Entropic Fluctuations in Quantum Statistical Mechanics

An Introduction

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Introduction

These lecture notes are the second instalment in a series of papers dealing with entropic fluctuations in non-equilibrium statistical mechanics. The first instalment [JPR] concerned classical statistical mechanics. This one deals with the quantum case and is an introduction to the results of [JOPP]. Although these lecture notes could be read independently of [JPR], a reader who wishes to get a proper grasp of the material is strongly encouraged to consult [JPR] for the classical analogs of the results presented here. In fact, to emphasize the link between the mathematical structure of classical and quantum theory of entropic fluctuations, we shall start the lectures with a *classical* example: a thermally driven harmonic chain. This example will serve as a prologue for the rest of the lecture notes.

The mathematical theory of entropic fluctuations developed in [JPR, JOPP] is axiomatic in nature. Starting with a general classical/quantum dynamical system, the basic objects of the theory—entropy production observable, finite time entropic functionals, finite time fluctuation theorems and relations, finite time linear response theory—are introduced/derived at a great level of generality. The axioms concern the large time limit $t \to \infty$, *i.e.*, the existence and the regularity properties of the limiting entropic functionals. The introduced axioms are natural and minimal (*i.e.*, necessary to have a meaningful theory), ergodic in nature, and typically difficult to verify in physically interesting models. Some of the quantum models for which the axioms have been verified (Spin-Fermion model, Electronic Black Box model) are described in Chapter 6.

However, apart for Chapter 5, we shall not discuss the axiomatic approach of [JOPP] here. The main body of the lecture notes is devoted to a pedagogical self-contained introduction to the finite time entropic functionals and fluctuation relations for *finite* quantum systems. A typical example the reader should have in mind is a quantum spin system or a Fermi gas with finite configuration space $\Lambda \subset \mathbb{Z}^d$. After the theory is developed, one proceeds by taking first the thermodynamic limit ($\Lambda \to \mathbb{Z}^d$), and then the large time limit $t \to \infty$. The thermodynamic limit of the finite time/finite volume theory is typically an easy exercise in the techniques developed in the 70's (the two volumes monograph of Bratteli and Robinson provides a good introduction to this subject). On the other hand, the large time limit, as to be expected, is typically a very difficult ergodic-type problem. In these notes we shall discuss the thermodynamic and the large time limits only in Chapter 5. This section is intended for more advanced readers who are familiar with our previous works and lectures notes. It may be entirely skipped, although even technically less prepared readers my benefit from Sections 5.1 and 5.6 up to and including the proof of Theorem 5.7.

Let us comment on our choice of the topic. From a mathematical point of view, there is a complete parallel between classical and quantum theory of entropic fluctuations. The quantum theory applied to commutative structures (algebras) reduces to the classical theory, *i.e.*, the classical theory is a special case of the quantum one. There is, however, a big difference in mathematical tools needed to describe the respective theories. Only basic results of measure theory are needed for the finite time theory in classical statistical mechanics. In the non-commutative setting these familiar tools are replaced by the Tomita-Takesaki modular theory of von Neumann algebras. For example, Connes cocycles and relative modular operators replace Radon-Nikodym derivatives. The quantum transfer operators act on Araki-Masuda non-commutative L^p-spaces which replace the familiar L^p-spaces of measure theory on which Ruelle-Perron-Frobenius (classical) transfer operators act, etc. The remarkably beautiful and powerful modular theory needed to describe quantum theory of entropic fluctuations has been developed in 1970's and 80's, primarily by Araki, Connes and Haagerup. Although modular theory has played a key role in the mathematical development of non-equilibrium quantum statistical mechanics over the last decade, the extent of its application to quantum theory of entropic fluctuations is somewhat striking. Practically all fundamental results of modular theory play a role. Some of them, like the Araki-Masuda theory of non-commutative L^p-spaces, have found in this context their first application to quantum statistical mechanics.

The power of modular theory is somewhat shadowed by its technical aspects. Out of necessity, a reader of [JOPP] must be familiar with the full machinery of algebraic quantum statistical mechanics and modular theory. Finite quantum systems, *i.e.*, quantum systems described by finite dimensional Hilbert spaces, are special since all the structures and results of this machinery can be described by elementary tools. The purpose of these lecture notes is to provide a self-contained pedagogical introduction to the algebraic structure of quantum statistical mechanics, finite time entropic functionals, and finite time fluctuation relations for *finite quantum systems*. For most part, the lecture notes should be easily accessible to an undergraduate student with basic training in linear algebra and analysis. Apart from occasional remarks/exercises and Chapter 5, more advanced tools enter only in the computations of the thermodynamic limit and the large time limit of the examples in Chapters 1 and 6. A student who has taken a course in quantum mechanics and/or operator theory should have no difficulties with those tools either.

Apart from from a few comments in Chapter 5 we shall not discuss here the Gallavotti-Cohen fluctuation theorem and the principle of regular entropic fluctuations. These important topics concern non-equilibrium steady states and require a technical machinery not covered in these notes.

The lecture notes are organized as follows. In the Prologue, Chapter 1, we describe the classical theory of entropic fluctuations on the example of a classical harmonic chain. The rest of the notes can be read independently of this section. Chapter 2 is devoted to the algebraic quantum statistical mechanics of finite quantum systems. In Chapters 3 and 4 this algebraic structure is applied to the study of entropic functionals and fluctuation relations of finite quantum systems. In Chapter 6 we illustrate the results of Chapters 3 and 4 on examples of fermionic systems. Large deviation theory and the Gärtner-Ellis theorem play a key role in entropic fluctuation theorems and for this reason we review the Gärtner-Ellis theorem in Appendix A. Another tool, a convergence result based on Vitali's theorem, will be often used in the lecture notes, and we provide its proof in Appendix B.

Acknowledgment. The research of V.J. was partly supported by NSERC. The research of Y.O. was supported by JSPS Grant-in-Aid for Young Scientists (B), Hayashi Memorial Foundation for Female Natural Scientists, Sumitomo Foundation, and Inoue Foundation. The research of C.-A.P. was partly supported by ANR (grant 09-BLAN-0098). A part of the lecture notes was written during the stay at the first author at IHES. V.J. wishes to thank D. Ruelle for hospitality and useful discussions. Various parts of the lecture notes have been presented by its authors in mini-courses at University of Cergy-Pontoise, Erwin Schrödinger Institute (Vienna), Centre de Physique Théorique (Marseille and Toulon), University of British Columbia (Vancouver), Ecole Polytechnique (Paris), Institut Henri Poincaré (Paris) and Ecole de Physique des Houches. The lecture notes have gained a lot from these presentations and we wish to thank the respective institutions and F. Germinet, J. Yngvanson, R. Froese, S. Kuksin, G. Stoltz, J. Fröhlich for making these mini-courses possible.

Chapter 1

Prologue: A thermally driven classical harmonic chain

In this section we will discuss a very simple *classical* example: a finite harmonic chain $\mathcal{C}$ coupled at its left and right ends to two harmonic heat reservoirs $\mathcal{R}_L$, $\mathcal{R}_R$. This model is exactly solvable and allows for a transparent review of the classical theory of entropic fluctuations developed in [JPR]. Needless to say, models of this type have a long history in the physics literature and we refer the reader to Lebowitz and Spohn [LS1] for references and additional information. The reader should compare Chapter 4, which deals with the non-equilibrium statistical mechanics of open quantum systems, with the example of open classical system described here. The same remark applies to Section 6.6, where we study the non-equilibrium statistical mechanics of ideal Fermi gases.

1.1 The finite harmonic chain

We start with the description of an isolated harmonic chain on the finite 1D-lattice $\Lambda = [A, B] \subset \mathbb{Z}$ (see Fig. 1.1 below). Its phase space is

$$\Gamma_\Lambda = \{(p, q) = (\{p_x\}_{x\in\Lambda}, \{q_x\}_{x\in\Lambda}) \,|\, p_x, q_x \in \mathbb{R}\} = \mathbb{R}^\Lambda \oplus \mathbb{R}^\Lambda,$$

and its Hamiltonian is given by

$$H_\Lambda(p, q) = \sum_{x\in\mathbb{Z}} \left(\frac{p_x^2}{2} + \frac{q_x^2}{2} + \frac{(q_x - q_{x-1})^2}{2} \right),$$

where we set $p_x = q_x = 0$ for $x \notin \Lambda$.

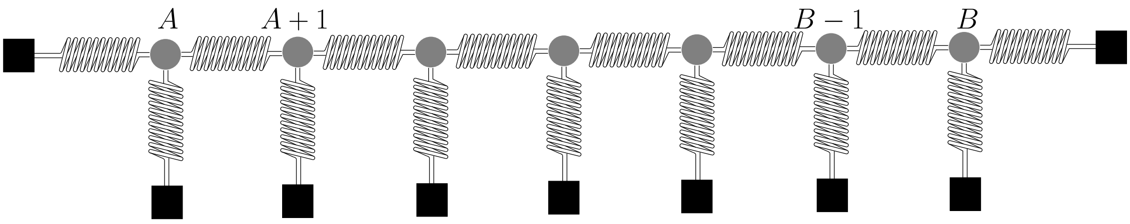

Figure 1.1: The finite harmonic chain on $\Lambda = [A, B]$.

Thus, w.r.t. the natural Euclidian structure of Γ_Λ, the function $2H_\Lambda(p, q)$ is the quadratic form associated to the symmetric matrix

$$h_\Lambda = \begin{bmatrix} \mathbb{1} & 0 \\ 0 & \mathbb{1} - \Delta_\Lambda \end{bmatrix},$$

where Δ_Λ denotes the discrete Laplacian on $\Lambda = [A, B]$ with Dirichlet boundary conditions

$$(-\Delta_\Lambda u)_x = \begin{cases} 2u_A - u_{A+1} & \text{for } x = A; \\ 2u_x - u_{x-1} - u_{x+1} & \text{for } x \in]A, B[; \\ 2u_B - u_{B-1} & \text{for } x = B. \end{cases} \tag{1.1}$$

The equations of motion of the chain,

$$\dot{p} = -(\mathbb{1} - \Delta_\Lambda)q, \qquad \dot{q} = p,$$

define a Hamiltonian flow on Γ_Λ, the one-parameter group $\mathrm{e}^{t\mathcal{L}_\Lambda}$ generated by

$$\mathcal{L}_\Lambda = jh_\Lambda, \qquad j = \left[\begin{array}{cc} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{array}\right].$$

This flow has two important properties:

(i) Energy conservation: $\mathrm{e}^{t\mathcal{L}_\Lambda^*} h_\Lambda \, \mathrm{e}^{t\mathcal{L}_\Lambda} = h_\Lambda$.

(ii) Liouville's theorem: $\det\left(\mathrm{e}^{t\mathcal{L}_\Lambda}\right) = \mathrm{e}^{t\,\mathrm{tr}(\mathcal{L}_\Lambda)} = 1$.

An observable of the harmonic chain is a real (or vector) valued function on its phase space Γ_Λ and a state is a probability measure on Γ_Λ. If f is an observable and ω a state, we denote by

$$\omega(f) = \int_{\Gamma_\Lambda} f(p, q) \, \mathrm{d}\omega(p, q),$$

the expectation of f w.r.t. ω. Under the flow of the Hamiltonian H_Λ the observables evolve as

$$f_t = f \circ \mathrm{e}^{t\mathcal{L}_\Lambda}.$$

In terms of the Poisson bracket

$$\{f, g\} = \nabla_p f \cdot \nabla_q g - \nabla_q f \cdot \nabla_p g,$$

the evolution of an observable f satisfies

$$\partial_t f_t = \{H_\Lambda, f_t\} = \{H_\Lambda, f\}_t.$$

The evolution of a state ω is given by duality

$$\omega_t(f) = \omega(f_t),$$

and satisfies

$$\partial_t \omega_t(f) = \omega_t(\{H_\Lambda, f\}).$$

ω is called steady state or stationary state if it is invariant under this evolution, *i.e.*, $\omega_t = \omega$ for all t. If ω has a density w.r.t. Liouville's measure on Γ_Λ, *i.e.*, $\mathrm{d}\omega(p, q) = \rho(p, q) \, \mathrm{d}p\mathrm{d}q$, then Liouville's theorem yields

$$\begin{aligned} \omega_t(f) &= \int_{\Gamma_\Lambda} f \circ \mathrm{e}^{t\mathcal{L}_\Lambda}(p, q) \rho(p, q) \, \mathrm{d}p\mathrm{d}q \\ &= \int_{\Gamma_\Lambda} f(p, q) \rho \circ \mathrm{e}^{-t\mathcal{L}_\Lambda}(p, q) \det\left(\mathrm{e}^{-t\mathcal{L}_\Lambda}\right) \, \mathrm{d}p\mathrm{d}q \\ &= \int_{\Gamma_\Lambda} f(p, q) \rho \circ \mathrm{e}^{-t\mathcal{L}_\Lambda}(p, q) \, \mathrm{d}p\mathrm{d}q, \end{aligned}$$

and so ω_t also has a density w.r.t. Liouville's measure given by $\rho \circ \mathrm{e}^{-t\mathcal{L}_\Lambda}$. If D is a positive definite matrix on Γ_Λ and ω is the centered Gaussian measure with covariance D,

$$\mathrm{d}\omega(p,q) = \det(2\pi D)^{-1/2}\,\mathrm{e}^{-D^{-1}[p,q]/2}\,\mathrm{d}p\mathrm{d}q,$$

where $D^{-1}[p,q]$ denotes the quadratic form associated to D^{-1}, then ω_t is the centered Gaussian measure with covariance $D_t = \mathrm{e}^{t\mathcal{L}_\Lambda} D \mathrm{e}^{t\mathcal{L}_\Lambda^*}$.

The thermal equilibrium state of the chain at inverse temperature β is the Gaussian measure with covariance $(\beta h_\Lambda)^{-1}$,

$$\mathrm{d}\omega_{\Lambda\beta}(p,q) = \sqrt{\det\left(\frac{\beta h_\Lambda}{2\pi}\right)}\,\mathrm{e}^{-\beta H_\Lambda(p,q)}\mathrm{d}p\mathrm{d}q.$$

Thermal equilibrium states are invariant under the Hamiltonian flow of H_Λ.

1.2 Coupling to the reservoirs

As a small system, we consider the harmonic chain $\mathcal{C}$ on $\Lambda = [-N, N]$. The left and right reservoirs are harmonic chains $\mathcal{R}_L$ and $\mathcal{R}_R$ on $\Lambda_L = [-M, -N-1]$ and $\Lambda_R = [N+1, M]$ respectively. In our discussion we shall keep N fixed, but eventually let $M \to \infty$. In any case, the reader should always have in mind that $M \gg N$.

The Hamiltonian of the joint but decoupled system is

$$H_0(p,q) = H_\Lambda(p,q) + H_{\Lambda_L}(p,q) + H_{\Lambda_R}(p,q).$$

The Hamiltonian of the coupled system is

$$H(p,q) = H_{\Lambda_L\cup\Lambda\cup\Lambda_R}(p,q) = H_0(p,q) + V_L(p,q) + V_R(p,q),$$

where $V_L(p,q) = -q_{-N-1}q_{-N}$ and $V_R(p,q) = -q_N q_{N+1}$.

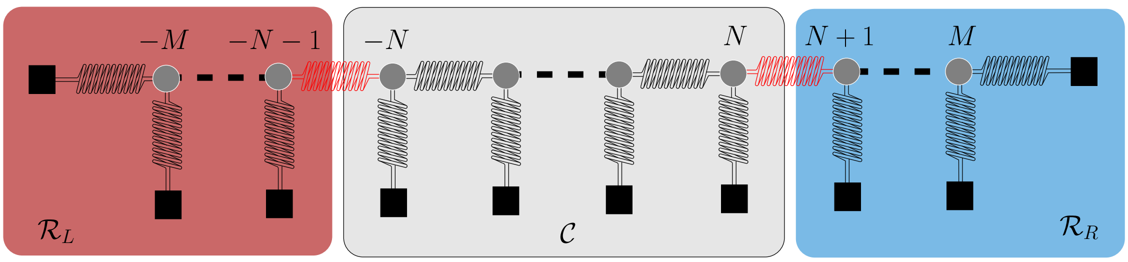

Figure 1.2: The chain $\mathcal{C}$ coupled at its left and right ends to the reservoirs $\mathcal{R}_L$ and $\mathcal{R}_R$.

We denote by h_0, h_L, h_R and h the symmetric matrices associated to the quadratic forms $2H_0$, $2H_L$, $2H_R$ and $2H$ and by $\mathcal{L}_0 = jh_0$ and $\mathcal{L} = jh$ the generators of the corresponding Hamiltonian flows. We also set $v = v_L + v_R = h - h_0$ where v_L and v_R are associated to $2V_L$ and $2V_R$ respectively.

1.3 Non-equilibrium reference measure

We shall assume that initially each subsystem is in thermal equilibrium, the reservoirs at temperatures $T_{L/R} = 1/\beta_{L/R}$, and the small system at temperature $T = 1/\beta$. The initial (reference) state is therefore

$$\mathrm{d}\omega_{\Lambda_L\beta_L} \otimes \mathrm{d}\omega_{\Lambda\beta} \otimes \mathrm{d}\omega_{\Lambda_R\beta_R}(p,q) = Z^{-1}\,\mathrm{e}^{-(\beta_L H_{\Lambda_L}(p,q) + \beta H_\Lambda(p,q) + \beta_R H_{\Lambda_R}(p,q))}\,\mathrm{d}p\mathrm{d}q. \tag{1.2}$$

If the temperatures of the reservoirs are different, the system is initially out of equilibrium. We set $X_L = \beta - \beta_L$, $X_R = \beta - \beta_R$ and $X = (X_L, X_R)$. We call X the thermodynamic force acting on the chain $\mathcal{C}$.

X_L and X_R are sometimes called affinities in non-equilibrium thermodynamics (see, *e.g.*, [dGM]). When $X = 0$, one has $\beta_L = \beta_R = \beta$ and the joint system is in equilibrium at inverse temperature β for the decoupled dynamics generated by H_0.

In view of the coupled dynamics generated by H, it will be more convenient to use a slightly modified initial state

$$\begin{aligned} \mathrm{d}\omega_X(p,q) &= Z_X^{-1}\,\mathrm{e}^{-(\beta_L H_{\Lambda_L}(p,q)+\beta H_\Lambda(p,q)+\beta_R H_{\Lambda_R}(p,q)+\beta V(p,q))}\mathrm{d}p\mathrm{d}q \\ &= Z_X^{-1}\,\mathrm{e}^{-(\beta H(p,q)-X_L H_{\Lambda_L}(p,q)-X_R H_{\Lambda_R}(p,q))}\mathrm{d}p\mathrm{d}q, \end{aligned}$$

which, for $X = 0$, reduces to the thermal equilibrium state at inverse temperature β of the joint system under the coupled dynamics. Note that ω_X is the Gaussian measure with covariance

$$D_X = (\beta h - k(X))^{-1}, \qquad k(X) = X_L h_L + X_R h_R,$$

whereas (1.2) is Gaussian with covariance $(\beta h_0 - k(X))^{-1}$. Since $h - h_0 = v$ is a rank 4 matrix which is well localized at the boundary of Λ, these two states describe the same thermodynamics.

1.4 Comparing states

Under the Hamiltonian flow of H, the state ω_X evolves into $\omega_{X,t}$, the Gaussian measure with covariance

$$D_{X,t} = \mathrm{e}^{t\mathcal{L}} D_X \mathrm{e}^{t\mathcal{L}^*} = \left(\beta h - \mathrm{e}^{-t\mathcal{L}^*} k(X)\mathrm{e}^{-t\mathcal{L}}\right)^{-1}.$$

As time goes on, the state $\omega_{X,t}$ diverges from the initial state ω_X. In order to quantify this divergence, we need a way to describe the "rate of change" of the state, *i.e.*, a concept of "distance" between states. Classical information theory provides several candidates for such a distance. In this section, we introduce two of them and explore their physical meaning.

Let ν and ω be two states. Recall that ν is said to be absolutely continuous w.r.t. ω, written $\nu \ll \omega$, if there exists a density, a non-negative function ρ satisfying $\omega(\rho) = 1$, such that $\nu(f) = \omega(\rho f)$ for all observables f. The function ρ is called Radon-Nikodym derivative of ν w.r.t. ω and is denoted $\mathrm{d}\nu/\mathrm{d}\omega$.

The relative entropy of ν w.r.t. ω is defined by

$$S(\nu|\omega) = \begin{cases} \nu\left(-\log\dfrac{\mathrm{d}\nu}{\mathrm{d}\omega}\right) & \text{if } \nu \ll \omega, \\ -\infty & \text{otherwise.} \end{cases} \tag{1.3}$$

Exercise 1.1.

1. Show that $\log(x^{-1}) \le x^{-1} - 1$ for $x > 0$, where equality holds iff $x = 1$.

2. Using the previous inequality, show that $S(\nu|\omega) \le 0$ with equality iff $\nu = \omega$. This justifies the use of relative entropy (or rather of $-S(\nu|\omega)$) as a measure of the "distance" between ν and ω. Note however that $-S(\nu|\omega)$ is not a metric in the usual sense since it is not symmetric and does not satisfy the triangle inequality.

Applying Definition (1.3) to $\omega_{X,t}$ and ω_X, we get

$$-\log\left(\frac{\mathrm{d}\omega_{X,t}}{\mathrm{d}\omega_X}\right) = X_L(H_{\Lambda_L} - H_{\Lambda_L,-t}) + X_R(H_{\Lambda_R} - H_{\Lambda_R,-t}), \tag{1.4}$$

and hence

$$
\begin{aligned}
S(\omega_{X,t}|\omega_X) &= \omega_{X,t}\left(X_L(H_{\Lambda_L} - H_{\Lambda_L,-t}) + X_R(H_{\Lambda_R} - H_{\Lambda_R,-t})\right) \\
&= X_L\omega_X\left(H_{\Lambda_L,t} - H_{\Lambda_L}\right) + X_R\omega_X\left(H_{\Lambda_R,t} - H_{\Lambda_R}\right).
\end{aligned}
$$

Since the observable $H_{\Lambda_R,t} - H_{\Lambda_R}$ measures the increase of the energy in the right reservoir during the time interval $[0,t]$ and

$$
H_{\Lambda_R,t} - H_{\Lambda_R} = \int_0^t \frac{\mathrm{d}}{\mathrm{d}s} H_{\Lambda_R,s}\,\mathrm{d}s = \int_0^t \{H, H_{\Lambda_R}\}_s\,\mathrm{d}s,
$$

we interpret

$$
\Phi_R = -\{H, H_{\Lambda_R}\} = \{H_{\Lambda_R}, V_R\} = -p_{N+1}q_N,
$$

as the energy flux out of the right reservoir. Similarly,

$$
\Phi_L = -\{H, H_{\Lambda_L}\} = \{H_{\Lambda_L}, V_L\} = -p_{-N-1}q_{-N},
$$

is the energy flux out of the left reservoir.

Exercise 1.2. Compare the equation of motion of the isolated reservoir $\mathcal{R}_R$ with that of the same reservoir coupled to $\mathcal{C}$. Deduce that the force exerted on the reservoir by the system $\mathcal{C}$ is given by q_N and therefore that q_Np_{N+1} is the power dissipated into the right reservoir.

In terms of fluxes, we have obtained the following *entropy balance relation*

$$
S(\omega_{X,t}|\omega_X) = -\int_0^t \omega_X(\sigma_{X,s})\,\mathrm{d}s, \tag{1.5}
$$

where

$$
\sigma_X = X_L\Phi_L + X_R\Phi_R.
$$

This bilinear expression in the thermodynamic forces and the corresponding fluxes has precisely the form of entropy production as derived in phenomenological non-equilibrium thermodynamics (see, *e.g.*, Section IV.3 of [dGM]). For this reason, we shall call σ_X the *entropy production* observable and

$$
\Sigma^t = \frac{1}{t}\int_0^t \sigma_{X,s}\,\mathrm{d}s, \tag{1.6}
$$

the *mean entropy production rate*[1] over the time interval $[0,t]$. The important fact is that the mean entropy production rate has non-negative expectation for $t > 0$:

$$
\omega_X(\Sigma^t) = \frac{1}{t}\int_0^t \omega_X(\sigma_{X,s})\,\mathrm{d}s = -\frac{1}{t}S(\omega_{X,t}|\omega_X) \geq 0. \tag{1.7}
$$

Another widely used measure of the discrepancy between two states ω and ν is Rényi relative α-entropy, defined for any $\alpha \in \mathbb{R}$ by

$$
S_\alpha(\nu|\omega) = \begin{cases} \log\omega\left(\left(\dfrac{\mathrm{d}\nu}{\mathrm{d}\omega}\right)^\alpha\right) & \text{if } \nu \ll \omega, \\ -\infty & \text{otherwise.} \end{cases}
$$

[1] Various other names are commonly used in the literature for the observable σ_X: phase space contraction rate, dissipation function, etc.

Starting from Equ. (1.4) one easily derives the formula

$$\log \frac{\mathrm{d}\omega_{X,t}}{\mathrm{d}\omega_X} = \int_0^{-t} \sigma_{X,s}\,\mathrm{d}s = t\Sigma^{-t}, \tag{1.8}$$

so that

$$e_t(\alpha) = S_\alpha(\omega_{X,t}|\omega_X) = \log \omega_X \left(\left(\frac{\mathrm{d}\omega_{X,t}}{\mathrm{d}\omega_X} \right)^\alpha \right) = \log \omega_X \left(\mathrm{e}^{\alpha t \Sigma^{-t}} \right). \tag{1.9}$$

Exercise 1.3.

1. Assuming $\nu \ll \omega$ and using Hölder's inequality, show that $\alpha \mapsto S_\alpha(\nu|\omega)$ is convex.
2. Show that $S_0(\nu|\omega) = S_1(\nu|\omega) = 0$ and conclude that $S_\alpha(\nu|\omega)$ is non-positive for $\alpha \in]0,1[$ and non-negative for $\alpha \notin]0,1[$.
3. Assuming also $\omega \ll \nu$, show that $S_{1-\alpha}(\nu|\omega) = S_\alpha(\omega|\nu)$.

1.5 Time reversal invariance

Our dynamical system is time reversal invariant: the map $\vartheta(p,q) = (-p,q)$ is an anti-symplectic involution, *i.e.*, $\{f\circ\vartheta, g\circ\vartheta\} = -\{f,g\}\circ\vartheta$ and $\vartheta\circ\vartheta = \mathrm{Id}$. Since $H\circ\vartheta = H$, it satisfies

$$\mathrm{e}^{t\mathcal{L}} \circ \vartheta = \vartheta \circ \mathrm{e}^{-t\mathcal{L}},$$

and leaves our reference state ω_X invariant,

$$\omega_X(f\circ\vartheta) = \omega_X(f).$$

It follows that $\omega_{X,t}(f\circ\vartheta) = \omega_{X,-t}(f)$, $\Phi_{L/R}\circ\vartheta = -\Phi_{L/R}$ and $\sigma_X\circ\vartheta = -\sigma_X$. Note in particular that $\omega_X(\Phi_{L/R}) = 0$ and $\omega_X(\sigma_X) = 0$. Applying time reversal to Definition (1.6) we further get

$$\begin{aligned}
\Sigma^t \circ \vartheta &= \frac{1}{t}\int_0^t \sigma_X \circ \mathrm{e}^{s\mathcal{L}} \circ \vartheta\,\mathrm{d}s = \frac{1}{t}\int_0^t \sigma_X \circ \vartheta \circ \mathrm{e}^{-s\mathcal{L}}\,\mathrm{d}s \\
&= -\frac{1}{t}\int_0^t \sigma_X \circ \mathrm{e}^{-s\mathcal{L}}\,\mathrm{d}s = \frac{1}{t}\int_0^{-t} \sigma_X \circ \mathrm{e}^{s\mathcal{L}}\,\mathrm{d}s \\
&= -\Sigma^{-t},
\end{aligned} \tag{1.10}$$

and Equ. (1.9) becomes

$$e_t(\alpha) = \log \omega_X \left(\mathrm{e}^{\alpha t \Sigma^{-t}\circ\vartheta} \right) = \log \omega_X \left(\mathrm{e}^{-\alpha t \Sigma^{t}} \right). \tag{1.11}$$

Thus, $\alpha \mapsto t^{-1}e_t(\alpha)$ is the cumulant generating function of the observable $-t\Sigma^t$ in the state ω_X, and in particular

$$\begin{aligned}
\left.\frac{\mathrm{d}}{\mathrm{d}\alpha} t^{-1} e_t(\alpha)\right|_{\alpha=0} &= -\omega_X\left(\frac{1}{t}\int_0^t \sigma_{X,s}\,\mathrm{d}s \right), \\
\left.\frac{\mathrm{d}^2}{\mathrm{d}\alpha^2} t^{-1} e_t(\alpha)\right|_{\alpha=0} &= \omega_X\left(\left(\frac{1}{\sqrt{t}}\int_0^t (\sigma_{X,s} - \omega_X(\sigma_{X,s}))\,\mathrm{d}s \right)^2 \right).
\end{aligned}$$

1.6 A universal symmetry

Let us look more closely at the positivity property (1.7). To this end, we introduce the distribution of the observable Σ^t induced by the state ω_X, *i.e.*, the probability measure P^t defined by

$$P^t(f) = \omega_X(f(\Sigma^t)).$$

To comply with (1.7), this distribution should be asymmetric and give more weight to positive values than to negative ones. Thus, let us compare P^t with the distribution $\overline{P}^t(f) = \omega_X(f(-\Sigma^t))$ of $-\Sigma^t$. Observing that

$$\begin{aligned}\Sigma^{-t} &= -\frac{1}{t}\int_0^{-t} \sigma_X \circ \mathrm{e}^{s\mathcal{L}}\,\mathrm{d}s = \frac{1}{t}\int_0^t \sigma_X \circ \mathrm{e}^{-s\mathcal{L}}\,\mathrm{d}s \\ &= \left(\frac{1}{t}\int_0^t \sigma_X \circ \mathrm{e}^{(t-s)\mathcal{L}}\,\mathrm{d}s\right) \circ \mathrm{e}^{-t\mathcal{L}} = \Sigma^t \circ \mathrm{e}^{-t\mathcal{L}},\end{aligned} \tag{1.12}$$

we obtain, using (1.8) and (1.10)

$$\begin{aligned}\overline{P}^t(f) &= \omega_X(f(-\Sigma^t)) = \omega_X(f(\Sigma^{-t}\circ\vartheta)) = \omega_X(f(\Sigma^{-t})) = \omega_X(f(\Sigma^t \circ \mathrm{e}^{-t\mathcal{L}})) \\ &= \omega_{X,-t}(f(\Sigma^t)) = \omega_X\left(\frac{\mathrm{d}\omega_{X,-t}}{\mathrm{d}\omega_X} f(\Sigma^t)\right) = \omega_X\left(\mathrm{e}^{-t\Sigma^t} f(\Sigma^t)\right),\end{aligned}$$

from which we conclude that $\overline{P}^t \ll P^t$ and

$$\frac{\mathrm{d}\overline{P}^t}{\mathrm{d}P^t}(s) = \mathrm{e}^{-ts}. \tag{1.13}$$

This relation shows that negative values of Σ^t are exponentially suppressed as $t \to \infty$. One easily deduces from (1.13) that

$$-s-\delta \le \frac{1}{t}\log\frac{\omega_X(\{\Sigma^t \in [-s-\delta, -s+\delta]\})}{\omega_X(\{\Sigma^t \in [s-\delta, s+\delta]\})} \le -s+\delta,$$

for $t, \delta > 0$ and any $s \in \mathbb{R}$. Such a property was discovered in numerical experiments on shear flows by Evans *et al.* [ECM]. Evans and Searles [ES] were the first to provide a theoretical analysis of the underlying mechanism. Since then, a large body of theoretical and experimental literature has been devoted to similar "fluctuation relations" or "fluctuation theorems". They have been derived for various types of systems: Hamiltonian and non-Hamiltonian mechanical systems, discrete and continuous time dynamical systems, Markov processes, ... We refer the reader to the review by Rondoni and Meíja-Monasterio [RM] for historical perspective and references and to [JPR] for a more mathematically oriented presentation.

We can rewrite Equ. (1.11) in terms of the Laplace transform of the measure P^t,

$$e_t(\alpha) = \log\int \mathrm{e}^{-\alpha ts}\,\mathrm{d}P^t(s).$$

Relation (1.13) is equivalent to

$$\int \mathrm{e}^{-(1-\alpha)ts}\,\mathrm{d}P^t(s) = \int \mathrm{e}^{\alpha ts}\,\mathrm{d}\overline{P}^t(s) = \int \mathrm{e}^{-\alpha ts}\,\mathrm{d}P^t(s),$$

and therefore can be expressed in the form

$$e_t(1-\alpha) = e_t(\alpha). \tag{1.14}$$

We shall call the last relation the *finite time Evans-Searles symmetry* of the function $e_t(\alpha)$. The above derivation directly extends to a general time-reversal invariant dynamical system, see [JPR].

1.7 A generalized Evans-Searles symmetry

Relation (1.13) deals with the mean entropy production rate Σ^t. It can be generalized to the mean energy flux, the vector valued observable

$$\mathbf{\Phi}^t = \frac{1}{t}\int_0^t \left(\Phi_L \circ \mathrm{e}^{s\mathcal{L}}, \Phi_R \circ \mathrm{e}^{s\mathcal{L}}\right) \mathrm{d}s.$$

Exercise 1.4. Denote by Q^t (respectively $\overline{Q}^t$) the distribution of $\mathbf{\Phi}^t$ (respectively $-\mathbf{\Phi}^t$) induced by the state ω_X, *i.e.*, $Q^t(f) = \omega_X(f(\mathbf{\Phi}^t))$ and $\overline{Q}^t(f) = \omega_X(f(-\mathbf{\Phi}^t))$. Using the fact that $X \cdot \mathbf{\Phi}^t = \Sigma^t$ and mimicking the proof of (1.13) show that

$$\frac{\mathrm{d}\overline{Q}^t}{\mathrm{d}Q^t}(\mathbf{s}) = \mathrm{e}^{-tX\cdot\mathbf{s}}. \tag{1.15}$$

Again, this derivation can be extended to an arbitrary time-reversal invariant dynamical system, see [JPR].

