. Note that both methods not only prove the absolute continuity of the spectrum but also yield important information on the resolvent. The former method implies that the resolvent can be analytically continued across the spectrum. The latter method yields the existence of boundary values of the resolvent at the spectrum, as a quadratic

form between appropriate weighted spaces. (The last statement goes under the name of *Limiting Absorption Principle*).

In both methods an important ingredient is the choice of the so-called *conjugate operator*. In the literature, there are two main choices for the conjugate operator. The first choice, introduced in [84], involves the *second quantization* of the *generator of translation* in the spectral variable. It is used mostly when the spectrum covers the whole real line and we can "glue" the negative and positive frequencies (the so-called *Jakšić–Pillet gluing*), see also [47]. The second choice is the second quantization of the *generator of dilations*, used e.g. in [29, 30].

### 18.2 Point Spectrum and the Fermi Golden Rule

There exist also results about the point spectrum of perturbed operators.

Consider the operator (18.2). Let us assume that $k$ is an eigenvalue of $K$, and hence an eigenvalue of $H$ for $\lambda = 0$. We attempt to compute the shift of this eigenvalue using the perturbation theory. For simplicity we assume that $k$ is a non-degenerate eigenvalue of $K$. The term linear in $\lambda$ vanishes. The second-order contribution to the eigenvalue shift is

$$\int |v(\xi)|^2 (k + \mathrm{i}0 - \omega(\xi))^{-1} \mathrm{d}\xi. \tag{18.3}$$

The imaginary part of (18.3) equals $-\mathrm{i}\pi |v(k)|^2$. If this quantity is non-zero, then it clearly it cannot arise in the perturbation expansion of an eigenvalue of a selfadjoint operator.

The formula (18.3) is an instance of the so-called *Fermi Golden Rule*. It can be readily generalized to the case where $k$ is a degenerate eigenvalue. In that situation, the scalar expression (18.3) is replaced by the so-called *level shift operator*. Heuristically, it is easy to see that, for small but nonzero $\lambda$, the number of eigenvalues of the perturbed operator in a neighborhood of a given unperturbed eigenvalue should be less than the dimension of the kernel of the level shift operator.

In many situations this heuristic picture can be made rigorous. More precisely, one can often show that there exists $\lambda_0 > 0$ such that, for $0 < |\lambda| < \lambda_0$, the above expectations are indeed fulfilled.

When the interaction is sufficiently analytic, one can study *resonances*, that is, eigenvalues of suitably analytically deformed operators. At positive temperatures, resonances can be introduced using the Jakšić–Pillet gluing construction together with analyticity with respect to translations [84]. At arbitrary temperature, one may attempt to define resonances using dilation analyticity. With this approach, resonances are not isolated eigenvalues of the deformed operator; rather, they are located at the tips of cuspidal regions of its spectrum. Such resonances have been analyzed using an iterative method based on the *renormalization group* in [29, 30].

Especially satisfactory results are available in the case of the *ground state*. Under quite general conditions, and for arbitrary values of the coupling constant, one can show that the Hamiltonian (18.2) or (18.1) has an eigenvalue at the bottom of its spectrum [62, 63].

### 18.3 Return to Equilibrium

Assume that the 1-particle excitation spectrum of the bosonic reservoir is given by $\omega(\xi) = |\xi|$, and fix a non-negative function $\gamma$. Consider the $W^*$-dynamical system $(\mathfrak{M}_\gamma, \tau_\gamma)$ introduced in Section 15. We would like to analyze its normal stationary states.

The stationary states of the decoupled system (the case $\lambda = 0$) are easy to analyze: they are all described by density matrices of the small system that commute with $K$, tensored with the vacuum state of the reservoir. We expect that, upon switching on the perturbation, most of these states disappear, since they correspond to embedded eigenvalues of the generator of the dynamics. Only the KMS state is stable.

This expectation can be turned into two rigorous theorems, that we describe below. We start with a theorem describing the thermal case:

**Theorem 18.1** *Assume that the reservoir is thermal at inverse temperature $\beta$. Suppose that the interaction is sufficiently regular and effective (effective means that it couples the reservoir to the small system sufficiently well). Then there exists $\lambda_0 > 0$ such that for $0 < |\lambda| \leq \lambda_0$ the system $(\mathfrak{M}_\gamma, \tau_\gamma)$ has a unique normal stationary state $\psi$. This state is $\beta$-KMS for $\tau_\gamma$. It satisfies the property of* return to equilibrium*: for any normal state $\phi$ and $A \in \mathfrak{M}_\gamma$*

$$\lim_{|t|\to\infty} \phi\left(\tau_{\gamma,t}(A)\right) = \psi(A).$$

In the nonthermal case, by analogous methods one can prove

**Theorem 18.2** *Assume that the reservoir consists of two parts, which are thermal at distinct temperatures. Suppose that the interaction is sufficiently regular and effective. Then there exists $\lambda_0 > 0$ such that for $0 < |\lambda| \leq \lambda_0$ the system $(\mathfrak{M}_\gamma, \tau_\gamma)$ has no normal stationary states.*

In order to prove these theorems it is convenient to use the so-called Liouvillean, which is a certain naturally defined selfadjoint operator implementing the dynamics $\tau_\gamma$ in the so-called *standard representation* of the $W^*$-algebra $\mathfrak{M}_\gamma$, see Section 2.

Note that for $\lambda = 0$, the Liouvillean has a degenerate eigenvalue at 0 and it has non-zero eigenvalues corresponding to differences of the eigenvalues of $K$ – the so-called *Bohr frequencies* of the small system. To prove Theorem 18.1 one needs to show that for small nonzero $\lambda$ the spectral properties of the Liouvillean change: it has a one-dimensional kernel and its spectrum away from zero is absolutely continuous.

This is achieved in two steps. The theory of KMS states, mentioned in Section 2, shows that the dimension of the kernel of the Liouvillean is at least one. Then one studies spectral properties of the Liouvillean, as sketched in Sections 18.1 and 18.2. In particular, an argument based on the Fermi Golden Rule shows that the remaining eigenvectors of the Liouvillean do not survive when we switch on the perturbation, and the dimension of the kernel of the Liouvillean is at most 1. There are several methods of a proof of this theorem that work under various assumptions – the original one goes back to [84]. See also [29, 47].

## Part V

**Equilibrium quantum statistical mechanics** Starting with the seminal work [69], the mathematical theory of equilibrium quantum statistical mechanics based on the KMS-condition has developed rapidly in the 1970s, resulting in a structure of rare unity and beauty. The summary of these developments can be found in the two volumes [33, 34]; see also the monographs [67, 71, 129, 137] and references therein. In parallel to the classical equilibrium theory of lattice spin systems based on the DLR equation, developed roughly at the same time, lattice quantum spin systems are the main paradigm of the quantum theory based on the KMS-condition[7].

## 19 General Setting

We start with the setting of a quantum system with finite-dimensional Hilbert space $\mathscr{K}$. We will refer to such quantum systems as *finite quantum systems*. $\mathscr{O}_{\mathscr{K}}$ denotes the $C^*$-algebra of all linear maps $A : \mathscr{K} \to \mathscr{K}$ and $\mathscr{S}_{\mathscr{K}} \subset \mathscr{O}_{\mathscr{K}}$ the set of all density matrices on $\mathscr{K}$. $\mathbb{1}$ denotes the identity in $\mathscr{O}_{\mathscr{K}}$. The observables of the system are identified with the elements of $\mathscr{O}_{\mathscr{K}}$ and its physical states with elements of $\mathscr{S}_{\mathscr{K}}$, with the usual duality $\nu(A) = \mathrm{tr}(\nu A)$, $\nu \in \mathscr{S}_{\mathscr{K}}$, $A \in \mathscr{O}_{\mathscr{K}}$. The number $\nu(A)$ is interpreted as the expectation value of the observable $A$ if the system is in the state $\nu$. A state $\nu$ is called faithful if $\nu > 0$. The dynamics is described by the system Hamiltonian $H = H^* \in \mathscr{O}_{\mathscr{K}}$ and the induced group $\tau = \{\tau^t \mid t \in \mathbb{R}\}$ of $*$-automorphisms of $\mathscr{O}_{\mathscr{K}}$, defined by

$$\tau^t(A) = \mathrm{e}^{\mathrm{i}tH} A \mathrm{e}^{-\mathrm{i}tH}.$$

We will sometimes write $A_t$ for $\tau^t(A)$ and call the map $A \mapsto A_t$ the dynamics in Heisenberg picture. In the dual Schrödinger picture, the states evolve in time as $\nu \to \nu_t$, where

$$\nu_t = \mathrm{e}^{-\mathrm{i}tH} \nu \mathrm{e}^{\mathrm{i}tH}.$$

Obviously, $\nu_t(A) = \nu(A_t)$. The time-correlations are quantified by the function

$$F_{\nu,A,B}(t) = \nu(AB_t).$$

A triple $(\mathscr{O}_{\mathscr{K}}, \tau, \omega)$, where $\omega$ is the initial (reference) state of the system, is called a finite quantum dynamical system. This system is said to be in thermal equilibrium at inverse temperature $\beta \in \mathbb{R}$ if its reference state is the Gibbs canonical ensemble

$$\omega_\beta = \mathrm{e}^{-\beta H} / \mathrm{tr}(\mathrm{e}^{-\beta H}). \tag{19.1}$$

The Gibbs ensemble (19.1) is the unique state in $\mathscr{S}_{\mathscr{K}}$ satisfying the:

[7] The equilibrium theory of quantum lattice spin systems is easily adapted to lattice fermions although a pedagogical exposition of this adaptation is lacking in the literature. A parallel exposition of the spin and fermion case, together with some far reaching generalizations, can be found in [4].

**Finite KMS-condition.** The time-correlation functions $F_{\nu,A,B}$ have the property

$$F_{\nu,A,B}(t + \mathrm{i}\beta) = F_{\nu,B,A}(t)$$

for all $A, B \in \mathscr{O}_{\mathscr{K}}$ and $t \in \mathbb{R}$.

Another fundamental characterization of the state (19.1) is given by the following result.

**Finite Gibbs Variational Principle.** Set $P(\beta) = \log \mathrm{tr}(\mathrm{e}^{-\beta H})$ and denote by $S(\nu) = -\mathrm{tr}(\nu \log \nu)$ the von Neumann entropy of $\nu \in \mathscr{S}_{\mathscr{K}}$. Then, for any $\nu \in \mathscr{S}_{\mathscr{K}}$,

$$S(\nu) - \beta\nu(H) \leq P(\beta),$$

with equality iff $\nu = \omega_\beta$.

The relative entropy of two states $\nu, \rho \in \mathscr{S}_{\mathscr{K}}$ is defined by[8]

$$\mathrm{Ent}(\nu|\rho) = \mathrm{tr}(\nu(\log \rho - \log \nu)). \tag{19.2}$$

Its basic property is that $\mathrm{Ent}(\nu|\rho) \leq 0$ with equality iff $\nu = \rho$. One computes

$$\mathrm{Ent}(\nu|\omega_\beta) = S(\nu) - \beta\nu(H) - P(\beta),$$

and so the finite Gibbs variational principle is an immediate consequence of the above property of relative entropy.

In the full generality of algebraic quantum statistical mechanics, observables of a quantum system are described by elements of a $C^*$-algebra $\mathscr{O}$ with unit $\mathbb{1}$. For a large part of the general theory, no other structure is imposed on $\mathscr{O}$. The set of selfadjoint elements in $\mathscr{O}$ is denoted by $\mathscr{O}_{\mathrm{sa}}$. Let $\mathscr{O}^*$ be the dual of $\mathscr{O}$ and $\mathscr{S}_{\mathscr{O}}$ the set of positive normalized elements in $\mathscr{O}^*$. We equip $\mathscr{O}^*$ with the weak$^*$-topology, with respect to which $\mathscr{S}_{\mathscr{O}}$ is a compact, convex subset of $\mathscr{O}^*$. The physical states are described by elements of $\mathscr{S}_{\mathscr{O}}$. If the system is in a state $\nu$, then the number $\nu(A)$ is interpreted as the expectation value of the observable $A$.

The notion of Hamiltonian is lost, and the dynamics in the Heisenberg picture is, from the outset, described by a strongly continuous[9] group $\tau = \{\tau^t \,|\, t \in \mathbb{R}\}$ of $*$-automorphisms of $\mathscr{O}$. The group $\tau$ is called $C^*$-dynamics and the pair $(\mathscr{O}, \tau)$ a $C^*$-dynamical system. Its dual action $\tau^*$ preserves $\mathscr{S}_{\mathscr{O}}$ and describes the dynamics in the Schrödinger picture. We write $A_t$ for $\tau^t(A)$ and $\nu_t$ for $\tau^{t*}(\nu) = \nu \circ \tau^t$. The function $F_{\nu,A,B}(t)$ is defined in the same way as in the finite case.

A state $\nu$ is called $\tau$-invariant (or stationary) if $\nu_t = \nu$ for all $t$. The set of all $\tau$-invariant states is denoted by $\mathscr{S}_\tau$ and is always non-empty. A triple $(\mathscr{O}, \tau, \omega)$, where $\omega$ is the initial (reference) state of the system, is called a $C^*$-quantum dynamical system.

[8] This relative entropy is finite iff $\mathrm{Ker}\,\rho \subseteq \mathrm{Ker}\,\nu$, otherwise it takes the value $-\infty$.

[9] $\lim_{t\to 0} \|\tau^t(A) - A\| = 0$ for all $A \in \mathscr{O}$

A state $\omega \in \mathscr{S}_\tau$ is called ergodic if

$$\lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} \omega(B^* A_t B)\mathrm{d}t = \omega(A)\omega(B^* B)$$

holds for all $A, B \in \mathscr{O}$. Upon passing to the GNS representation, it becomes clear that this definition is a special case of the one presented in Section 9.1.

Time-reversal plays an important role in statistical mechanics. An anti-linear involutive $*$-automorphism $\Theta$ of $\mathscr{O}$ is a time-reversal of the $C^*$-dynamical system $(\mathscr{O}, \tau)$ if

$$\Theta \circ \tau^t = \tau^{-t} \circ \Theta$$

for all $t \in \mathbb{R}$. A state $\omega$ is called time-reversal invariant if $\omega(\Theta(A)) = \omega(A^*)$ for all $A \in \mathscr{O}$. In the sequel we abbreviate time-reversal invariance by TRI.