Introducing the cumulant generating function

$$g_t(X,Y) = \log \omega_X\left(\mathrm{e}^{-tY\cdot\mathbf{\Phi}^t}\right), \tag{1.16}$$

and proceeding as in the previous section, we see that Relation (1.15) is equivalent to

$$\int \mathrm{e}^{-t(X-Y)\cdot\mathbf{s}}\,\mathrm{d}Q^t(\mathbf{s}) = \int \mathrm{e}^{tY\cdot\mathbf{s}}\,\mathrm{d}\overline{Q}^t(\mathbf{s}) = \int \mathrm{e}^{-tY\cdot\mathbf{s}}\,\mathrm{d}Q^t(\mathbf{s}),$$

which leads to the *generalized finite time Evans-Searles symmetry*

$$g_t(X, X-Y) = g_t(X,Y). \tag{1.17}$$

Exercise 1.5. Check that

$$g_t(X,Y) = -\frac{1}{2}\log\det\left(\mathbb{1} - D_X\left(\mathrm{e}^{t\mathcal{L}^*}k(Y)\mathrm{e}^{t\mathcal{L}} - k(Y)\right)\right), \tag{1.18}$$

where we adopt the convention that $\log x = -\infty$ whenever $x \le 0$. Using this formula verify directly Relation (1.17).

1.8 Thermodynamic limit

So far we were dealing with a finite dimensional harmonic system. Its Hamiltonian flow $\mathrm{e}^{t\mathcal{L}}$ is quasi-periodic and it is therefore not a surprise that entropy production vanishes in the large time limit,

$$\lim_{t\to\infty}\omega_X(\Sigma^t) = \lim_{t\to\infty}\frac{1}{2t}\mathrm{tr}\left(D_X\left(k(X) - \mathrm{e}^{t\mathcal{L}^*}k(X)\mathrm{e}^{t\mathcal{L}}\right)\right) = 0,$$

see also Figure 1.3. To achieve a strictly positive entropy production rate in the asymptotic regime $t \to \infty$, the thermodynamic limit of the reservoirs must be taken prior to the large time limit.

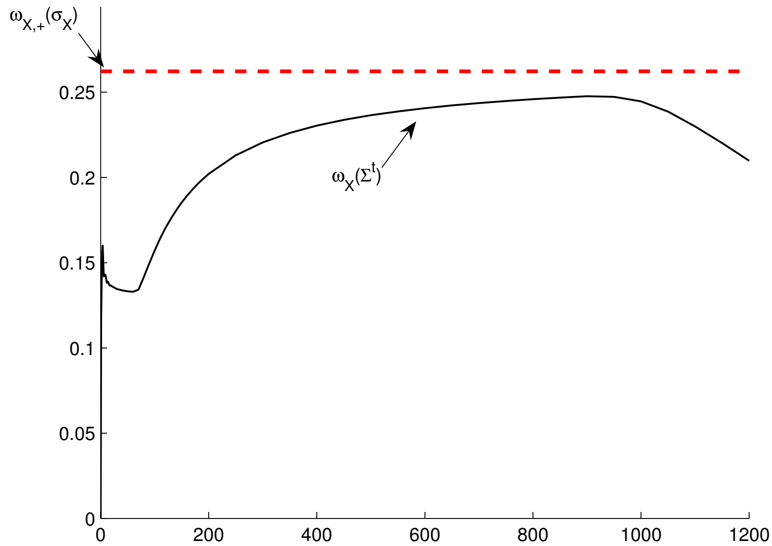

Figure 1.3: The typical behavior of the mean entropy production rate $t \mapsto \omega_X(\Sigma^t)$ for a finite system ($N = 20$, $M = 300$). The dashed line represent the steady state value $\omega_{X,+}(\sigma_X) = \lim_{t\to\infty} \omega_X(\Sigma^t)$ for the same finite chain ($N = 20$) coupled to two infinite reservoirs.

To take $M \to \infty$ while keeping N fixed we observe that the phase space $\Gamma_{[-M,M]}$ is naturally embeded in the real Hilbert space $\Gamma = \ell^2_{\mathbb{R}}(\mathbb{Z}) \oplus \ell^2_{\mathbb{R}}(\mathbb{Z})$ and that h_0, h_L, h_R and h are uniformly bounded and strongly convergent as operators on this space. For example

$$\mathrm{s}-\lim_{M\to\infty} h_0 = \left[\begin{array}{cc} \mathbb{1} & 0 \\ 0 & \mathbb{1}-\Delta_0 \end{array}\right],$$

where $\Delta_0 = \Delta_{]-\infty,-N-1]} \oplus \Delta_{[-N,N]} \oplus \Delta_{[N+1,\infty[}$ is the discrete Laplacian on $\mathbb{Z}$ with Dirichlet decoupling at $\pm N$ and

$$\mathrm{s}-\lim_{M\to\infty} h = \left[\begin{array}{cc} \mathbb{1} & 0 \\ 0 & \mathbb{1}-\Delta \end{array}\right],$$

where $\Delta = \Delta_{\mathbb{Z}}$ is the discrete Laplacian on $\mathbb{Z}$. It follows that $\mathcal{L}_0 = jh_0$ and $\mathcal{L} = jh$ are also strongly convergent. Hence, the Hamiltonian flows $\mathrm{e}^{t\mathcal{L}_0}$ and $\mathrm{e}^{t\mathcal{L}}$ converge strongly and uniformly on compact time intervals to the uniformly bounded, norm continuous groups on Γ generated by the strong limits of $\mathcal{L}_0$ and $\mathcal{L}$. Finally, since the covariance $D_X = (\beta h - k(X))^{-1}$ of the state ω_X converges strongly, the state ω_X converges weakly to the Gaussian measure with the limiting covariance. In the following, we shall use the same notation for these objects after the limit $M \to \infty$, *i.e.*, h, h_0, $\mathcal{L}$, $\mathcal{L}_0$, $k(X)$, ω_X, ... denote the thermodynamic limits of the corresponding finite volume objects.

After the thermodynamic limit, we are left with a linear dynamical system on the L^2-space of the Gaussian measure ω_X. Denoting by $\phi_{L/R}$ the finite rank operators corresponding to the flux observable $2\Phi_{L/R}$ and setting $\phi(Y) = Y_L\phi_L + Y_R\phi_R$, we can write

$$\mathrm{e}^{t\mathcal{L}^*} k(Y)\mathrm{e}^{t\mathcal{L}} - k(Y) = -\int_0^t \mathrm{e}^{s\mathcal{L}^*}\phi(Y)\mathrm{e}^{s\mathcal{L}}\,\mathrm{d}s. \tag{1.19}$$

Since the right hand side of this identity is trace class for every $Y \in \mathbb{R}^2$ and $t \in \mathbb{R}$, we conclude from

$$D_{X,t}^{-1} - D_X^{-1} = \mathrm{e}^{-t\mathcal{L}^*} k(X)\mathrm{e}^{-t\mathcal{L}} - k(X), \tag{1.20}$$

and the Feldman-Hajek-Shale theorem (see, *e.g.*, [Si]) that the Gaussian measure $\omega_{X,t}$ and ω_X are equivalent and that Relation (1.4) still holds in the following form

$$-\log\left(\frac{\mathrm{d}\omega_{X,t}}{\mathrm{d}\omega_X}\right) = \int_0^{-t} \sigma_{X,s}\,\mathrm{d}s.$$

For the same reason, Equ. (1.18) for the generalized Evans-Searles functional $g_t(X,Y)$ remains valid in the thermodynamic limit.

1.9 Large time limit I: Scattering theory

Taking the limit $t\to\infty$ in (1.19), (1.20) we obtain the formal result

$$D_{X,+}^{-1} = \lim_{t\to\infty} D_{X,t}^{-1} = D_X^{-1} + \int_{-\infty}^0 \mathrm{e}^{s\mathcal{L}^*}\phi(X)\mathrm{e}^{s\mathcal{L}}\,\mathrm{d}s,$$

which we can interpret in the following way: the state $\omega_{X,t}$, Gaussian with covariance $D_{X,t}$, converges as $t\to\infty$ towards a non-equilibrium steady state (NESS) $\omega_{X,+}$, Gaussian with covariance $D_{X,+}$, which formally writes

$$\mathrm{d}\omega_{X,+}(p,q) =$$

$$\frac{1}{Z_{X,+}}\mathrm{e}^{-\left(\beta H(p,q)-X_L H_{\Lambda_L}(p,q)-X_R H_{\Lambda_R}(p,q)+\int_{-\infty}^0 (X_L\Phi_{L,s}(p,q)+X_R\Phi_{R,s}(p,q))\,\mathrm{d}s\right)}\mathrm{d}p\mathrm{d}q.$$

This formal expression is a special case of the McLennan-Zubarev non-equilibrium ensemble (see [McL, Zu1, Zu2]). In this and the following sections we shall turn this formal argument into a rigorous construction.

The study of the limit $t\to\infty$ in our infinite dimensional harmonic system reduces to an application of trace class scattering theory. We refer to [RS3] for basic facts about scattering theory. We start with a few simple remarks:

(i) We denote by $\mathcal{H} = \ell^2_{\mathbb{C}}(\mathbb{Z})\oplus\ell^2_{\mathbb{C}}(\mathbb{Z}) \simeq \ell^2_{\mathbb{C}}(\mathbb{Z})\otimes\mathbb{C}^2$ the complexified phase space and extend all operators on Γ to $\mathcal{H}$ by $\mathbb{C}$-linearity. The inner product on the complex Hilbert space $\mathcal{H}$ is written $\langle\phi|\psi\rangle$.

(ii) $h-h_0=v$ is finite rank and hence trace class. Since $h_0\geq\mathbb{1}$ and $h\geq\mathbb{1}$, $h^{1/2}-h_0^{1/2}$ is also trace class.

(iii) $h^{1/2}h_0^{-1/2}-\mathbb{1} = (h^{1/2}-h_0^{1/2})h_0^{-1/2}$ is trace class. The same is true for $h_0^{1/2}h^{-1/2}-\mathbb{1}$, $h_0^{-1/2}h^{1/2}-\mathbb{1}$ and $h^{-1/2}h_0^{1/2}-\mathbb{1}$.

(iv) $L_0 = \mathrm{i}h_0^{1/2}jh_0^{1/2}$ and $L=\mathrm{i}h^{1/2}jh^{1/2}$ are self-adjoint, $L-L_0$ is trace class and

$$\mathrm{e}^{-\mathrm{i}tL_0} = h_0^{1/2}\mathrm{e}^{t\mathcal{L}_0}h_0^{-1/2}, \qquad \mathrm{e}^{-\mathrm{i}tL} = h^{1/2}\mathrm{e}^{t\mathcal{L}}h^{-1/2}.$$

Note that $\mathrm{i}L_0$ (respectively $\mathrm{i}L$) acting on $\mathcal{H}$ is unitarily equivalent to $\mathcal{L}_0$ (respectively $\mathcal{L}$) acting on the "energy" Hilbert space $\ell^2_{\mathbb{C}}(\mathbb{Z})\oplus\ell^2_{\mathbb{C}}(\mathbb{Z})$ equipped with the inner product $\langle\phi|\psi\rangle_{h_0} = \langle\phi|h_0|\psi\rangle$ (respectively $\langle\phi|\psi\rangle_h = \langle\phi|h|\psi\rangle$).

(v) L has purely absolutely continuous spectrum.

(vi) The Hilbert space $\mathcal{H}$ has a direct decomposition into three parts, $\mathcal{H}=\mathcal{H}_L\oplus\mathcal{H}_{\mathcal{C}}\oplus\mathcal{H}_R$, corresponding to the three subsystems $\mathcal{R}_L$, $\mathcal{C}$ and $\mathcal{R}_R$. We denote by P_L, $P_{\mathcal{C}}$ and P_R the corresponding orthogonal projections.

(vii) This decomposition reduces L_0 so that $L_0 = L_L \oplus L_{\mathcal{C}} \oplus L_R$. The operators L_L and L_R have purely absolutely continuous spectrum and $L_{\mathcal{C}}$ has purely discrete spectrum. In particular, $P_L + P_R$ is the spectral projection of L_0 onto its absolutely continuous part.

By Kato-Birman theory, the wave operators

$$W_\pm = \mathrm{s}-\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tL}\mathrm{e}^{-\mathrm{i}tL_0}(P_L + P_R)$$

exists and are complete, *i.e.*,

$$W_\pm^* = \mathrm{s}-\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tL_0}\mathrm{e}^{-\mathrm{i}tL},$$

also exists and satisfy $W_\pm^* W_\pm = P_L + P_R$, $W_\pm W_\pm^* = \mathbb{1}$. The scattering matrix $S = W_+^* W_-$ is unitary on $\mathcal{H}_L \oplus \mathcal{H}_R$. A few more remarks are needed to actually compute S:

(viii) One has

$$U^* L_0 U = \begin{bmatrix} \Omega_0 & 0 \\ 0 & -\Omega_0 \end{bmatrix}, \qquad U^* L U = \begin{bmatrix} \Omega & 0 \\ 0 & -\Omega \end{bmatrix},$$

where $\Omega = \sqrt{\mathbb{1} - \Delta}$ and $\Omega_0 = \sqrt{\mathbb{1} - \Delta_0}$ are discrete Klein-Gordon operators and U is the unitary

$$U = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & \mathrm{i} \\ \mathrm{i} & 1 \end{bmatrix}.$$

(ix) It follows that

$$W_\pm = U \begin{bmatrix} w_\pm & 0 \\ 0 & w_\mp \end{bmatrix} U^*,$$

where

$$w_\pm = \mathrm{s}-\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}t\Omega}\mathrm{e}^{-\mathrm{i}t\Omega_0}(P_L + P_R).$$

In particular, one has

$$S = U \begin{bmatrix} w_+^* w_- & 0 \\ 0 & w_-^* w_+ \end{bmatrix} U^*. \tag{1.21}$$

(x) By the invariance principle for wave operators, we have

$$\begin{aligned} w_\pm &= \mathrm{s}-\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}t\Omega^2}\mathrm{e}^{-\mathrm{i}t\Omega_0^2} P_{\mathrm{ac}}(\Omega_0^2) \\ &= \mathrm{s}-\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}t(-\Delta)}\mathrm{e}^{-\mathrm{i}t(-\Delta_0)} P_{\mathrm{ac}}(-\Delta_0). \end{aligned}$$

We proceed to compute the scattering matrix. A complete set of (properly normalized) generalized eigenfunctions for the absolutely continuous part of $-\Delta_0$ is given by

$$\phi_{\sigma,k}(x) = \sqrt{\frac{2}{\pi}}\,\theta(\sigma x - N)\sin k|\sigma x - N|, \qquad (\sigma,k) \in \{-,+\} \times [0,\pi],$$

where θ denotes the Heaviside step function and $-\Delta_0 \phi_{\sigma,k} = 2(1-\cos k)\phi_{\sigma,k}$. For the operator $-\Delta$, such a set is given by

$$\chi_{\sigma,k}(x) = \frac{1}{\sqrt{2\pi}}\,\mathrm{e}^{\mathrm{i}\sigma kx}, \qquad (\sigma,k) \in \{-,+\} \times [0,\pi].$$

Since

$$w_\pm \phi_{\sigma,k} = \mp\sigma \mathrm{i}\mathrm{e}^{\mp\mathrm{i}kN}\chi_{\pm\sigma,k},$$

we deduce that

$$w_\pm^* w_\mp \phi_{\sigma,k} = \mathrm{e}^{\pm 2\mathrm{i}kN}\phi_{-\sigma,k}. \tag{1.22}$$

We shall denote by $\mathfrak{h}_{k\pm}$ the 2-dimensional generalized eigenspace of L_0 to the "eigenvalue" $\pm\varepsilon(k) = \pm\sqrt{3-2\cos k}$. The space $\mathfrak{h}_{k+}$ is spanned by the two basis vectors

$$\psi_{\sigma,k,+} = U\begin{bmatrix}\phi_{\sigma,k}\\ 0\end{bmatrix}, \qquad \sigma\in\{-,+\},$$

and $\mathfrak{h}_{k-}$ is the span of

$$\psi_{\sigma,k,-} = U\begin{bmatrix}0\\ \phi_{\sigma,k}\end{bmatrix}, \qquad \sigma\in\{-,+\}.$$

In the direct integral representation

$$\mathcal{H}_L\oplus\mathcal{H}_R = \bigoplus_{\mu=\pm}\left(\int_{[0,\pi]}^{\oplus}\mathfrak{h}_{k\mu}\,\mathrm{d}k\right),$$

the scattering matrix is given by

$$S = \bigoplus_{\mu=\pm}\left(\int_{[0,\pi]}^{\oplus}S_\mu(k)\,\mathrm{d}k\right),$$

where, thanks to (1.21) and (1.22), the on-shell S-matrix $S_\mu(k)$ is given by

$$S_\pm(k) = S|_{\mathfrak{h}_{k\pm}} = \mathrm{e}^{\pm 2\mathrm{i}kN}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}. \tag{1.23}$$

1.10 Large time limit II: Non-equilibrium steady state

We shall now use scattering theory to compute the weak limit, as $t\to\infty$, of the state $\omega_{X,t}$. Setting $\widehat{X} = X_LP_L + X_RP_R$ for $X=(X_L,X_R)\in\mathbb{R}^2$, one has

$$k(X) = X_Lh_L + X_Rh_R = h_0^{1/2}\widehat{X}h_0^{1/2}.$$

Energy conservation yields $\mathrm{e}^{-t\mathcal{L}_0^*}k(X)\mathrm{e}^{-t\mathcal{L}_0} = k(X)$ and

$$\begin{aligned}
\mathrm{e}^{t\mathcal{L}^*}k(X)\mathrm{e}^{t\mathcal{L}} &= \mathrm{e}^{t\mathcal{L}^*}\mathrm{e}^{-t\mathcal{L}_0^*}h_0^{1/2}\widehat{X}h_0^{1/2}\mathrm{e}^{-t\mathcal{L}_0}\mathrm{e}^{t\mathcal{L}}\\
&= \mathrm{e}^{t\mathcal{L}^*}h_0^{1/2}\mathrm{e}^{-\mathrm{i}tL_0}\widehat{X}\mathrm{e}^{\mathrm{i}tL_0}h_0^{1/2}\mathrm{e}^{t\mathcal{L}}\\
&= \mathrm{e}^{t\mathcal{L}^*}h^{1/2}h^{-1/2}h_0^{1/2}\mathrm{e}^{-\mathrm{i}tL_0}\widehat{X}\mathrm{e}^{\mathrm{i}tL_0}h_0^{1/2}h^{-1/2}h^{1/2}\mathrm{e}^{t\mathcal{L}}\\
&= h^{1/2}\mathrm{e}^{\mathrm{i}tL}h^{-1/2}h_0^{1/2}\mathrm{e}^{-\mathrm{i}tL_0}\widehat{X}\mathrm{e}^{\mathrm{i}tL_0}h_0^{1/2}h^{-1/2}\mathrm{e}^{-\mathrm{i}tL}h^{1/2}.
\end{aligned}$$

By Property (ii) of the previous section, one has

$$\begin{aligned}
\mathrm{s}-\lim_{t\to\pm\infty}\mathrm{e}^{\mathrm{i}tL}h^{-1/2}h_0^{1/2}\mathrm{e}^{-\mathrm{i}tL_0}(P_L+P_R) &= W_\pm,\\
\mathrm{s}-\lim_{t\to\pm\infty}\mathrm{e}^{\mathrm{i}tL_0}h_0^{1/2}h^{-1/2}\mathrm{e}^{-\mathrm{i}tL} &= W_\pm^*,
\end{aligned}$$

and so

$$\mathrm{s}-\lim_{t\to\pm\infty}\mathrm{e}^{t\mathcal{L}^*}k(X)\mathrm{e}^{t\mathcal{L}} = h^{1/2}W_\pm\widehat{X}W_\pm^*h^{1/2}. \tag{1.24}$$

It follows that

$$\begin{aligned}
\mathrm{s}-\lim_{t\to\infty}D_{X,t} &= \mathrm{s}-\lim_{t\to\infty}(\beta h - \mathrm{e}^{-t\mathcal{L}^*}k(X)\mathrm{e}^{-t\mathcal{L}})^{-1}\\
&= (\beta h - h^{1/2}W_-\widehat{X}W_-^*h^{1/2})^{-1}\\
&= h^{-1/2}W_-(\beta-\widehat{X})^{-1}W_-^*h^{-1/2} = D_{X,+},
\end{aligned} \tag{1.25}$$

which implies that the state $\omega_{X,t}$ converges weakly to the Gaussian measure $\omega_{X,+}$ with covariance $D_{X,+}$. The state $\omega_{X,+}$ is invariant under the Hamiltonian flow $\mathrm{e}^{t\mathcal{L}}$ and is called the non-equilibrium steady state (NESS) associated to the reference state ω_X. Note that in the equilibrium case $\beta_L = \beta_R$ the operator $\widehat{X}$ is a multiple of the identity and

$$D_{X,+} = (\beta_L h)^{-1},$$

which means that the stationary state $\omega_{X,+}$ is the thermal equilibrium state of the coupled system at inverse temperature $\beta_L = \beta_R$.

Exercise 1.6. If $X_L \neq X_R$ then $\omega_{X,+}$ is singular w.r.t. ω_X, *i.e.,*

$$D_{X,+}^{-1} - D_X^{-1} = h_0^{1/2}\widehat{X}h_0^{1/2} - h^{1/2}W_-\widehat{X}W_-^* h^{1/2},$$

is not Hilbert-Schmidt. Prove this fact by deriving explicit formulas for $W_- P_{L/R} W_-^*$.

Exercise 1.7. Compute $\omega_{X,+}(\Phi_{L/R}) = \frac{1}{2}\mathrm{tr}(D_{X,+}\phi_{L/R})$ and show that

$$\omega_{X,+}(\Phi_L) = -\omega_{X,+}(\Phi_R) = \kappa(T_L - T_R),$$

where $T_{L/R} = \beta_{L/R}^{-1}$ is the temperature of the left/right reservoir and

$$\kappa = \frac{\sqrt{5}-1}{2\pi}.$$

Note in particular that $\omega_{X,+}(\Phi_L) + \omega_{X,+}(\Phi_R) = 0$. What is the physical origin of this fact ? Show that, more generally, if ω is a stationary state such that $\omega(p_x^2 + q_x^2) < \infty$ for all $x \in \mathbb{Z}$, then $\omega(\Phi_L) + \omega(\Phi_R) = 0$.

Using the result of Exercise 1.7 we conclude that

$$\begin{aligned}\omega_{X,+}(\sigma_X) &= X_L\omega_{X,+}(\Phi_L) + X_R\omega_{X,+}(\Phi_R)\\ &= (X_L - X_R)\omega_{X,+}(\Phi_L)\\ &= \kappa\frac{(T_L - T_R)^2}{T_L T_R} > 0,\end{aligned}$$

provided $T_L \neq T_R$. This implies that the mean entropy production rate in the state ω_X is strictly positive in the asymptotic regime[2],

$$\lim_{t\to\infty}\omega_X(\Sigma^t) = \lim_{t\to\infty}\frac{1}{t}\int_0^t \omega_X(\sigma_{X,s})\,\mathrm{d}s = \lim_{t\to\infty}\omega_{X,t}(\sigma_X) = \omega_{X,+}(\sigma_X) > 0,$$

and that it is constant and strictly positive in the NESS $\omega_{X,+}$,

$$\omega_{X,+}(\Sigma^t) = \frac{1}{t}\int_0^t \omega_{X,+}(\sigma_{X,s})\,\mathrm{d}s = \omega_{X,+}(\sigma_X) > 0.$$

[2]Recall that if $\lim_{t\to+\infty} f(t) = a$ exists then it coincide with the Cesáro limit of f at $+\infty$, $\lim_{T\to+\infty} T^{-1}\int_0^T f(t)\,\mathrm{d}t = a$, and with its Abel limit, $\lim_{\eta\downarrow 0}\eta\int_0^\infty \mathrm{e}^{-\eta t}f(t)\,\mathrm{d}t = a$.

1.11 Large time limit III: Generating functions

In this section we use scattering theory to study the large time asymptotic of the Evans-Searles functional $e_t(\alpha)$ (Equ. (1.11)) and the generalized Evans-Searles functional $g_t(X,Y)$ (Equ. (1.16)).

Starting from Equ. (1.18), and using (1.19) to write

$$T_t = -D_X \left(\mathrm{e}^{t\mathcal{L}^*} k(Y) \mathrm{e}^{t\mathcal{L}} - k(Y) \right) = \int_0^t D_X \mathrm{e}^{s\mathcal{L}^*} \phi(Y) \mathrm{e}^{s\mathcal{L}} \, \mathrm{d}s,$$

we get

$$\begin{aligned} \frac{1}{t} g_t(X,Y) &= -\frac{1}{2t} \log\det\left(\mathbb{1} + T_t\right) \\ &= -\frac{1}{2t} \mathrm{tr} \log\left(\mathbb{1} + T_t\right) \\ &= -\frac{1}{2t} \int_0^1 \frac{\mathrm{d}}{\mathrm{d}u} \mathrm{tr}\log\left(\mathbb{1} + uT_t\right) \mathrm{d}u. \end{aligned}$$

Using the result of Exercise 1.8, we further get

$$\begin{aligned} \frac{1}{t} g_t(X,Y) &= -\frac{1}{2t} \int_0^1 \mathrm{tr}\left(\left(\mathbb{1} + uT_t\right)^{-1} T_t \right) \mathrm{d}u \\ &= -\frac{1}{2t} \int_0^1 \int_0^t \mathrm{tr}\left(\left(\mathbb{1} + uT_t\right)^{-1} D_X \mathrm{e}^{s\mathcal{L}^*} \phi(Y) \mathrm{e}^{s\mathcal{L}} \right) \mathrm{d}s \, \mathrm{d}u \\ &= -\frac{1}{2t} \int_0^1 \int_0^t \mathrm{tr}\left[\left(D_X^{-1} - u\left(\mathrm{e}^{t\mathcal{L}^*} k(Y) \mathrm{e}^{t\mathcal{L}} - k(Y) \right) \right)^{-1} \mathrm{e}^{s\mathcal{L}^*} \phi(Y) \mathrm{e}^{s\mathcal{L}} \right] \mathrm{d}s \, \mathrm{d}u \\ &= -\frac{1}{2} \int_0^1 \int_0^1 \mathrm{tr}\left[\mathrm{e}^{st\mathcal{L}} \left(D_X^{-1} - u\left(\mathrm{e}^{t\mathcal{L}^*} k(Y) \mathrm{e}^{t\mathcal{L}} - k(Y) \right) \right)^{-1} \mathrm{e}^{st\mathcal{L}^*} \phi(Y) \right] \mathrm{d}s \, \mathrm{d}u. \end{aligned}$$

Writing

$$\begin{aligned} &\mathrm{e}^{st\mathcal{L}} \left(D_X^{-1} - u\left(\mathrm{e}^{t\mathcal{L}^*} k(Y) \mathrm{e}^{t\mathcal{L}} - k(Y) \right) \right)^{-1} \mathrm{e}^{st\mathcal{L}^*} \\ &\quad = \left(\mathrm{e}^{-st\mathcal{L}^*} D_X^{-1} \mathrm{e}^{-st\mathcal{L}} - u\, \mathrm{e}^{-st\mathcal{L}^*} \left(\mathrm{e}^{t\mathcal{L}^*} k(Y) \mathrm{e}^{t\mathcal{L}} - k(Y) \right) \mathrm{e}^{-st\mathcal{L}} \right)^{-1} \\ &\quad = \left(D_{X,st}^{-1} - u\left(\mathrm{e}^{(1-s)t\mathcal{L}^*} k(Y) \mathrm{e}^{(1-s)t\mathcal{L}} - \mathrm{e}^{-st\mathcal{L}^*} k(Y) \mathrm{e}^{-st\mathcal{L}} \right) \right)^{-1}, \end{aligned}$$

and using (1.24) and (1.25), we obtain

$$\begin{aligned} &\mathrm{s}-\lim_{t\to\infty} \mathrm{e}^{st\mathcal{L}} \left(D_X^{-1} - u\left(\mathrm{e}^{t\mathcal{L}^*} k(Y) \mathrm{e}^{t\mathcal{L}} - k(Y) \right) \right)^{-1} \mathrm{e}^{st\mathcal{L}^*} \\ &\quad = \left(D_{X,+}^{-1} - u h^{1/2} \left(W_+ \widehat{Y} W_+^* - W_- \widehat{Y} W_-^* \right) h^{1/2} \right)^{-1} \\ &\quad = \left(h^{1/2} \left(W_- (\beta - \widehat{X} + u\widehat{Y})^{-1} W_-^* - u W_+ \widehat{Y} W_+^* \right) h^{1/2} \right)^{-1} \\ &\quad = h^{-1/2} W_- \left(\beta - \widehat{X} - u(S^* \widehat{Y} S - \widehat{Y}) \right)^{-1} W_-^* \, h^{-1/2}, \end{aligned}$$

for all $s \in]0,1[$. Since $\phi(Y)$ is trace class (actually finite rank), we conclude that

$$g(X,Y) = \lim_{t\to\infty} \frac{1}{t} g_t(X,Y) = -\frac{1}{2} \int_0^1 \mathrm{tr}\left[\left(\beta - \widehat{X} - u(S^* \widehat{Y} S - \widehat{Y}) \right)^{-1} \mathcal{T} \right] \mathrm{d}u,$$

where

$$\mathcal{T} = W_-^* h^{-1/2} \phi(Y) h^{-1/2} W_-.$$

To evaluate the trace, we note that the scattering matrix S and the operators $\widehat{X}$, $\widehat{Y}$ all commute with L_0 while the trace class operator $\mathcal{T}$ acts non-trivially only on the absolutely continuous spectral subspace of L_0. It follows that

$$\begin{aligned}
&\mathrm{tr}\left[\left(\beta-\widehat{X}-u(S^*\widehat{Y}S-\widehat{Y})\right)^{-1}\mathcal{T}\right]\\
=&\mathrm{tr}\left[\left(\mathbb{1}-u(\beta-\widehat{X})^{-1}(S^*\widehat{Y}S-\widehat{Y})\right)^{-1}(\beta-\widehat{X})^{-1}\mathcal{T}\right]\\
=&\sum_{\mu=\pm}\int_0^\pi\sum_{\sigma=\pm}\langle\psi_{\sigma,k,\mu}|\left(\mathbb{1}-u(\beta-\widehat{X})^{-1}(S^*\widehat{Y}S-\widehat{Y})\right)^{-1}(\beta-\widehat{X})^{-1}\mathcal{T}|\psi_{\sigma,k,\mu}\rangle\,\mathrm{d}k.
\end{aligned}\tag{1.26}$$

Set

$$A(\eta)=\int_{-\infty}^{\infty}\mathrm{e}^{-\eta|t|}\langle\psi_{\sigma,k,\pm}|\mathrm{e}^{\mathrm{i}tL_0}\mathcal{T}\mathrm{e}^{-\mathrm{i}tL_0}|\psi_{\sigma',k',\pm}\rangle\frac{\mathrm{d}t}{2\pi},$$

$$B(\eta)=\eta\int_0^{\infty}\mathrm{e}^{-\eta t}\langle\psi_{\sigma,k,\pm}|\mathcal{F}|\psi_{\sigma',k',\pm}\rangle\frac{\mathrm{d}t}{2\pi},$$

where

$$\mathcal{F}=W_-^*h^{-1/2}\left(\mathrm{e}^{-t\mathcal{L}^*}k(Y)\mathrm{e}^{-t\mathcal{L}}-\mathrm{e}^{t\mathcal{L}^*}k(Y)\mathrm{e}^{t\mathcal{L}}\right)h^{-1/2}W_-.$$

By the intertwining property of the wave operator, we have

$$\begin{aligned}
\mathrm{e}^{\mathrm{i}tL_0}\mathcal{T}\mathrm{e}^{-\mathrm{i}tL_0}&=W_-^*\mathrm{e}^{\mathrm{i}tL}h^{-1/2}\phi(Y)h^{-1/2}\mathrm{e}^{-\mathrm{i}tL}W_-\\
&=W_-^*h^{-1/2}\mathrm{e}^{t\mathcal{L}^*}\phi(Y)\mathrm{e}^{t\mathcal{L}}h^{-1/2}W_-\\
&=-\frac{\mathrm{d}}{\mathrm{d}t}W_-^*h^{-1/2}\mathrm{e}^{t\mathcal{L}^*}k(Y)\mathrm{e}^{t\mathcal{L}}h^{-1/2}W_-,
\end{aligned}$$

and an integration by parts yields that

$$A(\eta)=B(\eta),\tag{1.27}$$

for any $\eta>0$. Let us now take the limit $\eta\downarrow 0$ in this formula. Since $\psi_{\sigma,k,\pm}$ is a generalized eigenfunction of L_0 to the eigenvalue $\pm\varepsilon(k)$, we get, on the left hand side of (1.27),

$$\langle\psi_{\sigma,k,\pm}|\mathcal{T}|\psi_{\sigma',k',\pm}\rangle\int_{-\infty}^{\infty}\mathrm{e}^{-\eta|t|\pm\mathrm{i}t(\varepsilon(k)-\varepsilon(k'))}\frac{\mathrm{d}t}{2\pi}\to\langle\psi_{\sigma,k,\pm}|\mathcal{T}|\psi_{\sigma',k,\pm}\rangle\delta(\varepsilon(k)-\varepsilon(k')).$$

Using (1.24), the Abel limit[3] on the right hand side of (1.27) yields

$$\begin{aligned}
&\frac{1}{2\pi}\langle\psi_{\sigma,k,\pm}|W_-^*h^{-1/2}\left(h^{1/2}W_-\widehat{Y}W_-^*h^{1/2}-h^{1/2}W_+\widehat{Y}W_+^*h^{1/2}\right)h^{-1/2}W_-|\psi_{\sigma',k',\pm}\rangle\\
&\qquad=\frac{1}{2\pi}\langle\psi_{\sigma,k,\pm}|\widehat{Y}-S^*\widehat{Y}S|\psi_{\sigma',k',\pm}\rangle\\
&\qquad=\frac{1}{2\pi}\langle\psi_{\sigma,k,\pm}|\widehat{Y}-S_\pm(k)^*\widehat{Y}S_\pm(k)|\psi_{\sigma',k,\pm}\rangle\delta(k-k'),
\end{aligned}$$

and we conclude that

$$\langle\psi_{\sigma,k,\pm}|\mathcal{T}|\psi_{\sigma',k,\pm}\rangle=\frac{1}{2\pi}\langle\psi_{\sigma,k,\pm}|\widehat{Y}-S_\pm(k)^*\widehat{Y}S_\pm(k)|\psi_{\sigma',k,\pm}\rangle\varepsilon'(k).\tag{1.28}$$

Note that the operator $\widehat{Y}$ acts on the fiber $\mathfrak{h}_{k\pm}$ as the matrix

$$\widehat{Y}\Big|_{\mathfrak{h}_{k\pm}}=\left[\begin{array}{cc}Y_L&0\\0&Y_R\end{array}\right].\tag{1.29}$$

[3] See footnote 2 on page 19

Relation (1.28) allows us to write

$$\begin{aligned}
&\sum_{\sigma=\pm}\langle\psi_{\sigma,k,\mu}|\left(I-u(\beta-\widehat{X})^{-1}(S^*\widehat{Y}S-\widehat{Y})\right)^{-1}(\beta-\widehat{X})^{-1}\mathcal{T}|\psi_{\sigma,k,\mu}\rangle\\
&\qquad=\operatorname{tr}_{\mathfrak{h}_{k\mu}}\left[\left(\mathbb{1}-u(\beta-\widehat{X})^{-1}(S_\mu(k)^*\widehat{Y}S_\mu(k)-\widehat{Y})\right)^{-1}\right.\\
&\qquad\qquad\left.\times\,(\beta-\widehat{X})^{-1}(\widehat{Y}-S_\mu(k)^*\widehat{Y}S_\mu(k))\right]\frac{\varepsilon'(k)}{2\pi}\\
&\qquad=\frac{\mathrm{d}}{\mathrm{d}u}\operatorname{tr}_{\mathfrak{h}_{k\mu}}\left[\log\left(\mathbb{1}-u(\beta-\widehat{X})^{-1}(S_\mu(k)^*\widehat{Y}S_\mu(k)-\widehat{Y})\right)\right]\frac{\varepsilon'(k)}{2\pi}.
\end{aligned}$$

Inserting the last identity into (1.26) and integrating over u we derive

$$\begin{aligned}
g(X,Y)&=-\sum_{\mu=\pm}\int_0^\pi\operatorname{tr}_{\mathfrak{h}_{k\mu}}\left[\log\left(\mathbb{1}-(\beta-\widehat{X})^{-1}(S_\mu(k)^*\widehat{Y}S_\mu(k)-\widehat{Y})\right)\right]\frac{\mathrm{d}\varepsilon(k)}{4\pi}\\
&=-\sum_{\mu=\pm}\int_0^\pi\log\det{}_{\mathfrak{h}_{k\mu}}\left(\mathbb{1}-(\beta-\widehat{X})^{-1}(S_\mu(k)^*\widehat{Y}S_\mu(k)-\widehat{Y})\right)\frac{\mathrm{d}\varepsilon(k)}{4\pi}.
\end{aligned}$$

Remark. The last formula retains its validity in a much broader context. It holds for an arbitrary number of infinite harmonic reservoirs coupled to a finite harmonic system as long as the scattering approach sketched here applies. Furthermore, the formal analogy between our Hilbert space treatment of harmonic dynamics and quantum mechanics suggests that quasi-free quantum systems could be also studied by a similar scattering approach. That is indeed the case, see Section 6.6.

Invoking (1.23) and (1.29) leads to our final result

$$g(X,Y)=-\kappa\log\left(1+\frac{(Y_R-Y_L)\left[(X_R-X_L)-(Y_R-Y_L)\right]}{(\beta-X_R)(\beta-X_L)}\right).\tag{1.30}$$

Note that $g(X,Y)$ is finite for $-T_R^{-1}<Y_R-Y_L<T_L^{-1}$ and $+\infty$ otherwise. Since $e_t(\alpha)=g_t(X,\alpha X)$, one has

$$e(\alpha)=\lim_{t\to\infty}\frac{1}{t}e_t(\alpha)=-\kappa\log\left(1+\frac{(T_L-T_R)^2}{T_LT_R}\alpha(1-\alpha)\right),$$

which is finite provided $2|\alpha-1/2|<(T_L+T_R)/|T_L-T_R|$ and $+\infty$ otherwise (see Figure 1.4). Note also the explicit symmetries $g(X,X-Y)=g(X,Y)$ and $e(1-\alpha)=e(\alpha)$ inherited from the finite time Evans-Searles symmetries (1.14) and (1.17).

Exercise 1.8. Let $\mathbb{R}\ni x\mapsto A(x)$ be a differentiable function with values in the trace class operators on a Hilbert space. Show that if $\|A(x_0)\|<1$ then $x\mapsto\operatorname{tr}\log(\mathbb{1}+A(x))$ is differentiable at x_0 and

$$\left.\frac{\mathrm{d}}{\mathrm{d}x}\operatorname{tr}\log(\mathbb{1}+A(x))\right|_{x=x_0}=\operatorname{tr}((\mathbb{1}+A(x_0))^{-1}A'(x_0)).$$

Hint: use the formula

$$\log(1+a)=\int_1^\infty\left(\frac{1}{t}-\frac{1}{t+a}\right)\mathrm{d}t,$$

valid for $|a|<1$.

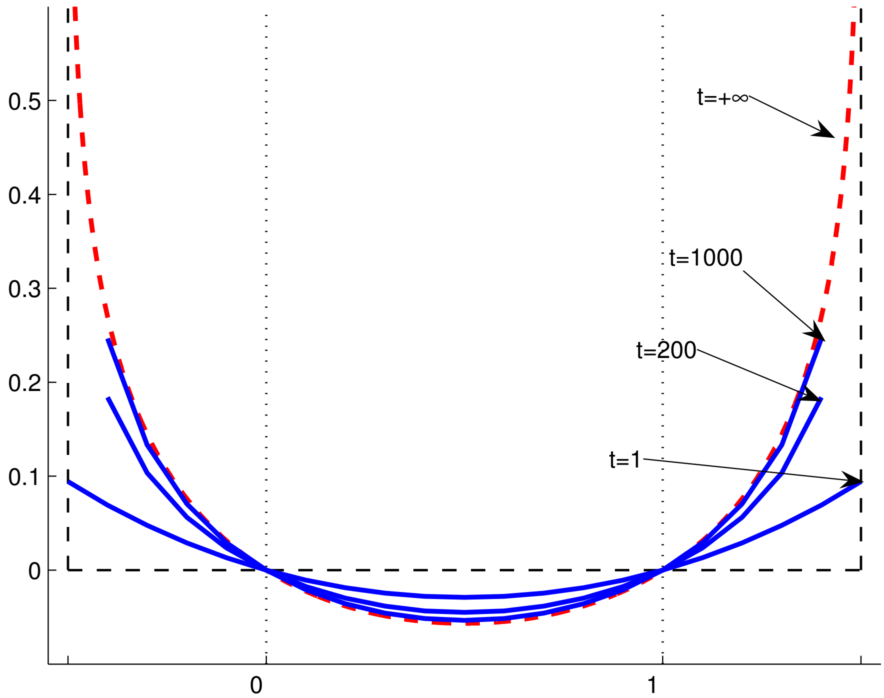

Figure 1.4: Solid lines: the generating function $\alpha \mapsto t^{-1}e_t(\alpha)$ for various values of t and finite reservoirs ($N = 20$, $M = 300$). The slope at $\alpha = 1$ is $\omega_X(\Sigma^t)$, compare with Figure 1.3. Dashed line: the limiting function $\alpha \mapsto e(\alpha)$ for infinite reservoirs.

1.12 The central limit theorem

As a first application of the generalized Evans-Searles functional $g(X,Y)$, we derive a central limit theorem (CLT) for the current fluctuations. To this end, let us decompose the mean currents into its expected value and a properly normalized fluctuating part, writing

$$\frac{1}{t}\int_0^t \Phi_{j,s}\,\mathrm{d}s = \frac{1}{t}\int_0^t \omega_X(\Phi_{j,s})\,\mathrm{d}s + \frac{1}{\sqrt{t}}\delta\Phi_j^t,$$

for $j \in \{L,R\}$. By Definition (1.16), the expected mean current is given by

$$\frac{1}{t}\int_0^t \omega_X(\Phi_{j,s})\,\mathrm{d}s = -\left.\partial_{Y_j}\frac{1}{t}g_t(X,Y)\right|_{Y=0},$$

while the fluctuating part is centered, $\omega_X(\delta\Phi_{j,t}) = 0$, with covariance

$$\omega_X(\delta\Phi_j^t\delta\Phi_k^t) = \left.\partial_{Y_k}\partial_{Y_j}\frac{1}{t}g_t(X,Y)\right|_{Y=0}.$$

For large t, the expected mean current converges to the NESS expectation

$$\lim_{t\to\infty}\frac{1}{t}\int_0^t \omega_X(\Phi_{j,s})\,\mathrm{d}s = \omega_{X,+}(\Phi_j).$$

To study the large time asymptotics of the current fluctuations $\delta\mathbf{\Phi}^t = (\delta\Phi_L^t, \delta\Phi_R^t)$ we consider the characteristic function

$$\omega_X\left(\mathrm{e}^{\mathrm{i}Y\cdot\delta\mathbf{\Phi}^t}\right) = \omega_X\left(\mathrm{e}^{\mathrm{i}\sum_j Y_j\frac{1}{\sqrt{t}}\int_0^t(\Phi_{j,s}-\omega_X(\Phi_{j,s}))\,\mathrm{d}s}\right), \tag{1.31}$$

i.e., the Fourier transform of their distribution. To control the limit $t\to\infty$, we need a technical result which is the object of the following exercise.

Exercise 1.9. Show that for a given $\beta_L > 0$ and $\beta_R > 0$ there exists $\epsilon > 0$ such that the function $Y \mapsto g_t(X,Y)$ is analytic in $D_\epsilon = \{Y = (Y_L, Y_R) \in \mathbb{C}^2 \,|\, |Y_L| < \epsilon, |Y_R| < \epsilon\}$ and satisfies

$$\sup_{\substack{Y\in D_\epsilon\\ t>0}}\left|\frac{1}{t}g_t(X,Y)\right| < \infty. \tag{1.32}$$

Hint: start with (1.18) and use the identity $\log\det(\mathbb{1}-T) = \mathrm{tr}(\log(\mathbb{1}-T))$ and the factorization $\log(\mathbb{1}-z) = -zf(z)$ to obtain the bound $|\log\det(\mathbb{1}-T)| \le \|T\|_1 f(\|T\|)$ where $\|T\|_1 = \mathrm{tr}(\sqrt{T^*T})$ denotes the trace norm of T.

The convergence result of the preceding section and the uniform bound (1.32) imply that

$$\lim_{t\to\infty}\frac{1}{t}g_t(X,Y) = g(X,Y),$$

uniformly for Y in compact subsets of D_ϵ, that all the derivatives w.r.t. Y of $\frac{1}{t}g_t(X,Y)$ are uniformly bounded on such compact subsets and converge uniformly to the corresponding derivatives of $g(X,Y)$ (see Theorem B.1 in Appendix B). For $Y \in \mathbb{C}^2$ and $t > 0$ large enough, Equ. (1.31) can be written as

$$\omega_X\left(\mathrm{e}^{\mathrm{i}Y\cdot\delta\mathbf{\Phi}^t}\right) = \exp\left[t\left(\frac{1}{t}g_t\left(X,\frac{Y}{\mathrm{i}\sqrt{t}}\right) - \frac{Y}{\mathrm{i}\sqrt{t}}\cdot\left(\mathbf{\nabla}_Y\frac{1}{t}g_t\right)(X,0)\right)\right],$$

and the Taylor expansion of $\frac{1}{t}g_t(X,Y)$ around $Y=0$ yields

$$\frac{1}{t}g_t\left(X,\frac{Y}{\mathrm{i}\sqrt{t}}\right) - \frac{Y}{\mathrm{i}\sqrt{t}}\cdot\left(\mathbf{\nabla}_Y\frac{1}{t}g_t\right)(X,0) = -\frac{1}{2t}\sum_{j,k}\left(\partial_{Y_j}\partial_{Y_k}\frac{1}{t}g_t\right)(X,0)Y_jY_k + O(t^{-3/2}),$$

from which we conclude that

$$\lim_{t\to\infty} \omega_X\left(\mathrm{e}^{\mathrm{i}Y\cdot\delta\mathbf{\Phi}^t}\right) = \mathrm{e}^{-\frac{1}{2}Y\cdot\mathbf{D}Y}, \tag{1.33}$$

with a covariance matrix $\mathbf{D} = [D_{jk}]$ given by

$$D_{jk} = \lim_{t\to\infty}\left(\partial_{Y_j}\partial_{Y_k}\frac{1}{t}g_t\right)(X,0) = \left(\partial_{Y_j}\partial_{Y_k}g\right)(X,0).$$

Evaluating the right hand side of these identities yields

$$D_{11} = D_{22} = -D_{12} = -D_{21} = \kappa\left(T_L^2 + T_R^2\right).$$

Since the right hand side of (1.33) is the Fourier transform of the centered Gaussian measure on $\mathbb{R}^2$ with covariance $\mathbf{D}$, the Lévy-Cramér continuity theorem (see *e.g.*, Theorem 7.6 in [Bi1]) implies that the current fluctuations $\delta\mathbf{\Phi}^t$ converge in law to this Gaussian, *i.e.*, that for all bounded continuous functions $f : \mathbb{R}^2 \to \mathbb{R}$

$$\lim_{t\to\infty}\omega_X(f(\delta\mathbf{\Phi}^t)) = \int f(\phi,-\phi)\mathrm{e}^{-\phi^2/2\mathfrak{d}}\frac{\mathrm{d}\phi}{\sqrt{2\pi\mathfrak{d}}}, \tag{1.34}$$

where $\mathfrak{d} = \kappa\left(T_L^2 + T_R^2\right)$. Note in particular that the fluctuations of the left and right mean currents are opposite to each other in this limit.

Exercise 1.10. Use the CLT (1.34) and the results of Exercise 1.7 to show that

$$\frac{1}{t}\int_0^t\left(\Phi_{L,s} + \Phi_{R,s}\right)\mathrm{d}s \longrightarrow 0,$$

in probability as $t\to\infty$, *i.e.*, that for any $\epsilon > 0$ the probability

$$\omega_X\left(\left\{\left|\frac{1}{t}\int_0^t\left(\Phi_{L,s}+\Phi_{R,s}\right)\mathrm{d}s\right| \geq \epsilon\right\}\right), \tag{1.35}$$

tends to zero as $t\to\infty$.

It is interesting to compare the equilibrium ($T_L = T_R$) and the non-equilibrium ($T_L \neq T_R$) case. In the first case the expected mean currents vanish (recall that in this case $\omega_{X,+}$ is the equilibrium state) while in the second they are non-zero. In both cases the fluctuations of the mean currents have similar qualitative features at the CLT scale $t^{-1/2}$. In particular they are always symmetrically distributed w.r.t. 0.

1.13 Linear response theory near equilibrium

The linear response theory for our harmonic chain model follows trivially from the formula for steady heat fluxes derived in Exercise 1.7. Our goal in this section, however, is to present a derivation of the linear response theory based on the functionals $g_t(X,Y)$ and $g(X,Y)$. This derivation, which follows the ideas of Gallavotti [Ga], is applicable to any time-reversal invariant dynamical system for which the conclusions of Exercise 1.9 hold. For additional information and a general axiomatic approach to derivation of linear response theory based on functionals $g_t(X,Y)$ and $g(X,Y)$ we refer the reader to [JPR].

Starting from

$$-\lim_{t\to\infty}\partial_{Y_{L/R}}\frac{1}{t}g_t(X,Y)\Big|_{Y=0} = \omega_{X,+}(\Phi_{L/R}),$$

and using the fact that the derivative and the limit can be interchanged (as we learned in the previous section) one gets

$$-\partial_{Y_{L/R}}g(X,Y)\big|_{Y=0} = \omega_{X,+}(\Phi_{L/R}). \tag{1.36}$$

Remark. The main result of Section 1.11, which expresses the Evans-Searles function $g(X, Y)$ in terms of the on-shell scattering matrix, immediately implies

$$\begin{aligned}
&\omega_{X,+}(\Phi_{L/R}) \\
&= \partial_{Y_{L/R}} \sum_{\mu=\pm} \int_0^\pi \mathrm{tr}_{\mathfrak{h}_{k\mu}} \left[\log \left(\mathbb{1} - (\beta - \widehat{X})^{-1} (S_\mu(k)^* \widehat{Y} S_\mu(k) - \widehat{Y}) \right) \right] \frac{\mathrm{d}\varepsilon(k)}{4\pi} \bigg|_{Y=0} \\
&= \sum_{\mu=\pm} \int_0^\pi \mathrm{tr}_{\mathfrak{h}_{k\mu}} \left[(\beta - \widehat{X})^{-1} (P_{L/R} - S_\mu(k)^* P_{L/R} S_\mu(k)) \right] \frac{\mathrm{d}\varepsilon(k)}{4\pi},
\end{aligned}$$

which can be interpreted as a classical version of the Landauer-Büttiker formula (see Exercise 6.13).

The Onsager matrix $\mathbf{L} = [L_{jk}]_{j,k \in \{L,R\}}$ defined by

$$L_{jk} = \partial_{X_k} \omega_{X,+}(\Phi_j)\big|_{X=0},$$

describes the response of the system to weak thermodynamic forces. Taylor's formula

$$\omega_{X,+}(\Phi_j) = \sum_k L_{jk} X_k + o(X), \qquad (X \to 0),$$

expresses the steady currents to the lowest order in the driving forces. From (1.36), we deduce that

$$L_{jk} = -\partial_{X_k} \partial_{Y_j} g(X, Y)\big|_{X=Y=0}.$$

The ES symmetry $g(X, X - Y) = g(X, Y)$ further leads to

$$\begin{aligned}
\partial_{X_k} \partial_{Y_j} g(X, Y) &= \partial_{X_k} \partial_{Y_j} g(X, X - Y) \\
&= -\partial_{X_k} (\partial_{Y_j} g)(X, X - Y) \\
&= -(\partial_{X_k} \partial_{Y_j} g)(X, X - Y) - (\partial_{Y_k} \partial_{Y_j} g)(X, X - Y),
\end{aligned}$$

so that

$$\partial_{X_k} \partial_{Y_j} g(X, Y)\big|_{X=Y=0} = -\frac{1}{2} \partial_{Y_k} \partial_{Y_j} g(X, Y)\bigg|_{X=Y=0}, \tag{1.37}$$

and hence

$$L_{jk} = \frac{1}{2} \partial_{Y_k} \partial_{Y_j} g(0, Y)\bigg|_{Y=0}. \tag{1.38}$$

Since the function $g(0, Y)$ is C^2 at $Y = 0$, we conclude from (1.38) that the Onsager reciprocity relation

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

hold.

Exercise 1.11. In regard to Onsager relation, open systems with *two* thermal reservoirs are special. Show that the Onsager relation follow from the conservation law

$$\omega_{X,+}(\Phi_L) + \omega_{X,+}(\Phi_R) = 0.$$

Time-reversal invariance plays no role in this argument! What is the physical origin of this derivation? Needless to say, the derivation of Onsager reciprocity relation described in this section directly extends to open classical systems coupled to more than 2 thermal reservoirs to which this exercise does not apply.

The positivity of entropy production implies

$$0 \leq \omega_{X,+}(\sigma_X) = \sum_j \omega_{X,+}(\Phi_j) X_j = \sum_{j,k} L_{jk} X_j X_k + o(|X|^2),$$

so that the Onsager matrix is positive semi-definite. In fact, looking back at Section 1.12, we observe that the Onsager matrix coincide, up to a constant factor, with the covariance of the current fluctuations at equilibrium,

$$\mathbf{L} = \frac{1}{2} \mathbf{D}\Big|_{X=0}.$$

This is of course the celebrated Einstein relation.

For our harmonic chain model the Green-Kubo formula for the Onsager matrix can be derived by an explicit computation. In the following exercises we outline a derivation that extends to general time-reversal invariant dynamical systems.

Exercise 1.12. Show that the Green-Kubo formula holds in the Cesàro sense

$$L_{jk} = \lim_{t\to\infty} \frac{1}{t} \int_0^t \left[\frac{1}{2} \int_{-s}^{s} \omega_0(\Phi_j \Phi_{k,\tau})\, \mathrm{d}\tau \right] \mathrm{d}s.$$

Hint: using the results of the previous section, rewrite (1.38) as

$$L_{jk} = \lim_{t\to\infty} \partial_{Y_k} \partial_{Y_j} \frac{1}{2t} g_t(0, Y)\Big|_{Y=0},$$

and work out the derivatives.

Exercise 1.13. Using the fact† that $\langle \delta_x | \mathrm{e}^{\mathrm{i}t\sqrt{I-\Delta}} | \delta_y \rangle = O(t^{-1/2})$ as $t \to \infty$ (δ_x is the Kronecker delta at $x \in \mathbb{Z}$), show that $\omega_0(\Phi_j \Phi_{k,t}) = O(t^{-1})$. Invoke the Hardy-Littlewood Tauberian theorem (see, *e.g.*, [Ko]) to conclude that the Kubo formula

$$L_{jk} = \lim_{t\to\infty} \frac{1}{2} \int_{-t}^{t} \omega_0(\Phi_j \Phi_{k,\tau})\, \mathrm{d}\tau,$$

holds.

†This follows from a simple stationary phase estimate.

1.14 The Evans-Searles fluctuation theorem

The central limit theorem derived in Section 1.12 shows that, for large t, typical fluctuations of the mean current $\mathbf{\Phi}^t$ with respect to its expected value $\omega_X(\mathbf{\Phi}^t)$ are small, of the order $t^{-1/2}$. In the same regime $t \to \infty$, the theory of large deviations provides information on the probability of occurrence of bigger fluctuations, of the order 1. More precisely, the existence of the limit[4],

$$g(X, Y) = \lim_{t\to\infty} \frac{1}{t} \log \int \mathrm{e}^{-tY\cdot s}\, \mathrm{d}Q^t(s), \tag{1.39}$$

[4]The distribution Q^t of the mean current $\mathbf{\Phi}^t$ was introduced in Exercise 1.4

and the regularity of the function $Y \mapsto g(X,Y)$ allow us to apply the Gärtner-Ellis theorem (see Exercise 1.15 below) to obtain the Large Deviation Principle (LDP)

$$-\inf_{s\in\mathrm{int}(G)} I_X(s) \leq \liminf_{t\to\infty} \frac{1}{t}\log Q^t(G) \leq \limsup_{t\to\infty}\frac{1}{t}\log Q^t(G) \leq -\inf_{s\in\mathrm{cl}(G)} I_X(s),$$

for any Borel set $G\subset\mathbb{R}^2$. Here, $\mathrm{int}(G)$ denotes the interior of G, $\mathrm{cl}(G)$ its closure, and the rate function $I_X:\mathbb{R}^2\to[-\infty,0]$ is given by

$$I_X(s) = -\inf_{Y\in\mathbb{R}^2}\left(Y\cdot s + g(X,Y)\right).$$

The symmetry $g(X,Y)=g(X,X-Y)$ implies

$$I_X(-s) = X\cdot s + I_X(s). \tag{1.40}$$

The last relation is sometimes called the Evans-Searles symmetry for the rate function.

Exercise 1.14. Show that

$$I_X(s_L,s_R) = \begin{cases} +\infty & \text{if } s_L+s_R\neq 0,\\ F(\theta) & \text{if } s_L=-s_R=\dfrac{\kappa}{\beta_0}\sinh\theta, \end{cases}$$

where

$$F(\theta)=\kappa\left[2\sinh^2\frac{\theta}{2}-\frac{\delta}{\beta_0}\sinh\theta-\log\left(\left(1-\frac{\delta^2}{\beta_0^2}\right)\cosh^2\frac{\theta}{2}\right)\right],$$

$\beta_0=\beta-(X_L+X_R)/2$ and $\delta=(X_L-X_R)/2$. Show that $I_X(s_L,s_R)$ is strictly positive (or $+\infty$) except for $s_L=-s_R=\omega_{X,+}(\Phi_L)$ where it vanishes. Compare with Figure 1.5.

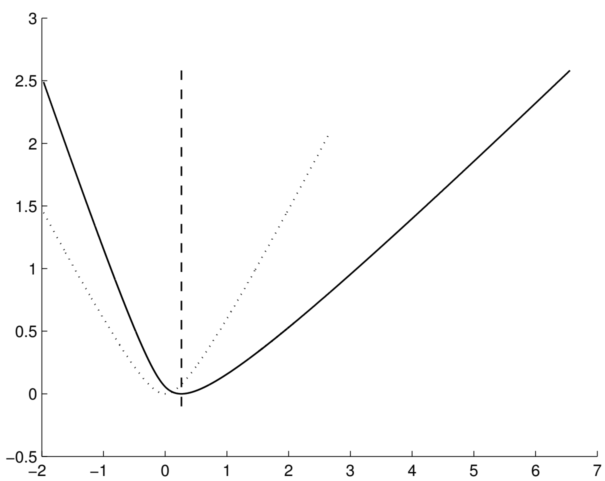

Figure 1.5: The rate function $I_X(s,-s)$ (solid line). Notice the asymmetry which reflects the fact that $X_L > X_R$. The dashed vertical line marks the position of the mean current $\omega_{X,+}(\Phi_L)>0$. In contrast, the rate function $I_X(s,-s)$ in the absence of forcing, $X_L=X_R$, (dotted line) is symmetric around zero.

The LDP provides the most powerful formulation of the Evans-Searles or transient fluctuation theorem. In particular, it gives fairly precise information on the rate at which the measure Q^t concentrates on the diagonal $\{(\phi, -\phi) \,|\, \phi \in \mathbb{R}\}$ (recall Exercise 1.10): the probability (1.35) decays super-exponentially as $t \to \infty$ for any $\epsilon > 0$. Taking this fact as well as the continuity of the function $F(\theta)$ into account, we observe that for any interval $J \subset \mathbb{R}$ one has

$$\lim_{t\to\infty} \frac{1}{t} \log Q^t(J \times \mathbb{R}) = -\inf_{s\in J} I_X(s, -s).$$

A rough interpretation of this formula

$$\omega_X \left(\left\{ \frac{1}{t} \int_0^t \Phi_{L,s}\, \mathrm{d}s = \phi \right\} \right) \sim \mathrm{e}^{-tI_X(\phi,-\phi)},$$

identifies $I_X(-\phi, \phi)$ as the rate of exponential decay of the probability for the mean current to deviate from its expected value $\omega_{X,+}(\Phi_L)$. More precisely, one has

$$\lim_{\delta\downarrow 0} \lim_{t\to\infty} \frac{1}{t} \log Q^t([\phi - \delta, \phi + \delta] \times \mathbb{R}) = -I_X(\phi, -\phi). \tag{1.41}$$

The symmetry (1.40) implies

$$I_X(-\phi, \phi) = I_X(\phi, -\phi) + (X_L - X_R)\phi \geq (X_L - X_R)\phi,$$

and it follows that

$$\lim_{\delta\downarrow 0} \lim_{t\to\infty} \frac{1}{t} \log \frac{Q^t([-\phi - \delta, -\phi + \delta] \times \mathbb{R})}{Q^t([\phi - \delta, \phi + \delta] \times \mathbb{R})} = -(X_L - X_R)\phi, \tag{1.42}$$

or, in a more sloppy notation,

$$\frac{\omega_X \left(\left\{ \frac{1}{t} \int_0^t \Phi_{L,s}\, \mathrm{d}s = -\phi \right\} \right)}{\omega_X \left(\left\{ \frac{1}{t} \int_0^t \Phi_{L,s}\, \mathrm{d}s = \phi \right\} \right)} \sim \mathrm{e}^{-t(X_L - X_R)\phi}.$$

This shows that the mean current is exponentially more likely to flow from the hotter to the colder reservoir than in the opposite direction, *i.e.*, on a large time scale, the probability of violating the second law of thermodynamics becomes exceedingly small. Note also that (1.42) is (essentially) a considerably weaker statement then (1.41). Relation (1.42), after replacing $\lim$ with $\limsup / \liminf$ can be derived directly from the finite time symmetry $g_t(X, Y) = g_t(X, X - Y)$ and without invoking the large deviation theory.

Exercise 1.15. Check that the Gärtner-Ellis theorem (Theorem A.6 in Appendix A.3 applies to (1.39), *i.e.*, show that the function $Y \mapsto g(X, Y)$ given in Equ. (1.30) is differentiable on the domain $\mathcal{D} = \{(Y_L, Y_R) \in \mathbb{R}^2 \,|\, -T_R^{-1} < Y_R - Y_L < T_L^{-1}\}$ where it is finite and that it is steep, *i.e.*,

$$\lim_{\mathcal{D}\ni Y\to Y_0} |\boldsymbol{\nabla}_Y g(X, Y)| = \infty,$$

for $Y_0 \in \partial\mathcal{D}$.

Exercise 1.16. Apply the Gärtner-Ellis theorem to the generating function $e(\alpha)$ to derive a LDP for the mean entropy production rate Σ^t, *i.e.*, for the probability distribution P^t of Section 1.6.

1.15 The Gallavotti-Cohen fluctuation theorem

In this section we briefly comment on the Gallavotti-Cohen fluctuation theorem for a thermally driven harmonic chain. Let us consider the cumulant generating function of the currents in the NESS $\omega_{X,+}$,

$$g_{+,t}(X,Y) = \omega_{X,+}\left(\mathrm{e}^{-tY\cdot\mathbf{\Phi}^t}\right).$$

Evaluating the Gaussian integral yields

$$g_{+,t}(X,Y) = -\frac{1}{2}\log\det\left(\mathbb{1} - D_{X,+}\left(\mathrm{e}^{t\mathcal{L}^*}k(Y)\mathrm{e}^{t\mathcal{L}} - k(Y)\right)\right).$$

Proceeding as in Section 1.11, one shows that

$$g_+(X,Y) = \lim_{t\to\infty}\frac{1}{t}g_{+,t}(X,Y) = \lim_{t\to\infty}\frac{1}{t}g_t(X,Y) = g(X,Y).$$

Hence, $g_+(X,Y)$ and the corresponding rate functions $I_{X,+}(s) = I_X(s)$ inherit the symmetries

$$g_+(X,Y) = g_+(X,X-Y), \qquad I_{X,+}(-s) = X\cdot s + I_{X,+}(s).$$

Via Gärtner-Ellis theorem, the functional $I_{X,+}(s)$ control the fluctuations of $\mathbf{\Phi}^t$ as $t\to\infty$ w.r.t. $\omega_{X,+}$ and, after replacing ω_X with $\omega_{X,+}$ (so now $Q^t(f) = \omega_{X,+}(f(\mathbf{\Phi}^t)$, etc) one can repeat the discussion of the previous section line by line. The obtained results are called the Gallavotti-Cohen fluctuation theorem.

Since $\omega_{X,+}$ is singular w.r.t. ω_X in the non-equilibrium case $X_L \neq X_R$, the Gallavotti-Cohen fluctuation theorem refers to configurations (points in the phase space) which are not seen by the Evans-Searles fluctuation theorem (and vice versa, of course). The identity $g_+(X,Y) = g(X,Y)$, which was for the first time observed in [JPR], may seem surprising on the first sight. It turned out, however, that it holds for any *non-trivial* model for which the existence of $g_+(X,Y)$ and $g(X,Y)$ has been established. This point has been raised in [JPR] to the *Principle of Regular Entropic Fluctuations*. Since we will not discuss quantum Gallavotti-Cohen fluctuation theorem in these lecture notes, we refer the reader to [JPR, JOPP] for additional discussion of these topics.

Chapter 2

Algebraic quantum statistical mechanics of finite systems

We now turn to the main topic of these lecture notes: quantum statistical mechanics. This section is devoted to a detailed exposition of the mathematical structure of algebraic quantum statistical mechanics of finite quantum systems.