Since the notion of Hamiltonian is lost, so is the notion of the Gibbs canonical ensemble (19.1). The KMS-condition, however, survives and extends to the general setting as:

**KMS-condition.** $\nu \in \mathscr{S}_\mathscr{O}$ is a $(\tau, \beta)$-KMS state if, for all $A, B \in \mathscr{O}$, the function $\mathbb{R} \ni t \mapsto F_{\nu,A,B}(t)$ has an analytic extension to the strip $0 < \mathrm{sign}(\beta)\,\mathrm{Im}\, z < |\beta|$ that is bounded and continuous on its closure and satisfies the KMS-boundary condition

$$F_{\nu,A,B}(t + \mathrm{i}\beta) = F_{\nu,B,A}(t)$$

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

We denote by $\mathscr{S}_{(\tau,\beta)}$ the set of all $(\tau, \beta)$-KMS states. At the current level of generality this set might be empty. One always has $\mathscr{S}_{(\tau,\beta)} \subset \mathscr{S}_\tau$. A quantum dynamical system $(\mathscr{O}, \tau, \omega)$ is said to be in thermal equilibrium at inverse temperature $\beta \in \mathbb{R}$ (or just thermal) if $\omega$ is a $(\tau, \beta)$-KMS state.

A state $\nu$ is called modular if there exists $C^*$-dynamics $\varsigma_\nu$ on $\mathscr{O}$ such that $\nu$ is $(\varsigma_\nu, -1)$-KMS state. $\varsigma_\nu$ is called modular dynamics of $\nu$ and is unique if it exists. We denote by $\delta_\nu$ the generator of $\varsigma_\nu$ with the convention $\varsigma_\nu^t = \mathrm{e}^{t\delta_\nu}$. If $\nu$ is a $(\tau, \beta)$-KMS state and $\beta \neq 0$, then $\varsigma_\nu^t = \tau^{-\beta t}$, or equivalently, $\delta_\nu = -\beta\delta$ where $\delta$ is the generator of $\tau$. The modular dynamics plays an important role in non-equilibrium statistical mechanics. In the equilibrium setting of quantum spin systems, its a priori existence allows for the formulation of the Gibbs condition as characterization of thermal equilibrium; we will briefly discuss this topic in the next section.

Given $(\mathscr{O}, \tau)$, the two basic questions of equilibrium statistical mechanics are:

**(QI)** Describe the properties of KMS-states and the structure of the sets $\mathscr{S}_{(\tau,\beta)}$.

**(QII)** Elucidate the dynamical, and in particular the ergodic, properties of thermal quantum dynamical systems.

Note that **(QI)** and **(QII)** have trivial answers in the finite setting: $\mathscr{S}_{(\tau,\beta)}$ is always a singleton and no thermal system is ergodic if $\dim(\mathscr{K}) > 1$. It is precisely this triviality that forces consideration of infinitely extended systems from the outset in the study of **(QI)** and **(QII)**.

From a general perspective, substantial progress has been made on **(QI)** and **(QII)** in the 1970s. The volumes [33, 34] are devoted to presenting these developments. The link between KMS-condition and Tomita-Takesaki's modular theory has played a central role in this progress. However, from the standpoint of concrete physically relevant models, advancement has been much slower, and comparatively little is known at a mathematically rigorous level.

The original definition of relative entropy of a pair $(\nu, \rho)$ of states on $\mathscr{O}$ goes back to Araki and is based on modular theory. This definition was discussed in Section 12.1 and we will review it again in Section 25. The relative entropy is also characterized by the Pusz-Woronowicz-Kosaki variational formula

$$\mathrm{Ent}(\nu|\rho) = \inf \int_0^\infty \left[ \frac{1}{t} \nu(x^*(t)x(t)) + \rho(y^*(t)y(t)) - \frac{1}{1+t} \right] \frac{\mathrm{d}t}{t}, \tag{19.3}$$

where $y(t) = \mathbb{1} - x(t)$ and the infimum is taken over all countably valued step functions $[0, \infty[ \ni t \mapsto x(t) \in \mathscr{O}$ vanishing in a neighborhood of zero; see [108, Section 5]. Its basic property is $\mathrm{Ent}(\nu|\rho) \leq 0$ with equality iff $\nu = \rho$. In the finite case (19.3) reduces to (19.2). The relative entropy plays a very important role in both equilibrium and non-equilibrium quantum statistical mechanics. In the equilibrium case and in the context of quantum lattice spin systems, relative entropy – through its relation with the specific entropy – plays a central role in the derivation of the Gibbs variational principle. This topic is discussed in detail in Section 6.2.3 of [33].

We conclude this section with three general remarks.

Modular theory and the closely related Araki's perturbation theory of KMS-structure play a central role in both equilibrium and non-equilibrium quantum statistical mechanics. A basic introduction to this subject can be found in [33, 34]; see also [48] and references therein for modern expositions. A pedagogical introduction to the modular theory in the context of finite quantum systems can be found in [72]

$W^*$-dynamical systems play a distinguished role in modular theory. A $W^*$-dynamical system is a pair $(\mathfrak{M}, \tau)$ where $\mathfrak{M}$ is a $W^*$-algebra and $\tau = \{\tau^t \mid t \in \mathbb{R}\}$ is a pointwise $\sigma$-weakly continuous group of $*$-automorphisms on $\mathfrak{M}$. We shall refer to such $\tau$ as $W^*$-dynamics. A triple $(\mathfrak{M}, \tau, \omega)$, where $\omega$ is a normal state on $\mathfrak{M}$, is called a $W^*$-dynamical system. In the general development of non-equilibrium quantum statistical mechanics, the $C^*$-quantum dynamical systems are preferred starting point since the central notion of non-equilibrium steady states cannot be naturally defined in the $W^*$-setting. In this context, the $W^*$-systems and modular structure emerge through the GNS-representation of $\mathscr{O}$ associated to the reference state $\omega$. This being said, there are important physical models that can be only described by $W^*$-dynamical system; a well-known example are Pauli-Fierz systems with bosonic reservoirs. It is most natural to develop the non-equilibrium statistical mechanics of such systems on a case-by-case basis.

The thermodynamic (often abbreviated TD) limit plays a distinguished role in statistical mechanics. It realizes infinitely extended systems through a limiting procedure involving only finite quantum system and is central for the identification of physically relevant objects in the extended setting. The precise way the TD limit is taken depends on the structure of the specific physical model under consideration, and often a num-

ber of different approximation routes are possible. This topic is well-understood and discussed on many places in the literature; see [33, 34, 126] and [72] for a pedagogical introduction to the topic. Since the early days it is well-known that the modular structure is stable under TD limit [2]; this fact plays an important role in the foundations of quantum statistical mechanics. The customary route in discussions of the structural theory is the following:

**Step 1.** A physical notion, introduced in the context of finite quantum systems, is expressed in a modular form, and through this form is directly extended, by definition, to a general $C^*$ or $W^*$-dynamical system. One basic example of such procedure is the introduction of the KMS-condition as characterization of thermal equilibrium states.

**Step 2.** In concrete physical models the definitions of Step 1 are justified by the TD limit.

Step 2 has been extensively studied in the early days of quantum statistical mechanics, and the wealth of obtained results make its implementation in modern literature most often a routine exercise. For this reason, this step is often skipped. There are rare exceptions to this rule, one of which emerged in the study of entropy production of open quantum systems [23, 25].

## 20 Lattice Quantum Spin Systems

We follow [33]; see also [71, 126, 129].

**$C^*$-algebra.** The lattice $G$ is taken to be a countably infinite set. At this stage, no additional structure on $G$ is assumed. The collection of all finite subsets of $G$ is denoted by $\mathfrak{G}_{\rm fin}$. If $(\Lambda_\alpha)$ is a net in $\mathfrak{G}_{\rm fin}$, $\Lambda_\alpha \to \infty$ means that $\Lambda_\alpha$ eventually contains any finite subset of $G$.

The single spin Hilbert space is finite dimensional and is denoted by $\mathfrak{h}$. To each $x \in G$ we associate a copy $\mathfrak{h}_x$ of $\mathfrak{h}$, and to each $\Lambda \in \mathfrak{G}_{\rm fin}$ the Hilbert space

$$\mathscr{K}_\Lambda = \bigotimes_{x\in\Lambda} \mathfrak{h}_x .$$

In the sequel, $\mathscr{O}_\Lambda$ stands for $\mathscr{O}_{\mathscr{K}_\Lambda}$. The $C^*$-algebra $\mathscr{O}_\Lambda$ describes observables of spins located at the points in $\Lambda$. For $\Lambda \subset \Lambda'$ one naturally identifies $\mathscr{O}_\Lambda$ with a $C^*$-subalgebra of $\mathscr{O}_{\Lambda'}$. The algebra of local observables is

$$\mathscr{O}_{\rm loc} = \bigcup_{\Lambda\in\mathfrak{G}_{\rm fin}} \mathscr{O}_\Lambda .$$

Finally, the $G$-lattice spin system $C^*$-algebra $\mathscr{O}_G$ is the completion of the $*$-algebra of local observables. The algebra $\mathscr{O}_G$ is unital, simple, and separable. For any $G_0 \subset G$ one has the natural identification $\mathscr{O}_G = \mathscr{O}_{G_0} \otimes \mathscr{O}_{G_0^c}$. Whenever $G$ is understood, we write $\mathscr{O}$ for $\mathscr{O}_G$.

**Dynamics.** An interaction is a map $\Phi : \mathfrak{G}_{\rm fin} \to \mathscr{O}_{\rm sa}$ such that $\Phi(X) \in \mathscr{O}_X$. For $\Lambda \in \mathfrak{G}_{\rm fin}$, the local Hamiltonians are defined by

$$H_\Lambda(\Phi) = \sum_{X \subset \Lambda} \Phi(X).$$

They generate the local $C^*$-dynamics $\tau_{\Phi,\Lambda}$ on $\mathscr{O}$, given by

$$\tau^t_{\Phi,\Lambda}(A) = \mathrm{e}^{\mathrm{i}tH_\Lambda(\Phi)} A \mathrm{e}^{-\mathrm{i}tH_\Lambda(\Phi)}.$$

To extend $\tau_{\Phi,\Lambda}$ to a $C^*$-dynamics on $\mathscr{O}$ in the limit $\Lambda \to \infty$, one needs a suitable regularity assumption. We choose the following one[10]

**(SR)** For some $\lambda > 0$,

$$\|\Phi\|_\lambda := \sum_{n \geq 0} \mathrm{e}^{\lambda n} \left( \sup_{x \in G} \sum_{\substack{X \ni x \\ |X| = n+1}} \|\Phi(X)\| \right) < \infty.$$

**Theorem 20.1** *Suppose that* **(SR)** *holds. Then:*

1. *For all $A \in \mathscr{O}$, the limit*
$$\tau^t_\Phi(A) := \lim_{\Lambda \to \infty} \tau^t_{\Phi,\Lambda}(A)$$
*exists and is uniform for $t$ in compacts sets.*
2. *$\tau_\Phi = \{\tau^t_\Phi \,|\, t \in \mathbb{R}\}$ is a $C^*$-dynamics on $\mathscr{O}$. We denote by $\delta_\Phi$ its generator.*
3. *$\mathscr{O}_{\rm loc} \subset \mathrm{Dom}(\delta_\Phi)$, and for $A \in \mathscr{O}_\Lambda$,*
$$\delta_\Phi(A) = \mathrm{i} \sum_{X \cap \Lambda \neq \emptyset} [\Phi(X), A].$$
*Moreover, $\mathscr{O}_{\rm loc}$ is a core for $\delta_\Phi$.*
4. *For $A \in \mathscr{O}_{\rm loc}$ and $n \geq 1$,*
$$\|\delta^n_\Phi(A)\| \leq \frac{2^n n!}{\lambda^n} \mathrm{e}^{\lambda|\Lambda|} \|\Phi\|^n_\lambda \|A\|,$$
*where $|\Lambda|$ denotes the cardinality of $\Lambda$. In particular, for all $A \in \mathscr{O}_{\rm loc}$, the map*
$$\mathbb{R} \ni t \mapsto \tau^t_\Phi(A) \in \mathscr{O}$$
*has an analytic extension to the strip $|\operatorname{Im} z| < \frac{\lambda}{2} \|\Phi\|^{-1}_\lambda$.*

[10] See Theorem 6.2.4 in [33].

For the proof, we refer the reader to [126, Lemma 7.6.1 and Theorem 7.6.2] and [33, Theorem 6.2.4].

Until the end of this section we assume that **(SR)** holds.

**KMS-states.** Let $\beta > 0$ be the inverse temperature. For $\Lambda \in \mathfrak{G}_{\rm fin}$, the local Gibbs state is defined by

$$\omega_{\Lambda,\beta} = \mathrm{e}^{-\beta H_\Lambda(\Phi)} / \operatorname{tr}(\mathrm{e}^{-\beta H_\Lambda(\Phi)}). \tag{20.1}$$

Using the identification $\mathscr{O} = \mathscr{O}_\Lambda \otimes \mathscr{O}_{\Lambda^c}$, one extends $\omega_{\Lambda,\beta}$ (in an arbitrary way) to a state on $\mathscr{O}$. Denoting this extension by the same letter, it is a basic result that any weak$^*$-limit point of the net $(\omega_\beta(\Lambda))_{\Lambda\in\mathfrak{G}_{\rm fin}}$ as $\Lambda \to \infty$ is a $(\tau_\Phi, \beta)$-KMS state on $\mathscr{O}$. The $(\tau_\Phi, \beta)$-KMS states that arise in this way are called thermodynamic-limit point $\beta$-KMS states.[11] This construction, in particular, shows that the set $\mathscr{S}_{(\tau_\Phi,\beta)}$ is non-empty.

If it happens that $\mathscr{S}_{(\tau_\Phi,\beta)}$ is a singleton, then all the nets $(\omega_\beta(\Lambda))_{\Lambda\in\mathfrak{G}_{\rm fin}}$ converge, as $\Lambda \to \infty$, to the unique $(\tau_\Phi, \beta)$-KMS state. This is known to be the case in the high-temperature regime, *i.e.*, for $\beta\|\Phi\|_\lambda$ small enough. For concrete estimates, see [33, Proposition 6.2.45], or [58] for more recent results.

If $\mathscr{S}_{(\tau_\Phi,\beta)}$ is not a singleton, one needs to take into account boundary conditions to reach all KMS-states by thermodynamic limit. That is our next topic.