2.1 Notation and basic facts

Let $\mathcal{K}$ be a finite dimensional complex Hilbert space with inner product $\langle\psi|\phi\rangle$ linear in the second argument[1]. Recall the Schwarz inequality $\langle\psi|\phi\rangle \leq \|\psi\|\,\|\phi\|$, where equality holds iff ψ and ϕ are collinear. In particular $\|\phi\| = \sup_{\|\psi\|=1}\langle\psi|\phi\rangle$. We will use Dirac's notation: for $\psi \in \mathcal{K}$, $\langle\psi|$ denotes the linear functional $\mathcal{K} \ni \phi \mapsto \langle\psi|\phi\rangle \in \mathbb{C}$ and $|\psi\rangle$ its adjoint $\mathbb{C} \ni \alpha \mapsto \alpha\psi \in \mathcal{K}$.

We denote by $\mathcal{O}$ the $*$-algebra[2] of all linear maps $A : \mathcal{K} \to \mathcal{K}$. For $A \in \mathcal{O}$, $\|A\| = \sup_{\|\psi\|=1} \|A\psi\|$ denotes its operator norm and $\mathrm{sp}(A)$ its spectrum, *i.e.*, the set of all eigenvalues of A. Let us recall some important properties of the operator norm. Since $\|A\psi\| \leq \|A\|\,\|\psi\|$, it follows that $\|AB\| \leq \|A\|\,\|B\|$ for all $A, B \in \mathcal{O}$. Since

$$\|A^*\phi\| = \sup_{\|\psi\|=1} \langle\psi|A^*\phi\rangle \sup_{\|\psi\|=1} \langle A\psi|\phi\rangle \leq \|A\|\,\|\phi\|,$$

and $A^{**} = A$, one has $\|A^*\| = \|A\|$ for all $A \in \mathcal{O}$. Finally, from the two inequalities $\|A^*A\| \leq \|A^*\|\,\|A\| = \|A\|^2$ and

$$\|A\|^2 = \sup_{\|\psi\|=1} \|A\psi\|^2 = \sup_{\|\psi\|=1} \langle A\psi|A\psi\rangle = \sup_{\|\psi\|=1} \langle\psi|A^*A\psi\rangle \leq \|A^*A\|,$$

on deduces the C^*-property $\|A^*A\| = \|A\|^2$.

The identity operator is denoted by $\mathbb{1}$ and, whenever the meaning is clear within the context, we shall write α for $\alpha\mathbb{1}$ and $\alpha \in \mathbb{C}$. Occasionally, we shall indicate the dependence on the underlying Hilbert space $\mathcal{K}$ by the subscript $_{\mathcal{K}}$ ($\mathcal{O}_{\mathcal{K}}$, $\mathbb{1}_{\mathcal{K}}$, etc).

To any orthonormal basis $\{e_1, \ldots, e_N\}$ of the Hilbert space $\mathcal{K}$ one can associate the basis $\{E_{ij} = |e_i\rangle\langle e_j| \,|\, i, j = 1, \ldots, N\}$ of $\mathcal{O}$ so that, for any $X \in \mathcal{O}$,

$$X = \sum_{i,j=1}^{N} X_{ij} E_{ij},$$

where $X_{ij} = \langle e_i|Xe_j\rangle$. Equipped with the inner product

$$(X|Y) = \mathrm{tr}(X^*Y),$$

[1] Many different Hilbert spaces will appear in the lecture notes and in latter parts we will often denote inner product by $(\,\cdot\,|\,\cdot\,)$

[2] See Exercise 2.1 below.

$\mathcal{O}$ becomes a Hilbert space and $\{E_{ij}\}$ an orthonormal basis of this space.

The self-adjoint and positive parts of $\mathcal{O}$ are the subsets

$$\mathcal{O}_{\rm self} = \{A \in \mathcal{O} \mid A^* = A\},$$
$$\mathcal{O}_+ = \{A \in \mathcal{O} \mid \langle\psi|A\psi\rangle \geq 0 \text{ for all } \psi \in \mathcal{K}\} \subset \mathcal{O}_{\rm self}.$$

We write $A \geq 0$ if $A \in \mathcal{O}_+$ and $A \geq B$ if $A-B \geq 0$. Note that $A \in \mathcal{O}_+$ iff $A \in \mathcal{O}_{\rm self}$ and $\mathrm{sp}(A) \subset [0,\infty[$. If $A \geq 0$ and $\mathrm{Ker}\, A = \{0\}$ we write $A > 0$.

A linear bijection $\vartheta : \mathcal{O} \to \mathcal{O}$ is called a $*$-automorphism of $\mathcal{O}$ if $\vartheta(AB) = \vartheta(A)\vartheta(B)$ and $\vartheta(A^*) = \vartheta(A)^*$. $\mathrm{Aut}(\mathcal{O})$ denotes the group of all $*$-automorphisms of $\mathcal{O}$ and id denotes its identity. Any $\vartheta \in \mathrm{Aut}(\mathcal{O})$ preserves $\mathcal{O}_{\rm self}$ and satisfies $\vartheta(\mathbb{1}) = \mathbb{1}$ and $\vartheta(A^{-1}) = \vartheta(A)^{-1}$ for all invertible $A \in \mathcal{O}$. In particular, $\vartheta((z-A)^{-1}) = (z-\vartheta(A))^{-1}$ and $\mathrm{sp}(\vartheta(A)) = \mathrm{sp}(A)$. It follows that ϑ preserves $\mathcal{O}_+$ and is isometric, *i.e.*, $\|\vartheta(A)\| = \|A\|$ for all $A \in \mathcal{O}$.

Let $\mathcal{K}_1$ and $\mathcal{K}_2$ be two complex Hilbert spaces of dimension N_1 and N_2. Let $\{e_1^{(1)}, \ldots, e_{N_1}^{(1)}\}$ and $\{e_1^{(2)}, \ldots, e_{N_2}^{(2)}\}$ be orthonormal basis of $\mathcal{K}_1$ and $\mathcal{K}_2$. The tensor product $\mathcal{K}_1 \otimes \mathcal{K}_2$ is defined, up to isomorphism, as the $N_1 \times N_2$-dimensional complex Hilbert space with orthonormal basis $\{e_{i_1}^{(1)} \otimes e_{i_2}^{(2)} \mid i_1 = 1, \ldots, N_1; i_2 = 1, \ldots, N_2\}$, *i.e.*, $\mathcal{K}_1 \otimes \mathcal{K}_2$ consists of all linear combinations

$$\psi = \sum_{i_1=1}^{N_1} \sum_{i_2=1}^{N_2} \psi_{i_1 i_2}\, e_{i_1}^{(1)} \otimes e_{i_2}^{(2)},$$

the inner product being determined by $\langle e_{i_1}^{(1)} \otimes e_{i_2}^{(2)} | e_{j_1}^{(1)} \otimes e_{j_2}^{(2)}\rangle = \delta_{i_1 j_1}\delta_{i_2 j_2}$. The *tensor product* of two vectors $\psi = \sum_{i=1}^{N_1} \psi_i e_i^{(1)} \in \mathcal{K}_1$ and $\phi = \sum_{i=1}^{N_2} \phi_i e_i^{(2)} \in \mathcal{K}_2$ is the vector in $\mathcal{K}_1 \otimes \mathcal{K}_2$ defined by

$$\psi \otimes \phi = \sum_{i_1=1}^{N_1} \sum_{i_2=1}^{N_2} \psi_{i_1}\phi_{i_2}\, e_{i_1}^{(1)} \otimes e_{i_2}^{(2)}.$$

The tensor product extends to a bilinear map from $\mathcal{K}_1 \times \mathcal{K}_2$ to $\mathcal{K}_1 \otimes \mathcal{K}_2$. We recall the characteristic property of the space $\mathcal{K}_1 \otimes \mathcal{K}_2$: for any Hilbert space $\mathcal{K}_3$, any bilinear map $F : \mathcal{K}_1 \times \mathcal{K}_2 \to \mathcal{K}_3$ uniquely extends to a linear map $\widehat{F} : \mathcal{K}_1 \otimes \mathcal{K}_2 \to \mathcal{K}_3$ by setting $\widehat{F}\psi \otimes \phi = F(\psi, \phi)$.

The tensor product of two linear operators $X \in \mathcal{O}_{\mathcal{K}_1}$ and $Y \in \mathcal{O}_{\mathcal{K}_2}$ is the linear operator on $\mathcal{K}_1 \otimes \mathcal{K}_2$ defined by

$$(X \otimes Y)\psi \otimes \phi = X\psi \otimes Y\phi,$$

and $\mathcal{O}_{\mathcal{K}_1} \otimes \mathcal{O}_{\mathcal{K}_2}$ is the $*$-algebra generated by such operators. Denoting by $\{E_{i_1 i_2}^{(1)}\}$ and $\{E_{j_1 j_2}^{(2)}\}$ the basis of $\mathcal{O}_{\mathcal{K}_1}$ and $\mathcal{O}_{\mathcal{K}_2}$ corresponding to the orthonormal basis $\{e_i^{(1)}\}$ and $\{e_j^{(2)}\}$ of $\mathcal{K}_1$ and $\mathcal{K}_2$, the $N_1^2 \times N_2^2$ operators

$$E_{i_1 i_2, j_1 j_2} = E_{i_1 j_1}^{(1)} \otimes E_{i_2 j_2}^{(2)} = |e_{i_1}^{(1)} \otimes e_{i_2}^{(2)}\rangle\langle e_{j_1}^{(1)} \otimes e_{j_2}^{(2)}|,$$

form a basis of $\mathcal{O}_{\mathcal{K}_1 \otimes \mathcal{K}_2}$. This leads to a natural identification of $\mathcal{O}_{\mathcal{K}_1 \otimes \mathcal{K}_2}$ and $\mathcal{O}_{\mathcal{K}_1} \otimes \mathcal{O}_{\mathcal{K}_2}$.

If $\lambda \in \mathrm{sp}(A)$ we denote by P_λ the associated spectral projection. When we wish to indicate its dependence on A we shall write $P_\lambda(A)$. If $A \in \mathcal{O}_{\rm self}$, we shall denote by $\lambda_j(A)$ the eigenvalues of A listed with *multiplicities* and in *decreasing* order.

If $f(z) = \sum_{n=0}^{\infty} a_n z^n$ is analytic in the disk $|z| < r$ and $\|A\| < r$, then $f(A)$ is defined by the analytic functional calculus,

$$f(A) = \sum_{n=0}^{\infty} a_n A^n = \oint_{|w|=r'} f(w)(w-A)^{-1} \frac{\mathrm{d}w}{2\pi\mathrm{i}},$$

for any $\|A\| < r' < r$. If $A \in \mathcal{O}_{\rm self}$ and $f : \mathbb{R} \to \mathbb{C}$, then $f(A)$ is defined by the spectral theorem, *i.e.*,

$$f(A) = \sum_{\lambda \in \mathrm{sp}(A)} f(\lambda) P_\lambda.$$

In particular, for $A \in \mathcal{O}_+$,

$$\log A = \sum_{\lambda \in \mathrm{sp}(A)} \log(\lambda) P_\lambda,$$

where $\log$ denotes the natural logarithm. We shall always use the following conventions: $\log 0 = -\infty$ and $0 \log 0 = 0$. By the Lie product formula, for any $A, B \in \mathcal{O}$,

$$\mathrm{e}^{A+B} = \lim_{n \to \infty} \left(\mathrm{e}^{A/n} \mathrm{e}^{B/n} \right)^n = \lim_{n \to \infty} \left(\mathrm{e}^{A/2n} \mathrm{e}^{B/n} \mathrm{e}^{A/2n} \right)^n . \tag{2.1}$$

For any $A \in \mathcal{O}$, $A^* A \geq 0$ and we set $|A| = \sqrt{A^* A} \in \mathcal{O}_+$ and denote by $\mu_j(A)$ the singular values of A (the eigenvalues of $|A|$) listed with multiplicities and in decreasing order. Since $\|A\psi\|^2 = \||A|\psi\|^2$ one has $\mathrm{Ker}\,|A| = \mathrm{Ker}\,A$ and $\mathrm{Ran}\,|A| = \mathrm{Ran}\,A^*$. It follows that the map $U : \mathrm{Ran}\,A^* \ni |A|\psi \mapsto A\psi \in \mathrm{Ran}\,A$ is well defined and isometric. It provides the polar decomposition $A = U|A|$.

Exercise 2.1. A *complex algebra* is a complex vector space $\mathcal{A}$ with a product $\mathcal{A} \times \mathcal{A} \to \mathcal{A}$ satisfying the following axioms: for any $A, B, C \in \mathcal{A}$ and any $\alpha \in \mathbb{C}$,
(1) $A(BC) = (AB)C$.
(2) $A(B + C) = AB + AC$.
(3) $\alpha(AB) = (\alpha A)B = A(\alpha B)$.
The algebra $\mathcal{A}$ is called *abelian* or *commutative* if $AB = BA$ for all $A, B \in \mathcal{A}$ and *unital* if there exists $\mathbb{1} \in \mathcal{A}$ such that $A\mathbb{1} = \mathbb{1}A = A$ for all $A \in \mathcal{A}$.

A $*$-*algebra* is a complex algebra with a map $\mathcal{A} \ni A \mapsto A^* \in \mathcal{A}$ such that, for any $A, B \in \mathcal{A}$ and any $\alpha \in \mathbb{C}$,
(4) $A^{**} = A$.
(5) $(AB)^* = B^* A^*$.
(6) $(\alpha A + B)^* = \overline{\alpha} A^* + B^*$.

A norm on a $*$-algebra $\mathcal{A}$ is a norm on the vector space $\mathcal{A}$ satisfying $\|AB\| \leq \|A\|\,\|B\|$ and $\|A^*\| = \|A\|$ for all $A, B \in \mathcal{A}$. A finite dimensional normed $*$-algebra $\mathcal{A}$ is a C^**-algebra* if $\|A^* A\| = \|A\|^2$ for all $A \in \mathcal{A}$. (If $\mathcal{A}$ is infinite dimensional, one additionally requires $\mathcal{A}$ to be complete w.r.t. the norm topology).

Show that if $\mathcal{K}$ is a finite dimensional Hilbert space then the set $\mathcal{O}$ of all linear maps $A : \mathcal{K} \to \mathcal{K}$ is a unital C^*-algebra.

Exercise 2.2. Prove the Löwner-Heinz inequality: if $A, B \in \mathcal{O}_+$ are such that $A \geq B$ then $A^s \geq B^s$ for any $s \in [0, 1]$.
Hint: show that $(B + t)^{-1} \geq (A + t)^{-1}$ for all $t > 0$ and use the identity

$$A^s - B^s = \frac{\sin \pi s}{\pi} \int_0^\infty t^s \left(\frac{1}{B + t} - \frac{1}{A + t} \right) \mathrm{d}t.$$

Exercise 2.3.

1. Let $A, B \in \mathcal{O}$. Prove Duhamel's formula

$$\mathrm{e}^B - \mathrm{e}^A = \int_0^1 \mathrm{e}^{sB} (B - A) \mathrm{e}^{(1-s)A} \, \mathrm{d}s.$$

Hint: integrate the derivative of the function $f(s) = \mathrm{e}^{sB}\mathrm{e}^{(1-s)A}$.

2. Iterating Duhamel's formula, prove the second order Duhamel expansion

$$\mathrm{e}^B - \mathrm{e}^A = \int_0^1 \mathrm{e}^{sB}(B-A)\mathrm{e}^{(1-s)B}\,\mathrm{d}s + \int_0^1\int_0^s \mathrm{e}^{uB}(B-A)\mathrm{e}^{(s-u)A}(A-B)\mathrm{e}^{(1-s)B}\,\mathrm{d}u\mathrm{d}s.$$

3. Let P be a projection and set $Q = \mathbb{1} - P$. Apply the previous formula to the case $B = PAP$ to show that

$$P\mathrm{e}^A P = P\mathrm{e}^{PAP}P + \int_0^1\int_0^u \mathrm{e}^{(u-s)PAP}PAQ\mathrm{e}^{(1-u)A}QAP\mathrm{e}^{sPAP}\,\mathrm{d}s\mathrm{d}u.$$

Exercise 2.4. Let $\vartheta \in \mathrm{Aut}(\mathcal{O})$. Show that there exists unitary $U_\vartheta \in \mathcal{O}$, unique up to a phase, such that $\vartheta(A) = U_\vartheta A U_\vartheta^{-1}$.
Hint: show first that if P is an orthogonal projection, then so is $\vartheta(P)$ and $\mathrm{tr}(P) = \mathrm{tr}(\vartheta(P))$. Pick an orthonormal basis $\{e_1, \cdots, e_N\}$ of $\mathcal{K}$ and show that $\vartheta(|e_i\rangle\langle e_j|) = |e_i'\rangle\langle e_j'|$, where $\{e_1', \cdots, e_N'\}$ is also an orthonormal basis of $\mathcal{K}$. Set $U_\vartheta e_i = e_i'$ and complete the proof.

Exercise 2.5.

1. Let $A \in \mathcal{O}_{\mathrm{self}}$. Prove the min-max principle: for $j = 1, \ldots, \dim\mathcal{K}$,

$$\lambda_j(A) = \sup_S \inf_{\substack{\psi\perp S\\ \|\psi\|=1}} \langle\psi|A\psi\rangle,$$

where supremum is taken over all subspaces $S \subset \mathcal{K}$ such that $\dim S = \dim\mathcal{K} - j$ (recall our convention $\lambda_1(A) \geq \lambda_2(A) \geq \cdots \geq \lambda_{\dim\mathcal{K}}(A)$.

2. Using the min-max principle, prove that for $A, B \in \mathcal{O}_{\mathrm{self}}$,

$$|\lambda_j(A) - \lambda_j(B)| \leq \|A - B\|.$$

2.2 Trace inequalities

Let $\{\psi_j\}$ be an orthonormal basis of $\mathcal{K}$. We recall that the trace of $A \in \mathcal{O}$, denoted $\mathrm{tr}(A)$, is defined by

$$\mathrm{tr}(A) = \sum_j \langle\psi_j|A\psi_j\rangle.$$

For any unitary $U \in \mathcal{O}$, $\mathrm{tr}(A) = \mathrm{tr}(UAU^{-1})$ and $\mathrm{tr}(A)$ is independent of the choice of the basis. In particular, if A is self-adjoint then $\mathrm{tr}(A) = \sum_j \lambda_j(A) \in \mathbb{R}$ and if $A \in \mathcal{O}_+$ then $\mathrm{tr}\,(A) \geq 0$.

For $p \in]0, \infty[$ we set

$$\|A\|_p = (\mathrm{tr}|A|^p)^{1/p} = \left(\sum_j \mu_j(A)^p\right)^{1/p}. \tag{2.2}$$

$\|A\|_\infty = \max_j \mu_j(A)$ is the usual operator norm of A. The function $]0, \infty[\ni p \mapsto \|A\|_p$ is real analytic, monotonically decreasing, and

$$\lim_{p\to\infty} \|A\|_p = \|A\|_\infty. \tag{2.3}$$

For $p \in [1, \infty]$, the map $\mathcal{O} \ni A \mapsto \|A\|_p$ is a unitary invariant norm. Since $\dim \mathcal{K} < \infty$, all these norms are equivalent and induce the same topology on $\mathcal{O}$.

Let $A = U|A|$ be the polar decomposition of A and denote by $\{\psi_j\}$ an orthonormal basis of eigenvectors of $|A|$. Then

$$\operatorname{tr}(BA) = \sum_j \langle \psi_j | BU|A|\psi_j\rangle = \sum_j \mu_j(A)\langle \psi_j | BU\psi_j\rangle,$$

from which we conclude that

$$|\operatorname{tr}(BA)| \leq \sum_j \mu_j(A)|\langle \psi_j | BU\psi_j\rangle| \leq \|B\| \sum_j \mu_j(A) = \|B\|\, \|A\|_1. \tag{2.4}$$

In particular,

$$|\operatorname{tr}(A)| \leq \|A\|_1.$$

The basic trace inequalities are:

Theorem 2.1 (1) *The Peierls-Bogoliubov inequality: for $A, B \in \mathcal{O}_{\mathrm{self}}$,*

$$\log \frac{\operatorname{tr}(\mathrm{e}^A \mathrm{e}^B)}{\operatorname{tr}(\mathrm{e}^B)} \geq \frac{\operatorname{tr}(A\mathrm{e}^B)}{\operatorname{tr}(\mathrm{e}^B)}.$$

(2) *The Klein inequality: for $A, B \in \mathcal{O}_+$,*

$$\operatorname{tr}(A \log A - A \log B) \geq \operatorname{tr}(A - B),$$

with equality iff $A = B$.

(3) *The Hölder inequality: for $A, B \in \mathcal{O}$ and $p, q \in [1, \infty]$ satisfying $p^{-1} + q^{-1} = 1$,*

$$\|AB\|_1 \leq \|A\|_p \|B\|_q.$$

(4) *The Minkowski inequality: for $A, B \in \mathcal{O}$ and $p \in [1, \infty]$,*

$$\|A + B\|_p \leq \|A\|_p + \|B\|_p.$$

Proof. (1) For $\lambda \in \operatorname{sp}(A)$ we set

$$p_\lambda = \frac{\operatorname{tr}(P_\lambda(A)\mathrm{e}^B)}{\operatorname{tr}(\mathrm{e}^B)},$$

so that $p_\lambda \in [0, 1]$ and $\sum_\lambda p_\lambda = 1$. The convexity of the exponential function and Jensen's inequality imply

$$\frac{\operatorname{tr}(\mathrm{e}^A \mathrm{e}^B)}{\operatorname{tr}(\mathrm{e}^B)} = \sum_\lambda \mathrm{e}^\lambda p_\lambda \geq \mathrm{e}^{\sum_\lambda \lambda p_\lambda} = \mathrm{e}^{\operatorname{tr}(A\mathrm{e}^B)/\operatorname{tr}(\mathrm{e}^B)}.$$

(2) If $\operatorname{Ker} B \not\subset \operatorname{Ker} A$, then the left-hand side in (2) is $+\infty$ and the inequality holds trivially. Assuming $\operatorname{Ker} B \subset \operatorname{Ker} A$, we set

$$p_{\lambda,\mu} = \operatorname{tr}(P_\lambda(A) P_\mu(B)),$$

for $(\lambda, \mu) \in \operatorname{sp}(A) \times \operatorname{sp}(B)$ so that $p_{\lambda,\mu} \in [0, 1]$, $\sum_{\lambda,\mu} p_{\lambda,\mu} = 1$ and $p_{\lambda,0} = \delta_{\lambda,0} p_{0,0}$. Then, we can write

$$\operatorname{tr}(A \log A - A \log B) = \sum_{\substack{\lambda,\mu \\ \mu \neq 0}} \lambda \log(\lambda/\mu) p_{\lambda,\mu}.$$

The inequality $x \log x \geq x - 1$, which holds for $x \geq 0$, implies that for $\lambda \geq 0$ and $\mu > 0$,

$$\lambda \log \frac{\lambda}{\mu} = \mu \frac{\lambda}{\mu} \log \frac{\lambda}{\mu} \geq \mu \left(\frac{\lambda}{\mu} - 1 \right) = \lambda - \mu,$$

and so

$$\mathrm{tr}(A\log A - A\log B) \geq \sum_{\substack{\lambda,\mu \\ \mu\neq 0}} (\lambda-\mu)p_{\lambda,\mu} = \sum_{\lambda,\mu}(\lambda-\mu)p_{\lambda,\mu} = \mathrm{tr}(A-B).$$

If the equality holds, then we must have

$$\sum_{\substack{\lambda,\mu \\ \mu\neq 0}} \mu\left[\frac{\lambda}{\mu}\log\frac{\lambda}{\mu} - \left(\frac{\lambda}{\mu}-1\right)\right]p_{\lambda,\mu} = 0,$$

where all the terms in the sum are non-negative. Since $x\log x = x-1$ iff $x=1$, it follows that $p_{\lambda,\mu}=0$ for $\lambda\neq\mu\neq 0$. We have already noticed that $p_{\lambda,0}=0$ for $\lambda\neq 0$, hence we have $p_{\lambda,\mu}=0$ for $\lambda\neq\mu$ and it follows that

$$P_\lambda(A)P_\mu(B)P_\lambda(A) = 0 = P_\mu(B)P_\lambda(A)P_\mu(B),$$

for $\lambda\neq\mu$. Since

$$P_\lambda(A) = \sum_\mu P_\lambda(A)P_\mu(B)P_\lambda(A) = P_\lambda(A)P_\lambda(B)P_\lambda(A),$$

we must have $P_\lambda(B)\geq P_\lambda(A)$ and $\mathrm{sp}(A)\subset\mathrm{sp}(B)$. By symmetry, the reverse inequalities also hold and hence $B=A$.

(3) Equ. (2.3) implies that it suffices to consider the case $1<p<\infty$. Denote by $AB=U|AB|$, $A=V|A|$ and $B=W|B|$ the polar decompositions of AB, A and B. Then

$$\|AB\|_1 = \mathrm{tr}|AB| = \mathrm{tr}(U^*AB) = \mathrm{tr}(U^*V|A|W|B|) = \lim_{\epsilon\downarrow 0}\mathrm{tr}(U^*V(|A|+\epsilon)W(|B|+\epsilon)).$$

The function

$$F_\epsilon(z) = \mathrm{tr}(U^*V(|A|+\epsilon)^{pz}W(|B|+\epsilon)^{q(1-z)}),$$

is entire analytic and bounded on the strip $0\leq\mathrm{Re}\,z\leq 1$. For any $y\in\mathbb{R}$, the bound (2.4) yields

$$|F_\epsilon(\mathrm{i}y)|\leq\mathrm{tr}((|B|+\epsilon)^q), \qquad |F_\epsilon(1+\mathrm{i}y)|\leq\mathrm{tr}((|A|+\epsilon)^p).$$

Hence, by Hadamard's three lines theorem (see, *e.g.*, [RS2]), for any z in the strip $0\leq\mathrm{Re}\,z\leq 1$,

$$|F_\epsilon(z)|\leq\left[\mathrm{tr}((|A|+\epsilon)^p)\right]^{\mathrm{Re}\,z}\left[\mathrm{tr}((|B|+\epsilon)^q)\right]^{1-\mathrm{Re}\,z}.$$

Substituting $z=1/p$ we get

$$|\mathrm{tr}(U^*V(|A|+\epsilon)W(|B|+\epsilon))|\leq\||A|+\epsilon\|_p\||B|+\epsilon\|_q,$$

and the limit $\epsilon\downarrow 0$ yields the statement.

(4) Again, it suffices to consider the case $1<p<\infty$. Let q be such that $p^{-1}+q^{-1}=1$. We first observe that

$$\|A\|_p = \sup_{\|C\|_q=1}|\mathrm{tr}(AC)|. \tag{2.5}$$

Indeed, the Hölder inequality implies

$$\sup_{\|C\|_q=1}|\mathrm{tr}(AC)|\leq\sup_{\|C\|_q=1}\|AC\|_1\leq\|A\|_p.$$

On the other hand, if $C=\|A\|_p^{-p/q}|A|^{p/q}U^*$ where $A=U|A|$ denotes the polar decomposition of A, then $\|C\|_q=1$ and $\mathrm{tr}(AC)=\|A\|_p$, and so (2.5) holds. Finally, (2.5) implies

$$\|A+B\|_p = \sup_{\|C\|_q=1}|\mathrm{tr}((A+B)C)|\leq\sup_{\|C\|_q=1}|\mathrm{tr}(AC)|+\sup_{\|C\|_q=1}|\mathrm{tr}(BC)| = \|A\|_p+\|B\|_p.$$

□

We shall also need:

Theorem 2.2 *The Araki-Lieb-Thirring inequality: for $A, B \in \mathcal{O}_+$, $p > 0$ and $r \geq 1$,*

$$\operatorname{tr}\left((A^{1/2}BA^{1/2})^{rp}\right) \leq \operatorname{tr}\left((A^{r/2}B^r A^{r/2})^p\right).$$

Proof. By an obvious limiting argument (replacing A and B with $A+\epsilon$ and $B+\epsilon$) it suffices to prove the theorem in the case $A, B > 0$. We split the proof into four steps.

Step 1. If $A, B > 0$, then for $0 \leq s \leq 1$, $\|A^s B^s\| \leq \|AB\|^s$.
Proof. Let $\phi, \psi \in \mathcal{K}$ be unit vectors and

$$F(z) = \frac{(\phi|A^z B^z \psi)}{\|AB\|^z}.$$

The function $F(z)$ is entire analytic and bounded on the strip $0 \leq \operatorname{Re} z \leq 1$. For $y \in \mathbb{R}$ one has $|F(\mathrm{i}y)| \leq 1$, $|F(1+\mathrm{i}y)| \leq 1$, and so by the three lines theorem, $|F(z)| \leq 1$ for $0 \leq \operatorname{Re} z \leq 1$. Taking $z = s$, we deduce that

$$|(\phi|A^s B^s \psi)| \leq \|AB\|^s,$$

and

$$\|A^s B^s\| = \sup_{\|\phi\|=\|\psi\|=1} |(\phi|A^s B^s \psi)| \leq \|AB\|^s.$$

Step 2. If $A, B > 0$, then for $s \geq 1$, $\|A^s B^s\| \geq \|AB\|^s$.
Proof. Let $\tilde{A} = A^s$, $\tilde{B} = B^s$. Then by Step 1, $\|\tilde{A}^{1/s}\tilde{B}^{1/s}\| \leq \|\tilde{A}\tilde{B}\|^{1/s}$, and the result follows.
Step 3. Set $X_r = B^{r/2}A^{r/2}$, $Y_r = X_r^* X_r = A^{r/2}B^r A^{r/2}$. Let $N = \dim \mathcal{K}$ and denote by $\lambda_1(r) \geq \cdots \geq \lambda_N(r)$ the eigenvalues of Y_r listed with multiplicities. Then for $1 \leq n \leq N$,

$$\prod_{j=1}^n \lambda_j(r) \geq \prod_{j=1}^n \lambda_j(1)^r. \tag{2.6}$$

Proof. Let $\mathcal{H} = \mathcal{K}^{\wedge n}$ be the n-fold anti-symmetric tensor product of $\mathcal{K}$ and $\Gamma_n(Y_q) = Y_q^{\wedge n}$ (the reader not familiar with this concept may consult Section 6.1). Step 2 yields the inequality

$$\begin{aligned}\|\Gamma_n(Y_r)\| &= \|\Gamma_n(X_r)^*\Gamma_n(X_r)\| = \|\Gamma_n(X_r)\|^2 = \|\Gamma_n(B)^{r/2}\Gamma_n(A)^{r/2}\|^2 \\ &\geq \|\Gamma_n(B)^{1/2}\Gamma_n(A)^{1/2}\|^{2r} = \|\Gamma_n(X_1)\|^{2r} = \|\Gamma_n(Y_1)\|^r,\end{aligned}$$

Since $\|\Gamma_n(Y_r)\| = \prod_{j=1}^n \lambda_j(r)$, (2.6) follows.

Step 4. For $1 \leq n \leq N$,

$$\sum_{j=1}^n \lambda_j(r)^p \geq \sum_{j=1}^n \lambda_j(1)^{rp}. \tag{2.7}$$

Proof. Set $a_j(r) = \log \lambda_j(r)$. Then, by Step 3, $a_j(r)$ is a decreasing sequence of real numbers satisfying

$$\sum_{j=1}^n a_j(r) \geq \sum_{j=1}^n r a_j(1),$$

for all n. We have to show that for all n,

$$\sum_{j=1}^n \mathrm{e}^{p a_j(r)} \geq \sum_{j=1}^n \mathrm{e}^{p r a_j(1)}. \tag{2.8}$$

Let $y_+ = \max(y, 0)$. We claim that for all $y \in \mathbb{R}$ and all n,

$$\sum_{j=1}^n (a_j(r) - y)_+ \geq \sum_{j=1}^n (r a_j(1) - y)_+. \tag{2.9}$$

This relation is obvious if $ra_1(1) - y \le 0$. Otherwise, let $k \le n$ be such that

$$ra_1(1) - y \ge \cdots \ge ra_k(1) - y \ge 0 \ge ra_{k+1}(1) - y \ge \cdots \ge ra_n(1) - y.$$

Then $\sum_{j=1}^n (ra_j(1) - y)_+ = \sum_{j=1}^k (ra_j(1) - y)$ and it follows that

$$\sum_{j=1}^n (a_j(r) - y)_+ \ge \sum_{j=1}^k (a_j(r) - y)_+ \ge \sum_{j=1}^k (a_j(r) - y)$$

$$\ge \sum_{j=1}^k (ra_j(1) - y) = \sum_{j=1}^n (ra_j(1) - y)_+.$$

The relation (2.9) and the identity

$$\mathrm{e}^{px} = p^2 \int_{\mathbb{R}} (x - y)_+ \mathrm{e}^{py} \mathrm{d}y,$$

imply (2.8) and (2.7) follows. In the case $n = N$ the relation (2.7) reduces to the Araki-Lieb-Thirring inequality. □

Theorem 2.2 and the Lie product formula (2.1) imply:

Corollary 2.3 *For $A, B \in \mathcal{O}_{\mathrm{self}}$ the function*

$$[1, \infty[\ni p \mapsto \|\mathrm{e}^{B/p}\mathrm{e}^{A/p}\|_p^p = \mathrm{tr}([\mathrm{e}^{A/p}\mathrm{e}^{2B/p}\mathrm{e}^{A/p}]^{p/2})$$

is monotonically decreasing and

$$\lim_{p\to\infty} \|\mathrm{e}^{B/p}\mathrm{e}^{A/p}\|_p^p = \mathrm{tr}(\mathrm{e}^{A+B}).$$

In particular, the Golden-Thompson inequality holds,

$$\mathrm{tr}(\mathrm{e}^A\mathrm{e}^B) = \|\mathrm{e}^{B/2}\mathrm{e}^{A/2}\|_2^2 \ge \mathrm{tr}(\mathrm{e}^{A+B}).$$

Exercise 2.6.

1. Prove the following generalization of Hölder's inequality:

$$\|AB\|_r \le \|A\|_p \, \|B\|_q, \tag{2.10}$$

for $p, q, r \in [1, \infty]$ such that $p^{-1} + q^{-1} = r^{-1}$.
Hint: use the polar decomposition $B = U|B|$ to write $|AB|^2 = |B|C^2|B|$ with $C = \sqrt{U^*|A|^2U}$. Invoke the Araki-Lieb-Thirring inequality to show that $\mathrm{tr}(|AB|^r) \le \mathrm{tr}(|C^r|B|^r|) = \|C^r|B|^r\|_1$. Conclude the proof by applying the Hölder inequality.

2. Using (2.10), show that

$$\|A_1 \cdots A_n\|_r \le \prod_{j=1}^n \|A_j\|_{p_j},$$

provided $\sum_j p_j^{-1} = r^{-1}$.

Exercise 2.7. Show that for any $A \in \mathcal{O}$ and $p \in [1, \infty]$ one has $\|A^*\|_p = \|A\|_p$. In particular, if $A, B \in \mathcal{O}_{\mathrm{self}}$ then

$$\|AB\|_p = \|BA\|_p. \tag{2.11}$$

Exercise 2.8. Let $A, B \in \mathcal{O}_{\rm self}$. Prove that the function

$$[1,\infty[\ni p \mapsto \|e^{B/p}e^{A/p}\|_p^p = \mathrm{tr}([e^{A/p}e^{2B/p}e^{A/p}]^{p/2})$$

is strictly decreasing unless A and B commute (in which case the function is constant). Deduce that the Golden-Thompson inequality is strict unless A and B commute.
Hint: show first that the function is real analytic. Hence, if the function is not strictly decreasing, it must be constant. If the function is constant, then its values at $p = 2$ and $p = 4$ are equal and

$$\mathrm{tr}(e^A e^B) = \mathrm{tr}(e^{A/2}e^{B/2}e^{A/2}e^{B/2}).$$

This identity is equivalent to $\mathrm{tr}([e^{A/2}e^{B/2} - e^{B/2}e^{A/2}][e^{A/2}e^{B/2} - e^{B/2}e^{A/2}]^*) = 0$, and so $e^{A/2}e^{B/2} = e^{B/2}e^{A/2}$.

Corollary 2.4 *For $A, B \in \mathcal{O}_+$ and $p \geq 1$ the function*

$$\mathbb{R} \ni \alpha \mapsto \log \|A^\alpha B^{1-\alpha}\|_p^p,$$

is convex.

Proof. As in the proof of Theorem 2.2 we can assume that A and B are non-singular. We first note that for any $s \in]0,1[$ the Araki-Lieb-Thirring inequality implies

$$\|A^s B^s\|_p^p = \mathrm{tr}\left(\left[B^s A^{2s} B^s\right]^{p/2}\right) = \mathrm{tr}\left(\left[\left(B^s A^{2s} B^s\right)^{1/s}\right]^{ps/2}\right)$$

$$\leq \mathrm{tr}\left(\left[BA^2B\right]^{ps/2}\right) = \|AB\|_{ps}^{ps}.$$

Applying the Hölder inequality (2.10), the identity (2.11) and the previous inequality one gets, for $\alpha, \beta \in \mathbb{R}$ and $\lambda \in]0,1[$,

$$\begin{aligned}
\|A^{\lambda\alpha+(1-\lambda)\beta}B^{1-(\lambda\alpha+(1-\lambda)\beta)}\|_p^p &= \|A^{\lambda\alpha}A^{(1-\lambda)\beta}B^{(1-\lambda)(1-\beta)}B^{\lambda(1-\alpha)}\|_p^p \\
&= \|B^{\lambda(1-\alpha)}A^{\lambda\alpha}A^{(1-\lambda)\beta}B^{(1-\lambda)(1-\beta)}\|_p^p \\
&\leq \|B^{\lambda(1-\alpha)}A^{\lambda\alpha}\|_{p/\lambda}^p \|A^{(1-\lambda)\beta}B^{(1-\lambda)(1-\beta)}\|_{p/(1-\lambda)}^p \\
&= \|A^{\lambda\alpha}B^{\lambda(1-\alpha)}\|_{p/\lambda}^p \|A^{(1-\lambda)\beta}B^{(1-\lambda)(1-\beta)}\|_{p/(1-\lambda)}^p \\
&\leq \|A^\alpha B^{1-\alpha}\|_p^{\lambda p} \|A^\beta B^{1-\beta}\|_p^{(1-\lambda)p}.
\end{aligned}$$

Taking the logarithm of both sides yields the result. □

2.3 Positive and completely positive maps on $\mathcal{O}$

Denoting by $\{e_1, \ldots, e_N\}$ the standard basis of $\mathbb{C}^N$, a vector $\psi \in \mathcal{K} \otimes \mathbb{C}^N$ has a unique representation

$$\psi = \sum_{j=1}^N \psi_j \otimes e_j,$$

where $\psi_j \in \mathcal{K}$ is completely determined by $\langle\phi|\psi_j\rangle = \langle\phi \otimes e_j|\psi\rangle$ for all $\phi \in \mathcal{K}$. Accordingly, an operator $X \in \mathcal{O}_{\mathcal{K}\otimes\mathbb{C}^N}$ can be represented as a $N \times N$ block matrix

$$X = \begin{bmatrix} X_{11} & X_{12} & \cdots & X_{1N} \\ X_{21} & X_{22} & \cdots & X_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ X_{N1} & X_{N2} & \cdots & X_{NN} \end{bmatrix},$$

where $X_{ij} \in \mathcal{O}_{\mathcal{K}}$ is completely determined by $\langle \phi | X_{ij} \psi \rangle = \langle \phi \otimes e_i | X \psi \otimes e_j \rangle$ for all $\phi, \psi \in \mathcal{K}$, so that

$$X\psi = \sum_{i,j=1}^{N} (X_{ij}\psi_j) \otimes e_i.$$

In particular, X is non-negative iff

$$\sum_{i,j} \langle \psi_i | X_{ij} \psi_j \rangle \geq 0,$$

for all $\psi_1, \ldots, \psi_N \in \mathcal{K}$. Note that since $\mathcal{O}_{\mathcal{K}} \otimes \mathcal{O}_{\mathbb{C}^N}$ is isomorphic to $\mathcal{O}_{\mathcal{K} \otimes \mathbb{C}^N}$, the same block matrix representation holds for $X \in \mathcal{O}_{\mathcal{K}} \otimes \mathcal{O}_{\mathbb{C}^N}$.

Let $\Phi : \mathcal{O}_{\mathcal{K}} \to \mathcal{O}_{\mathcal{K}'}$ be a linear map. Φ is called *positive* if $\Phi(\mathcal{O}_{\mathcal{K}+}) \subset \mathcal{O}_{\mathcal{K}'+}$. One easily shows that if Φ is positive, then $\Phi(X^*) = \Phi(X)^*$ for all $X \in \mathcal{O}_{\mathcal{K}}$. Φ is called *N-positive* if the map $\Phi \otimes \mathbb{1}_N : \mathcal{O}_{\mathcal{K}} \otimes \mathcal{O}_{\mathbb{C}^N} \to \mathcal{O}_{\mathcal{K}'} \otimes \mathcal{O}_{\mathbb{C}^N}$ is positive, where $\mathbb{1}_N$ is the identity map on $\mathcal{O}_{\mathbb{C}^N}$. Note that if $X \in \mathcal{O}_{\mathcal{K}} \otimes \mathcal{O}_{\mathbb{C}^N}$ has the block matrix representation $[X_{ij}]$, then $\Phi \otimes \mathbb{1}_N(X) \in \mathcal{O}_{\mathcal{K}'} \otimes \mathcal{O}_{\mathbb{C}^N}$ is represented by the block matrix $[\Phi(X_{ij})]$. If Φ is N-positive for all N, then it is called *completely positive* (CP). Φ is called *unital* if $\Phi(\mathbb{1}_{\mathcal{K}}) = \mathbb{1}_{\mathcal{K}'}$ and *trace preserving* if $\mathrm{tr}\,(\Phi(X)) = \mathrm{tr}\,(X)$ for all $X \in \mathcal{O}_{\mathcal{K}}$.

Example 2.1 Suppose that $\mathcal{K} = \mathcal{K}_1 \otimes \mathcal{K}_2$ and let $\Phi : \mathcal{O}_{\mathcal{K}} \to \mathcal{O}_{\mathcal{K}_1}$ be the unique map satisfying

$$\mathrm{tr}_{\mathcal{K}}((B \otimes \mathbb{1}_{\mathcal{K}_2})A) = \mathrm{tr}_{\mathcal{K}_1}(B\Phi(A)),$$

for all $A \in \mathcal{O}_{\mathcal{K}}$, $B \in \mathcal{O}_{\mathcal{K}_1}$. $\Phi(A)$ is called the partial trace of A over $\mathcal{K}_2$ and we shall denote it by $\mathrm{tr}_{\mathcal{K}_2}(A)$. If $\{\chi_j\}$ is an orthonormal basis of $\mathcal{K}_2$, then the matrix elements of $\mathrm{tr}_{\mathcal{K}_2}(A)$ are

$$\langle \psi | \mathrm{tr}_{\mathcal{K}_2}(A) \varphi \rangle = \sum_k \langle \psi \otimes \chi_k | A\, \varphi \otimes \chi_k \rangle.$$

The map $A \mapsto \mathrm{tr}_{\mathcal{K}_2}(A)$ is obviously linear, positive (in fact $A > 0$ implies that $\mathrm{tr}_{\mathcal{K}_2}(A) > 0$) and trace preserving. To show that it is completely positive, we note that if $[X_{ij}]$ is a positive block matrix then

$$\sum_{i,j} \langle \psi_i | \mathrm{tr}_{\mathcal{K}_2}(X_{ij}) \psi_j \rangle = \sum_k \sum_{i,j} \langle \psi_i \otimes \chi_k | X_{ij}\, \psi_j \otimes \chi_k \rangle \geq 0.$$

Exercise 2.9. Show that the following maps are completely positive:
1. A $*$-automorphism $\vartheta : \mathcal{O} \to \mathcal{O}$.
2. $\mathcal{O}_{\mathcal{K}} \ni X \mapsto \Phi(X) = X \otimes \mathbb{1}_{\mathcal{K}'} \in \mathcal{O}_{\mathcal{K} \otimes \mathcal{K}'}$.
3. $\mathcal{O}_{\mathcal{K}} \ni X \mapsto \Phi(X) = VXV^* \in \mathcal{O}_{\mathcal{K}}$, where $V \in \mathcal{O}_{\mathcal{K}}$.

The following result, due to Stinespring, gives a characterization of CP maps.

Proposition 2.5 *The linear map $\Phi : \mathcal{O}_{\mathcal{K}} \to \mathcal{O}_{\mathcal{K}'}$ is completely positive iff there exists a finite family of operators $V_\alpha : \mathcal{K} \to \mathcal{K}'$ such that*

$$\Phi(X) = \sum_\alpha V_\alpha X V_\alpha^*, \tag{2.12}$$

for all $X \in \mathcal{O}_{\mathcal{K}}$. Moreover, Φ is unital iff $\sum_\alpha V_\alpha V_\alpha^* = \mathbb{1}_{\mathcal{K}'}$ and trace preserving iff $\sum_\alpha V_\alpha^* V_\alpha = \mathbb{1}_{\mathcal{K}}$.

Remark. The right hand side of (2.12) is called a Kraus representation of the completely positive map Φ. Such a representation is not unique.

Example 2.2 Let U be a unitary operator on $\mathcal{K}_1 \otimes \mathcal{K}_2$. By Example 2.1 and Exercise 2.9, the map

$$\Phi(X) = \frac{\mathrm{tr}_{\mathcal{K}_2}(U(X \otimes \mathbb{1}_{\mathcal{K}_2})U^*)}{\dim \mathcal{K}_2},$$

is completely positive and unital on $\mathcal{O}_{\mathcal{K}_1}$. A Kraus representation is given by

$$\Phi(X) = \sum_{i,j=1}^{\dim \mathcal{K}_2} V_{i,j} X V_{i,j}^*,$$

where

$$V_{i,j} = \frac{1}{\sqrt{\dim \mathcal{K}_2}} \sum_{k,l=1}^{\dim \mathcal{K}_1} |e_k\rangle\langle e_k \otimes f_i | U e_l \otimes f_j\rangle\langle e_l|,$$

and $\{e_j\}$, $\{f_k\}$ are orthonormal basis of $\mathcal{K}_1$ and $\mathcal{K}_2$.

Proof of Proposition 2.5. The fact that a map Φ defined by Equ. (2.12) is completely positive follows from Part 2 of Exercise 2.9. To prove the reverse implication, let $\Phi : \mathcal{O}_{\mathcal{K}} \to \mathcal{O}_{\mathcal{K}'}$ be completely positive and denote by $E_{ij} = |\chi_i\rangle\langle\chi_j|$ the basis of $\mathcal{O}_{\mathcal{K}}$ associated to the orthonormal basis $\{\chi_i\}$ of $\mathcal{K}$. Since

$$\sum_{i,j=1}^{\dim \mathcal{K}} \langle \psi_i | E_{ij} \psi_j \rangle = \left| \sum_{i=1}^{\dim \mathcal{K}} \langle \psi_i | \chi_i \rangle \right|^2 \geq 0,$$

the block matrix $[E_{ij}]$ is positive and hence so is the block matrix $M = [\Phi(E_{ij})]$, an operator on $\mathcal{K}' \otimes \mathbb{C}^{\dim \mathcal{K}}$. Let e_i be the standard basis of $\mathbb{C}^{\dim \mathcal{K}}$ and define the operator $Q_i : \mathcal{K}' \otimes \mathbb{C}^{\dim \mathcal{K}} \to \mathcal{K}'$ by $Q_i \sum_j \psi_j \otimes e_j = \psi_i$, so that $\Phi(E_{ij}) = Q_i M Q_j^*$. If

$$M = \sum_{k=1}^{\dim \mathcal{K} \times \dim \mathcal{K}'} \lambda_k |\phi_k\rangle\langle\phi_k|,$$

is a spectral representation of M, then

$$\Phi(E_{ij}) = \sum_{k=1}^{\dim \mathcal{K} \times \dim \mathcal{K}'} \lambda_k Q_i |\phi_k\rangle\langle\phi_k| Q_j^*. \tag{2.13}$$

For each $k = 1, \ldots, \dim \mathcal{K} \times \dim \mathcal{K}'$ define a linear operator $V_k : \mathcal{K} \to \mathcal{K}'$ by $V_k e_i = \sqrt{\lambda_k} Q_i \phi_k$ for $i = 1, \ldots, \dim \mathcal{K}$. Then, we can rewrite (2.13) as

$$\Phi(E_{ij}) = \sum_{k=1}^{\dim \mathcal{K} \times \dim \mathcal{K}'} V_k E_{ij} V_k^*,$$

and since any $X \in \mathcal{O}_{\mathcal{K}}$ can be written as $X = \sum_{i,j} X_{ij} E_{ij}$ we have

$$\Phi(X) = \sum_{k=1}^{\dim \mathcal{K} \times \dim \mathcal{K}'} V_k X V_k^*.$$

The last statement of Proposition 2.5 is obvious. □

Definition 2.6 *A linear map $\Phi : \mathcal{O}_{\mathcal{K}} \to \mathcal{O}_{\mathcal{K}'}$ such that, for all $X \in \mathcal{O}_{\mathcal{K}}$,*

$$\Phi(X)^*\Phi(X) \leq \Phi(X^*X), \tag{2.14}$$

is called a Schwarz map and (2.14) is called the Schwarz inequality.

Proposition 2.7 *Any 2-positive map $\Phi : \mathcal{O}_{\mathcal{K}} \to \mathcal{O}_{\mathcal{K}'}$ is a Schwarz map.*

Proof. For any $X \in \mathcal{O}_{\mathcal{K}}$, the 2×2 block matrix

$$[A_{ij}] = \left[\begin{array}{cc} \mathbb{1} & X \\ X^* & X^*X \end{array} \right],$$

is non-negative. Indeed, for any $\psi_1, \psi_2 \in \mathcal{K}$ one has

$$\sum_{i,j} \langle \psi_i | A_{ij} \psi_j \rangle = \|\psi_1 + X\psi_2\|^2 \geq 0.$$

If Φ is 2-positive, then the block matrix $[\Phi(A_{ij})]$ is also non-negative and hence

$$\sum_{i,j} \langle \phi_i | A_{ij} \phi_j \rangle = \|\phi_1 + \Phi(X)\phi_2\|^2 + \langle \phi_2 | (\Phi(X^*X) - \Phi(X)^*\Phi(X))\phi_2 \rangle \geq 0,$$

for all $\phi_1, \phi_2 \in \mathcal{K}'$. Setting $\phi_1 = -\Phi(X)\phi_2$ yields the Schwarz inequality. □

Exercise 2.10. Let $\Phi : \mathcal{O}_{\mathcal{K}} \to \mathcal{O}_{\mathcal{K}'}$ be a linear map and denote by Φ^* its adjoint w.r.t. the inner product $(\,\cdot\,|\,\cdot\,)$, that is

$$(X|\Phi(Y)) = \mathrm{tr}_{\mathcal{K}'}(X^*\Phi(Y)) = \mathrm{tr}_{\mathcal{K}}(\Phi^*(X)^*Y) = (\Phi^*(X)|Y).$$

1. Show that Φ^* is positive iff Φ is positive.
2. Show that Φ^* is N-positive iff Φ is N-positive.
3. Show that Φ^* is trace preserving iff Φ is unital.

2.4 States

An element $\rho \in \mathcal{O}_+$ is called a density matrix or a *state* if $\mathrm{tr}(\rho) = 1$. We denote by $\mathfrak{S}$ the collection of all states. We shall identify a state ρ with the linear functional

$$\begin{array}{rccc} \rho : & \mathcal{O} & \to & \mathbb{C} \\ & A & \mapsto & \mathrm{tr}(\rho A). \end{array}$$

With this identification, $\mathfrak{S}$ can be characterized as the set of all linear functionals $\phi : \mathcal{O} \to \mathbb{C}$ which are positive ($\phi(A) \geq 0$ for all $A \in \mathcal{O}_+$) and normalized ($\phi(\mathbb{1}) = 1$). In models that arise in physics the elements of $\mathcal{O}$ describe observables of the physical system under consideration. The physical states are described by elements of $\mathfrak{S}$. If A is self-adjoint and $A = \sum_{\alpha \in \mathrm{sp}(A)} \alpha P_\alpha$ is its spectral decomposition, then the possible outcomes of a measurement of A are the eigenvalues of A. If the system is in a state ρ, the probability that α is observed is $\mathrm{tr}(\rho P_\alpha) = \mathrm{tr}(P_\alpha \rho P_\alpha) \in [0, 1]$. In particular,

$$\rho(A) = \mathrm{tr}(\rho A),$$

is the expectation value of the observable A and its variance is

$$\Delta_\rho(A) = \rho((A - \rho(A))^2) = \rho(A^2) - \rho(A^2).$$

Note that if $A \in \mathcal{O}_+$, then $\rho(A) \geq 0$. For $A, B \in \mathcal{O}_{\mathrm{self}}$ the Heisenberg uncertainty principle takes the form

$$\frac{1}{2}|\rho(\mathrm{i}[A, B])| \leq \sqrt{\Delta_\rho(A)}\sqrt{\Delta_\rho(B)}.$$

If $\Phi : \mathcal{O}_{\mathcal{K}} \to \mathcal{O}_{\mathcal{K}'}$ is a positive, unit preserving map, then its adjoint Φ^* is positive and trace preserving. In particular, it maps states $\rho \in \mathfrak{S}_{\mathcal{K}'}$ into states $\Phi^*(\rho) \in \mathfrak{S}_{\mathcal{K}}$ in such a way that

$$\rho(\Phi(A)) = \Phi^*(\rho)(A),$$

i.e., $\Phi^*(\rho) = \rho \circ \Phi$.

2.5 Entropy

Let ρ be a state. The orthogonal projection on the subspace $\operatorname{Ran}\rho = (\operatorname{Ker}\rho)^\perp$ is called the support of ρ and is denoted $\mathrm{s}(\rho)$. We shall use the notation $\rho \ll \nu$ iff $\mathrm{s}(\rho) \le \mathrm{s}(\nu)$, that is, iff $\operatorname{Ran}\rho \subset \operatorname{Ran}\nu$, and $\rho \perp \nu$ iff $\mathrm{s}(\rho) \perp \mathrm{s}(\nu)$, that is, iff $\operatorname{Ran}\rho \subset \operatorname{Ker}\nu$. Two states ρ and ν are called equivalent if $\rho \ll \nu$ and $\nu \ll \rho$. A state ρ is called faithful if $\mathrm{s}(\rho) = \mathbb{1}$, *i.e.*, if $\rho > 0$. The set $\mathfrak{S}$ and the set of all faithful states $\mathfrak{S}_{\mathrm{f}}$ are convex subsets of $\mathcal{O}_+$. A state ρ is called pure if $\rho = |\psi\rangle\langle\psi|$ for some unit vector ψ. The state

$$\rho_{\mathrm{ch}} = \frac{\mathbb{1}}{\dim \mathcal{K}}, \tag{2.15}$$

is called chaotic. If A is self-adjoint, we denote

$$\rho_A = \frac{\mathrm{e}^A}{\operatorname{tr}(\mathrm{e}^A)}.$$

The state ρ_A is faithful and $\rho_A = \rho_B$ iff A and B differ by a constant. If $\mathcal{K} = \mathcal{K}_1 \otimes \mathcal{K}_2$ and $\rho \in \mathfrak{S}_{\mathcal{K}}$, then $\rho_{\mathcal{K}_1} = \operatorname{tr}_{\mathcal{K}_2}(\rho) \in \mathfrak{S}_{\mathcal{K}_1}$ and $\rho_{\mathcal{K}_2} = \operatorname{tr}_{\mathcal{K}_1}(\rho) \in \mathfrak{S}_{\mathcal{K}_2}$.

The von Neumann entropy of a state ρ, defined by

$$S(\rho) = -\operatorname{tr}(\rho \log \rho) = -\sum_{\lambda \in \operatorname{sp}(\rho)} \lambda \log \lambda.$$

is the non-commutative extension of the Gibbs or Shannon entropy of a probability distribution. It is characterized by the following dual variational principles.

Theorem 2.8 (1) *For any $\rho \in \mathfrak{S}$, one has*

$$S(\rho) = \min_{A \in \mathcal{O}_{\mathrm{self}}} \log \operatorname{tr}(\mathrm{s}(\rho)\mathrm{e}^A) - \rho(A).$$

(2) *For any $A \in \mathcal{O}_{\mathrm{self}}$, one has*

$$\log \operatorname{tr}(\mathrm{e}^A) = \max_{\rho \in \mathfrak{S}} \rho(A) + S(\rho).$$

Remark. Adopting the decomposition $\mathcal{K} = \operatorname{Ran}\rho \oplus \operatorname{Ker}\rho$, the minimum in (1) is achieved at A iff $A = (\log(\rho|_{\operatorname{Ran}\rho}) \oplus B) + c$ where B is an arbitrary self-adjoint operator on $\operatorname{Ker}\rho$ and c an arbitrary real constant. An alternative formulation of (1) is

$$S(\rho) = \inf_{A \in \mathcal{O}_{\mathrm{self}}} \log \operatorname{tr}(\mathrm{e}^A) - \rho(A).$$

The maximizer in (2) is unique and given by $\rho = \rho_A$.

Proof. (2) Let $G_A(\rho) = \rho(A) + S(\rho)$. Since $\log \rho_A = A - \log \operatorname{tr}(\mathrm{e}^A)$, Klein's inequality implies

$$\log \operatorname{tr}(\mathrm{e}^A) - G_A(\rho) = \operatorname{tr}(\rho(\log \rho - \log \rho_A)) \ge \operatorname{tr}(\rho - \rho_A) = 0,$$

for any $\rho \in \mathfrak{S}$, with equality iff $\rho = \rho_A$. Thus,

$$G_A(\rho) \le \log \operatorname{tr}(\mathrm{e}^A), \tag{2.16}$$

with equality iff $\rho = \rho_A$.

(1) We decompose $\mathcal{K} = \operatorname{Ran}\rho \oplus \operatorname{Ker}\rho$ and set $P = \mathrm{s}(\rho)$ and $Q = \mathbb{1} - P$. Since $G_A(\rho) = G_{PAP}(\rho)$, we can invoke (2.16) within the subspace $\operatorname{Ran}\rho$ to write

$$G_A(\rho) \le \log \operatorname{tr}(P\mathrm{e}^{PAP}P),$$

where equality holds iff $\rho = P\mathrm{e}^{PAP}P/\mathrm{tr}(P\mathrm{e}^{PAP}P)$, *i.e.*, $PAP = \log(\rho|_{\mathrm{Ran}\,\rho}) + c$ for some real constant c. A second order Duhamel expansion (see Part 3 of Exercise 2.3) further yields

$$\mathrm{tr}(P\mathrm{e}^{A}P) = \mathrm{tr}(P\mathrm{e}^{PAP}P) + \int_0^1 u\,\mathrm{tr}\left(\mathrm{e}^{uPAP/2}PAQ\mathrm{e}^{(1-u)A}QAP\mathrm{e}^{uPAP/2}\right)\,\mathrm{d}u,$$

so that $\mathrm{tr}(P\mathrm{e}^{PAP}P) \le \mathrm{tr}(P\mathrm{e}^{A}P)$ with equality iff $QAP = 0$. We conclude that $G_A(\rho) \le \log\mathrm{tr}(P\mathrm{e}^{A}P)$ and hence $S(\rho) \le \log\mathrm{tr}(P\mathrm{e}^{A}P) - \rho(A)$ where equality holds iff $A = (\log(\rho|_{\mathrm{Ran}\,\rho}) \oplus B) + c$. □

An immediate consequence of Theorem 2.8 is

Corollary 2.9 (1) *The function $\mathfrak{S} \ni \rho \mapsto S(\rho)$ is concave.*
(2) *The function $\mathcal{O}_{\mathrm{self}} \ni A \mapsto \log\mathrm{tr}(\mathrm{e}^{A})$ is convex.*

Further basic properties of the entropy functional are:

Theorem 2.10 (1) *The map $\mathfrak{S} \ni \rho \mapsto S(\rho)$ is continuous.*
(2) $0 \le S(\rho) \le \log\dim\mathcal{K}$. *Moreover, $S(\rho) = 0$ iff ρ is pure and $S(\rho) = \log\dim\mathcal{K}$ iff ρ is chaotic.*
(3) *For any unitary U, $S(U\rho U^{-1}) = S(\rho)$.*
(4) $S(\rho_A) = \log\mathrm{tr}(\mathrm{e}^{A}) - \mathrm{tr}(A\rho_A)$.
(5) *If $\mathcal{K} = \mathcal{K}_1 \otimes \mathcal{K}_2$, then $S(\rho) \le S(\rho_{\mathcal{K}_1}) + S(\rho_{\mathcal{K}_2})$ where the equality holds if and only if $\rho = \rho_{\mathcal{K}_1} \otimes \rho_{\mathcal{K}_2}$ (recall that $\rho_{\mathcal{K}_1} = \mathrm{tr}_{\mathcal{K}_2}(\rho)$).*

Remark. To (1): the Fannes inequality

$$|S(\rho) - S(\nu)| \le \|\rho - \nu\|_1 \log\frac{\dim\mathcal{K}}{\|\rho - \nu\|_1},$$

holds provided $\|\rho - \nu\|_1 < 1/3$. See, e.g., [OP].

Proof. The proofs of (1)–(4) are easy and left to the reader. To prove (5) we invoke the variational principle to write

$$S(\rho) \le \min_{(A,B)\in\mathcal{O}_1\times\mathcal{O}_2} \log\mathrm{tr}(\mathrm{s}(\rho)\mathrm{e}^{A\otimes\mathbb{1}+\mathbb{1}\otimes B}) - \rho(A\otimes\mathbb{1} + \mathbb{1}\otimes B).$$

Setting $\rho_j = \rho_{\mathcal{K}_j}$, the support $\mathrm{s}(\rho_1)$ satisfies $1 = \mathrm{tr}_{\mathcal{K}_1}(\mathrm{s}(\rho_1)\rho_1) = \mathrm{tr}_{\mathcal{K}}((\mathrm{s}(\rho_1)\otimes\mathbb{1})\rho)$ and, by the definition of the support, we must have $\mathrm{s}(\rho_1)\otimes\mathbb{1} \ge \mathrm{s}(\rho)$ and a similar inequality for $\mathrm{s}(\rho_2)$. It follows that $\mathrm{s}(\rho_1)\otimes\mathrm{s}(\rho_2) \ge \mathrm{s}(\rho)$ and therefore

$$\mathrm{tr}(\mathrm{s}(\rho)\mathrm{e}^{A\otimes\mathbb{1}+\mathbb{1}\otimes B}) \le \mathrm{tr}(\mathrm{s}(\rho_1)\mathrm{e}^{A}\otimes\mathrm{s}(\rho_2)\mathrm{e}^{B}).$$

Thus, we can write

$$\begin{aligned} S(\rho) &\le \min_{(A,B)\in\mathcal{O}_1\times\mathcal{O}_2} \log\mathrm{tr}(\mathrm{s}(\rho_1)\mathrm{e}^{A}) + \log\mathrm{tr}(\mathrm{s}(\rho_2)\mathrm{e}^{B}) - \rho_1(A) - \rho_2(B) \\ &= S(\rho_1) + S(\rho_2). \end{aligned}$$

Moreover, equality holds iff the variational principle has a minimizer of the form $A\otimes\mathbb{1} + \mathbb{1}\otimes B$, which, by the remark after Theorem 2.10, is possible only if $\rho = \rho_1\otimes\rho_2$. □

2.6 Relative entropies

The Rényi relative entropy (or α-relative entropy) of two states ρ, ν is defined for $\alpha \in]0,1[$ by

$$S_\alpha(\rho|\nu) = \log\mathrm{tr}(\rho^\alpha\nu^{1-\alpha}).$$

This quantity will play an important role in these lecture notes. According to our convention $\log(\rho|_{\mathrm{Ker}\,\rho}) = -\infty$, and

$$\rho^\alpha = \mathrm{e}^{\alpha \log \rho} = \mathrm{e}^{\alpha \log(\rho|_{\mathrm{Ran}\,\rho})} \oplus 0|_{\mathrm{Ker}\,\rho}.$$

The Hölder inequality implies that $S_\alpha(\rho|\nu) \in [-\infty, 0]$. $S_\alpha(\rho|\nu) = -\infty$ iff $\rho \perp \nu$ (that is, if ρ and ν are mutually singular). In terms of the spectral data of ρ and ν,

$$S_\alpha(\rho|\nu) = \log \left[\sum_{\substack{(\lambda,\mu)\in \mathrm{sp}(\rho)\times\mathrm{sp}(\nu) \\ \lambda\neq 0, \mu\neq 0}} \lambda^\alpha \mu^{1-\alpha} \mathrm{tr}(P_\lambda(\rho)P_\mu(\nu)) \right], \tag{2.17}$$

and so if $\rho \not\perp \nu$, then $]0,1[\ni \alpha \mapsto S_\alpha(\rho|\nu) \in]-\infty, 0]$ extends to a real-analytic function on $\mathbb{R}$. The basic properties of Rényi's relative entropy are:

Proposition 2.11 *Suppose that $\rho \not\perp \nu$. Then:*

(1) $S_0(\rho|\nu) = \log \nu(\mathrm{s}(\rho))$ *and* $S_1(\rho|\nu) = \log \rho(\mathrm{s}(\nu))$.

(2) *The map $\mathbb{R} \ni \alpha \mapsto S_\alpha(\rho|\nu)$ is convex.*

(3) $S_\alpha(U\rho U^{-1}|U\nu U^{-1}) = S_\alpha(\rho|\nu)$ *for any unitary U.*

(4) *Suppose that $\mathrm{s}(\rho) = \mathrm{s}(\nu)$. Then the map $\mathbb{R} \ni \alpha \mapsto S_\alpha(\rho|\nu)$ is strictly convex iff $\rho \neq \nu$.*

(5) $S_\alpha(\rho|\nu) = S_{1-\alpha}(\nu|\rho)$.

Proof. (1), (3) and (5) are obvious. (2) Follows from the following facts, easily derived from (2.17),

$$\partial_\alpha S_\alpha(\rho|\nu) = \sum_{(\lambda,\mu)\in \mathrm{sp}(\rho)\times\mathrm{sp}(\nu)} p_{\lambda,\mu} \log(\lambda/\mu) = \theta_\alpha,$$

$$\partial_\alpha^2 S_\alpha(\rho|\nu) = \sum_{(\lambda,\mu)\in \mathrm{sp}(\rho)\times\mathrm{sp}(\nu)} p_{\lambda,\mu} \left[\log(\lambda/\mu) - \theta_\alpha\right]^2 \geq 0,$$

where

$$p_{\lambda,\mu} = \frac{\lambda^\alpha \mu^{1-\alpha} \mathrm{tr}(P_\lambda(\rho)P_\mu(\nu))}{\sum\limits_{(\lambda,\mu)\in \mathrm{sp}(\rho)\times\mathrm{sp}(\nu)} \lambda^\alpha \mu^{1-\alpha} \mathrm{tr}(P_\lambda(\rho)P_\mu(\nu))} \geq 0,$$

$$\sum_{(\lambda,\mu)\in \mathrm{sp}(\rho)\times\mathrm{sp}(\nu)} p_{\lambda,\mu} = 1.$$

(4) Invoking analyticity, we further deduce that either $\partial_\alpha^2 S_\alpha(\rho|\nu) = 0$ for all $\alpha \in \mathbb{R}$, or $\partial_\alpha^2 S_\alpha(\rho|\nu) > 0$ except possibly on a discrete subset of $\mathbb{R}$. In the former case $S_\alpha(\rho|\nu) = (1-\alpha)S_0(\rho|\nu) + \alpha S_1(\rho|\nu)$ is an affine function of α. In the latter case $S_\alpha(\rho|\nu)$ is strictly convex.