**Araki-Gibbs Condition.** For any $\Lambda \in \mathfrak{G}_{\rm fin}$, the so called surface energies

$$W_\Lambda(\Phi) := \sum_{\substack{X\cap\Lambda\neq\emptyset \\ X\cap\Lambda^c\neq\emptyset}} \Phi(X)$$

are in $\mathscr{O}_{\rm sa}$. Let $\beta > 0$ and $V_\Lambda = \beta W_\Lambda(\Phi)$. Suppose that $\omega$ is a modular state on $\mathscr{O}$ and let $\delta_\omega$ be the generator of its modular $C^*$-dynamics $\varsigma_\omega$, $\varsigma_\omega^t = \mathrm{e}^{t\delta_\omega}$. Consider the perturbed dynamics $\varsigma_{\omega,V_\Lambda}$ generated by $\delta_\omega + \mathrm{i}[V_\Lambda, \cdot\,]$, and let $\omega_{V_\Lambda}$ be the $(\varsigma_{\omega,V_\Lambda}, -1)$-KMS state associated to $\omega$ by Araki's perturbation theory. We say that $\omega$ satisfies $(\beta, \Phi)$ Gibbs condition if, for all $\Lambda \in \mathfrak{G}_{\rm fin}$, the restriction of $\omega_{V_\Lambda}$ to $\mathscr{O}_\Lambda$ is given by (20.1). The Gibbs condition is the quantum counterpart of the DLR equation in the equilibrium theory of classical spin systems. For the proofs, see [33, Proposition 6.2.17].

**Theorem 20.2** *Suppose that $\omega$ is a modular state on $\mathscr{O}$ and $\beta > 0$. The following statements are equivalent.*

1. *$\omega$ is a $(\tau_\Phi, \beta)$-KMS state.*
2. *$\omega$ satisfies the $(\beta, \Phi)$ Gibbs condition.*

**Gibbs Variational Principle.** We will discuss the Gibbs variational principle only in the translation invariant setting; for a general lattice theory see [33, Section 6.2.3]. Suppose that $G = \mathbb{Z}^d$, and let $\varphi = \{\varphi^x \mid x \in \mathbb{Z}^d\} \subset \mathrm{Aut}(\mathscr{O})$ denote the natural action of the translation group $\mathbb{Z}^d$ on $\mathscr{O}$. We denote by $\mathscr{S}_{\rm I}$ the set of all translation-invariant (that is, $\varphi$-invariant) states on $\mathscr{O}$. For any $\nu \in \mathscr{S}_{\rm I}$, the limit

$$s(\nu) = \lim_{\Lambda\to\infty} \frac{S(\nu_\Lambda)}{|\Lambda|}$$

[11] We follow the terminology introduced in [33, Section 6.2.2.].

exists, where $\nu_\Lambda$ denotes the restriction of $\nu$ to $\mathscr{O}_\Lambda$ and $S(\nu_\Lambda)$ is its von Neumann entropy. $s(\nu)$ is the specific entropy of the state $\nu$. The entropy map $\mathscr{S}_1 \ni \nu \mapsto s(\nu)$ is affine, upper-semicontinuous, and takes values in $[0, \log \dim \mathfrak{h}]$. An interaction $\Phi$ is translation invariant if

$$\varphi^x(\Phi(X)) = \Phi(X + x)$$

holds for all finite subsets $X \subset \mathbb{Z}^d$ and all $x \in \mathbb{Z}^d$. For translation invariant interactions,

$$\|\Phi\|_\lambda = \sum_{X \ni 0} \mathrm{e}^{\lambda(|X|-1)} \|\Phi(X)\|.$$

In what follows we fix a translation invariant $\Phi$ satisfying $\|\Phi\|_\lambda < \infty$ for some $\lambda > 0$. The specific energy observable of $\Phi$ is

$$E_\Phi = \sum_{X \ni 0} \frac{\Phi(X)}{|X|},$$

and for any $\omega \in \mathscr{S}_1$,

$$\lim_{\Lambda \to \infty} \frac{1}{|\Lambda|} \omega(H_\Lambda(\Phi)) = \omega(E_\Phi).$$

Finally, the finite limit

$$P(\Phi) = \lim_{\Lambda \to \infty} \frac{1}{|\Lambda|} \log \mathrm{tr} \left( \mathrm{e}^{-H_\Lambda(\Phi)} \right)$$

exists and is called the pressure of $\Phi$. The next theorem is known as the Gibbs variational principle.

**Theorem 20.3** *For any $\beta > 0$,*

$$P(\beta\Phi) = \sup_{\nu \in \mathscr{S}_1} (s(\nu) - \beta\nu(E_\Phi)).$$

*Moreover,*

$$\mathscr{S}_{\mathrm{eq}}(\beta\Phi) = \{\nu \in \mathscr{S}_1 \mid P(\beta\Phi) = s(\nu) - \beta\nu(E_\Phi)\}$$

*is a non-empty convex compact subset of $\mathscr{S}_1$. The elements of $\mathscr{S}_{\mathrm{eq}}(\beta\Phi)$ are called equilibrium states for interaction $\Phi$ at inverse temperature $\beta$.*

Finally, equilibrium states and KMS states are related by

**Theorem 20.4** *For any $\beta > 0$ the following statements are equivalent.*

1. *$\omega \in \mathscr{S}_{\mathrm{eq}}(\beta\Phi)$.*
2. *$\omega$ is a translation invariant $(\tau_\Phi, \beta)$-KMS state.*

For further discussion of Theorems 20.3 and 2, we refer the reader to [33, Proposition 6.2.39 and Theorem 6.2.40], and [33, Theorem 6.2.42].

## Part VI

**Non-equilibrium Quantum Statistical Mechanics** The works [79, 110, 122, 123][12] initiated modern developments in non-equilibrium quantum statistical mechanics by introducing the notions of entropy production observable and non-equilibrium steady states (NESS). The concept of quantum entropy production observable goes back at least to [112],[13] and was re-introduced independently in the literature several times since; see [105–107]. The concept of NESS in the quantum setting was novel and motivated by developments in classical non-equilibrium statistical mechanics; see [127]. The introduction of the quantum entropy production observable in conjunction with NESS has spurred rapid developments in non-equilibrium quantum statistical mechanics–both in structural theory and in the study of concrete models–that continue to this day. For a non-exhaustive list of references, we refer the reader to [23].

## 21 General Setting

We follow [79]. Let $(\mathscr{O}, \tau, \omega)$ be a $C^*$-quantum dynamical system whose reference state $\omega$ is not $\tau$-invariant. The NESS of $(\mathscr{O}, \tau, \omega)$ are the limit points of the net

$$\left\{\frac{1}{T}\int_0^T \omega \circ \tau^t \mathrm{d}t\right\}_{T>0}$$

as $T \uparrow \infty$. The set $\mathscr{S}_{\tau+}(\omega)$ of NESS is non-empty and its elements are $\tau$-invariant.

To introduce the entropy production observable, we assume that the state $\omega$ is modular. Recall that $\delta_\omega$ denotes the generator of the modular dynamics $\varsigma_\omega$. We further assume that the generator $\delta$ of $\tau$ has the form

$$\delta = \delta_{\mathrm{fr}} + \mathrm{i}[V, \cdot],$$

where $V \in \mathscr{O}_{\mathrm{sa}}$ and $\delta_{\mathrm{fr}}$ generates a "free" $C^*$-dynamics $\tau_{\mathrm{fr}}$ for which $\omega \in \mathscr{S}_{\tau_{\mathrm{fr}}}$. Lacking a better terminology, we shall say that such a system $(\mathscr{O}, \tau, \omega)$ is locally perturbed (abbreviated LP). If $V \in \mathrm{Dom}(\delta_\omega)$, the entropy production observable of a LP system is defined by

$$\sigma := \delta_\omega(V).$$

When we wish to indicate the dependence of $\tau$ and $\sigma$ on $V$ we will write $\tau_V, \sigma_V$.

The starting point of the theory is the entropy balance equation

$$\mathrm{Ent}(\omega_t|\omega) = -\int_0^t \omega_s(\sigma)\mathrm{d}s. \tag{21.1}$$

Since the relative entropy is non-positive, it follows that

$$\omega_+(\sigma) \geq 0$$

[12] The work [66], although focused on the concrete exactly solvable non-equilibrium $XY$-spin chain, foreshadowed these developments.

[13] See the Remark on page 281 of this paper. Another pioneering work on the subject is [130].

for any NESS $\omega_+ \in \mathscr{S}_{\tau+}(\omega)$.

The two basic questions of non-equilibrium quantum statistical mechanics are:

**(QIII)** Describe the structure of the set $\mathscr{S}_{\tau+}$ and the properties of its elements.

**(QIV)** Elucidate dynamical mechanisms that ensure $\omega_+(\sigma) > 0$ for all $\omega_+ \in \mathscr{S}_{\tau+}$.

There are two general approaches to **(QIII)**. The first is the $C^*$-scattering method that goes back to Robinson [116] and in the context of NESS was further developed by Ruelle [122]; see also [14]. In this method the goal is to prove that for $A \in \mathscr{O}$ the limit

$$\gamma^+(A) := \lim_{t\to\infty} \tau_{\rm fr}^{-t} \circ \tau^t(A)$$

exists. In this case $\gamma^+ \in \mathrm{Aut}(\mathscr{O})$, $\lim_{t\to\infty} \omega_t = \omega_+ = \omega \circ \gamma^+$, and $\mathscr{S}_{\tau+} = \{\omega_+\}$. A sufficient condition that ensures the existence of the Møller morphism $\gamma^+$ is that there exists a dense subset $\mathscr{A} \subset \mathscr{O}$ such that for all $A \in \mathscr{A}$,

$$\int_0^\infty \|[\tau^t(A), V]\| \mathrm{d}t < \infty.$$

Conditions of this type are called $L^1$-asymptotic Abelianness and have been extensively used in the literature; see [33]. For some physically important models where this condition has been verified, see [31, 56, 78].

The second general approach to **(QIII)** was developed in [81] based on the spectral theory of quantum transfer operators. It is a quantum extension of Ruelle transfer operator method; see [18]. For a pedagogical introduction to quantum transfer operators in finite quantum system setting, see [72]. For modern developments, see [24].

Regarding **(QIV)**, we refer the reader to [14, 80] and references therein. Both questions **(QIII)** and **(QIV)** remain poorly understood and much work remains to be done.

A special class of LP systems, the so-called open quantum systems, play a privileged role in the study of non-equilibrium quantum statistical mechanics and we proceed to describe them.

Consider finitely many, say $M$, thermal reservoirs $\mathscr{R}_j$ described by $C^*$-quantum dynamical systems $(\mathscr{O}_j, \tau_j, \omega_j)$. We denote by $\delta_j$ the generator of $\tau_j$. The reservoir $\mathscr{R}_j$ is assumed to be in thermal equilibrium at inverse temperature $\beta_j > 0$, that is, we assume that $\omega_j$ is a $(\tau_j, \beta_j)$-KMS state on $\mathscr{O}_j$. In the absence of interaction, the combined reservoir system $\mathscr{R} = \mathscr{R}_1 + \cdots + \mathscr{R}_M$ is described by the quantum dynamical system $(\mathscr{O}_\mathscr{R}, \tau_\mathscr{R}, \omega_\mathscr{R})$, where[14]

$$\mathscr{O}_\mathscr{R} := \mathscr{O}_1 \otimes \cdots \otimes \mathscr{O}_M,$$
$$\tau_{\rm fr} := \tau_1 \otimes \cdots \otimes \tau_M,$$
$$\omega_\mathscr{R} := \omega_1 \otimes \cdots \otimes \omega_M.$$

[14] Whenever the meaning is clear within the context, we write $A$ for $A \otimes \mathbb{1}$ and $\mathbb{1} \otimes A$, $\delta_j$ for $\delta_j \otimes \mathrm{Id}$, $\mathrm{Id} \otimes \delta_j$, etc.

There are two ways to couple the reservoirs. In the first case of directly coupled reservoirs, $\tau_{\rm fr} = \tau_{\mathscr{R}}$, the interaction is described by $V \in \mathscr{O}_{\mathscr{R},\rm sa}$, and the interacting dynamics $\tau$ is generated by $\delta = \delta_{\mathscr{R}} + \mathrm{i}[V, \cdot\,]$.

The reservoirs can be also coupled through a finite quantum system $\mathscr{S}$ with Hilbert space $\mathscr{K}_{\mathscr{S}}$. Let $(\mathscr{O}_{\mathscr{S}}, \tau_{\mathscr{S}}, \omega_{\mathscr{S}})$ be a finite-dimensional quantum system dynamical describing $\mathscr{S}$[15], where we assume that $\omega_{\mathscr{S}} > 0$. The generator of $\tau_{\mathscr{S}}$ is $\delta_{\mathscr{S}} = \mathrm{i}[H_{\mathscr{S}}, \cdot\,]$, where $H_{\mathscr{S}}$ is the Hamiltonian of $\mathscr{S}$. In the absence of interaction, the joint system $\mathscr{S} + \mathscr{R}$ is described by the $C^*$-quantum dynamical system $(\mathscr{O}, \tau_{\rm fr}, \omega)$ where

$$\mathscr{O} = \mathscr{O}_{\mathscr{S}} \otimes \mathscr{O}_{\mathscr{R}}, \qquad \tau_{\rm fr} = \tau_{\mathscr{S}} \otimes \tau_{\mathscr{R}}, \qquad \omega = \omega_{\mathscr{S}} \otimes \omega_{\mathscr{R}}.$$

The interaction of $\mathscr{S}$ with $\mathscr{R}_j$ is described by a selfadjoint $V_j \in \mathscr{O}_{\mathscr{S}} \otimes \mathscr{O}_j$, and the full interaction by $V := \sum_j V_j$. The interacting dynamics $\tau$ is generated by $\delta := \delta_{\rm fr} + \mathrm{i}[V, \cdot\,]$. We assume that $V_j \in \mathrm{Dom}(\delta_j)$ for all $j$, which ensures that the entropy production observable is well-defined.

In what follows, we will always take

$$\omega_{\mathscr{S}} = \mathbb{1}/\dim \mathscr{K}_{\mathscr{S}} \tag{21.2}$$

for the reference state of $\mathscr{S}$. This choice is made for convenience. It is easy to show that none of the asymptotic results of this paper depend on the choice of $\omega_{\mathscr{S}}$ as long as $\omega_{\mathscr{S}}$ is faithful. With the choice (21.2),

$$\sigma = -\sum \beta_j \mathscr{J}_j,$$

where the observable $\mathscr{J}_j := \delta_j(V_j)$ describes the energy flux out of the $j$-th reservoir.