Suppose now that $\mathrm{s}(\rho) = \mathrm{s}(\nu)$. Without loss of generality, we can assume that ρ and ν are faithful. If $\rho = \nu$ then $S_\alpha(\rho|\nu) = 0$ for all $\alpha \in \mathbb{R}$. Reciprocally, if $\partial_\alpha^2 S_\alpha(\rho|\nu)$ vanishes identically then $\theta = \partial_\alpha S_\alpha(\rho|\nu)$ is constant and $\lambda = \mathrm{e}^\theta \mu$ whenever $\mathrm{tr}(P_\lambda(\rho)P_\mu(\nu)) \neq 0$. It follows from

$$1 = \mathrm{tr}(\rho) = \sum_{\lambda,\mu} \lambda\, \mathrm{tr}(P_\lambda(\rho)P_\mu(\nu)) = \mathrm{e}^\theta \sum_{\lambda,\mu} \mu\, \mathrm{tr}(P_\lambda(\rho)P_\mu(\nu)) = \mathrm{e}^\theta \mathrm{tr}(\nu) = \mathrm{e}^\theta,$$

that $\theta = 0$. Repeating the argument in the proof of Part (2) of Theorem 2.1 leads to the conclusion that $\rho = \nu$. $\square$

The following theorem, a variant of the celebrated Kosaki's variational formula ([Kos, OP]), is deeper. The result and its proof were communicated to us by R. Seiringer (unpublished). The proof will be given in Section 2.12 as an illustration of the power of the modular structure to be introduced there.

Theorem 2.12 *For* $\alpha \in]0,1[$,

$$S_\alpha(\rho|\nu) = \inf_{A\in C(\mathbb{R}_+,\mathcal{O})} \log\left[\frac{\sin\pi\alpha}{\pi}\int_0^\infty t^{\alpha-1}\left(\frac{1}{t}\rho(|A(t)^*|^2)+\nu(|\mathbb{1}-A(t)|^2)\right)\mathrm{d}t\right],$$

where $C(\mathbb{R}_+,\mathcal{O})$ *denotes the set of all continuous functions* $\mathbb{R}_+\ni t\mapsto A(t)\in\mathcal{O}$. *Moreover, the infimum is achieved for*

$$A(t) = t\int_0^\infty \mathrm{e}^{-s\rho}\nu\mathrm{e}^{-st\nu}\mathrm{d}s,$$

and this is the unique minimizer if either ρ *or* ν *is faithful.*

An immediate consequence of Kosaki's variational formula is *Uhlmann's monotonicity theorem*, [Uh]:

Theorem 2.13 *If* $\Phi:\mathcal{O}_\mathcal{K}\to\mathcal{O}_{\mathcal{K}'}$ *is a unital Schwarz map, then*

$$S_\alpha(\rho\circ\Phi|\nu\circ\Phi)\geq S_\alpha(\rho|\nu),$$

for all $\alpha\in[0,1]$ *and* $\rho,\nu\in\mathfrak{S}_{\mathcal{K}'}$.

Proof. With $\hat\rho=\rho\circ\Phi$ and $\hat\nu=\nu\circ\Phi$, Kosaki's formula reads

$$S_\alpha(\hat\rho|\hat\nu) = \inf_{A\in C(\mathbb{R}_+,\mathcal{O}_\mathcal{K})} \log\left[\frac{\sin\pi\alpha}{\pi}\int_0^\infty t^{\alpha-1}\left(\frac{1}{t}\hat\rho(|A(t)^*|^2)+\hat\nu(|\mathbb{1}-A(t)|^2)\right)\mathrm{d}t\right].$$

Since Φ is a unital Schwarz map, for any $A\in\mathcal{O}_\mathcal{K}$ one has

$$\hat\rho(|A^*|^2)=\rho(\Phi(AA^*))\geq\rho(\Phi(A)\Phi(A)^*)=\rho(|\Phi(A)^*|^2),$$

as well as

$$\begin{aligned}\hat\nu(|\mathbb{1}-A|^2)&=\nu(\Phi((\mathbb{1}-A)^*(\mathbb{1}-A)))\\&\geq\nu(\Phi(\mathbb{1}-A)^*\Phi(\mathbb{1}-A))\\&=\nu((\mathbb{1}-\Phi(A))^*(\mathbb{1}-\Phi(A)))=\nu(|\mathbb{1}-\Phi(A)|^2).\end{aligned}$$

It follows that

$$\begin{aligned}S_\alpha(\hat\rho|\hat\nu)&\geq\inf_{A\in C(\mathbb{R}_+,\mathcal{O}_\mathcal{K})}\log\left[\frac{\sin\pi\alpha}{\pi}\int_0^\infty t^{\alpha-1}\left(\frac{1}{t}\rho(|\Phi(A(t))^*|^2)+\nu(|\mathbb{1}-\Phi(A(t))|^2)\right)\mathrm{d}t\right]\\&=\inf_{A\in\Phi(C(\mathbb{R}_+,\mathcal{O}_\mathcal{K}))}\log\left[\frac{\sin\pi\alpha}{\pi}\int_0^\infty t^{\alpha-1}\left(\frac{1}{t}\rho(|A(t)^*|^2)+\nu(|\mathbb{1}-A(t)|^2)\right)\mathrm{d}t\right],\end{aligned}$$

where $\Phi(C(\mathbb{R}_+,\mathcal{O}_\mathcal{K}))=\{\Phi\circ A\,|\,A\in C(\mathbb{R}_+,\mathcal{O}_\mathcal{K})\}$. Since Φ is continuous, one has $\Phi(C(\mathbb{R}_+,\mathcal{O}_\mathcal{K}))\subset C(\mathbb{R}_+,\mathcal{O}_{\mathcal{K}'})$, and the result follows from Kosaki's formula. □

Another consequence of Theorem 2.12 is the celebrated Lieb's concavity theorem.

Theorem 2.14 *For* $\alpha\in[0,1]$, *the map* $\mathfrak{S}\times\mathfrak{S}\ni(\rho,\nu)\mapsto S_\alpha(\rho|\nu)$ *is jointly concave, i.e.,*

$$S_\alpha(\lambda\rho+(1-\lambda)\rho'|\lambda\nu+(1-\lambda)\nu')\geq\lambda S_\alpha(\rho|\nu)+(1-\lambda)S_\alpha(\rho'|\nu'),$$

for any $\rho,\rho',\nu,\nu'\in\mathfrak{S}$ *and any* $\lambda\in[0,1]$.

Proof. The result is obvious for $\lambda=0$ and for $\lambda=1$. Hence, we assume $\lambda\in]0,1[$ in the following. For $\alpha=0$ and for $\alpha=1$, the result follows from Part (1) of Proposition 2.11, the concavity of the logarithm, and the fact that $\mathrm{s}(\lambda\rho+(1-\lambda)\rho')\geq\mathrm{s}(\rho)$. For $\alpha\in]0,1[$ and $A\in C(\mathbb{R}_+,\mathcal{O})$, the map

$$(\rho,\nu)\mapsto F_A(\rho,\nu)=\frac{\sin\pi\alpha}{\pi}\int_0^\infty t^{\alpha-1}\left(\frac{1}{t}\rho(|A(t)^*|^2)+\nu(|\mathbb{1}-A(t)|^2)\right)\mathrm{d}t,$$

is affine. The concavity of the logarithm implies that the map $(\rho,\nu)\mapsto\log F_A(\rho,\nu)$ is concave. Therefore, the function $(\rho,\nu)\mapsto S_\alpha(\rho|\nu)$ being the infimum of a family of concave functions, it is itself concave (see the following exercise). $\square$

Exercise 2.11. Let $C\subset\mathbb{R}^n$ be a convex set and $\mathcal{F}$ a nonempty set of real valued functions on C. Set $F(x)=\inf\{f(x)\,|\,f\in\mathcal{F}\}$.

1. Show that if the elements of $\mathcal{F}$ are concave then F is concave.
2. Show that if the elements of $\mathcal{F}$ are continuous then F is upper semi-continuous, *i.e.,*

$$\limsup_{x\to x_0}F(x)\leq F(x_0),$$

for all $x_0\in\mathbb{R}^n$.

3. Show that the function $(\rho,\nu)\mapsto S_\alpha(\rho|\nu)$ is upper semi-continuous on $\mathfrak{S}\times\mathfrak{S}$.

The relative entropy of the state ρ w.r.t. the state ν is defined by

$$S(\rho|\nu)=\begin{cases}\operatorname{tr}(\rho(\log\nu-\log\rho)) & \text{if } \rho\ll\nu.\\ -\infty & \text{otherwise.}\end{cases}$$

Equivalently, in terms of the spectral data of ρ and ν, one has

$$S(\rho|\nu)=\sum_{(\lambda,\mu)\in\operatorname{sp}(\rho)\times\operatorname{sp}(\nu)}\lambda(\log\mu-\log\lambda)\operatorname{tr}(P_\lambda(\rho)P_\mu(\nu)).$$

For $\nu\in\mathfrak{S}$ and $A\in\mathcal{O}_{\rm self}$, we define

$$\mathrm{e}^{A+\log\nu}=\lim_{n\to\infty}\left(\mathrm{e}^{A/n}\nu^{1/n}\right)^n.$$

It s not difficult to show that, according to the decomposition $\mathcal{K}=\operatorname{Ran}\nu\oplus\operatorname{Ker}\nu$,

$$\mathrm{e}^{A+\log\nu}=\mathrm{e}^{\mathrm{s}(\nu)A\mathrm{s}(\nu)|_{\operatorname{Ran}\nu}+\log(\nu|_{\operatorname{Ran}\nu})}\oplus 0_{\operatorname{Ker}\nu}.$$

With this definition, the relative entropy functional has the following variational characterizations:

Theorem 2.15 (1) *For any $\rho,\nu\in\mathfrak{S}$, one has*

$$S(\rho|\nu)=\inf_{A\in\mathcal{O}_{\rm self}}\log\operatorname{tr}(\mathrm{e}^{A+\log\nu})-\rho(A).$$

(2) *For any $A\in\mathcal{O}_{\rm self}$ and $\nu\in\mathfrak{S}$, one has*

$$\log\operatorname{tr}(\mathrm{e}^{A+\log\nu})=\max_{\rho\in\mathfrak{S}}S(\rho|\nu)+\rho(A).$$

Remark. If ρ and ν are equivalent, then the infimum in (1) is achieved at A iff $\mathrm{s}(\nu)A\mathrm{s}(\nu)|_{\operatorname{Ran}\nu}=\log(\rho|_{\operatorname{Ran}\nu})-\log(\nu|_{\operatorname{Ran}\nu})+c$ where c is an arbitrary real constant. The maximizer in (2) is unique and given by $\rho=\mathrm{e}^{A+\log\nu}/\operatorname{tr}(\mathrm{e}^{A+\log\nu})$.

Proof. (2) Set $G_{\nu,A}(\rho)=S(\rho|\nu)+\rho(A)$ and $\widetilde{\nu}=\mathrm{e}^{A+\log\nu}/\operatorname{tr}(\mathrm{e}^{A+\log\nu})$. Note that $G_{\nu,A}(\rho)=-\infty$ if $\rho\not\ll\nu$ while $G_{\nu,A}(\nu)=\nu(A)>-\infty$. Thus, it suffices to consider $\rho\ll\nu$ in which case one has

$$\rho\left(\log\widetilde{\nu}\right)=\rho(A)+\rho(\log\nu)-\log\operatorname{tr}(\mathrm{e}^{A+\log\nu}).$$

Klein's inequality yields

$$\log \operatorname{tr}(\mathrm{e}^{A+\log\nu}) - G_{\nu,A}(\rho) = \operatorname{tr}\left(\rho\left(\log\rho - \log\widetilde{\nu}\right)\right) \geq \operatorname{tr}(\rho - \widetilde{\nu}) = 0,$$

with equality iff $\rho = \widetilde{\nu}$.

(1) We first consider the case $\rho \not\ll \nu$. Then, there exists a projection P such that $\operatorname{Ran} P \perp \operatorname{Ran}\nu$ and $\rho(P) > 0$. Since $\mathrm{e}^{\lambda P+\log\nu} = \nu$, it follows that

$$\log \operatorname{tr}(\mathrm{e}^{\lambda P+\log\nu}) - \rho(\lambda P) = -\lambda\rho(P) \to -\infty = S(\rho|\nu),$$

as $\lambda \to \infty$. On the other hand, for any $\rho \ll \nu$ and $A \in \mathcal{O}_{\mathrm{self}}$, (2) implies that

$$S(\rho|\nu) \leq \log \operatorname{tr}(\mathrm{e}^{A+\log\nu}) - \rho(A),$$

with equality iff $\rho = \mathrm{e}^{A+\log\nu}/\operatorname{tr}(\mathrm{e}^{A+\log\nu})$. If $\nu \ll \rho$, this means that equality holds iff $\mathrm{s}(\nu)A\mathrm{s}(\nu)|_{\operatorname{Ran}\nu} = \log(\rho|_{\operatorname{Ran}\nu}) - \log(\nu|_{\operatorname{Ran}\nu})$ up to an arbitrary additive constant. If $\nu \not\ll \rho$, *i.e.*, if $\mathrm{s}(\rho) < \mathrm{s}(\nu)$, then $A_\lambda = \log(\rho|_{\operatorname{Ran}\rho}) \oplus \lambda\mathbb{1}_{\operatorname{Ker}\rho} - \log(\nu|_{\operatorname{Ran}\nu}) \oplus 0_{\operatorname{Ker}\nu}$ is such that, with $d = \dim\operatorname{Ran}\nu - \dim\operatorname{Ran}\rho$,

$$\log \operatorname{tr}(\mathrm{e}^{A_\lambda+\log\nu}) - \rho(A_\lambda) = \log\left(1 + \mathrm{e}^{\lambda}d\right) + S(\rho|\nu) \to S(\rho|\nu),$$

as $\lambda \to -\infty$. □

As an immediate consequence of Theorem 2.15 we note, for later reference

Corollary 2.16 *For any state $\nu \in \mathfrak{S}$ and any self-adjoint observable $A \in \mathcal{O}$ one has*

$$\operatorname{tr}(\mathrm{e}^{\log\nu+A}) \geq \mathrm{e}^{\nu(A)}.$$

The basic properties of the relative entropy functional are:

Proposition 2.17 (1) *$S(\rho|\nu) \leq 0$ with equality iff $\rho = \nu$.*

(2) *$S(\rho|\rho_{\mathrm{ch}}) = S(\rho) - \log\dim\mathcal{K}$.*

(3) *$S(U\rho U^{-1}|U\nu U^{-1}) = S(\rho|\nu)$ for any unitary U.*

(4)

$$S(\rho_A|\rho_B) = \log\frac{\operatorname{tr}(\mathrm{e}^A)}{\operatorname{tr}(\mathrm{e}^B)} - \operatorname{tr}(\rho_A(A-B)).$$

(5) *For any $\rho, \nu \in \mathfrak{S}$ one has*

$$S(\rho|\nu) = \lim_{\alpha\downarrow 0}\frac{S_\alpha(\nu|\rho)}{\alpha} = \lim_{\alpha\uparrow 1}\frac{S_\alpha(\rho|\nu)}{1-\alpha}. \tag{2.18}$$

In particular, if $\rho \ll \nu$ then $S_0(\nu|\rho) = S_1(\rho|\nu) = 0$ and

$$S(\rho|\nu) = \left.\frac{\mathrm{d}}{\mathrm{d}\alpha}S_\alpha(\nu|\rho)\right|_{\alpha=0} = -\left.\frac{\mathrm{d}}{\mathrm{d}\alpha}S_\alpha(\rho|\nu)\right|_{\alpha=1}. \tag{2.19}$$

(6) *If $\Phi : \mathcal{O}_{\mathcal{K}} \to \mathcal{O}_{\mathcal{K}'}$ is a unital Schwarz map then, for any $\rho, \nu \in \mathfrak{S}_{\mathcal{K}}$,*

$$S(\rho\circ\Phi|\nu\circ\Phi) \geq S(\rho|\nu).$$

(7) *The map $(\rho, \nu) \mapsto S(\rho|\nu)$ is continuous on $\mathfrak{S} \times \mathfrak{S}_{\mathrm{f}}$ and upper semi-continuous on $\mathfrak{S} \times \mathfrak{S}$.*

(8) *If $\mathrm{s}(\nu) = \mathrm{s}(\rho)$, then $S_\alpha(\rho|\nu) \geq \alpha S(\nu|\rho)$.*

Proof. Part (1) follows from Klein's inequality. Parts (2), (3) and (4) are obvious. Part (5) is easy and left to the reader. Part (6) follows from (2.18) and Uhlmann's monotonicity theorem (Theorem 2.13). The upper semi-continuity of the map $(\rho,\nu)\mapsto S(\rho|\nu)$ follows from (5) and part 3 of Exercise 2.11. A direct proof goes as follows. Let us fix $(\rho_0,\nu_0)\in\mathfrak{S}\times\mathfrak{S}$. Define $\lambda_0=\min\{\lambda\in\mathrm{sp}(\nu_0)\,|\,\lambda>0\}$, and for $\nu\in\mathfrak{S}$ set

$$Q_\nu=\sum_{\substack{\lambda\in\mathrm{sp}(\nu)\\ \lambda>\lambda_0/2}}P_\lambda(\nu).$$

Let $0<\varepsilon<\lambda_0/2$. We know from perturbation theory that

$$\lim_{\nu\to\nu_0}Q_\nu=\mathrm{s}(\nu_0),\qquad \lim_{\nu\to\nu_0}\nu Q_\nu=\nu_0,$$

and that

$$\nu^{(\varepsilon)}=\nu Q_\nu+(\mathbb{1}-Q_\nu)\varepsilon\geq\nu,$$

provided ν is close enough to ν_0. It follows that

$$S(\rho|\nu)=\rho(\log\nu)-S(\rho)\leq\rho(\log\nu^{(\varepsilon)})-S(\rho).$$

Since $\nu^{(\varepsilon)}\geq\epsilon>0$ it follows from the analytic functional calculus that

$$\lim_{\nu\to\nu_0}\log\nu^{(\varepsilon)}=\log\left(\lim_{\nu\to\nu_0}\nu^{(\varepsilon)}\right)=\log(\nu_0|_{\mathrm{Ran}\,\nu_0})\oplus\log\varepsilon|_{\mathrm{Ker}\,\nu_0},$$

and hence, using Theorem 2.10 (1), we deduce

$$\begin{aligned}\limsup_{(\rho,\nu)\to(\rho_0,\nu_0)}S(\rho|\nu)&\leq\lim_{(\rho,\nu)\to(\rho_0,\nu_0)}\rho(\log\nu^{(\varepsilon)})-S(\rho)\\&=\rho_0(\log\nu_0|_{\mathrm{Ran}\,\nu_0}\oplus 0|_{\mathrm{Ker}\,\nu_0})-S(\rho_0)+(1-\rho_0(\mathrm{s}(\nu_0)))\log\varepsilon.\end{aligned}$$

If $\rho_0\not\ll\nu_0$ then $1-\rho_0(\mathrm{s}(\nu_0))>0$ and letting $\varepsilon\downarrow 0$ we conclude that

$$\limsup_{(\rho,\nu)\to(\rho_0,\nu_0)}S(\rho|\nu)\leq-\infty=S(\rho_0|\nu_0).$$

If $\rho_0\ll\nu_0$ then $1-\rho_0(\mathrm{s}(\nu_0))=0$ and $\mathrm{Ker}\,\nu_0\subset\mathrm{Ker}\,\rho_0$ so that

$$\limsup_{(\rho,\nu)\to(\rho_0,\nu_0)}S(\rho|\nu)\leq\rho_0(\log\nu_0)-S(\rho_0)=S(\rho_0|\nu_0).$$

Finally, we observe that if $\nu_0>0$, then $\nu\geq\lambda_0/2$ for all ν sufficiently close to ν_0. Hence $\lim_{\nu\to\nu_0}\log\nu=\log\nu_0$ and

$$\lim_{(\rho,\nu)\to(\rho_0,\nu_0)}S(\rho|\nu)=S(\rho_0|\nu_0).$$

Property (8) is a direct consequence of the convexity of $\alpha\mapsto S_\alpha(\rho|\nu)$ and Equ. (2.19). $\square$

Remark. The following example shows that the function $(\rho,\nu)\mapsto S(\rho|\nu)$ is not continuous on $\mathfrak{S}\times\mathfrak{S}$. Setting

$$\rho_n=\begin{bmatrix}1-1/n & 0\\ 0 & 1/n\end{bmatrix},\qquad \nu_n=\begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix},$$

one has $S(\rho_n|\nu_n)=-\infty$ for all $n\in\mathbb{N}^*$, so

$$\lim_{n\to\infty}S(\rho_n|\nu_n)=-\infty\neq S(\lim_{n\to\infty}\rho_n|\lim_{n\to\infty}\nu_n)=0.$$

As a direct consequence of Theorem 2.14 and Relation (2.18), we have:

Theorem 2.18 *The map $\mathfrak{S}\times\mathfrak{S}\ni(\rho,\nu)\mapsto S(\rho|\nu)$ is jointly concave, that is, for $\lambda\in[0,1]$ and $\rho,\rho',\nu,\nu'\in\mathfrak{S}$,*

$$S(\lambda\rho+(1-\lambda)\rho'|\lambda\nu+(1-\lambda)\nu')\geq\lambda S(\rho|\nu)+(1-\lambda)S(\rho'|\nu').$$

Exercise 2.12. Use Uhlmann's monotonicity theorem to show that

$$S_\alpha(\rho \circ \vartheta | \nu \circ \vartheta) = S_\alpha(\rho|\nu),$$

for all $\rho, \nu \in \mathfrak{S}$ and $\vartheta \in \mathrm{Aut}(\mathcal{O})$.

2.7 Quantum hypothesis testing

Since the pioneering work of Pearson [Pe], hypothesis testing has played an important role in theoretical and applied statistics (see, *e.g.*, [Be]). In the last decade, the mathematical structure and basic results of classical hypothesis testing have been extended to the non-commutative setting. A clear exposition of the basic results of quantum hypothesis testing can be found in [ANSV, HMO].

It was recently observed in [JOPS] that there is a close relation between recent developments in the field of quantum hypothesis testing and the developments in non-equilibrium statistical mechanics. In this section we describe the setup of quantum hypothesis testing following essentially [ANSV]. We will discuss the relation to non-equilibrium statistical mechanics in Section 5.6.

Let ν and ρ be two states and $p \in]0,1[$. Suppose that we know a priori that the system is with probability p in the state ρ and with probability $1-p$ in the state ν. By performing a measurement we wish to decide with minimal error probability what is the true state of the system. The following procedure is known as *quantum hypothesis testing*. A *test* P is an orthogonal projection in $\mathcal{O}$. On the basis of the outcome of the test (that is, a measurement of P) one decides whether the system is in the state ρ or ν. More precisely, if the outcome of the test is 1, one decides that the system is in the state ρ (Hypothesis I) and if the outcome is 0, one decides that the system is in the state ν (Hypothesis II). $\rho(\mathbb{1}-P)$ is the error probability of accepting II if I is true and $\nu(P)$ is the error probability of accepting I if II is true. The average error probability is

$$D_p(\rho, \nu, P) = p\rho(\mathbb{1} - P) + (1-p)\nu(P),$$

and we are interested in minimizing $D_p(\rho, \nu, P)$ w.r.t. P. Let

$$D_p(\rho, \nu) = \inf\{D_p(\rho, \nu, P) \,|\, P \in \mathcal{O}_{\mathrm{self}},\, P^2 = P\}.$$

The set of all orthogonal projections is a norm closed subset of $\mathcal{O}$ and so the infimum on the right-hand side is achieved at some projection P. The quantum Bayesian distinguishability problem is to identify the orthogonal projections P such that $D_p(\rho, \nu, P) = D_p(\rho, \nu)$. Let P_{opt} be the orthogonal projection onto the range of

$$((1-p)\nu - p\rho)_+\,,$$

where $x_+ = (|x| + x)/2$ denotes the positive part of x. The following result was proven in [ANSV], where the reader can find references to the previous works on the subject.

Theorem 2.19 (1)

$$D_p(\rho, \nu) = D_p(\rho, \nu, P_{\mathrm{opt}}) = \frac{1}{2}\left(1 - \|(1-p)\nu - p\rho\|_1\right).$$

Moreover, P_{opt} is the unique minimizer of the functional $P \mapsto D_p(\rho, \nu, P)$.

(2)

$$D_p(\rho, \nu) = \min\{D_p(\rho, \nu, T) \,|\, T \in \mathcal{O}_{\mathrm{self}}, 0 \le T \le \mathbb{1}\}.$$

(3) *For $\alpha \in [0,1]$,*

$$D_p(\rho, \nu) \le p^\alpha (1-p)^{1-\alpha} \mathrm{tr}(\rho^\alpha \nu^{1-\alpha}).$$

Remark. Part (1) is the quantum version of the Neyman-Pearson lemma. Part (3) is the quantum analog of the Chernoff bound in classical hypothesis testing. In quantum information theory the quantity

$$\zeta_{QCB}(\rho,\nu) = -\log \min_{\alpha\in[0,1]} \operatorname{tr}(\rho^\alpha \nu^{1-\alpha}) = -\min_{\alpha\in[0,1]} S_\alpha(\rho|\nu),$$

is called the Chernoff distance between the states ρ and ν. We shall prove a lower bound on the function $D_p(\rho,\nu)$ in Section 2.12.

Proof. (1)–(2) Set $A = (1-p)\nu - p\rho$ so that, for $T \in \mathcal{O}_{\rm self}$, $0 \le T \le \mathbb{1}$, we can write

$$D_p(\rho,\nu,T) = \operatorname{tr}\left(p\rho(\mathbb{1}-T) + (1-p)\nu T\right) = p + \operatorname{tr}(TA) \ge p + \operatorname{tr}(TA_+),$$

where equality holds iff $\operatorname{Ran} T \subset \operatorname{Ker} A_- = \operatorname{Ran} A_+$. It follows that $P_{\rm opt}$ is the unique minimizer and

$$D_p(\rho,\nu,P_{\rm opt}) = p + \operatorname{tr}(A_+) = p + \frac{1}{2}\operatorname{tr}\left(A + |A|\right) = \frac{1}{2}(1 + \operatorname{tr}\left(|A|\right)).$$

(3) (Following S. Ozawa, private communication. The original proof can be found in [ANSV]). Setting $B = p\rho$ and $C = (1-p)\nu$ and given (1), one has to show that

$$\operatorname{tr}(B^\alpha C^{1-\alpha}) \ge \frac{1}{2}\operatorname{tr}(B + C - |B - C|),$$

for all $B, C \in \mathcal{O}_+$ and $\alpha \in [0,1]$. With $A = C - B$, one clearly has

$$B \le B + A_+, \tag{2.20}$$

and since $C - B \le (C-B)_+$, one also has

$$C \le B + A_+. \tag{2.21}$$

We shall make repeated use of the Löwner-Heinz inequality (Exercise 2.2). From (2.20) and the fact that $B^\alpha \ge 0$ we get

$$\operatorname{tr}(B^\alpha(B^{1-\alpha} - C^{1-\alpha})) \le \operatorname{tr}(B^\alpha((B + A_+)^{1-\alpha} - C^{1-\alpha})). \tag{2.22}$$

From (2.21) we deduce that

$$(B + A_+)^{1-\alpha} - C^{1-\alpha} \ge 0.$$

Thus, (2.20) and (2.22) imply

$$\begin{aligned}\operatorname{tr}(B^\alpha(B^{1-\alpha} - C^{1-\alpha})) &\le \operatorname{tr}((B + A_+)^\alpha((B + A_+)^{1-\alpha} - C^{1-\alpha}))\\ &= \operatorname{tr}(B + A_+) - \operatorname{tr}((B + A_+)^\alpha C^{1-\alpha}).\end{aligned}$$

Using again Inequality (2.21), and the fact that $C \ge 0$, we obtain

$$\operatorname{tr}(B^\alpha(B^{1-\alpha} - C^{1-\alpha})) \le \operatorname{tr}(B + A_+) - \operatorname{tr}(C^\alpha C^{1-\alpha}) = \operatorname{tr}(B - C + A_+).$$

This inequality can be rewritten as

$$\operatorname{tr}(B^\alpha C^{1-\alpha}) \ge \operatorname{tr}(C - A_+),$$

and since $A_+ = A + A_-$,

$$\operatorname{tr}(B^\alpha C^{1-\alpha}) \ge \operatorname{tr}(C - A - A_-) = \operatorname{tr}(C - (C - B) - A_-) = \operatorname{tr}(B - A_-).$$

Combining the last two inequalities we finally get

$$\operatorname{tr}(B^\alpha C^{1-\alpha}) \ge \frac{1}{2}\operatorname{tr}(B + C - A_+ - A_-) = \frac{1}{2}\operatorname{tr}(B + C - |B - C|),$$

as required. □

2.8 Dynamical systems

A *dynamics* on the $*$-algebra $\mathcal{O}$ is a continuous one-parameter subgroup of $\mathrm{Aut}(\mathcal{O})$, *i.e.*, a map $\mathbb{R} \ni t \mapsto \tau^t \in \mathrm{Aut}(\mathcal{O})$ satisfying $\tau^t \circ \tau^s = \tau^{t+s}$ for all $t, s \in \mathbb{R}$ and $\lim_{t\to 0} \|\tau^t(A) - A\| = 0$ for all $A \in \mathcal{O}$. Such a map automatically satisfies $\tau^0 = \mathrm{id}$ and $(\tau^t)^{-1} = \tau^{-t}$ for all $t \in \mathbb{R}$. Moreover, since τ^t is isometric and $\mathcal{O}$ is a finite dimensional vector space, the continuity is uniform

$$\lim_{\epsilon\to 0} \sup_{\substack{\|A\|=1\\ t\in\mathbb{R}}} \|\tau^{t+\epsilon}(A) - \tau^t(A)\| = 0,$$

and the map $t \mapsto \tau^t(A)$ is differentiable (in fact entire analytic). In terms of the generator

$$\delta(A) = \left.\frac{\mathrm{d}}{\mathrm{d}t}\tau^t(A)\right|_{t=0},$$

one has $\tau^t(A) = \mathrm{e}^{t\delta}(A)$. Clearly, $\delta(\mathbb{1}) = 0$, $\delta(AB) = \delta(A)B + A\delta(B)$ and $\delta(A)^* = \delta(A^*)$ hold for all $A, B \in \mathcal{O}$. We call *dynamical system* a pair $(\mathcal{O}, \tau^t)$, where τ^t is a dynamics on $\mathcal{O}$.

If $H \in \mathcal{O}_{\mathrm{self}}$, then

$$\tau^t(A) = \mathrm{e}^{\mathrm{i}tH} A \mathrm{e}^{-\mathrm{i}tH}, \tag{2.23}$$

is a dynamics on $\mathcal{O}$. One of the special features of finite quantum systems is that the converse is true. Given a dynamical system $(\mathcal{O}, \tau^t)$, there exists $H \in \mathcal{O}_{\mathrm{self}}$ such that (2.23) holds for all $t \in \mathbb{R}$. Moreover, H is uniquely determined up to a constant. It can be explicitly constructed as follows. Let δ be the generator of τ^t. Let $\{\psi_j\}$ be an orthonormal basis of $\mathcal{K}$ and $E_{ij} = |\psi_i\rangle\langle\psi_j|$ the corresponding basis of $\mathcal{O}$. Let

$$H = \frac{1}{\mathrm{i}} \sum_j \delta(E_{ji}) E_{ij}.$$

The relation $\sum_j E_{ji}E_{ij} = \sum_j E_{jj} = \mathbb{1}$ implies

$$\sum_j \delta(E_{ji})E_{ij} + \sum_j E_{ji}\delta(E_{ij}) = \delta(\mathbb{1}) = 0,$$

and

$$\begin{aligned}\mathrm{i}[H, E_{kl}] &= \sum_j \delta(E_{ji})E_{ij}E_{kl} + E_{kl}E_{ji}\delta(E_{ij})\\ &= \delta(E_{ki})E_{il} + E_{ki}\delta(E_{il}) = \delta(E_{ki}E_{il}) = \delta(E_{kl}).\end{aligned}$$

Hence $\mathrm{i}[H, X] = \delta(X)$ for all $X \in \mathcal{O}$ and (2.23) follows.

Remark. From the above discussion, the reader familiar with the theory of Lie groups will recognize that $\mathrm{Aut}(\mathcal{O})$ is a simply connected Lie group with Lie algebra

$$\mathfrak{aut}(\mathcal{O}) = \{\mathrm{d}_X = \mathrm{i}[X, \cdot\,] \,|\, X \in \mathcal{O}_{\mathrm{self}}\},$$

and bracket $[\mathrm{d}_X, \mathrm{d}_Y] = \mathrm{d}_{\mathrm{i}[X,Y]}$. Since $\mathrm{d}_X = \mathrm{d}_Y$ iff $X - Y$ is a real multiple of the identity, the dimension of $\mathrm{Aut}(\mathcal{O})$ is given by $\dim_{\mathbb{R}}(\mathcal{O}_{\mathrm{self}}) - 1 = (\dim \mathcal{K})^2 - 1$.

According to the basic principles of quantum mechanics, if H is the energy observable of the system, *i.e.*, its Hamiltonian, then the group $\tau^t(A) = \mathrm{e}^{\mathrm{i}tH} A \mathrm{e}^{-\mathrm{i}tH}$ describes its time evolution in the Heisenberg picture. If the system was in the state ρ at time $t = 0$ then the expectation value of the observable A at time t is given by

$$\mathrm{tr}(\rho\tau^t(A)) = \rho(\tau^t(A)) = \rho \circ \tau^t(A).$$

In the Schrödinger picture the state ρ evolves in time as $\tau^{-t}(\rho)$ and in what follows we adopt the shorthands

$$A_t = \tau^t(A), \qquad \rho_t = \tau^{-t}(\rho) = \rho \circ \tau^t.$$

Clearly, $\rho_t(A) = \rho(A_t)$.

2.9 Gibbs states, KMS condition and variational principle

For the dynamical system $(\mathcal{O}, \tau^t)$, with Hamiltonian H, the state of thermal equilibrium at inverse temperature β is described by the Gibbs canonical ensemble

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

Note that, for any $A, B \in \mathcal{O}$, one has

$$\rho_\beta(AB) = \frac{\mathrm{tr}(\mathrm{e}^{-\beta H}AB)}{\mathrm{tr}(\mathrm{e}^{-\beta H})} = \frac{\mathrm{tr}(B\mathrm{e}^{-\beta H}A)}{\mathrm{tr}(\mathrm{e}^{-\beta H})} = \frac{\mathrm{tr}(\mathrm{e}^{-\beta H}\tau^{-\mathrm{i}\beta}(B)A)}{\mathrm{tr}(\mathrm{e}^{-\beta H})} = \rho_\beta(\tau^{-\mathrm{i}\beta}(B)A).$$

We say that a state ρ satisfies the Kubo-Martin-Schwinger (KMS) condition at inverse temperature β, or, for short, that ρ is a β-KMS state if

$$\rho(AB) = \rho(\tau^{-\mathrm{i}\beta}(B)A), \tag{2.24}$$

holds for all $A, B \in \mathcal{O}$. The β-KMS condition (2.24) plays a central role in algebraic quantum statistical mechanics. For the finite quantum system considered in this section it is a characterization of the Gibbs state ρ_β.

Proposition 2.20 *ρ is a β-KMS state iff $\rho = \rho_\beta$.*

Proof. It remains to show that if ρ is β-KMS, then $\rho = \rho_\beta$. Setting $X = \rho\mathrm{e}^{\beta H}$ and $A = \mathrm{e}^{\beta H}C$ in the KMS condition

$$\mathrm{tr}(\rho\mathrm{e}^{\beta H}B\mathrm{e}^{-\beta H}A) = \mathrm{tr}(\rho AB),$$

yields $\mathrm{tr}(XBC) = \mathrm{tr}(XCB)$ for all $B, C \in \mathcal{O}$. Since this is equivalent to $\mathrm{tr}([X, B]C) = 0$, we conclude that $[X, B] = 0$ for all $B \in \mathcal{O}$ and hence that $X = \alpha\mathbb{1}$ for some constant α. This means that $\rho = \alpha\mathrm{e}^{-\beta H}$. The constant α is now determined by the normalization condition $\mathrm{tr}(\rho) = 1$. □

The Gibbs canonical ensemble can be also characterized by a variational principle. The number $E = \rho_\beta(H)$ is the expectation value of the energy in the state ρ_β. Since

$$\frac{\mathrm{d}}{\mathrm{d}\beta}\rho_\beta(H) = -\rho_\beta((H-E)^2) \le 0,$$

the function $\beta \mapsto \rho_\beta(H)$ is decreasing and is strictly decreasing unless H is constant. If $E_{\min} = \min \mathrm{sp}(H)$ and $E_{\max} = \max \mathrm{sp}(H)$, then

$$\lim_{\beta\to-\infty} \rho_\beta(H) = E_{\max}, \qquad \lim_{\beta\to\infty} \rho_\beta(H) = E_{\min}.$$

Note also that $\lim_{\beta\to\pm\infty} \rho_\beta = \rho_{\pm\infty}$ where

$$\rho_{+\infty/-\infty} = \frac{P_{\min\,/\,\max}}{\mathrm{tr}(P_{\min\,/\,\max})},$$

and $P_{\min\,/\,\max}$ denote the spectral projection of H associated to its eigenvalue $E_{\min\,/\,\max}$. Hence to any $E \in [E_{\min}, E_{\max}]$ one can associate a unique $\beta \in [-\infty, \infty]$ such that

$$\rho_\beta(H) = E. \tag{2.25}$$

We adopt the shorthands

$$S(\beta) = S(\rho_\beta), \qquad P(\beta) = \log \mathrm{tr}(\mathrm{e}^{-\beta H}).$$

The function $P(\beta)$ is called the *pressure* (or *free energy*). Note that

$$S(\beta) = \beta E + P(\beta). \tag{2.26}$$

If $\mathfrak{S}_E = \{\rho \in \mathfrak{S} \,|\, \rho(H) = E\}$ and $\nu \in \mathfrak{S}_E$, then

$$S(\nu) = S(\nu) - \beta\nu(H) + \beta E \le \max_{\rho\in\mathfrak{S}}\{S(\rho) - \beta\rho(H)\} + \beta E = \log \mathrm{tr}(\mathrm{e}^{-\beta H}) + \beta E,$$

and so

$$S(\nu) \le S(\beta),$$

where equality holds iff $\nu = \rho_\beta$. Hence, we have proven the Gibbs variational principle:

Theorem 2.21 *Let $E \in [E_{\min}, E_{\max}]$ and let β be given by (2.25). Then*

$$\max_{\rho\in\mathfrak{S}_E} S(\rho) = S(\beta),$$

and the unique maximizer is the Gibbs state ρ_β.

Note that neither the KMS condition nor the Gibbs variational principle require β to be positive. The justification of the physical restriction $\beta > 0$ typically involves some form of the second law of thermodynamics. Recall that $\beta = \beta(E)$ is uniquely specified by (2.25). Considering $S(E) = S(\beta(E))$ as the function of E, the differentiation of relation (2.26) w.r.t. E yields

$$\frac{\mathrm{d}S}{\mathrm{d}E} = \beta,$$

and the second law $\frac{\mathrm{d}S}{\mathrm{d}E} \ge 0$ (the increase of entropy with energy) requires $\beta \ge 0$. An alternative approach goes as follows. Let an external force act on the system during the time interval $[0, T]$ so that its Hamiltonian becomes time dependent, $H(t) = H + V(t)$. We assume that $V(t)$ depends continuously on t and vanishes for $t \notin]0, T[$. Let $U(t)$ be the corresponding unitary propagator, *i.e.*, the solution of the time-dependent Schrödinger equation

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}U(t) = H(t)U(t), \qquad U(0) = \mathbb{1}.$$

Suppose that at $t = 0$ the system was in the Gibbs state ρ_β. At the later time $t > 0$, its state is given by $\rho_{\beta,t} = U(t)\rho_\beta U(t)^*$ and the work performed on the system by the external force during the time interval $[0, T]$ is

$$\Delta E = \rho_{\beta,T}(H) - \rho_\beta(H) = \int_0^T \frac{\mathrm{d}}{\mathrm{d}t}\rho_{\beta,t}(H)\,\mathrm{d}t.$$

The change of relative entropy $S(\rho_{\beta,t}|\rho_\beta)$ over the time interval $[0, T]$ equals

$$\Delta S = S(\rho_{\beta,T}|\rho_\beta) - S(\rho_\beta|\rho_\beta) = \int_0^T \frac{\mathrm{d}}{\mathrm{d}t}S(\rho_{\beta,t}|\rho_\beta)\,\mathrm{d}t = -\beta\int_0^T \frac{\mathrm{d}}{\mathrm{d}t}\rho_{\beta,t}(H)\,\mathrm{d}t,$$

and so

$$\Delta S = -\beta\Delta E.$$

If $V(t)$ is non-trivial in the sense that $\rho_{\beta,T} \ne \rho_\beta$, then $\Delta S = S(\rho_{\beta,T}|\rho_\beta) < 0$. The second law of thermodynamics, more precisely the fact that one can not extract work from a system in thermal equilibrium, requires that $\Delta E \ge 0$. Hence, negative values of β are not allowed by thermodynamics.

The above discussion can be generalized as follows. Let $N \in \mathcal{O}_{\mathrm{self}}$ be an observable such that $[H, N] = 0$ (N is colloquially called a *charge*). Let β and μ be real parameters and let

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

be the β-KMS state for the dynamics generated by $H - \mu N$. Denote $\rho_{\beta,\mu}(H) = E$, $\rho_{\beta,\mu}(N) = \varrho$, $S(\beta,\mu) = S(\rho_{\beta,\mu})$, $P(\beta,\mu) = \log \mathrm{tr}(\mathrm{e}^{-\beta(H-\mu N)})$. Then

$$S(\beta,\mu) = \beta(E - \mu\varrho) + P(\beta,\mu). \tag{2.27}$$

If $\mathfrak{S}_{E,\varrho} = \{\rho \in \mathfrak{S} \,|\, \rho(H) = E, \rho(N) = \varrho\}$, then

$$\max_{\rho\in\mathfrak{S}_{E,\varrho}} S(\rho) = S(\beta, \mu),$$

with unique maximizer $\rho_{\beta,\mu}$. The parameter μ is interpreted as chemical potential associated to the charge N and the state $\rho_{\beta,\mu}$ describes the system in thermal equilibrium at inverse temperature β and chemical potential μ. Considering $\beta = \beta(E, \varrho)$ and $\mu = \mu(E, \varrho)$ as functions of E and ϱ we see from (2.27) that

$$\frac{\partial S}{\partial E} = \beta, \qquad \frac{\partial S}{\partial \varrho} = -\beta\mu.$$

Although in general $\rho_{\beta,\mu}$ is not a β-KMS state for the dynamics τ^t, if A and B commute with N, then $\tau^t(A) = \mathrm{e}^{\mathrm{i}t(H-\mu N)} A \mathrm{e}^{-\mathrm{i}t(H-\mu N)}$ and the β-KMS condition

$$\rho_{\beta,\mu}(\tau^{-\mathrm{i}\beta}(B)A) = \rho_{\beta,\mu}(AB),$$

is satisfied. In other words, if $\mu \neq 0$, the physical observables must be invariant under the gauge group $\gamma^\theta(A) = \mathrm{e}^{\mathrm{i}\theta N} A \mathrm{e}^{-\mathrm{i}\theta N}$. The generalization of these results to the case of several charges is straightforward.

2.10 Perturbation theory

Let $(\mathcal{O}, \tau^t)$ be a dynamical system with Hamiltonian H and let $V \in \mathcal{O}_{\text{self}}$ be a perturbation. In this section we consider the perturbed dynamics τ_V^t generated by the Hamiltonian $H + V$,

$$\tau_V^t(A) = \mathrm{e}^{\mathrm{i}t(H+V)} A \mathrm{e}^{-\mathrm{i}t(H+V)}.$$

If δ denotes the generator of τ^t, then the generator of τ_V^t is given by

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

and one easily checks that the map $\mathbb{R} \ni t \mapsto \gamma_V^t \in \mathrm{Aut}(\mathcal{O})$ defined by

$$\gamma_V^t = \tau_V^t \circ \tau^{-t} = \mathrm{e}^{t(\delta+\mathrm{d}_V)} \circ \mathrm{e}^{-t\delta},$$

has the following properties:

(1) $\tau_V^t = \gamma_V^t \circ \tau^t$.

(2) $(\gamma_V^t)^{-1} = \tau^t \circ \gamma_V^{-t} \circ \tau^{-t}$.

(3) $\gamma_V^{t+s} = \gamma_V^s \circ \tau^s \circ \gamma_V^t \circ \tau^{-s}$.

(4) $\gamma_V^0 = \mathrm{id}$ and $\partial_t \gamma_V^t = \gamma_V^t \circ \mathrm{d}_{\tau^t(V)}$.

Integration of Relation (4) yields the integral equation

$$\gamma_V^t = \mathrm{id} + \int_0^t \gamma_V^s \circ \mathrm{d}_{\tau^s(V)}\, \mathrm{d}s,$$

which can be iterated to obtain

$$\begin{aligned}\gamma_V^t = \mathrm{id} + \sum_{n=1}^{N-1} \int_{0\le s_1\le\cdots\le s_n\le t} \mathrm{d}_{\tau^{s_n}(V)} \circ \cdots \circ \mathrm{d}_{\tau^{s_1}(V)}\, \mathrm{d}s_1 \cdots \mathrm{d}s_n \\ + \int_{0\le s_1\le\cdots\le s_N\le t} \gamma_V^{s_N} \circ \mathrm{d}_{\tau^{s_N}(V)} \circ \cdots \circ \mathrm{d}_{\tau^{s_1}(V)}\, \mathrm{d}s_1 \cdots \mathrm{d}s_N.\end{aligned}$$

Since γ_V^t is isometric and $\|d_{\tau^t(V)}\| = \|\mathrm{i}[\tau^t(V), \cdot\,]\| \le 2\|V\|$, we can bound the norm of the last term by

$$\int_{0\le s_1\le\cdots\le s_N\le t} (2\|V\|)^N\, \mathrm{d}s_1 \cdots \mathrm{d}s_N \le \frac{(2\|V\|t)^N}{N!},$$

and conclude that the Dyson expansion

$$\gamma_V^t = \mathrm{id} + \sum_{n=1}^{\infty} \int_{0\le s_1\le\cdots\le s_n\le t} \mathrm{d}_{\tau^{s_n}(V)} \circ \cdots \circ \mathrm{d}_{\tau^{s_1}(V)} \,\mathrm{d}s_1 \cdots \mathrm{d}s_n,$$

converges in norm for all $t \in \mathbb{R}$, and uniformly for t in compact intervals. Using Relation (1), we conclude that

$$\tau_V^t = \tau^t + \sum_{n=1}^{\infty} \int_{0\le s_1\le\cdots\le s_n\le t} \mathrm{d}_{\tau^{s_n}(V)} \circ \cdots \circ \mathrm{d}_{\tau^{s_1}(V)} \circ \tau^t \,\mathrm{d}s_1 \cdots \mathrm{d}s_n,$$

which we can rewrite as

$$\tau_V^t(A) = \sum_{n=0}^{\infty} (\mathrm{i}t)^n \int_{0\le s_1\le\cdots\le s_n\le 1} [\tau^{ts_n}(V), [\cdots, [\tau^{ts_1}(V), \tau^t(A)]\cdots]] \,\mathrm{d}s_1 \cdots \mathrm{d}s_n.$$

Finally, we note that since $\tau^z(V)$, $\tau^z(A)$ and $\tau_V^z(A)$ are entire analytic functions of z and $\|\tau^z\| \le \mathrm{e}^{2|\mathrm{Im}\, z|\,\|H\|}$, the above expression provides an expansion of $\tau_V^z(A)$ which converges uniformly for z in compact subsets of $\mathbb{C}$.

Similar conclusions hold for the interaction picture propagator

$$\mathrm{E}_V(t) = \mathrm{e}^{\mathrm{i}t(H+V)}\mathrm{e}^{-\mathrm{i}tH}.$$

It satisfies:

(1') $\mathrm{e}^{\mathrm{i}t(H+V)} = \mathrm{E}_V(t)\mathrm{e}^{\mathrm{i}tH}$ and $\tau_V^t(A) = \mathrm{E}_V(t)\tau^t(A)\mathrm{E}_V(t)^{-1}$.

(2') $\mathrm{E}_V(t)^{-1} = \mathrm{E}_V(t)^* = \tau^t(\mathrm{E}_V(-t))$.

(3') $\mathrm{E}_V(t+s) = \mathrm{E}_V(s)\tau^s(\mathrm{E}_V(t))$.

(4') $\mathrm{E}_V(0) = \mathbb{1}$ and $\partial_t \mathrm{E}_V(t) = \mathrm{i}\mathrm{E}_V(t)\tau^t(V)$.

Integrating relation (4') yields, after iteration,

$$\mathrm{E}_V(t) = \sum_{n=0}^{\infty} (\mathrm{i}t)^n \int_{0\le s_1\le\cdots\le s_n\le 1} \tau^{ts_n}(V)\cdots\tau^{ts_1}(V) \,\mathrm{d}s_1 \cdots \mathrm{d}s_n.$$

This expansion is uniformly convergent for t in compact subsets of $\mathbb{C}$. In particular,

$$\mathrm{E}_V(\mathrm{i}\beta) = \sum_{n=0}^{\infty} (-\beta)^n \int_{0\le s_1\le\cdots\le s_n\le 1} \tau^{\mathrm{i}\beta s_n}(V)\cdots\tau^{\mathrm{i}\beta s_1}(V) \,\mathrm{d}s_1 \cdots \mathrm{d}s_n. \tag{2.28}$$

Using Relation (1') with $t = \mathrm{i}\beta$ we can express the perturbed KMS-state

$$\rho_{\beta V} = \frac{\mathrm{e}^{-\beta(H+V)}}{\mathrm{tr}(\mathrm{e}^{-\beta(H+V)})},$$

in terms of the unperturbed one $\rho_\beta = \mathrm{e}^{-\beta H}/\mathrm{tr}(\mathrm{e}^{-\beta H})$ as

$$\rho_{\beta V}(A) = \frac{\rho_\beta(A\,\mathrm{E}_V(\mathrm{i}\beta))}{\rho_\beta(\mathrm{E}_V(\mathrm{i}\beta))}. \tag{2.29}$$

Using this last formula one can compute the perturbative expansion of $\rho_{\beta V}(A)$ w.r.t. V. To control this expansion, we need the following estimate.

Proposition 2.22 *The bound*

$$|\rho_\beta(\mathrm{E}_{\alpha V}(\mathrm{i}\beta)) - 1| \le \mathrm{e}^{|\alpha\beta|\|V\|} - 1, \tag{2.30}$$

holds for any $\beta \in \mathbb{R}$*,* $V \in \mathcal{O}_{\mathrm{self}}$ *and* $\alpha \in \mathbb{C}$*.*

Proof. Using Duhamel formula

$$\frac{\mathrm{d}}{\mathrm{d}s}\,\mathrm{e}^{-\beta(H+s\alpha V)} = -\alpha\int_0^\beta \mathrm{e}^{-(\beta-u)(H+s\alpha V)}V\mathrm{e}^{-u(H+s\alpha V)}\,\mathrm{d}u,$$

we can write

$$\rho_\beta(\mathrm{E}_{\alpha V}(\mathrm{i}\beta)-\mathbb{1}) = \int_0^1 \frac{\mathrm{d}}{\mathrm{d}s}\rho_\beta(\mathrm{E}_{s\alpha V}(\mathrm{i}\beta))\,\mathrm{d}s = -\alpha\beta\int_0^1 f_\beta(s)\,\mathrm{d}s, \tag{2.31}$$

where

$$f_\beta(s) = \frac{\mathrm{tr}(V\mathrm{e}^{-\beta(H+s\alpha V)})}{\mathrm{tr}(\mathrm{e}^{-\beta H})}.$$

Starting with the simple bound

$$|f_\beta(s)| \le \|V\|\frac{\|\mathrm{e}^{-\beta(H+s\alpha V)}\|_1}{\mathrm{tr}(\mathrm{e}^{-\beta H})},$$

and setting $\alpha = a + ib$ with $a, b \in \mathbb{R}$, we estimate the numerator on the right hand side by the Hölder inequality (Part 2 of Exercise 2.6) applied to the Lie product formula,

$$\begin{aligned}\|\mathrm{e}^{-\beta(H+saV+\mathrm{i}sbV)}\|_1 &= \lim_{n\to\infty}\|(\mathrm{e}^{-\beta(H+saV)/n}\mathrm{e}^{-\mathrm{i}\beta sbV/n})^n\|_1\\ &\le \limsup_{n\to\infty}\|\mathrm{e}^{-\beta(H+saV)/n}\|_n^n\,\|\mathrm{e}^{-\mathrm{i}\beta sbV/n}\|_\infty^n = \mathrm{tr}(\mathrm{e}^{-\beta(H+saV)}).\end{aligned}$$

For $s \in [0,1]$, the Golden-Thompson inequality further leads to

$$\frac{\mathrm{tr}(\mathrm{e}^{-\beta(H+saV)})}{\mathrm{tr}(\mathrm{e}^{-\beta H})} \le \frac{\mathrm{tr}(\mathrm{e}^{-\beta H}\mathrm{e}^{-\beta saV})}{\mathrm{tr}(\mathrm{e}^{-\beta H})} = \rho_\beta(\mathrm{e}^{-\beta saV}) \le \mathrm{e}^{s|\beta\alpha|\,\|V\|},$$

so that, finally,

$$|f_\beta(s)| \le \|V\|\,\mathrm{e}^{s|\beta\alpha|\,\|V\|}.$$

Using Equ. (2.31), we derive

$$|\rho_\beta(\mathrm{E}_V(\mathrm{i}\beta))-1| \le |\alpha\beta|\|V\|\int_0^1 \mathrm{e}^{s|\alpha\beta|\|V\|}\mathrm{d}s = \mathrm{e}^{|\alpha\beta|\|V\|}-1.$$

□

Replacing V with αV and using the expansion (2.28), we can write

$$\rho_\beta(A\,\mathrm{E}_{\alpha V}(\mathrm{i}\beta)) = \sum_{n=0}^\infty \alpha^n c_n(A),$$

where $c_0(A) = \rho_\beta(A)$ and

$$c_n(A) = (-\beta)^n\int_{0\le s_1\le\cdots\le s_n\le 1}\rho_\beta(A\tau^{\mathrm{i}\beta s_n}(V)\cdots\tau^{\mathrm{i}\beta s_1}(V))\,\mathrm{d}s_1\cdots\mathrm{d}s_n.$$

It follows from the estimate (2.30) that the entire function $\mathbb{C}\ni\alpha\mapsto\rho_\beta(\mathrm{E}_{\alpha V}(\mathrm{i}\beta))$ has no zero in the disk

$$|\alpha| < \frac{\log 2}{|\beta|\|V\|}.$$

Hence, Equ. (2.29) shows that the function $\mathbb{C}\ni\alpha\mapsto\rho_{\beta(\alpha V)}(A)$ is analytic on this disk. Writing

$$\rho_{\beta(\alpha V)}(A) = \sum_{n=0}^\infty \alpha^n b_n(A),$$

Relation (2.29) yields

$$\sum_{n=0}^{\infty} \alpha^n c_n(A) = \left(\sum_{n=0}^{\infty} \alpha^n b_n(A)\right)\left(\sum_{n=0}^{\infty} \alpha^n c_n(\mathbb{1})\right),$$

and we conclude that for all n,

$$c_n(A) = \sum_{j=0}^{n} b_j(A) c_{n-j}(\mathbb{1}).$$

Thus, with coefficients $b_n(A)$ given by the recursive formula

$$b_0(A) = c_0(A) = \rho_\beta(A), \qquad b_n(A) = c_n(A) - \sum_{j=0}^{n-1} b_j(A) c_{n-j}(\mathbb{1}),$$

we can write

$$\rho_{\beta V}(A) = \sum_{n=0}^{\infty} b_n(A), \tag{2.32}$$

provided $|\beta|\, \|V\| < \log 2$.

Exercise 2.13. Show that the expression

$$\langle A|B\rangle_\beta = \int_0^1 \rho_\beta(A^* \tau^{\mathrm{i}\beta s}(B))\, \mathrm{d}s = \frac{1}{\beta}\int_0^\beta \rho_\beta(A^* \tau^{\mathrm{i}s}(B))\, \mathrm{d}s, \tag{2.33}$$

defines an inner product on $\mathcal{O}$. It is called Kubo-Mari or Bogoliubov scalar product, Duhamel two point function or canonical correlation.

Exercise 2.14. Show that the first coefficients $b_1(A)$ and $b_2(A)$ can be written as

$$b_1(A) = -\beta\langle V|\widehat{A}\rangle_\beta,$$

$$b_2(A) = \beta^2 \int_0^1 \mathrm{d}s \int_0^s \mathrm{d}s' \left[\rho_\beta(\widehat{A}\tau^{\mathrm{i}\beta s}(V)\tau^{\mathrm{i}\beta s'}(V)) - \rho_\beta(\widehat{A}\tau^{\mathrm{i}\beta s}(V))\rho_\beta(V) - \rho_\beta(\widehat{A}\tau^{\mathrm{i}\beta s'}(V))\rho_\beta(V)\right],$$

where $\widehat{A} = A - \rho_\beta(A)$.

2.11 The standard representations of $\mathcal{O}$

In this and the following sections we introduce the so called modular structure associated with the $*$-algebra $\mathcal{O} = \mathcal{O}_\mathcal{K}$. Historically, the structure was unveiled in the work of Araki and Woods [AWo] on the equilibrium states of a free Bose gas and linked to the KMS condition by Haag, Hugenholtz and Winnink [HHW]. After the celebrated works of Tomita [To] and Takesaki [Ta], modular theory became an essential tool in the study of operator algebras.

For us, the main purpose of modular theory is to provide a framework which will allow us to describe a quantum system in a way that is robust enough to survive the thermodynamic limit. While familiar objects like Hamiltonians or density matrices will lose their meaning in this limit, the notions that we are about to introduce: standard representation, modular groups and operators, Connes cocycles, relative Hamiltonians, Liouvilleans, etc, will continue to make sense in the context of extended quantum systems. As a *rule of thumb*, a result that holds for finite quantum systems and can be formulated in terms of robust objects of modular theory will remain valid for extended systems.

Let $\mathcal{H}$ be an auxiliary Hilbert space and denote by $\mathcal{L}(\mathcal{H})$ the $*$-algebra of all linear operators on $\mathcal{H}$. A subset $\mathcal{A} \subset \mathcal{L}(\mathcal{H})$ is called *self-adjoint*, written $\mathcal{A}^* = \mathcal{A}$, if $A^* \in \mathcal{A}$ for all $A \in \mathcal{A}$. A self-adjoint subset $\mathcal{A} \subset \mathcal{L}(\mathcal{H})$ is a *$*$-subalgebra* if it is a vector subspace such that $AB \in \mathcal{A}$ for all $A, B \in \mathcal{A}$. A *representation* of $\mathcal{O}$ in $\mathcal{H}$ is a linear map $\phi : \mathcal{O} \to \mathcal{L}(\mathcal{H})$ such that $\phi(AB) = \phi(A)\phi(B)$ and $\phi(A^*) = \phi(A)^*$ for all $A, B \in \mathcal{O}$. A representation is *faithful* if the map ϕ is injective, *i.e.*, if $\mathrm{Ker}\,\phi = \{0\}$. A faithful representation of $\mathcal{O}$ in $\mathcal{H}$ is therefore an isomorphism between $\mathcal{O}$ and the $*$-subalgebra $\phi(\mathcal{O}) \subset \mathcal{L}(\mathcal{H})$. A vector $\psi \in \mathcal{H}$ is called *cyclic* for the representation ϕ if $\mathcal{H} = \phi(\mathcal{O})\psi$. It is called *separating* if $\phi(A)\psi = 0$ implies that $A = 0$. Two representations $\phi_1 : \mathcal{O} \to \mathcal{L}(\mathcal{H}_1)$ and $\phi_2 : \mathcal{O} \to \mathcal{L}(\mathcal{H}_2)$ are called *equivalent* if there exists a unitary $U : \mathcal{H}_1 \to \mathcal{H}_2$ such that $U\phi_1(A) = \phi_2(A)U$ for all $A \in \mathcal{O}$.

Let $\mathcal{A}$ and $\mathcal{B}$ be subsets of $\mathcal{L}(\mathcal{H})$. $\mathcal{A} \vee \mathcal{B}$ denotes the smallest $*$-subalgebra of $\mathcal{L}(\mathcal{H})$ containing $\mathcal{A}$ and $\mathcal{B}$. $\mathcal{A}'$ denotes the *commutant* of $\mathcal{A}$, *i.e.*, the set of all elements of $\mathcal{L}(\mathcal{H})$ which commute with all elements of $\mathcal{A}$. If $\mathcal{A}$ is self-adjoint, then $\mathcal{A}'$ is a $*$-subalgebra.

A *cone* in the Hilbert space $\mathcal{H}$ is a subset $\mathcal{C} \subset \mathcal{H}$ such that $\lambda\psi \in \mathcal{C}$ for all $\lambda \geq 0$ and all $\psi \in \mathcal{C}$. If $\mathcal{M} \subset \mathcal{H}$, then

$$\widehat{\mathcal{M}} = \{\phi \in \mathcal{H} \,|\, \langle\psi|\phi\rangle \geq 0 \text{ for all } \psi \in \mathcal{M}\},$$

is a cone. A cone $\mathcal{C} \subset \mathcal{H}$ is called *self-dual* if $\widehat{\mathcal{C}} = \mathcal{C}$. We have already noticed that $\mathcal{O}$, viewed as a complex vector space, becomes a Hilbert space when equipped with the inner product

$$(\xi|\eta) = \mathrm{tr}\,(\xi^*\eta).$$

In the sequel, in order to distinguish this Hilbert space from the $*$-algebra $\mathcal{O}$ we shall denote the former by $\mathcal{H}_\mathcal{O}$. Thus, $\mathcal{O}$ and $\mathcal{H}_\mathcal{O}$ are the same set, but carry distinct algebraic structures. We will use lower case greeks $\xi, \eta, \ldots$ to denote elements of the Hilbert space $\mathcal{H}_\mathcal{O}$ and upper case romans $A, B, \ldots$ to denote elements of the $*$-algebra $\mathcal{O}$.

Remark. Let $\psi \mapsto \overline{\psi}$ denote an arbitrary complex conjugation (*i.e.*, an anti-unitary involution) on the Hilbert space $\mathcal{K}$. One easily checks that the map $|\psi\rangle\langle\varphi| \mapsto \psi \otimes \overline{\varphi}$ extends to a unitary operator from $\mathcal{H}_{\mathcal{O}_\mathcal{K}}$ to $\mathcal{K} \otimes \mathcal{K}$. Thus, the Hilbert space $\mathcal{H}_{\mathcal{O}_\mathcal{K}}$ is isomorphic to $\mathcal{K} \otimes \mathcal{K}$.

To any $A \in \mathcal{O}$ we can associate two elements $L(A)$ and $R(A)$ of $\mathcal{L}(\mathcal{H}_\mathcal{O})$ by

$$L(A) : \xi \mapsto A\xi, \qquad R(A) : \xi \mapsto \xi A^*.$$

The map $\mathcal{O} \ni A \mapsto L(A) \in \mathcal{L}(\mathcal{H}_\mathcal{O})$ is clearly linear and satisfies $L(AB) = L(A)L(B)$. Moreover, for all $\xi, \eta \in \mathcal{H}_\mathcal{O}$ one has

$$(\xi|L(A)\eta) = \mathrm{tr}\,(\xi^* A\eta) = \mathrm{tr}\,((A^*\xi)^*\eta) = (L(A^*)\xi|\eta),$$

so that $L(A^*) = L(A)^*$. In short, L is a representation of the $*$-algebra $\mathcal{O}$ on the Hilbert space $\mathcal{H}_\mathcal{O}$. In the same way one checks that $R : \mathcal{O} \to \mathcal{L}(\mathcal{O})$ is antilinear and satisfies $R(AB) = R(A)R(B)$ as well as $R(A^*) = R(A)^*$.

Proposition 2.23 (1) *The maps L and R are isometric and hence injective.*

(2) $L(\mathcal{O}) = \{L(A) \,|\, A \in \mathcal{O}\}$ *and* $R(\mathcal{O}) = \{R(A) \,|\, A \in \mathcal{O}\}$ *are $*$-subalgebras of $\mathcal{L}(\mathcal{H}_\mathcal{O})$ isomorphic to $\mathcal{O}$.*

(3) $L(\mathcal{O}) \cap R(\mathcal{O}) = \mathbb{C}\mathbb{1}$.

(4) $L(\mathcal{O}) \vee R(\mathcal{O}) = \mathcal{L}(\mathcal{H}_\mathcal{O})$.

(5) $L(\mathcal{O})' = R(\mathcal{O})$.

(6) $R(\mathcal{O})' = L(\mathcal{O})$.

Proof. (1)–(2) For $A \in \mathcal{O}$, one has

$$\begin{aligned}\|L(A)\|^2 = \sup_{\|\xi\|=1} \|L(A)\xi\|^2 &= \sup_{\mathrm{tr}\,(\xi^*\xi)=1} \mathrm{tr}((A\xi)^*(A\xi)) \\ &= \sup_{\mathrm{tr}\,(\xi\xi^*)=1} \mathrm{tr}\,((\xi\xi^*)(A^*A)) \leq \|A^*A\| = \|A\|^2.\end{aligned}$$

On the other hand, if ψ is a normalized eigenvector of A^*A to its maximal eigenvalue $\|A^*A\|$ and $\xi = |\psi\rangle\langle\psi|$, then $\|\xi\| = 1$ and

$$\|L(A)\xi\| = \|A\xi\| = \langle\psi|A^*A\psi\rangle = \|A^*A\|,$$

so that we can conclude that $\|L(A)\| = \|A\|$. L is a linear map and $\mathrm{Ker}\, L = \{0\}$. Thus, L is injective and is an $*$-isomorphism between $\mathcal{O}$ and its image $L(\mathcal{O})$. The same argument holds for R.

(3) If $T \in L(\mathcal{O}) \cap R(\mathcal{O})$, then there exists $A, B \in \mathcal{O}$ such that $A\xi = \xi B$ for all $\xi \in \mathcal{H}_\mathcal{O}$. Setting $\xi = \mathbb{1}$ we deduce $A = B$. It follows that $[A, \xi] = 0$ for all $\xi \in \mathcal{O}$ and hence A must be a multiple of the identity.