The above description of open quantum system needs to be adapted in the case of fermionic systems. The modifications are straightforward; see [14, 78].

## 22 Open Lattice Quantum Spin Systems

We follow [123], and consider the lattice quantum spin system of Section 20, the interaction $\Phi$ satisfying Assumption **(SR)**. We further assume:

**(a)** For some finite $M$,

$$G = S \cup \left( \bigcup_{j=1}^{M} R_j \right)$$

where $S$ is a finite set and each $R_j$ is an infinite set. The sets $S, R_1, \ldots, R_M$ are assumed to be disjoint.

[15] We abbreviate $\mathscr{O}_{\mathscr{K}_{\mathscr{S}}}$ by $\mathscr{O}_{\mathscr{S}}$

We adapt the notation of Section 20 to that of Section 21 by setting $\mathscr{O}_{\mathscr{R}_j} = \mathscr{O}_{R_j}$ for $j \in \{1, \dots, M\}$, $\mathscr{O}_{\mathscr{S}} = \mathscr{O}_S$, and $\mathscr{K}_{\mathscr{S}} := \otimes_{x\in S}\mathfrak{h}_x$. One then has the decomposition

$$\mathscr{O} = \mathscr{O}_{\mathscr{S}} \otimes \mathscr{O}_{\mathscr{R}} = \mathscr{O}_{\mathscr{S}} \otimes \mathscr{O}_{\mathscr{R}_1} \otimes \cdots \otimes \mathscr{O}_{\mathscr{R}_M}.$$

In the framework of Section 21, the subsystems described by the subalgebras $\mathscr{O}_{\mathscr{R}_j}$ act as reservoirs, and the next assumption forbids direct coupling between these reservoirs.

**(b)** For any $X \in \mathfrak{G}_{\rm fin}$, if $X \cap R_i \neq \emptyset$, $X \cap R_j \neq \emptyset$ for some $i \neq j$ , then $\Phi(X) = 0$.

We denote by $\mathfrak{G}_{j,\rm fin}$ the collection of all finite subsets of $R_j$, and by $\Phi_j$ the restriction of $\Phi$ to $\mathfrak{G}_{j,\rm fin}$. $\tau_{\mathscr{R}_j}$ denotes the $C^*$-dynamics on $\mathscr{O}_{\mathscr{R}_j}$ generated by $\Phi_j$ and $\delta_{\mathscr{R}_j}$ its generator. The coupling of the finite subsystem $\mathscr{S}$ with the $j$-th reservoir is given by

$$V_j := \sum_{X\cap S\neq\emptyset, X\cap R_j\neq\emptyset} \Phi(X),$$

and we set $V := \sum_j V_j$. The "free" $C^*$-dynamics $\tau_{\rm fr}$ on $\mathscr{O}$ is generated by

$$\delta_{\rm fr} = \delta_{\mathscr{S}} + \sum_j \delta_{\mathscr{R}_j},$$

where $\delta_{\mathscr{S}} = \mathrm{i}[H_S(\Phi), \cdot\,]$. The fully coupled dynamics $\tau = \tau_\Phi$ on $\mathscr{O}$ is generated by

$$\delta_\Phi = \delta_{\rm fr} + \mathrm{i}[V, \cdot\,].$$

The model is completed by a choice of $(\tau_{\mathscr{R}_j}, \beta_j)$-KMS state $\omega_{\beta_j}$ on $\mathscr{O}_{\mathscr{R}_j}$ for $j = 1, \dots, M$, and by taking[16]

$$\omega = \omega_{\mathscr{S}} \otimes \omega_{\beta_1} \otimes \cdots \otimes \omega_{\beta_M}$$

for the reference state of $(\mathscr{O}, \tau)$. $(\mathscr{O}, \tau, \omega)$ is an example of open quantum system discussed in Section 21.

Assumption **(SR)** ensures that

$$\sum_j \sum_Y \sum_{X\cap S\neq\emptyset, X\cap R_j\neq\emptyset} \|[\Phi(Y), \Phi(X)]\| < \infty.$$

Since $\delta_\omega = -\sum_j \beta_j \delta_{\mathscr{R}_j}$, we deduce that $V \in \mathrm{Dom}(\delta_\omega)$, the entropy production observable being given by

$$\sigma = \delta_\omega(V) = \sum_j \sum_{Y\subset R_j} \sum_{X\cap S\neq\emptyset, X\cap R_j\neq\emptyset} -\mathrm{i}\beta_j[\Phi(Y), \Phi(X)].$$

[16] $\omega_{\mathscr{S}}$ is given by (21.2).

We now turn to the discussion of the thermodynamic limit of open lattice quantum spin systems. One starts with $\Lambda \in \mathfrak{G}_{\rm fin}$ of the form

$$\Lambda = S \cup \left( \bigcup_{j=1}^{M} \Lambda_j \right),$$

where $\Lambda_j \in \mathfrak{G}_{j,\rm fin}$, and

$$\mathscr{O}_\Lambda = \mathscr{O}_{\mathscr{S}} \otimes \mathscr{O}_{\Lambda_1} \otimes \cdots \otimes \mathscr{O}_{\Lambda_M}.$$

The finite volume dynamics $\tau_\Lambda$ is generated by the Hamiltonian

$$H_\Lambda(\Phi) = H_{{\rm fr},\Lambda} + V_\Lambda,$$

where

$$H_{{\rm fr},\Lambda} := H_S(\Phi) + \sum_j H_{\Lambda_j}(\Phi_j), \qquad V_\Lambda := \sum_j V_{j,\Lambda},$$

with

$$V_{j,\Lambda} := \sum_{\substack{X \subseteq S \cup \Lambda_j \\ X \cap S \neq \emptyset, X \cap \Lambda_j \neq \emptyset}} \Phi(X).$$

The finite volume reference state has a product structure

$$\omega_\Lambda = \omega_{\mathscr{S}} \otimes \omega_{\Lambda_1} \otimes \cdots \otimes \omega_{\Lambda_M}, \tag{22.1}$$

where

$$\omega_{\Lambda_j} = {\rm e}^{-\beta_j H_{\Lambda_j}(\Phi_j)} / \operatorname{tr}({\rm e}^{-\beta_j H_{\Lambda_j}(\Phi_j)}). \tag{22.2}$$

The first basic question regarding the thermodynamic limit in the present setting concerns the entropy production observable. In a finite volume $\Lambda$, the entropy production observable is given by

$$\sigma_\Lambda = -{\rm i} \sum_j \beta_j [H_{\Lambda_j}(\Phi_j), V_{j,\Lambda}] = {\rm i} \sum_j \beta_j [H_\Lambda(\Phi), H_{\Lambda_j}(\Phi_j)]. \tag{22.3}$$

The finite volume entropy balance equation takes the form

$$\operatorname{Ent}(\omega_\Lambda \circ \tau_\Lambda^t | \omega_\Lambda) = -\int_0^t \omega_\Lambda(\tau_\Lambda^s(\sigma_\Lambda)) {\rm d}s,$$

and of course has an elementary proof.

**Theorem 22.1** *1.* $\lim_{\Lambda \to \infty} \sigma_\Lambda = \sigma$.

2. *Suppose that each $\omega_{\beta_j}$ is a thermodynamic-limit point $\beta_j$-KMS state on $\mathscr{O}_{\mathscr{R}_j}$. Let*

$$\Lambda_\alpha = S \cup \left( \bigcup_{j=1}^{M} \Lambda_{j,\alpha} \right),$$

*be a net in $\mathfrak{G}_{\rm fin}$ such that for each $j$,*

$$\lim_{\Lambda_{j,\alpha}\to\infty} \omega_{\Lambda_{j,\alpha}} = \omega_{\beta_j}.$$

*Then*

$$\begin{aligned} \mathrm{Ent}(\omega \circ \tau^t|\omega) &= \lim_{\Lambda_\alpha\to\infty} \mathrm{Ent}(\omega_{\Lambda_\alpha} \circ \tau^t_{\Lambda_\alpha}|\omega_{\Lambda_\alpha}) \\ &= -\lim_{\Lambda_\alpha\to\infty} \int_0^t \omega_{\Lambda_\alpha}(\tau^s_{\Lambda_\alpha}(\sigma_{\Lambda_\alpha}))\mathrm{d}s \\ &= -\int_0^t \omega(\tau^s(\sigma))\mathrm{d}s. \end{aligned}$$

In [123], Ruelle considered a somewhat more general setting by allowing for suitable "boundary terms" in (22.2). The reason for introducing these "boundary terms" is to reach a broader class of reservoir KMS-states than the "free boundary condition" (22.2) allows. To address this issue more generally, one can start with an arbitrary $(\tau_{\mathscr{R}_j}, \beta_j)$-KMS state $\omega_{\beta_j}$ on $\mathscr{O}_{\mathscr{R}_j}$, set $\omega_{\Lambda_j} = \omega_{\beta_j} \restriction_{\mathscr{O}_{\Lambda_j}}$, and take (22.1) defined with these new $\omega_{\Lambda_j}$. The entropy production observable $\sigma_\Lambda$ remains defined by (22.3). In this case, the total entropy production over the time-interval $[0, t]$,

$$-\int_0^t \omega_\Lambda(\tau^s_\Lambda(\sigma_\Lambda))\mathrm{d}s,$$

cannot be directly linked to the relative entropy and *does not need* to be non-negative. However, since

$$-\lim_{\Lambda} \int_0^s \omega_\Lambda(\tau^t_\Lambda(\sigma_\Lambda))\mathrm{d}t = -\int_0^s \omega_t(\sigma)\mathrm{d}t = \mathrm{Ent}(\omega_s|\omega),$$

the basic properties of entropy production are restored in the thermodynamic limit. For further discussion of this topic, we refer the reader to [25, Section 3.4].

## 23 Equilibrium Versus Non-Equilibrium

There are good reasons why our understanding of equilibrium quantum statistical mechanics vastly surpasses its non-equilibrium counterpart. Perhaps the most

important reasons concern the role of dynamics, the variational principle, and the thermodynamic limit. Although thermal equilibrium states have dynamical characterization in terms of the KMS-condition, in the concrete setting of lattice spin or fermionic systems the KMS condition is equivalent to the Gibbs variational principle and Gibbs condition. The latter two, in conjunction with thermodynamic limit, provide powerful tools in the study of the question **(QI)** and sharply separate it from the much less understood question **(QII)**. There is no such separation in the non-equilibrium case, and a detailed understanding of the dynamics is central to both **(QIII)** and **(QIV)**.

Another important reason concerns the relation of **(QIV)** with the singularity of NESS. If $\omega_+ = \omega_{\rm n} + \omega_{\rm s}$ is the decomposition of a NESS into its $\omega$-normal part $\omega_{\rm n}$ and its $\omega$-singular part $\omega_{\rm s}$, then $\omega_{\rm n}(\sigma) = 0$, and so $\omega_+(\sigma) > 0$ iff $\omega_{\rm s}(\sigma) > 0$. Moreover, if the following boundedness condition holds,

$$\sup_{T>0} \left| \int_0^T (\omega(\tau^t(\sigma)) - \omega_+(\sigma)) \mathrm{d}t \right| < \infty,$$

then $\omega_+(\sigma) > 0$ iff $\omega_{\rm s} \neq 0$; see [81, Theorem 1.1]. Although physically natural, the fact that the entropy production of NESS is carried by its singular part makes its study particularly delicate. This emergence of singularity is specific to non-equilibrium: if $\omega$ is a $(\tau_{\rm fr}, \beta)$-KMS state, then the NESS is unique and $\omega$-normal. These points are discussed in detail in [14, 80].

All the reasons discussed above are common to the classical and quantum case, underscoring that the conceptual difficulty of non-equilibrium statistical mechanics is not a specifically quantum phenomenon.

### Part VII

**Quantum phase space contraction** In open (classical or quantum) systems entropy production is directly related to the heat generation. The phase-space contraction reflects the loss of microscopic information as the system evolves, in the large-time limit, to a singular NESS. These two notions are closely related. Much of this section follows [24].

## 24 Classical Setting

We consider a classical dynamical system $(\mathscr{X}, \phi)$ where $\mathscr{X}$ is a compact metric space and $\phi = \{\phi^t \mid t \in \mathbb{R}\}$ is a group of homeomorphisms of $\mathscr{X}$ such that the map

$$\mathbb{R} \times \mathscr{X} \ni (t, x) \mapsto \phi^t(x) \in \mathscr{X}$$

is continuous. We denote by $C(\mathscr{X})$ the vector space of all continuous complex-valued functions on $\mathscr{X}$ and equip it with the sup norm $\|f\|_\infty := \sup_{x\in\mathscr{X}} |f(x)|$. The observables are functions $f \in C(\mathscr{X})$ and they evolve in time as $f \mapsto f_t := f \circ \phi^t$. The states are Borel probability measures on $\mathscr{X}$ and we write $\nu(f) = \int_{\mathscr{X}} f \mathrm{d}\nu$. They evolve in time as $\nu \mapsto \nu_t := \nu \circ \phi^{-t}$. A state $\nu$ is $\phi$-invariant if $\nu_t = \nu$ for all $t$. The

classical relative entropy of two states $\nu$ and $\rho$ is defined by

$$\mathrm{Ent}(\nu|\rho) = \int_{\mathscr{X}} \log \frac{\mathrm{d}\rho}{\mathrm{d}\nu} \mathrm{d}\nu$$

if $\rho \ll \nu$, and is set to $-\infty$ otherwise. Its basic property is $\mathrm{Ent}(\nu|\rho) \leq 0$ with equality iff $\nu = \rho$.

A time-reversal of $(\mathscr{X}, \phi)$ is an involutive homeomorphism $\vartheta : \mathscr{X} \to \mathscr{X}$ such that

$$\vartheta \circ \phi^t = \phi^{-t} \circ \vartheta$$

for all $t \in \mathbb{R}$. A state $\nu$ is called time-reversal invariant (TRI) if $\nu \circ \vartheta = \nu$.

The starting point is a classical dynamical system $(\mathscr{X}, \phi, \omega)$, assuming that the initial (reference) state $\omega$ is not $\phi$-invariant. The system is TRI if $\omega$ is TRI for some time-reversal of $(\mathscr{X}, \phi)$.

We set the regularity assumptions. First, throughout this section we assume

**(C1)** For all $t \in \mathbb{R}$ the measures $\omega$ and $\omega_t$ are equivalent,*i.e.*, have the same sets of measure zero.

Let

$$\Delta_{\omega_t|\omega} := \frac{\mathrm{d}\omega_t}{\mathrm{d}\omega}, \qquad \ell_{\omega_t|\omega} := \log \Delta_{\omega_t|\omega}.$$

**(C2)** $\ell_{\omega_t|\omega} \in C(\mathscr{X})$ for all $t \in \mathbb{R}$.

We set

$$c^t := \ell_{\omega_t|\omega} \circ \phi^t,$$

and denote by $Q_t$ the law of $c^t$ w.r.t. $\omega$. For $\alpha \in \mathbb{C}$, let

$$\mathfrak{F}_t(\alpha) := \int_{\mathbb{R}} \mathrm{e}^{-\alpha s} \mathrm{d}Q_t(s).$$

**(C3)** The map

$$\mathbb{R} \ni t \mapsto \ell_{\omega_t|\omega} \in C(\mathscr{X})$$

is differentiable at $t = 0$.

The entropy production observable, or the phase space contraction rate, is defined by

$$\sigma = \frac{\mathrm{d}}{\mathrm{d}t} \ell_{\omega_t|\omega}\big|_{t=0} = \frac{\mathrm{d}}{\mathrm{d}t} c^t\big|_{t=0}.$$

**Proposition 24.1** *Suppose that* **(C1)**–**(C2)** *hold.*

1. *For all* $t, s \in \mathbb{R}$,

$$\Delta_{\omega_{t+s}|\omega} = \Delta_{\omega_s|\omega} \circ \phi^{-t} \Delta_{\omega_t|\omega}$$

$$\ell_{\omega_{t+s}|\omega} = \ell_{\omega_s|\omega} \circ \phi^{-t} + \ell_{\omega_t|\omega},$$

$$c^{t+s} = c^s + c^t \circ \phi^s.$$

2. $\mathrm{Ent}(\omega_t|\omega) = -\omega(c^t)$.

*In the remaining statements we assume that* **(C3)** *also holds.*

3. $$\ell_{\omega_t|\omega} = \int_0^t \sigma_{-s}\mathrm{d}s, \qquad c^t = \int_0^t \sigma_s \mathrm{d}s,$$
*and*
$$\mathrm{Ent}(\omega_t|\omega) = -\int_0^t \omega_s(\sigma)\mathrm{d}s.$$
4. $\omega(\sigma) = 0$.

*In the remaining statements we assume that, in addition,* $(\mathscr{X}, \phi, \omega)$ *is* TRI *with time-reversal* $\vartheta$.

5. $c^t \circ \vartheta = c^{-t}$ *and* $\sigma \circ \vartheta = -\sigma$.
6. *For all* $t \in \mathbb{R}$ *and* $\alpha \in \mathbb{C}$,
$$\mathfrak{F}_t(\alpha) = \mathfrak{F}_t(1-\bar{\alpha}).$$
7. *Let* $\mathfrak{r} : \mathbb{R} \to \mathbb{R}$ *be the reflection* $\mathfrak{r}(s) = -s$ *and* $\overline{Q}_t = Q_t \circ \mathfrak{r}$. *Then, for any* $t \in \mathbb{R}$, *the measures* $Q_t$ *and* $\overline{Q}_t$ *are equivalent, and*
$$\frac{\mathrm{d}\overline{Q}_t}{\mathrm{d}Q_t}(s) = \mathrm{e}^{-s}. \tag{24.1}$$

The NESS of $(\mathscr{X}, \phi, \omega)$ are defined as the weak-limit points of the net

$$\left\{ \frac{1}{T}\int_0^T \omega_t \mathrm{d}t \mid T > 0 \right\}_{T>0}.$$

The set of NESS is non-empty and any NESS is $\phi$-invariant. Moreover, for any NESS $\omega_+$ one has

$$\omega_+(\sigma) \geq 0.$$

The two basic questions **(QIII)** and **(QIV)** of Section 21 have the same formulation in the classical case. In fact, the classical case can be directly embedded in the quantum case by considering commutative $C^*$-dynamical systems, see [24].

## 25 GNS-representation and Modular Structure

Some of the material below has been already discussed; see in particular Sections 5 and 12.

We denote by $(\mathscr{H}_\omega, \pi_\omega, \Omega_\omega)$ the GNS-representation of $\mathscr{O}$ associated to $\omega$ and by $\mathfrak{M}_\omega = \pi_\omega(\mathscr{O})''$ the enveloping von Neumann algebra of bounded operators on $\mathscr{H}_\omega$. We drop subscript $\omega$ when no confusion is possible. Since the state $\omega$ is assumed to

be modular, the vector $\Omega$ is separating for $\mathfrak{M}$,[17] and in particular $\|\pi(A)\| = \|A\|$ for all $A \in \mathscr{O}$. Whenever the meaning is clear from the context, we will denote $\pi(A)$ by $A$.

$\mathscr{N}$ denotes the set of all normal states on $\mathfrak{M}$, *i.e.*, the states described by density matrices on $\mathscr{H}$. Obviously elements of $\mathscr{N}$ also define states on $\mathscr{O}$. Any state on $\mathscr{O}$ that arises in this way is called $\omega$-normal. Again, whenever the meaning is clear from the context, we will denote such states by the same letter. In particular, the vector state $\mathfrak{M} \ni A \mapsto \langle \Omega, A\Omega \rangle$ is denoted by $\omega$.

We will assume that the reader is familiar with the basic notions of Tomita-Takesaki modular theory; see Section 5 and any of the references [33, 34, 47, 67, 108, 133]. We will use the same notation and terminology as in Section 5.3. $\mathscr{H}_+$ and $J$ denote the natural cone and modular conjugation associated to the pair $(\mathfrak{M}, \Omega)$. The unique vector representative of $\nu \in \mathscr{N}$ in the natural cone is denoted by $\Omega_\nu$. The modular operator of $\nu \in \mathscr{N}$ is denoted by $\Delta_\nu$. The relative modular operator of a pair $(\nu, \rho)$ of normal states is denoted by $\Delta_{\nu|\rho}$. The following perturbative result [82] is behind the entropy balance equation (21.1).

**Theorem 25.1** *Let $\nu$ be a modular state on $\mathscr{O}$ and $U \in \mathrm{Dom}(\delta_\nu)$ a unitary. Consider the state $\nu_U(\,\cdot\,) = \nu(U^* \cdot U)$ and let $P = -\mathrm{i}U\delta_\nu(U^*)$. Then*

$$\log \Delta_{\nu_U|\nu} = \log \Delta_\nu + P.$$

The relative entropy of a pair $(\nu, \rho)$ of normal faithful states is

$$\mathrm{Ent}(\nu|\rho) = \langle \Omega_\nu, \log \Delta_{\rho|\nu} \Omega_\nu \rangle.$$

This is the original definition of Araki [10], with the sign and ordering convention of [33]; see also Section 12.

Since $\omega$ is $\varsigma_\omega$ invariant, the family $\{\pi \circ \varsigma_\omega^t \,|\, t \in \mathbb{R}\}$ extends to a $W^*$-dynamics on $\mathfrak{M}$ which we again denote by $\varsigma_\omega$.[18] For $A \in \mathfrak{M}$,

$$\varsigma_\omega^t(A) = \Delta_\omega^{\mathrm{i}t} A \Delta_\omega^{-\mathrm{i}t}.$$

More generally, to any faithful $\nu \in \mathscr{N}$ one associates a $W^*$-dynamics $\varsigma_\nu$ by

$$\varsigma_\nu^t(A) = \Delta_\nu^{\mathrm{i}t} A \Delta_\nu^{-\mathrm{i}t}.$$

$\varsigma_\nu$ is called the modular dynamics of $\nu$, and $\nu$ is a $(\varsigma_\nu, -1)$-KMS state on $\mathfrak{M}$.

We make the assumption:

**(St)** The family $\{\pi \circ \tau^t \,|\, t \in \mathbb{R}\}$ extends to a $W^*$-dynamics on $\mathfrak{M}$ which we again denote by $\tau$.

[17] See [33, Corollary 5.3.9].

[18] Pointwise $\sigma$-weakly continuous groups of $*$-automorphisms on $\mathfrak{M}$.

This assumption is automatically satisfied for LP systems discussed in Section 21. It ensures that $\omega_t$ is a faithful $\omega$-normal state on $\mathfrak{M}$, and that there exists a unique selfadjoint operator $\mathscr{L}$ on $\mathscr{H}$, called the standard Liouvillean of $\tau$, such that for all $A \in \mathfrak{M}$ and $t \in \mathbb{R}$,

$$\tau^t(A) = \mathrm{e}^{\mathrm{i}t\mathscr{L}} A \mathrm{e}^{-\mathrm{i}t\mathscr{L}}, \qquad \mathrm{e}^{-\mathrm{i}t\mathscr{L}} \mathscr{H}_+ = \mathscr{H}_+.$$

The vector representative of $\omega_t$ in $\mathscr{H}_+$ is $\mathrm{e}^{-\mathrm{i}t\mathscr{L}}\Omega$. The standard Liouvillean is a basic example of a quantum transfer operator. Note that the standard Liouvillean of $\varsigma_\omega$ is $\log \Delta_\omega$.

The basic properties of the standard Liouvillean are summarized in:

**Theorem 25.2** *1.* $\mathrm{e}^{\mathrm{i}t\mathscr{L}} J = J\mathrm{e}^{\mathrm{i}t\mathscr{L}}$.

2. *The standard Liouvillean of an LP system is*

$$\mathscr{L} = \mathscr{L}_{\mathrm{fr}} + V - JVJ,$$

*where* $\mathscr{L}_{\mathrm{fr}}$ *is the standard Liouvillean of* $\tau_{\mathrm{fr}}$.

3. $\omega \in \mathscr{S}_\tau$ *iff* $\mathscr{L}\Omega = 0$.
4. *Suppose that* $\omega \in \mathscr{S}_\tau$. *Then the quantum dynamical system* $(\mathscr{O}, \tau, \omega)$ *is ergodic iff* 0 *is a simple eigenvalue of* $\mathscr{L}$.

The following well-known results identifies ergodicity with the so-called property of return to equilibrium.

**Theorem 25.3** *Suppose that* $\omega$ *is* $\tau$*-invariant. Then the quantum dynamical system* $(\mathscr{O}, \tau, \omega)$ *is ergodic iff, for any* $\omega$*-normal state* $\nu$ *and* $A \in \mathscr{O}$, *one has*

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \nu(\tau^t(A))\mathrm{d}t = \omega(A).$$

To any two faithful normal states $\nu$ and $\rho$ one associates a family of unitary operators called Connes' cocycle

$$[D\nu : D\rho]_{\mathrm{i}t} := \Delta_{\nu|\rho}^{\mathrm{i}t} \Delta_\rho^{-\mathrm{i}t}, \qquad t \in \mathbb{R}.$$

Its basic properties are summarized in:

**Theorem 25.4** *1. For all* $t \in \mathbb{R}$, $[D\nu : D\rho]_{\mathrm{i}t}$ *is a unitary element of* $\mathfrak{M}$.

2. $[D\nu : D\rho]_{\mathrm{i}t}^* = [D\rho : D\nu]_{\mathrm{i}t}$ *for all* $t \in \mathbb{R}$.
3. *The* $\varsigma_\rho$*-cocycle relation*

$$[D\nu : D\rho]_{\mathrm{i}s}\, \varsigma_\rho^s([D\nu : D\rho]_{\mathrm{i}t}) = [D\nu : D\rho]_{\mathrm{i}(s+t)},$$

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

4. *The intertwining relation*

$$[D\nu : D\rho]_{\mathrm{i}t}\varsigma_\rho^t(A)[D\nu : D\rho]_{\mathrm{i}t}^* = \varsigma_\nu^t(A),$$

*holds for any* $A \in \mathfrak{M}$ *and* $t \in \mathbb{R}$.

5. *If* $\mu$ *is another faithful normal state, then the chain rule*

$$[D\nu : D\rho]_{\mathrm{i}t}[D\rho : D\mu]_{\mathrm{i}t} = [D\nu : D\mu]_{\mathrm{i}t},$$

*holds for any* $t \in \mathbb{R}$.

For the proof we refer the reader to [5].

The family of Connes cocycles $([D\omega_t : D\omega]_\alpha)_{\alpha\in\mathrm{i}\mathbb{R}}$ will be crucial for the identification of quantum phase space contraction in the next section. The following proposition describes its basic property, which is the quantum counterpart of the first relation in Theorem 24.1(i).

**Proposition 25.5** *For all* $t, s \in \mathbb{R}$ *and* $\alpha \in \mathrm{i}\mathbb{R}$,

$$[D\omega_{t+s} : D\omega]_\alpha = \tau^{-t}([D\omega_s : D\omega]_\alpha)[D\omega_t : D\omega]_\alpha.$$

In the development of non-equilibrium quantum statistical mechanics, the following regularity assumption plays an important role:

**(Reg1)** For all $t \in \mathbb{R}$ and $\alpha \in \mathrm{i}\mathbb{R}$,

$$[D\omega_t : D\omega]_\alpha \in \pi(\mathscr{O}).$$

When **(Reg1)** holds, we will denote $\pi^{-1}([D\omega_t : D\omega]_\alpha)$ by $[D\omega_t : D\omega]_\alpha$. For LP systems, **(Reg1)** holds if $V \in \mathrm{Dom}(\delta_\omega)$.

## 26 Quantum Phase Space Contraction

As in the classical case, our starting point is Proposition 25.5. We make two additional regularity assumptions:

**(Reg2)** For all $t \in \mathbb{R}$ the map

$$\mathrm{i}\mathbb{R} \ni \alpha \mapsto [D\omega_t : D\omega]_\alpha \in \mathscr{O}$$

is differentiable at $\alpha = 0$.

Let

$$\ell_{\omega_t|\omega} := \frac{\mathrm{d}}{\mathrm{d}\alpha}[D\omega_t : D\omega]_\alpha\big|_{\alpha=0},$$

and

$$c^t := \tau^t(\ell_{\omega_t|\omega}).$$

Note that $\ell_{\omega_t|\omega}$, and consequently $c^t$, are selfadjoint elements of $\mathscr{O}$.

**(Reg3)** The map

$$\mathbb{R} \ni t \mapsto \ell_{\omega_t|\omega} \in \mathscr{O},$$

is differentiable at $t = 0$.

Let

$$\sigma = \frac{\mathrm{d}}{\mathrm{d}t}\ell_{\omega_t|\omega}\big|_{t=0} = \frac{\mathrm{d}}{\mathrm{d}t}c^t\big|_{t=0}. \tag{26.1}$$

**Proposition 26.1** *1. For all $t, s \in \mathbb{R}$, one has*

$$\ell_{\omega_{t+s}|\omega} = \tau^{-t}(\ell_{\omega_s|\omega}) + \ell_{\omega_t|\omega},$$
$$c^{t+s} = c^s + \tau^s(c^t).$$

*2. For all $t \in \mathbb{R}$, $\log \Delta_{\omega_t|\omega} = \log \Delta_\omega + \ell_{\omega_t|\omega}$, and for $\alpha \in \mathrm{i}\mathbb{R}$,*

$$[D\omega_t : D\omega]_\alpha = \mathrm{e}^{\alpha(\log \Delta_\omega + \ell_{\omega_t|\omega})}\mathrm{e}^{-\alpha \log \Delta_\omega}.$$

*3. For all $t \in \mathbb{R}$, $\mathrm{Ent}(\omega_t|\omega) = -\omega(c^t)$.*
*4. Setting $\sigma_t = \tau^t(\sigma)$ for $t \in \mathbb{R}$, one has*

$$\ell_{\omega_t|\omega} = \int_0^t \sigma_{-s}\mathrm{d}s, \qquad c^t = \int_0^t \sigma_s \mathrm{d}s,$$

*and*

$$\mathrm{Ent}(\omega_t|\omega) = -\int_0^t \omega_s(\sigma)\mathrm{d}s. \tag{26.2}$$

*5. $\omega(\sigma) = 0$.*
*6. If $(\mathscr{O}, \tau, \omega)$ is* TRI *with time-reversal $\Theta$, then $\Theta(c^t) = c^{-t}$ and $\Theta(\sigma) = -\sigma$.*

This proposition is the direct quantum analogue of Proposition 24.1. $\sigma$ is the entropy production observable of $(\mathscr{O}, \tau, \omega)$ and (26.2) is the entropy balance equation.

Theorem 26.1 sheds light on the introduction to non-equilibrium quantum statistical mechanics presented in Section 21 in the context of the LP systems.

**Proposition 26.2** *Suppose that $(\mathscr{O}, \tau, \omega)$ is an LP system and that $V \in \mathrm{Dom}(\delta_\omega)$. Then* **(Reg1)**, **(Reg2)** *and* **(Reg3)** *hold, and $\sigma$ in* (26.1) *is equal to $\delta_\omega(V)$.*

The two basic questions of non-equilibrium quantum statistical mechanics, **(QIII)** and **(QIV)** formulated in Section 21, extend in the obvious way to the more general setting considered here.

Motivated by the analogies between Theorem 24.1 and Theorem 26.1, we consider the map

$$\mathrm{i}\mathbb{R} \ni \alpha \mapsto [D\omega_{-t} : D\omega]_\alpha \in \mathscr{O}$$

as the quantum analogue characterization of phase space contraction for $(\mathscr{O}, \tau, \omega)$ at time $t$.

## Part VIII

**How should one define quantum entropy production?** Entropy production quantifies irreversibility and information loss and is directly linked to the Second Law of Thermodynamics. While entropy production is a well-defined concept in classical physics, its interpretation becomes multifaceted and subtler in the quantum domain. In particular, multiple non-equivalent notions of entropy production arise.

## 27 Quantum Phase Space Contraction and Entropy Production Observable

The most direct approach to defining quantum entropy production proceeds by quantizing the corresponding classical entropy production observable, and has been described in Sections 21 and 26. This route has been adopted in [79, 123] and played an important role in the development of the subject.

The main criticism of this approach concerns the following two points:

1. The experimental status of the selfadjoint observable $c^t = \int_0^t \sigma_s \mathrm{d}s$ is questionable.
2. The finite time fluctuation relation, the quantum analog of (24.1), fails for $c^t$ as an operator-valued observable. More precisely, if $Q_t$ is the spectral measure for $\omega$ and $c^t$, the relation
$$\frac{\mathrm{d}\overline{Q}_t}{\mathrm{d}Q_t}(s) = \mathrm{e}^{-s}.$$
*does not hold* except in special cases; see [72, Exercise 3.3].

Point **(a)** is connected to several perennial aspects of the so-called standard (or orthodox) view of the conceptual foundations of quantum mechanics. There are many excellent discussions of this view in the literature, beginning with the classical book of von Neumann [103]. Here we limit ourselves to two further references: [67, Section 7] and [140]. Point **(b)**, on the other hand, was emphasized forcefully in [138].

We do not think that the validity of the finite time fluctuation relation can be raised to a fundamental principle of what is observable in quantum statistical mechanics, and hence we do not find criticism **(b)** tenable. Although **(a)** obviously must be taken more seriously, it is reasonable to accept that any proposal for the average entropy production over a time interval $[0, t]$ of $(\mathscr{O}, \tau, \omega)$ gives the same value $\omega(c^t)$, and this is certainly true for all the known proposals. Thus, the questions **(QIII)** and **(QIV)** of Section 21 are unaffected by **(a)**. The entropy production observable is also a natural starting point in the study of the linear response theory, Onsager reciprocity relations, and near-equilibrium fluctuation-dissipation mechanism [75–78]; see also Section 12. It is the analysis of far from equilibrium entropy production fluctuations that brings **(a)** to focus.

We however emphasize that some foundational issues about the choice of entropy production observable $\sigma$ remain, even if one focuses only on the averages $\omega(c^t)$. One of them is our next topic.

## 28 Ruelle's Decomposition of Entropy Production

Shortly after the introduction of NESS and entropy production observable in [79, 123], David Ruelle wrote an important but little known paper [124] concerning the interpretation of the quantum entropy production. We start with a brief summary of [124] adjusting certain points to allow for a clearer comparison with subsequent developments.

Consider a finite open quantum system on the Hilbert space $\mathscr{K} = \otimes_{j=1}^{M} \mathscr{K}_j$, in the directly coupled reservoir setting. With a more involved notation the arguments easily extend to a general open quantum system. For $j = 1, \ldots, M$ we set $\mathscr{K}_{\setminus j} := \bigotimes_{i \neq j} \mathscr{K}_i$. Let[19]

$$\omega_{tj} := \mathrm{tr}_{\mathscr{K}_{\setminus j}} \omega_t$$

be the state of the $j$-th reservoir at the time $t$ and

$$\omega_t^{\mathrm{dec}} := \bigotimes_{j=1}^{M} \omega_{tj}.$$

Note that $\omega_0^{\mathrm{dec}} = \omega$. Let[20]

$$\Delta S(t) := S(\omega_t^{\mathrm{dec}}) - S(\omega),$$

and

$$\Delta \mathfrak{S}(t) := -\mathrm{Ent}(\omega_t^{\mathrm{dec}}|\omega).$$

Obviously, $\Delta \mathfrak{S}(t) \geq 0$. Moreover, since $S(\omega_t^{\mathrm{dec}}) = -\mathrm{tr}(\omega_t^{\mathrm{dec}} \log \omega_t^{\mathrm{dec}}) = -\mathrm{tr}(\omega_t \log \omega_t^{\mathrm{dec}})$ and $S(\omega) = S(\omega_t)$, one has

$$\Delta S(t) = -\mathrm{tr}(\omega_t(\log \omega_t^{\mathrm{dec}} - \log \omega_t)) = -\mathrm{Ent}(\omega_t|\omega_t^{\mathrm{dec}}) \geq 0.$$

The starting point of [124] is the identity

$$\begin{aligned} \int_0^t \omega_s(\sigma)\mathrm{d}s &= -\mathrm{Ent}(\omega_t|\omega) = \mathrm{tr}(\omega_t(\log \omega_t - \log \omega)) \\ &= \mathrm{tr}(\omega_t(\log \omega_t - \log \omega_t^{\mathrm{dec}})) + \mathrm{tr}(\omega_t(\log \omega_t^{\mathrm{dec}} - \log \omega)) \qquad (28.1) \\ &= -\mathrm{Ent}(\omega_t|\omega_t^{\mathrm{dec}}) - \mathrm{Ent}(\omega_t^{\mathrm{dec}}|\omega) = \Delta S(t) + \Delta \mathfrak{S}(t), \end{aligned}$$

expressing the mean entropy production over the time interval $[0, t]$ as the sum of *mutual information* $\Delta S(t)$ and a relative entropy-cost $\Delta \mathfrak{S}(t)$ associated with the reduced reservoir dynamics.

[19] $\mathrm{tr}_{\mathscr{K}_{\setminus j}}$ denotes the partial trace over $\mathscr{K}_{\setminus j}$.

[20] We recall that $S(\nu) = -\mathrm{tr}(\nu \log \nu)$ denotes the von Neumann entropy of $\nu$.

The decomposition (28.1) remains valid for infinitely extended reservoirs and can be justified either by a thermodynamic limit argument or directly by an application of Corollary 5.20 and identity (5.22) of [108]

In [124], Ruelle proposes a heuristic framework in which $\Delta S(t)$ is expected to dominate (28.1). This perspective touches on foundational issues in non-equilibrium statistical mechanics, particularly concerning the role and structure of thermal reservoirs in open quantum systems. Ruelle's program remains only partially understood, and much work remains to be done.

Finally, we note that the Ruelle program is not specific to the quantum setting; the same analysis applies, and the same questions arise, in open classical systems, where equally little is known.

## 29 Two-Time Measurement Entropy Production (TTMEP)

In the finite dimensional setting, the notion of *two-times entropy production* goes back to [91, 136]. Our presentations follows [72].

Consider a finite quantum dynamical system $(\mathscr{O}_{\mathscr{K}}, \tau, \omega)$. The observable to be measured is described by a partition of unity $(P_a)_{a\in\mathscr{A}}$ on $\mathscr{K}$[21] indexed by a finite alphabet $\mathscr{A}$ labeling the possible outcomes of the measurement. The two-times measurement protocol goes as follows. At time $t = 0$, when the system was in the state $\omega$, the first measurement is performed and the outcome $a \in \mathscr{A}$ is observed with probability

$$p(a) = \mathrm{tr}(\omega P_a).$$

After this first measurement, the system is in the reduced state

$$\frac{1}{p(a)} P_a \omega P_a,$$

which evolves over the time interval $[0, t]$[22] to

$$\frac{1}{p(a)} \mathrm{e}^{-\mathrm{i}tH} P_a \omega P_a \mathrm{e}^{\mathrm{i}tH}.$$

The second measurement, at the time $t$, yields the outcome $a' \in \mathscr{A}$ with probability

$$p_t(a'|a) = \frac{1}{p(a)} \mathrm{tr}\left(\mathrm{e}^{-\mathrm{i}tH} P_a \omega P_a \mathrm{e}^{\mathrm{i}tH} P_{a'}\right).$$

Finally, the probability of observing the pair $(a, a')$ in the two-times measurement protocol is

$$p_t(a, a') = p_t(a'|a)p(a) = \mathrm{tr}\left(\mathrm{e}^{-\mathrm{i}tH} P_a \omega P_a \mathrm{e}^{\mathrm{i}tH} P_{a'}\right).$$

[21] The $P_a$ are orthogonal projections such that $\sum_{a\in\mathscr{A}} P_a = \mathbb{1}$.

[22] We allow for $t < 0$.

Starting with the above protocol, there are two distinct routes to define measurement based entropy production. We describe here the one which is the main topic of this section. The second route involving repeated measurements is reviewed in Section 34.

Assume that $\omega > 0$ and consider the partition of unity $(P_a)_{a\in\mathscr{A}}$ that arises through the spectral decomposition of $\omega$,

$$\omega = \sum_{a\in\mathscr{A}} \lambda_a P_a,$$

where the eigenvalues $\lambda_a$ are assumed to be distinct. The entropy production random variable $\mathscr{E} : \mathscr{A} \times \mathscr{A} \to \mathbb{R}$ is defined by

$$\mathscr{E}(a, a') = \log \lambda_{a'} - \log \lambda_a,$$

and its probability distribution with respect to $p_t$ is denoted by $Q_t$,

$$Q_t(s) = \sum_{\mathscr{E}(a,a')=s} p_t(a, a').$$

The statistics of TTMEP over the time interval $[0, t]$ is described by $Q_t$. For $\alpha \in \mathbb{C}$, we set

$$\mathfrak{F}_t^{\mathrm{ttm}}(\alpha) := \int_{\mathbb{R}} \mathrm{e}^{-\alpha s} \mathrm{d}Q_t(s).$$

We then have:

**Proposition 29.1** *1.*

$$\mathfrak{F}_t^{\mathrm{ttm}}(\alpha) = \omega([D\omega_{-t} : D\omega]_\alpha) = \mathrm{tr}(\omega_{-t}^\alpha \omega^{1-\alpha}). \tag{29.1}$$

*2.*

$$\int_{\mathbb{R}} s \, \mathrm{d}Q_t(s) = -\mathrm{Ent}(\omega_t|\omega).$$

*In particular* $\int_{\mathbb{R}} s \, \mathrm{d}Q_t(s) \geq 0$ *with equality iff* $\omega = \omega_t$.

*In the remaining statements we assume that the system is* TRI.

*3.*

$$\mathfrak{F}_t^{\mathrm{ttm}}(\alpha) = \mathfrak{F}_t^{\mathrm{ttm}}(1 - \bar{\alpha}).$$

*4.*

$$Q_t(-s) = \mathrm{e}^{-s} Q_t(s). \tag{29.2}$$

The identity (29.2) is sometimes called *finite time fluctuation relation*.

We now turn to a general modular quantum dynamical system $(\mathscr{O}, \tau, \omega)$ satisfying **(Reg1)**, **(Reg2)** and **(Reg3)**. For $t \in \mathbb{R}$ and $\alpha \in \mathrm{i}\mathbb{R}$, we set

$$\mathfrak{F}_t^{\mathrm{ttm}}(\alpha) := \omega\left([D\omega_{-t} : D\omega]_\alpha\right).$$

When $(\mathscr{O}, \tau, \omega)$ is finite, this reduces to (29.1).

**Proposition 29.2** *1. There exists unique probability measure $Q_t$ on $\mathbb{R}$ such that*

$$\mathfrak{F}_t^{\mathrm{ttm}}(\alpha) = \int_{\mathbb{R}} \mathrm{e}^{-\alpha s} \mathrm{d}Q_t(s).$$

*2. $\int_{\mathbb{R}} s \, \mathrm{d}Q_t(s) = -\mathrm{Ent}(\omega_t|\omega)$. In particular, $\int_{\mathbb{R}} s \, \mathrm{d}Q_t(s) \geq 0$ with equality iff $\omega = \omega_t$.*

*3. For $\alpha \in \mathrm{i}\mathbb{R}$,*

$$\mathfrak{F}_t^{\mathrm{ttm}}(\alpha) = \langle \Omega, \Delta_{\omega_{-t}|\omega}^{\alpha} \Omega \rangle.$$

*In particular, $Q_t$ is the spectral measure of the selfadjoint operator $-\log \Delta_{\omega_{-t}|\omega}$ for the vector $\Omega$.*

*In the remaining statements we assume that $(\mathscr{O}, \tau, \omega)$ is* TRI.

*4. The map $\mathrm{i}\mathbb{R} \ni \alpha \mapsto \mathfrak{F}_t^{\mathrm{ttm}}(\alpha)$ has an analytic extension to the vertical strip $0 < \mathrm{Re}\, z < 1$ that is bounded and continuous on its closure.*

*5. For any $\alpha$ satisfying $0 \leq \mathrm{Re}\, \alpha \leq 1$,*

$$\mathfrak{F}_t^{\mathrm{ttm}}(\alpha) = \mathfrak{F}_t^{\mathrm{ttm}}(1 - \bar{\alpha}).$$

*6. Let $\mathfrak{r} : \mathbb{R} \to \mathbb{R}$ be the reflection $\mathfrak{r}(s) = -s$ and $\overline{Q}_t = Q_t \circ \mathfrak{r}$. Then the measures $Q_t$ and $\overline{Q}_t$ are equivalent and*

$$\frac{\mathrm{d}\overline{Q}_t}{\mathrm{d}Q_t}(s) = \mathrm{e}^{-s}.$$

The measure $Q_t$ describes the statistics of the two-time measurement entropy production of $(\mathscr{O}, \tau, \omega)$ over the time interval $[0, t]$.

## 30 Thermodynamic Limit of TTMEP in Open Quantum Spin Systems

The general modular theoretic approach to $Q_t$ described in the previous section requires justification of the thermodynamic limit for concrete models. In this section we address this question in the context of open quantum lattice spin systems introduced in Section 22. We denote by $Q_{t,\Lambda}$ the law of the TTMEP for $(\mathscr{O}_\Lambda, \tau_\Lambda, \omega_\Lambda)$ over the time interval $[0, t]$ with $\omega_\Lambda$ defined by (22.1) and (22.2). Convergence of probability measures is understood in the weak sense.

**Theorem 30.1** *Suppose that each $\omega_{\beta_j}$ is a thermodynamic limit point $\beta_j$-KMS state on $\mathscr{O}_{R_j}$. Let*

$$\Lambda_a = S \cup \left( \bigcup_{j=1}^{M} \Lambda_{j,a} \right)$$

*be a net in $\mathfrak{G}_{\mathrm{fin}}$ such that for each $j$,*

$$\lim_{\Lambda_{j,a} \to \infty} \overline{\omega}_{\Lambda_{j,a}} = \omega_{\beta_j}.$$

*Then, for all* $t \in \mathbb{R}$,

$$\lim_{\Lambda_a \to \infty} Q_{t,\Lambda_a} = Q_t.$$

For the proof and additional information, see [25].

## 31 Ancilla State Tomography

*Ancilla state tomography* is a technique which extracts information on the state of a quantum system from the outcome of measurements performed on an auxiliary system, the *ancilla*, coupled to the system of interest. In this section, following [24], we show how this technique allows for an indirect measurement of the function $\mathfrak{F}_t^{\mathrm{ttm}}$.

We start with the finite system of Section 29. The state of the ancilla is described by a spin 1/2 on $\mathbb{C}^2$. We denote by $v_\pm$ the eigenvectors of the Pauli matrix $\sigma_z$ associated to the eigenvalues $\pm 1$. The state of ancilla is described by a density matrix $\rho_a$ such that $\langle v_+, \rho_a v_- \rangle \neq 0$. The Hilbert space of the coupled system is $\widehat{\mathscr{K}} = \mathscr{K} \otimes \mathbb{C}^2$, and its initial state is $\widehat{\omega} = \omega \otimes \rho_a$. We introduce the following family of Hamiltonians, indexed by $\alpha \in \mathrm{i}\mathbb{R}$,

$$\widehat{H}_\alpha = \mathrm{e}^{\frac{\alpha}{2} \log \omega \otimes \sigma_z} (H \otimes \mathbb{1}) \, \mathrm{e}^{-\frac{\alpha}{2} \log \omega \otimes \sigma_z}.$$

Setting $N := |v_-\rangle\langle v_+|$, a computation gives

$$\mathrm{tr}\left( \mathrm{e}^{-\mathrm{i}t\widehat{H}_\alpha} \widehat{\omega} \mathrm{e}^{\mathrm{i}t\widehat{H}_\alpha} (\mathbb{1} \otimes N) \right) = \langle v_+, \rho_a v_- \rangle \, \mathfrak{F}_t^{\mathrm{ttm}}(\alpha). \tag{31.1}$$

The left-hand side in (31.1) is interpreted as *entropic ancilla state tomography* of the finite quantum system over the interval $[0, t]$.

In the particular case of a finite LP system where $H = H_{\mathrm{fr}} + V$ with $[\log \omega, H_{\mathrm{fr}}] = 0$, one has

$$\widehat{H}_\alpha = H \otimes \mathbb{1} + \widehat{W}_\alpha,$$

where

$$\widehat{W}_\alpha = \tfrac{1}{2} W_\alpha \otimes (\mathbb{1} + \sigma_z) + \tfrac{1}{2} W_{-\alpha} \otimes (\mathbb{1} - \sigma_z), \tag{31.2}$$

and

$$W_\alpha = \varsigma_\omega^{-\mathrm{i}\alpha/2}(V) - V. \tag{31.3}$$

Turning to the general modular quantum dynamical system of Section 29, we now consider a LP system satisfying $V \in \mathrm{Dom}(\delta_\omega)$. Let $\widehat{\mathscr{O}} := \mathscr{O} \otimes \mathscr{O}_{\mathbb{C}^2}$ and $\widehat{\tau}^t = \tau^t \otimes \mathrm{Id}$. For $\alpha \in \mathrm{i}\mathbb{R}$, $\widehat{W}_\alpha$ and $W_\alpha$ are given by (31.2) and (31.3). Note that $W_\alpha \in \mathscr{O}_{\mathrm{sa}}$ and $\widehat{W}_\alpha \in \widehat{\mathscr{O}}_{\mathrm{sa}}$. Let $\widehat{\tau}_\alpha$ be the perturbation of $\widehat{\tau}$ by $\widehat{W}_\alpha$. Let $N$ as above and $\widehat{\omega} = \omega \otimes \rho_a$. Then, again, for all $t \in \mathbb{R}$,

$$\widehat{\omega}\left( \widehat{\tau}_\alpha^t (\mathbb{1} \otimes N) \right) = \langle v_+, \rho_a v_- \rangle \, \mathfrak{F}_t^{\mathrm{ttm}}(\alpha).$$

We refer the reader to [37, 39, 49, 65, 74, 98, 113] for related theoretical studies in the physics literature and to [6, 19, 20, 109] for experimental implementations.

## 32 Limitations of TTMEP

The statistics of the two-time measurement entropy production was initially introduced in the context of finite quantum systems (or, slightly more generally, confined quantum systems with a possibly infinite discrete energy spectra). Experimental studies have been carried out in this same setting, often relying on ancilla state tomography. The thermodynamic limit of these statistics is stable and preserves the connection with modular theory and ancilla state tomography, although – to the best of our knowledge – the statistics of the two-time measurement entropy production of infinitely extended system has not been experimentally explored. Obviously, the ancilla state tomography link is central to the physical relevance of the two-time measurement protocol for large quantum systems. It tells us that if the protocol could have been implemented, then the resulting statistics would coincide with those predicted by the ancilla-based tomography. This is certainly satisfactory.

On the other hand, the TTMEP exhibits a surprising degree stability (or rigidity) with respect to the instant of the first measurement – an effect with no classical counterpart – which has been recently investigated in [23–25, 27]. Suppose that the first measurement of the entropy production observable is not performed at $t = 0$, when the system was in the reference state $\omega$ from which the observable is defined, but instead at the later time $T$, when the system is in the state $\omega \circ \tau_T$. A second measurement is then performed at time $T + t$. After passing to the thermodynamic limit, and under a general and natural dynamical ergodicity assumption, the statistics of the TTMEP turn out to be independent of the instant $T$ of the first measurement. This effect arises from the invasive decoherence induced by the first measurement, which dominates the resulting statistics in the thermodynamic limit. This stability should be further examined both theoretically and experimentally before drawing any final conclusions regarding the foundational role of TTMEP in large quantum systems.

## 33 Bessis-Moussa-Villani Entropy Production

To motivate the introduction of this notion of entropy production, we return to the classical setting of Section 24. The variational formula for the classical relative entropy[23] gives that for $\alpha \in \mathbb{R}$,

$$\log\left[\int_{\mathscr{X}} \mathrm{e}^{-\alpha \int_0^t \sigma_s \mathrm{d}s} \mathrm{d}\omega\right] = \sup_{\nu}\left[S(\nu|\omega) - \alpha \int_{\mathscr{X}} \int_0^t \sigma_s \mathrm{d}s \mathrm{d}\nu\right],$$

where the supremum is taken over all Borel probability measures $\nu$ on $\mathscr{X}$. For finite quantum systems, one has

$$\log \mathrm{tr}\left[\mathrm{e}^{\log \omega - \alpha \int_0^t \sigma_s \mathrm{d}s}\right] = \sup_{\nu}\left[S(\nu|\omega) - \alpha \int_0^t \nu(\sigma_s)\mathrm{d}s\right],$$

[23] See [108] or Theorem 2.1 in [85].

where the supremum is taken over all density matrices $\nu$ on the system Hilbert space $\mathscr{K}$. We set

$$\mathfrak{F}_t^{\mathrm{BMV}}(\alpha) = \mathrm{tr}\left[\mathrm{e}^{\log\omega - \alpha\int_0^t \sigma_s \mathrm{d}s}\right]. \tag{33.1}$$

This function has been introduced and studied in [72]. The acronym BMV in (33.1) reflects the connection of the right-hand side with the celebrated Bessis–Moussa–Villani conjecture [32][24], which was proved by Herbert Stahl [132] in 2013.

**Theorem 33.1** *Let $A$ and $B$ be $n \times n$ Hermitian matrices, and assume that $B$ is positive semidefinite. Define*

$$[0,\infty) \ni \alpha \mapsto f(\alpha) = \mathrm{tr}\left(\mathrm{e}^{A-\alpha B}\right).$$

*Then there exists a non-negative Borel measure $\mu$ on $[0,\infty)$ such that*

$$f(\alpha) = \int_0^\infty \mathrm{e}^{-\alpha s}\, d\mu(s)$$

*for all $\alpha \geq 0$.*

Stahl's theorem gives that there exists a Borel probability measure $Q_t^{\mathrm{BMV}}$ on $\mathbb{R}$ such that, for $\alpha \in \mathbb{C}$,

$$\mathfrak{F}_t^{\mathrm{BMV}}(\alpha) = \int_{\mathbb{R}} \mathrm{e}^{-\alpha s}\mathrm{d}Q_t^{\mathrm{BMV}}(s). \tag{33.2}$$

We will refer to $Q_t^{\mathrm{BMV}}$ as the statistics of the BMV entropy production over the time interval $[0,t]$. Except in trivial cases, the measure $Q_t^{\mathrm{BMV}}$ is not atomic. We have

**Proposition 33.2** *1.* $\int_{\mathbb{R}} s\,\mathrm{d}Q_t^{\mathrm{BMV}}(s) = -\mathrm{Ent}(\omega_t|\omega)$.

*In the remaining statements we assume that the finite quantum system $(\mathscr{C}_\mathscr{K}, \tau, \omega)$ is* TRI.

2. *For $\alpha \in \mathbb{C}$,*
$$\mathfrak{F}_t^{\mathrm{BMV}}(\alpha) = \mathfrak{F}_t^{\mathrm{BMV}}(1-\bar{\alpha}).$$

3. *Let $\mathfrak{r} : \mathbb{R} \to \mathbb{R}$ be the reflection $\mathfrak{r}(s) = -s$ and $\overline{Q}_t^{\mathrm{BMV}} = Q_t^{\mathrm{BMV}} \circ \mathfrak{r}$. Then the measures $Q_t^{\mathrm{BMV}}$ and $\overline{Q}_t^{\mathrm{BMV}}$ are equivalent and*
$$\frac{\mathrm{d}\overline{Q}_t^{\mathrm{BMV}}}{\mathrm{d}Q_t^{\mathrm{BMV}}}(s) = \mathrm{e}^{-s}.$$

In the general setting of a modular $C^*$-quantum dynamical systems satisfying **(Reg1)**, **(Reg2)**, and **(Reg3)**, one has, for $\alpha \in \mathbb{R}$,

$$\log\|\mathrm{e}^{\frac{1}{2}(\log\Delta_\omega - \alpha\int_0^t \sigma_s \mathrm{d}s)}\Omega\|^2 = \sup_\nu\left[S(\nu|\omega) - \alpha\int_0^t \nu(\sigma_s)\mathrm{d}s\right], \tag{33.3}$$

[24] See also [95].

where the supremum is taken over all states $\nu$ on $\mathscr{O}$. For finite quantum systems the left-hand side of (33.3) is a rewriting of (33.3) in modular terms. For $\alpha \in \mathbb{R}$, we define

$$\mathfrak{F}_t^{\mathrm{BMV}}(\alpha) = \|\mathrm{e}^{\frac{1}{2}(\log \Delta_\omega - \alpha \int_0^t \sigma_s \mathrm{d}s)}\Omega\|^2.$$

It follows from Araki's perturbation theory of the KMS structure that $\mathfrak{F}_t^{\mathrm{BMV}}(\alpha)$ is finite for all $\alpha \in \mathbb{R}$, and that the map $\mathbb{R} \ni \alpha \mapsto \mathfrak{F}_t^{\mathrm{BMV}}(\alpha)$ extends to an entire analytic function. We also have

$$\frac{\partial}{\partial \alpha}\mathfrak{F}_t^{\mathrm{BMV}}(\alpha)\Big|_{\alpha=0} = \mathrm{Ent}(\omega_t|\omega).$$

In addition, if $(\mathscr{O}, \tau, \omega)$ is TRI, then for all $\alpha \in \mathbb{C}$,

$$\mathfrak{F}_t^{\mathrm{BMV}}(\alpha) = \mathfrak{F}_t^{\mathrm{BMV}}(1-\bar{\alpha}). \tag{33.4}$$

The existence of the BMV measure satisfying (33.2) is not known except for finite quantum systems and in the thermodynamic limit setting; see the conjecture at the end of this section.

Returning to the thermodynamic limit of non-equilibrium open quantum spin systems, we have

**Theorem 33.3** *Suppose that each $\omega_{\beta_j}$ is a thermodynamic limit point $\beta_j$-KMS state on $\mathscr{O}_{R_j}$. Let*

$$\Lambda_a = S \cup \left(\bigcup_{j=1}^{M} \Lambda_{j,a}\right)$$

*be a net in $\mathfrak{G}_{\mathrm{fin}}$ such that for each $j$,*

$$\lim_{\Lambda_{j,a}\to\infty} \omega_{\Lambda_{j,a}}, = \omega_{\beta_j}.$$

*where $\omega_{\Lambda_{j,a}}$ is the same as in Theorem 22.1. Then, for all $t \in \mathbb{R}$, the limit*

$$Q_t^{\mathrm{BMV}} := \lim_{\Lambda_a\to\infty} Q_{t,\Lambda_a}^{\mathrm{BMV}}$$

*exists and for all $\alpha \in \mathbb{R}$,*

$$\mathfrak{F}_t^{\mathrm{BMV}}(\alpha) = \int_{\mathbb{R}} \mathrm{e}^{-\alpha s}\mathrm{d}Q_t^{\mathrm{BMV}}.$$

The proof of this result is implicit in [25].

The BMV entropy possesses several appealing features. By Proposition 33.2(i), it correctly predicts the entropy production of NESS, and the symmetry (33.4), with its suitable generalization, leads to the linear response theory of NESS; see [72]. The

function $\mathfrak{F}_t^{\mathrm{BMV}}$ is entire analytic without invoking any additional regularity assumptions.

Many interesting questions remain open; we mention here perhaps the two most important ones.

**Question 1** For finite quantum systems, the physical status of the statistics $Q_t^{\mathrm{BMV}}$ is unclear. Are these statistics experimentally accessible?

**Question 2** At present, for infinitely extended systems the existence of the probability measures $Q_t^{\mathrm{BMV}}$ can only be justified by thermodynamic limit arguments. These measures would exist for any modular $C^*$-dynamical system $(\mathscr{O}, \tau, \omega)$ provided that the following KMS extension of the BMV conjecture holds.

**Conjecture.** Let $(\mathfrak{M}, \tau)$ be a $W^*$-dynamical system on a Hilbert space $\mathscr{H}$ and $\omega(A) = (\Omega, A\Omega)$ a faithful $(\tau, \beta)$-KMS vector state on $\mathfrak{M}$. Let $\mathscr{L}$ be the standard Liouvillean of $\tau$, $V \in \mathfrak{M}$ selfadjoint, and consider the perturbed $W^*$-dynamics on $\mathfrak{M}$ given by

$$\tau_V^t(A) = \mathrm{e}^{\mathrm{i}t(\mathscr{L}+V)} A \mathrm{e}^{-\mathrm{i}t(\mathscr{L}+V)}.$$

Let

$$\omega_V(A) = \frac{(\Omega_V, A\Omega_V)}{\|\Omega_V\|^2}, \qquad \Omega_V = \mathrm{e}^{-\frac{\beta}{2}(\mathscr{L}+V)}\Omega,$$

be the perturbed $(\tau_V, \beta)$-KMS vector state on $\mathfrak{M}$. Then there exists a Borel probability measure $P$ on $\mathbb{R}$ such that for all $\alpha \in \mathbb{R}$,

$$\|\Omega_{\alpha V}\|^2 = \int_{\mathbb{R}} \mathrm{e}^{-\alpha s} \mathrm{d}P(s).$$

In finite dimension, the above conjecture is equivalent to the BMV conjecture positively resolved by Stahl [132]. The Stahl method, however, is restricted to finite-dimensional matrices, and novel ideas are needed to address the above general conjecture.

The material discussed in this section has not previously appeared in print.

## 34 Entropy Production of Repeated Quantum Measurements

Besides the dynamical system approach to classical entropy production, in which the reference state plays an important role, an altogether different random path approach has been developed in [92, 96, 97], that does not make use of the reference state and is applicable to stochastic processes. Its quantum formulation in the setting of repeated quantum measurement processes goes back to [38], and was elaborated in [21, 22]. The advent of experimental methods in cavity and circuit QED, and in particular the experimental breakthroughs of the Haroche–Raimond and Wineland groups [68, 70, 141], make this complementary approach particularly relevant.

Let $\mathscr{H}$ be a Hilbert space and let $\mathscr{B}(\mathscr{H})$ denote the algebra of bounded operators on $\mathscr{H}$. A linear completely positive map

$$\Phi : \mathscr{B}(\mathscr{H}) \to \mathscr{B}(\mathscr{H})$$

is called a *quantum channel*. The channel $\Phi$ is said to be *unital* if it preserves the identity operator, *i.e.*, satisfies $\Phi(\mathbb{1}) = \mathbb{1}$. The predual of a quantum channel $\Phi$ is the map $\Phi^*$ on the trace class operators on $\mathscr{H}$ such that

$$\mathrm{tr}(\rho\Phi(A)) = \mathrm{tr}(\Phi^*(\rho)A)$$

for all $A \in \mathscr{B}(\mathscr{H})$. If $\Phi$ is unital, then $\Phi^*$ is trace preserving and maps density matrices to density matrices.

**Definition 34.1** Given a unital quantum channel $\Phi$ on a separable Hilbert space $\mathscr{H}$ and a Polish space $\mathbf{A}$, a **$(\Phi, A)$-instrument** is a $\sigma$-additive map $\mathscr{J}$ from the Borel $\sigma$-algebra $\mathscr{A}$ of $\mathbf{A}$ to the set of completely positive maps on $\mathscr{B}(\mathscr{H})$ satisfying

$$\mathscr{J}(\mathbf{A}) = \Phi.$$

An instrument models a repeatable quantum measurement as follows. Let the system be in the state (density matrix) $\rho$ at time $t = 1$. A measurement is performed, and a random outcome $\omega_1 \in \mathbf{A}$ is observed with the law $\mathrm{tr}(\mathscr{J}(\mathrm{d}\omega_1)^*(\rho))$. After the measurement, the system state conditioned on $\omega_1 \in A_1$ is

$$\rho_{A_1} = \frac{\mathscr{J}(A_1)^*(\rho)}{\mathrm{tr}(\mathscr{J}(A_1)^*(\rho))}.$$

The law of the outcome $\omega_2$ of the next measurement at time $t = 2$ is $\mathrm{tr}(\mathscr{J}(\mathrm{d}\omega_2)^*(\rho_{A_1}))$, and the state of the system after the second measurement conditioned on $(\omega_1, \omega_2) \in A_1 \times A_2$ is

$$\rho_{A_1A_2} = \frac{\mathscr{J}(A_2)^*(\rho_{A_1})}{\mathrm{tr}(\mathscr{J}(A_2)^*(\rho_{A_1}))}.$$

The probability that the observed $(\omega_1, \omega_2)$ is in $A_1 \times A_2$ is

$$\begin{aligned}&\mathrm{tr}(\mathscr{J}(A_1)^*(\rho))\,\mathrm{tr}(\mathscr{J}(A_2)^*(\rho_{A_1})) = \mathrm{tr}(\mathscr{J}(A_2)^* \circ \mathscr{J}(A_1)^*(\rho))\\ &\quad = \mathrm{tr}(\rho\,\mathscr{J}(A_1) \circ \mathscr{J}(A_2)(\mathbb{1})).\end{aligned}$$

Continuing in this way, one derives that, after $n$ repeated measurements, the probability of observing a sequence of outcomes $(\omega_1, \ldots, \omega_n) \in A_1 \times \cdots \times A_n$ is given by

$$\mathbb{P}_n(A_1 \times \cdots \times A_n) = \mathrm{tr}\left(\rho\,\mathscr{J}(A_1) \circ \cdots \circ \mathscr{J}(A_n)(\mathbb{1})\right).$$

This defines a probability measure $\mathbb{P}_n$ on $\Omega_n = \mathbf{A}^n$, and the unitality of $\mathscr{J}(\mathbf{A}) = \Phi$ implies that the family $(\mathbb{P}_n)_{n\in\mathbb{N}}$ is consistent. Let $\mathbb{P}$ be the unique probability measure

induced on $\Omega = \mathbf{A}^{\mathbb{N}}$, equipped with the usual product $\sigma$-algebra $\mathscr{F}$, and the filtration $(\mathscr{F}_n)_{n\in\mathbb{N}}$ generated by the cylinders

$$[A_1, \ldots, A_n] = \{\omega \in \Omega \mid (\omega_1, \ldots, \omega_n) \in A_1 \times \cdots \times A_n\}, \qquad A_1, \ldots, A_n \in \mathscr{A}.$$

We assume that the state $\rho$ is $\Phi$-invariant. Then $\mathbb{P}\circ\phi^{-1} = \mathbb{P}$ where $\phi$ is the left shift on $\Omega$. The dynamical system $(\Omega, \phi, \mathbb{P})$ thus describes the outcomes of the repeated measurement process. The measure $\mathbb{P}$ is sometimes called the *$\rho$-statistics* of the instrument $\mathscr{J}$.

A *local reversal* on $\mathbf{A}$ is a measurable involution $\theta : \mathbf{A} \to \mathbf{A}$. The associated $\theta$-time reversal on $\Omega_n$ is the involution

$$\theta_n(\omega_1, \ldots, \omega_n) = (\theta(\omega_n), \ldots, \theta(\omega_1)).$$

The family of probability measures $(\widehat{\mathbb{P}}_n)_{n\in\mathbb{N}}$ defined by

$$\widehat{\mathbb{P}}_n = \mathbb{P}_n \circ \theta_n$$

is also consistent. By Kolmogorov's extension theorem, there exists a unique $\phi$-invariant $\widehat{\mathbb{P}} \in \mathscr{P}_\phi(\Omega)$ which describes the statistics of the $\theta$-time reversal of the dynamical system $(\Omega, \phi, \mathbb{P})$.

We shall say that the pair $(\Omega, \mathbb{P})$ is *$\theta$-time-reversal invariant* if $\mathbb{P} = \widehat{\mathbb{P}}$, *i.e.,* if $\mathbb{P}_n = \widehat{\mathbb{P}}_n$ for all $n \in \mathbb{N}$.

The relative entropy of two probability measures $\mathbb{P}$ and $\mathbb{Q}$ on $(\Omega, \mathscr{F})$, defined by

$$\mathrm{Ent}(\mathbb{P}|\mathbb{Q}) = \begin{cases} \displaystyle\int_\Omega \log \frac{\mathrm{d}\mathbb{P}}{\mathrm{d}\mathbb{Q}}(\omega)\, \mathrm{d}\mathbb{P}(\omega) & \text{if } \mathbb{P} \ll \mathbb{Q}; \\ \infty & \text{otherwise,} \end{cases}$$

is non-negative and vanishes iff $\mathbb{P} = \mathbb{Q}$. The *$\theta$-entropy production* of $(\Omega, \phi, \mathbb{P})$ in the discrete-time interval $[\![1, n]\!]$ is defined by

$$\mathrm{Ep}(\mathbb{P}_n, \theta) = \mathrm{Ent}(\mathbb{P}_n|\widehat{\mathbb{P}}_n).$$

The (possibly infinite) non-negative number

$$\mathrm{ep}(\mathbb{P}, \theta) = \limsup_{n\to\infty} \tfrac{1}{n} \mathrm{Ep}(\mathbb{P}_n, \theta)$$

is called the *$\theta$-entropy production rate* of $(\Omega, \phi, \mathbb{P})$.

At the current level of generality, the $\theta$-entropy production rate can exhibit pathological behavior; see [7]. The following *upper-decoupling* property excludes these pathologies, ensuring that $\theta$-time-reversal invariance is equivalent to the vanishing of entropy production, and in this sense is characteristic of equilibrium.

**(UD)** There is a constant $C > 0$ such that for any $n \in \mathbb{N}$, $A \in \mathscr{F}_n$ and $B \in \mathscr{F}$,

$$\mathbb{P}(A \cap \phi^{-n}(B)) \leq C\, \mathbb{P}(A)\mathbb{P}(B).$$

Note that if **(UD)** holds for $\mathbb{P}$, then it also holds for $\widehat{\mathbb{P}}$. **(UD)** automatically holds if $\dim \mathscr{H} < \infty$, $\rho > 0$, and the set $\mathbf{A}$ is finite.[25]

The following result is an immediate extension of Theorem 2.1 and Proposition 2.2 in [21] using the Donsker–Varadhan variational formula for the relative entropy. For details see [26, Proposition 1.3]

**Proposition 34.2** *Suppose that* **(UD)** *holds. Then:*

1. *The following (possibly infinite) limit exists:*

$$\mathrm{ep}(\mathbb{P}, \theta) = \lim_{n\to\infty} \tfrac{1}{n} \mathrm{Ep}(\mathbb{P}_n, \theta).$$

2. *Assume in addition that* $\mathbb{P}$ *is* $\phi$*-ergodic. Then* $\mathrm{ep}(\mathbb{P}, \theta) = 0$ *iff* $\mathbb{P} = \widehat{\mathbb{P}}$.

This result is a starting point of [21, 22] which focus on the non-equilibrium case $\mathrm{ep}(\mathbb{P}, \theta) > 0$. In [26] the vanishing of $\mathrm{ep}(\mathbb{P}, \theta)$ for a suitable class of instruments is linked to the detailed balance condition induced by the inner product (16.2).

## 35 Conclusion

The study of entropy production in the setting of $C^*$-quantum dynamical systems has revealed a somewhat unexpected structural richness of non-equilibrium quantum statistical mechanics. There exist several distinct notions that correctly predict the mean entropy production of NESS and its linear response theory, while at the same time capturing different facets of the subject. The richness of the subject is further enhanced by the study of entropic fluctuations in the large-deviations regime and their links to quantum fluctuation theorems [24] and to hypothesis testing of the arrow of time [73].

In Parts V–VIII, we have touched on the complexities and subtleties that arise in the study of quantum entropy production; much theoretical and experimental work remains to be done to achieve a deeper understanding of this notion.

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[25] These assumptions cover many cases of physical interest.

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