(4) Let $T \in \mathcal{L}(\mathcal{H}_\mathcal{O})$ and denote by $\{E_{ij}\}$ the orthogonal basis of $\mathcal{H}_\mathcal{O}$ associated to some orthogonal basis $\{e_i\}$ of $\mathcal{K}$. Setting $T_{ij,kl} = (E_{ij}|TE_{kl})$, one has

$$TE_{kl} = \sum_{i,j,k,l} T_{ij,kl}E_{ij}.$$

Since $E_{ij} = |e_i\rangle\langle e_j| = |e_i\rangle\langle e_k|e_k\rangle\langle e_l|e_l\rangle\langle e_j| = E_{ik}E_{kl}E_{lj} = L(E_{ik})R(E_{jl})E_{kl}$, we can write

$$T = \sum_{i,j,k,l} T_{ij,kl}L(E_{ik})R(E_{jl}),$$

which shows that the subalgebras $L(\mathcal{O})$ and $R(\mathcal{O})$ generate all of $\mathcal{L}(\mathcal{H}_\mathcal{O})$.

(5)–(6) For any $A, B \in \mathcal{O}$ and $\xi \in \mathcal{H}_\mathcal{O}$ on has $L(A)R(B)\xi = A\xi B = R(B)L(A)\xi$ which shows that $R(\mathcal{O}) \subset L(\mathcal{O})'$ and $L(\mathcal{O}) \subset R(\mathcal{O})'$. Let $T \in L(\mathcal{O})'$ so that $[T, L(A)] = 0$ for all $A \in \mathcal{O}$. Set $B = T\mathbb{1}$, then

$$T\xi = TL(\xi)\mathbb{1} = L(\xi)T\mathbb{1} = L(\xi)B = \xi B = R(B^*)\xi,$$

for all $\xi \in \mathcal{H}_\mathcal{O}$. Hence, $T = R(B^*)$ and we conclude that $L(\mathcal{O})' \subset R(\mathcal{O})$. A similar argument shows that $R(\mathcal{O})' \subset L(\mathcal{O})$. □

Proposition 2.24 (1) *The map $J : \xi \mapsto \xi^*$ is a anti-unitary involution of the Hilbert space $\mathcal{H}_\mathcal{O}$.*

(2) *$JL(\mathcal{O})J^* = L(\mathcal{O})'$.*

(3) *$\mathcal{H}_\mathcal{O}^+ = \mathcal{O}_+$ is a self-dual cone of the Hilbert space $\mathcal{H}_\mathcal{O}$.*

(4) *$J\xi = \xi$ for all $\xi \in \mathcal{H}_\mathcal{O}^+$.*

(5) *$JXJ = X^*$ for all $X \in L(\mathcal{O}) \cap L(\mathcal{O})'$.*

(6) *$L(A)JL(A)\mathcal{H}_\mathcal{O}^+ \subset \mathcal{H}_\mathcal{O}^+$ for all $A \in \mathcal{O}$.*

Proof. (1) J is clearly antilinear and involutive. Since

$$(\xi|J\eta) = \mathrm{tr}\,(\xi^*\eta^*) = \overline{\mathrm{tr}\,(\xi\eta)} = \overline{(J\xi|\eta)},$$

J is also antiunitary.

(2) For all $A \in \mathcal{O}$ and $\xi \in \mathcal{H}_\mathcal{O}$ one has $JL(A)J\xi = (A\xi^*)^* = \xi A^* = R(A)\xi$ which implies $JL(A)J = R(A)$.

(3) The fact that $\mathcal{H}_\mathcal{O}^+ = \mathcal{O}_+$ is a cone is obvious. It is also clear that if $\xi, \eta \in \mathcal{H}_\mathcal{O}^+$ then $(\xi|\eta) \geq 0$ so that $\mathcal{H}_\mathcal{O}^+ \subset \widehat{\mathcal{H}_\mathcal{O}^+}$. To prove the reverse inclusion, let $\xi \in \widehat{\mathcal{H}_\mathcal{O}^+}$. Then $(\eta|\xi) \geq 0$ for all $\eta \in \mathcal{H}_\mathcal{O}^+$. In particular, with $\eta = |\psi\rangle\langle\psi|$, we get $(\eta|\xi) = \langle\psi|\xi\psi\rangle \geq 0$ from which we conclude that $\xi \in \mathcal{H}_\mathcal{O}^+$.

(4)–(5) are obvious and (6) follows from the fact that

$$L(A)JL(A)\xi = A\xi A^* \geq 0,$$

for all $\xi \geq 0$. □

The faithful representation $L : \mathcal{O} \to \mathcal{L}(\mathcal{H}_\mathcal{O})$ is called *standard representation* of $\mathcal{O}$, J is called the *modular conjugation* and the cone $\mathcal{H}_\mathcal{O}^+$ is called the *natural cone*. The map

$$\mathfrak{S} \ni \nu \mapsto \xi_\nu = \nu^{1/2} \in \mathcal{H}_\mathcal{O}^+,$$

is clearly a bijection between the set of states and the unit vectors in $\mathcal{H}_\mathcal{O}^+$. For all $A \in \mathcal{O}$, one has

$$(\xi_\nu | L(A)\xi_\nu) = \mathrm{tr}\,(\nu^{1/2} A \nu^{1/2}) = \nu(A).$$

ξ_ν is called the*vector representative* of the state ν in the standard representation. Note that a unit vector $\xi \in \mathcal{H}_\mathcal{O}^+$ is cyclic for the standard representation iff $\xi > 0$, *i.e.*, iff the corresponding state is faithful and in this case, for any $\eta \in \mathcal{H}_\mathcal{O}$, one has $\eta = L(A)\xi$ with $A = \eta\xi^{-1}$. Since $L(A)\xi = 0$ iff $\mathrm{Ran}\,\xi \subset \mathrm{Ker}\,A$, ξ is a separating vector iff $\xi > 0$.

Exercise 2.15. *(The GNS representation)* Let ν be a state and define $\mathcal{H}_\nu$ to be the vector space of all linear maps $\xi : \mathrm{Ran}\,\nu \to \mathcal{K}$, equipped with the inner product

$$(\xi|\eta)_\nu = \mathrm{tr}_{\mathrm{Ran}\,\nu}(\nu\xi^*\eta) = \mathrm{tr}_\mathcal{K}(\eta\nu\xi^*).$$

1. Show that $\mathcal{H}_\nu$ is a Hilbert space and that $\pi_\nu : \mathcal{O} \to \mathcal{L}(\mathcal{H}_\nu)$ defined by $\pi_\nu(A)\xi = A\xi$ is a representation of $\mathcal{O}$ in $\mathcal{H}_\nu$.

2. Denote by $\eta_\nu : \mathrm{Ran}\,\nu \hookrightarrow \mathcal{K}$ the canonical injection $\eta_\nu\psi = \psi$. Show that η_ν is a cyclic vector for the representation π_ν and that

$$\nu(A) = (\eta_\nu|\pi_\nu(A)\eta_\nu)_\nu,$$

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

3. A cyclic representation of $\mathcal{O}$ associated to a state ν is a representation π of $\mathcal{O}$ in a Hilbert space $\mathcal{H}$ such that:
(i) there exists a vector $\psi \in \mathcal{H}$ which is cyclic for π.
(ii) $\nu(A) = (\psi|\pi(A)\psi)$ for all $A \in \mathcal{O}$.
Show that any cyclic representation of $\mathcal{O}$ associated to the state ν is equivalent to the above representation π_ν.
Hint: show that $\pi(A)\psi \mapsto \pi_\nu(A)\eta_\nu$ defines a unitary map from $\mathcal{H}$ to $\mathcal{H}_\nu$.

Thus, up to equivalence, there is only one cyclic representation of $\mathcal{O}$ associated to a state ν. This representation is called the Gelfand-Naimark-Segal (GNS) representation of $\mathcal{O}$ induced by ν.

4. Show that the map $U : \mathcal{H}_\nu \ni \xi \mapsto \xi\nu^{1/2} \in \mathcal{H}_\mathcal{O}$ is a partial isometry which intertwine the GNS representation and the standard representation

$$U\pi_\nu(A)\xi = L(A)U\xi.$$

Show that if ν is faithful, then U is unitary so that these two representations are equivalent.

5. Let $\psi \mapsto \overline{\psi}$ be a complex conjugation on $\mathcal{K}$. We have already remarked that the map $U(|\psi\rangle\langle\varphi|) = \psi \otimes \overline{\varphi}$ extends to a unitary operator from $\mathcal{H}_{\mathcal{O}_\mathcal{K}}$ to $\mathcal{K} \otimes \mathcal{K}$. Show that under this unitary the standard representation transforms as follows.
(i) $UR(A)U^{-1} = A \otimes \mathbb{1}$ and $UL(A)U^{-1} = \mathbb{1} \otimes A$.
(ii) $UJU^{-1}\psi \otimes \phi = \overline{\phi} \otimes \overline{\psi}$.
(iii) $U\xi_\nu = \sum_j \lambda_j^{1/2}\psi_j \otimes \overline{\psi_j}/\mathrm{tr}(\nu)^{1/2}$, where λ_j's are the eigenvalues of ν listed with multiplicities and ψ_j's are the corresponding eigenfuntions.

Let τ^t be a dynamics on $\mathcal{O}$ generated by the Hamiltonian H. Since

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

the self-adjoint operator $L(H)$ seems to play the role of the Hamiltonian in the standard representation. If ν is a state and $\xi_\nu \in \mathcal{H}_\mathcal{O}^+$ its vector representative, then

$$\nu(\tau^t(A)) = (\xi_\nu|L(\tau^t(A))\xi_\nu) = (\mathrm{e}^{-\mathrm{i}tL(H)}\xi_\nu|L(A)\mathrm{e}^{-\mathrm{i}tL(H)}\xi_\nu).$$

The state vector thus evolves according to $\mathrm{e}^{-\mathrm{i}tL(H)}\xi_\nu = \mathrm{e}^{-\mathrm{i}tH}\xi_\nu$. Note that this vector is generally not an element of the natural cone. Indeed, since $\nu_t = \mathrm{e}^{-\mathrm{i}tH}\nu\mathrm{e}^{\mathrm{i}tH}$, its vector representative is given by

$$\xi_{\nu_t} = \nu_t^{1/2} = \mathrm{e}^{-\mathrm{i}tH}\nu^{1/2}\mathrm{e}^{\mathrm{i}tH} = L(\mathrm{e}^{-\mathrm{i}tH})R(\mathrm{e}^{-\mathrm{i}tH})\xi_\nu,$$

which is generally distinct from $\mathrm{e}^{-\mathrm{i}tH}\xi_\nu$. On the other hand, by Part (5) of Proposition 2.23, one has

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

so that the unitary group (recall that R is anti-linear)

$$L(\mathrm{e}^{\mathrm{i}tH})R(\mathrm{e}^{\mathrm{i}tH}) = \mathrm{e}^{\mathrm{i}tL(H)}\mathrm{e}^{-\mathrm{i}tR(H)} = \mathrm{e}^{\mathrm{i}t(L(H)-R(H))},$$

also implements the dynamics τ^t in the standard representation. We call the self-adjoint generator

$$K = L(H) - R(H) = [H, \cdot\,],$$

the *standard Liouvillean* of the dynamics.

Exercise 2.16.

1. Show that if ν is a faithful state on $\mathcal{O}$ then the natural cone of $\mathcal{H}_\mathcal{O}$ can be written as

$$\mathcal{H}_\mathcal{O}^+ = \{L(A)JL(A)\xi_\nu \,|\, A \in \mathcal{O}\}.$$

Conclude that the unitary group $\mathrm{e}^{\mathrm{i}tX}$ preserves the natural cone iff $JX + XJ = 0$.

2. Show that the standard Liouvillean K is the only self-adjoint operator on $\mathcal{H}_\mathcal{O}$ such that, for all $A \in \mathcal{O}$ and $t \in \mathbb{R}$,

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

with the additional property that $\mathrm{e}^{-\mathrm{i}tK}\mathcal{H}_\mathcal{O}^+ \subset \mathcal{H}_\mathcal{O}^+$. (See Proposition 3.4 for a generalization of this result.)

3. Show that the spectrum of K is given by

$$\mathrm{sp}(K) = \{\lambda - \mu \,|\, \lambda, \mu \in \mathrm{sp}(H)\}.$$

Note in particular that if $\dim \mathcal{K} = n$ then 0 is at least n-fold degenerate eigenvalue of K.

2.12 The modular structure of $\mathcal{O}$

2.12.1 Modular group and modular operator

In Section 2.9 we have shown that, given a dynamics τ^t generated by the Hamiltonian H, $\mathrm{e}^{-\beta H}/\mathrm{tr}(\mathrm{e}^{-\beta H})$ is the unique β-KMS state. Modular theory starts with the reverse point of view. Given a faithful state ρ, the dynamics generated by the Hamiltonian $-\beta^{-1}\log\rho$ is the unique dynamics with respect to which ρ is a β-KMS state. This dynamics might not be in itself physical but it will lead to a remarkable mathematical structure with profound physical implications. For historical reasons the reference value of β is taken to be -1. The dynamics

$$\varsigma_\rho^t(A) = \mathrm{e}^{\mathrm{i}t\log\rho}A\mathrm{e}^{-\mathrm{i}t\log\rho},$$

is called the *modular dynamics* or *modular group* of the state ρ. Its generator is given by

$$\delta_\rho(A) = \mathrm{i}[\log\rho, A].$$

The $(\beta = -1)$-KMS condition can be written as

$$\rho(AB) = \rho(\varsigma_\rho^{\mathrm{i}}(B)A).$$

According to the previous section, the standard Liouvillean of the modular dynamics is the self-adjoint operator on $\mathcal{H}_\mathcal{O}$ defined by

$$K_\rho = L(\log\rho) - R(\log\rho),$$

and one has

$$L(\varsigma_\rho^t(A)) = \Delta_\rho^{\mathrm{i}t} L(A)\Delta_\rho^{-\mathrm{i}t},$$

where the positive operator $\Delta_\rho = \mathrm{e}^{K_\rho}$ is called the *modular operator* of the state ρ. Its action on a vector $\xi \in \mathcal{H}_\mathcal{O}$ is described by

$$\Delta_\rho\xi = \mathrm{e}^{L(\log\rho)-R(\log\rho)}\xi = L(\rho)R(\rho^{-1})\xi = \rho\xi\rho^{-1}.$$

More generally, for $z \in \mathbb{C}$,

$$\Delta_\rho^z\xi = \mathrm{e}^{z(L(\log\rho)-R(\log\rho))}\xi = L(\rho^z)R(\rho^{-z})\xi = \rho^z\xi\rho^{-z},$$

and in particular

$$J\Delta_\rho^{1/2}A\xi_\rho = (\Delta_\rho^{1/2}A\xi_\rho)^* = (\rho^{1/2}(A\rho^{1/2})\rho^{-1/2})^* = A^*\xi_\rho, \tag{2.34}$$

for any $A \in \mathcal{O}$. The last relation completely characterizes the modular conjugation J and the square root of the modular operator $\Delta_\rho^{1/2}$ as the anti-unitary and positive factors of the (unique) polar decomposition of the anti-linear map $A\xi_\rho \mapsto A^*\xi_\rho$.

Generalizing the Kubo-Mari inner product (2.33), we shall call

$$\langle A|B\rangle_\rho = \int_0^1 \rho(A^*\varsigma_\rho^{-\mathrm{i}u}(B))\mathrm{d}u,$$

the standard correlation of $A, B \in \mathcal{O}$ w.r.t. ρ

2.12.2 Connes cocycle and relative modular operator

The modular groups of two faithful states ρ and ν are related by their *Connes' cocycle*, the family of unitary elements of $\mathcal{O}$ defined by

$$[D\rho : D\nu]^t = \rho^{\mathrm{i}t}\nu^{-\mathrm{i}t} = \mathrm{e}^{\mathrm{i}t\log\rho}\mathrm{e}^{-\mathrm{i}t\log\nu}.$$

Indeed, one has

$$[D\rho : D_\nu]^t\varsigma_\nu^t(A)[D\nu : D\rho]^t = \varsigma_\rho^t(A), \tag{2.35}$$

for all $A \in \mathcal{O}$ and any $t \in \mathbb{R}$. The Connes cocycles have the following immediate properties:

(1) $[D\rho : D\nu]^t[D\nu : D\omega]^t = [D\rho : D\omega]^t$.

(2) $([D\rho : D\nu]^t)^{-1} = [D\nu : D\rho]^t$.

(3) $[D\rho : D\nu]^t\varsigma_\nu^t([D\rho : D_\nu]^s) = [D\rho : D\nu]^{t+s}$.

They are obviously defined for any $t \in \mathbb{C}$ and (2.35) as well as (1)–(3) remain valid. The operator

$$[D\rho : D\nu]^{-\mathrm{i}} = \rho\nu^{-1},$$

satisfies

$$\nu(A[D\rho : D\nu]^{-\mathrm{i}}) = \rho(A),$$

and is the non-commutative Radon-Nikodym derivative of ρ w.r.t. ν. The Rényi relative entropy can be expressed in terms of the Connes cocycle as

$$S_\alpha(\rho|\nu) = \log \nu([D\rho : D\nu]^{-\mathrm{i}\alpha}).$$

The *relative modular dynamics* of two faithful states ρ and ν is defined by

$$\varsigma^t_{\rho|\nu}(A) = \rho^{\mathrm{i}t} A \nu^{-\mathrm{i}t} = \mathrm{e}^{\mathrm{i}t\log\rho} A \mathrm{e}^{-\mathrm{i}t\log\nu}.$$

It is related to the modular dynamics of ρ and ν by the Connes cocycles,

$$\varsigma^t_{\rho|\nu}(A) = [D\rho : D\nu]^t \varsigma^t_\nu(A) = \varsigma^t_\rho(A)[D\rho : D\nu]^t.$$

Its standard Liouvillean is given by

$$K_{\rho|\nu} = L(\log\rho) - R(\log\nu),$$

and the corresponding *relative modular operator* $\Delta_{\rho|\nu} = \mathrm{e}^{K_{\rho|\nu}}$ is a positive operator acting in $\mathcal{H}_\mathcal{O}$ as

$$\Delta_{\rho|\nu}\xi = L(\rho)R(\nu^{-1})\xi = \rho\xi\nu^{-1}.$$

More generally, for $z \in \mathbb{C}$,

$$\Delta^z_{\rho|\nu}\xi = L(\rho^z)R(\nu^{-z})\xi = \rho^z\xi\nu^{-z},$$

and in particular

$$J\Delta^{1/2}_{\rho|\nu}A\xi_\nu = A^*\xi_\rho,$$

for any $A \in \mathcal{O}$. Again, this relation characterizes completely $\Delta^{1/2}_{\rho|\nu}$ as the positive factor of the polar decomposition of the anti-linear map $A\xi_\nu \mapsto A^*\xi_\rho$.

In the standard representation of $\mathcal{O}$ the relative modular dynamics is described by

$$L(\varsigma^t_{\rho|\nu}(A)) = \Delta^{\mathrm{i}t}_{\rho|\nu} L(A) \Delta^{-\mathrm{i}t}_{\rho|\nu},$$

and the relative entropies of ρ w.r.t. ν are given by

$$S_\alpha(\rho|\nu) = \log(\xi_\nu|\Delta^\alpha_{\rho|\nu}\xi_\nu),$$

$$S(\rho|\nu) = (\xi_\rho|\log\Delta_{\nu|\rho}\xi_\rho).$$

The *relative Hamiltonian* of ρ with respect to ν is the self-adjoint element of $\mathcal{O}$ defined by

$$\ell_{\rho|\nu} = \frac{1}{\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}t}[D\rho : D\nu]^t\bigg|_{t=0} = \log\rho - \log\nu. \tag{2.36}$$

Since $\delta_\rho = \delta_\nu + \mathrm{i}[\ell_{\rho|\nu}, \cdot\,]$, $\ell_{\rho|\nu}$ is the perturbation that links the modular dynamics ς^t_ν and ς^t_ρ, *i.e.*, with the notation of Section 2.10,

$$\varsigma^t_{\nu\ell_{\rho|\nu}} = \varsigma^t_\rho.$$

Further immediate properties of the relative Hamiltonian are:

(1) For any $\vartheta \in \mathrm{Aut}(\mathcal{O})$, $\ell_{\rho\circ\vartheta^{-1}|\nu\circ\vartheta^{-1}} = \vartheta(\ell_{\rho|\nu})$.

(2) $S(\rho|\nu) = -\rho(\ell_{\rho|\nu})$.

(3) $\log\Delta_{\rho|\nu} = \log\Delta_\nu + L(\ell_{\rho|\nu})$.

(4) $\log\Delta_\rho = \log\Delta_\nu + L(\ell_{\rho|\nu}) - R(\ell_{\rho|\nu})$.

(5) $\ell_{\rho|\nu} + \ell_{\nu|\omega} = \ell_{\rho|\omega}$.

At this point, the reader could ask about the need for such abstract constructions. To answer these concerns let us make more precise the introductory remarks made at the beginning of Section 2.11. After taking the thermodynamic limit, the Hamiltonian H generating the dynamics and the density matrices defining the states will lose their meaning. So will any expression explicitly involving H or density matrices. What will remain is an infinite dimensional algebra $\mathcal{O}$ describing the quantum observables of the system, a group τ^t of $*$-automorphisms of $\mathcal{O}$ describing quantum dynamics and states, positive, normalized linear functionals on $\mathcal{O}$. The modular group ς_ρ will also survive as a group of $*$-automorphisms of $\mathcal{O}$ and the modular operator Δ_ρ will survive as a positive self-adjoint operator on the Hilbert space carrying the standard representation of $\mathcal{O}$. In the same way, relative modular groups and operators will be available after the thermodynamic limit. These objects will become our handles to manipulate states. Modular theory allows us to recover, in the infinite dimensional case, the algebraic structure of the set of states which is clearly visible in the finite dimensional case. For example, the formula

$$[0,1] \ni \alpha \mapsto S_\alpha(\rho|\nu) = \log \operatorname{tr}(\rho^\alpha \nu^{1-\alpha}),$$

obviously makes sense if ρ and ν are density matrices (even in an infinite dimensional Hilbert space—it follows from Hölder's inequality that the product $\rho^\alpha\nu^{1-\alpha}$ is trace class). Thinking of ρ and ν as linear functionals, it is not clear how to make sense of such a product. The alternative formula

$$S_\alpha(\rho|\nu) = \log(\xi_\nu|\Delta_{\rho|\nu}^\alpha \xi_\nu),$$

provides a more general expression which makes sense even if ρ and ν are not associated to density matrices.

From a purely mathematical point of view, modular theory unravels the structures hidden in the traditional presentations of quantum statistical mechanics. These structures often allow for simpler and mathematically more natural proofs of classical results in quantum statistical mechanics with an additional advantage that the proofs typically extend to the general von Neumann algebra setting. We should illustrate this point on three examples at the end of this section[3].

Exercise 2.17. Let ρ and ν be two faithful states on $\mathcal{O}$.

1. Show that $\Delta_{\rho|\nu}^{-1} = J\Delta_{\nu|\rho}J$.

2. Let τ^t be a dynamics on $\mathcal{O}$. Show that

$$\Delta_{\rho\circ\tau^t|\nu\circ\tau^t} = \mathrm{e}^{-\mathrm{i}tK}\Delta_{\rho|\nu}\mathrm{e}^{\mathrm{i}tK}.$$

where K is the standard Liouvillean of τ^t.

2.12.3 Non-commutative L^p-spaces

For $p \in [1,\infty]$, we denote by $L^p(\mathcal{O})$ the Banach space $\mathcal{O}$ equipped with the p-norm (2.2). It follows from Hölder's inequality (Part (3) of Theorem 2.1) that if $p^{-1}+q^{-1}=1$ then $L^q(\mathcal{O})$ is the dual Banach space to $L^p(\mathcal{O})$ with respect to the duality $(\xi|\eta) = \operatorname{tr}(\xi^*\eta)$. Note in particular that $L^2(\mathcal{O}) = \mathcal{H}_\mathcal{O}$.

While the standard representation will provide a natural extension of $L^2(\mathcal{O})$ in the infinite dimensional setting that arises in the thermodynamic limit, there are no such extensions for the Banach spaces $L^p(\mathcal{O})$ for $p \neq 2$. Infinite dimensional extensions of those spaces which depend on a reference state were introduced by Araki and Masuda [AM]. We describe here their finite dimensional counterparts and relate them to the spaces $L^p(\mathcal{O})$.

Let ω be a faithful state. For $p \in [2,\infty]$ we set

$$\|\xi\|_{\omega,p} = \max_{\nu\in\mathfrak{S}} \|\Delta_{\nu|\omega}^{\frac{1}{2}-\frac{1}{p}}\xi\|_2.$$

[3] A perhaps most famous application of modular theory in mathematics is Alain Connes work on the general classification and structure theorem of type III factors for which he was awarded the Fields medal in 1982.

One easily checks that this is a norm on $\mathcal{O}$ and we denote by $L^p(\mathcal{O},\omega)$ the corresponding Banach space. Note that $\|\xi\|_{\omega,2} = \|\xi\|_2$ so that $L^2(\mathcal{O},\omega) = L^2(\mathcal{O}) = \mathcal{H}_{\mathcal{O}}$ for any faithful state ω. For $p \in [1,2]$, we define $L^p(\mathcal{O},\omega)$ to be the dual Banach space of $L^q(\mathcal{O},\omega)$ for $p^{-1}+q^{-1} = 1$ w.r.t. the duality $(\xi|\eta) = \mathrm{tr}(\xi^*\eta)$.

Theorem 2.25 *For $p \in [1,\infty]$ one has $\|\xi\|_{\omega,p} = \|\xi\omega^{1/p-1/2}\|_p$, i.e., the map*

$$\begin{array}{ccc} L^p(\mathcal{O}) & \to & L^p(\mathcal{O},\omega) \\ \xi & \mapsto & \xi\omega^{1/2-1/p}, \end{array}$$

is a surjective isometry.

Proof. For $p \in [2,\infty]$ one has $r = p/(p-2) \in [1,\infty]$ and if $\nu \in \mathfrak{S}$, then $\nu^{(p-2)/p} \in L^r(\mathcal{O})$ with $\|\nu^{(p-2)/p}\|_r = \|\nu\|_1 = 1$. By definition of the relative modular operator, one further has

$$\|\Delta_{\nu|\omega}^{\frac{p-2}{2p}}\xi\|_2^2 = (\nu^{\frac{p-2}{2p}}\xi\omega^{-\frac{p-2}{2p}}|\nu^{\frac{p-2}{2p}}\xi\omega^{-\frac{p-2}{2p}}) = \mathrm{tr}(\nu^{\frac{p-2}{p}}\xi^*\omega^{-\frac{p-2}{p}}\xi).$$

Noting that $1-1/r = 2/p$, we can write

$$\|\xi\|_{\omega,p}^2 = \max_{\|\eta\|_r=1}\mathrm{tr}(\eta\xi^*\omega^{-\frac{p-2}{p}}\xi) = \|\xi^*\omega^{-\frac{p-2}{p}}\xi\|_{p/2} = \|\omega^{-\frac{p-2}{2p}}\xi\|_p^2.$$

We conclude using the fact that $\|\omega^{-\frac{p-2}{2p}}\xi\|_p = \|\xi\omega^{-\frac{p-2}{2p}}\|_p$ (recall Exercise 2.7). For $p \in [1,2]$ we have, with $q^{-1} = 1-p^{-1} \in [2,\infty]$,

$$\|\xi\|_{\omega,p} = \sup_{\eta\neq 0}\frac{|\mathrm{tr}(\xi^*\eta)|}{\|\eta\|_{\omega,q}} = \sup_{\eta\neq 0}\frac{|\mathrm{tr}(\xi^*\eta)|}{\|\omega^{-\frac{q-2}{2q}}\eta\|_q} = \sup_{\nu\neq 0}\frac{|\mathrm{tr}(\xi^*\omega^{\frac{q-2}{2q}}\nu)|}{\|\nu\|_q} = \|\xi^*\omega^{\frac{q-2}{2q}}\|_p.$$

Since $(q-2)/2q = -(p-2)/2p$, we get

$$\|\xi\|_{\omega,p} = \|\xi^*\omega^{-\frac{p-2}{2p}}\|_p = \|\omega^{-\frac{p-2}{2p}}\xi\|_p = \|\xi\omega^{-\frac{p-2}{2p}}\|_p.$$

□

Exercise 2.18.

1. Denote by $L^p_+(\mathcal{O},\omega)$ the image of the cone $L^p_+(\mathcal{O}) = \{\xi \in L^p(\mathcal{O})\,|\,\xi \geq 0\}$ by the isometry of Theorem 2.25,

$$L^p_+(\mathcal{O},\omega) = \{A\omega^{1/2-1/p}\,|\,A \in \mathcal{O}_+\}.$$

Show that, with $p^{-1}+q^{-1} = 1$, the dual cone to $L^p_+(\mathcal{O},\omega)$ is $L^q_+(\mathcal{O},\omega)$, i.e., that

$$(\eta|\xi) \geq 0$$

for all $\xi \in L^p_+(\mathcal{O},\omega)$ iff $\eta \in L^q_+(\mathcal{O},\omega)$. (Note that $L^2_+(\mathcal{O},\omega) = \mathcal{H}^+_{\mathcal{O}}$, the natural cone.)

2. Show that

$$L^p_+(\mathcal{O},\omega) = \{\lambda\Delta_{\rho|\omega}^{1/p}\xi_\omega\,|\,\rho \in \mathfrak{S}, \lambda > 0\}.$$

We finish this section with several examples of applications of the modular structure. The first one is a proof of Kosaki's variational formula.

Proof of Theorem 2.12. We extend the definition of the relative modular operator to pairs of non-faithful states. As already noticed (just before Exercise 2.15), if $\nu \in \mathfrak{S}$ is not faithful then its vector representative

$\xi_\nu \in \mathcal{H}_\mathcal{O}$ is not cyclic for the standard representation. In fact $\mathcal{O}\xi_\nu = \{A\xi_\nu \,|\, A \in \mathcal{O}\}$ is the proper subspace of $\mathcal{H}_\mathcal{O}$ given by

$$\mathcal{O}\xi_\nu = \{\eta \in \mathcal{H}_\mathcal{O} \,|\, \mathrm{Ker}\,\eta \supset \mathrm{Ker}\,\nu\} = \{\eta \in \mathcal{H}_\mathcal{O} \,|\, \eta(\mathbb{1} - \mathrm{s}(\nu)) = 0\}.$$

Accordingly, one has the orthogonal decomposition

$$\mathcal{H}_\mathcal{O} = \mathcal{O}\xi_\nu \oplus [\mathcal{O}\xi_\nu]^\perp,$$

where

$$[\mathcal{O}\xi_\nu]^\perp = \{\eta \in \mathcal{H}_\mathcal{O} \,|\, \mathrm{Ker}\,\eta \supset \mathrm{Ran}\,\nu\} = \{\eta \in \mathcal{H}_\mathcal{O} \,|\, \eta\mathrm{s}(\nu) = 0\}.$$

For $\rho, \nu \in \mathfrak{S}$, we define the linear operator $\Delta_{\rho|\nu}$ on $\mathcal{H}_\mathcal{O}$ by

$$\Delta_{\rho|\nu} : \xi \mapsto \rho\xi[(\nu|_{\mathrm{Ran}\,\nu})^{-1} \oplus 0|_{\mathrm{Ker}\,\nu}].$$

One easily checks that $\Delta_{\rho|\nu}$ is non-negative, with $\mathrm{Ker}\,\Delta_{\rho|\nu} = \{\xi \in \mathcal{H}_\mathcal{O} \,|\, \mathrm{s}(\rho)\xi\mathrm{s}(\nu) = 0\}$. We note in particular that

$$J\Delta_{\rho|\nu}^{1/2}(L(A)\xi_\nu \oplus \eta) = \mathrm{s}(\nu)L(A)^*\xi_\rho, \tag{2.37}$$

for any $A \in \mathcal{O}$ and $\eta \in [\mathcal{O}\xi_\nu]^\perp$.

Starting from the identity $\mathrm{tr}(\rho^\alpha\nu^{1-\alpha}) = (\xi_\nu|\Delta_{\rho|\nu}^\alpha\xi_\nu)$ and using the integral formula of Exercise 2.2 we write, for $\alpha \in]0,1[$,

$$\mathrm{tr}(\rho^\alpha\nu^{1-\alpha}) = \frac{\sin\pi\alpha}{\pi}\int_0^\infty t^{\alpha-1}\left(\xi_\nu|\Delta_{\rho|\nu}(\Delta_{\rho|\nu}+t)^{-1}\xi_\nu\right)\mathrm{d}t.$$

For $A \in \mathcal{O}$ one has,

$$\rho(|A^*|^2) = \|L(A)^*\xi_\rho\|^2 = \|\mathrm{s}(\nu)L(A)^*\xi_\rho\|^2 + \|QL(A)^*\xi_\rho\|^2,$$

where $Q = \mathbb{1} - \mathrm{s}(\nu)$ is the orthogonal projection on $\mathrm{Ker}\,\nu$. By Equ. (2.37), we obtain

$$\begin{aligned}\rho(|A^*|^2) &= \|J\Delta_{\rho|\nu}^{1/2}L(A)\xi_\nu\|^2 + \|QL(A)^*\xi_\rho\|^2 \\ &= (\xi_\nu|L(A^*)\Delta_{\rho|\nu}L(A)\xi_\nu) + \rho(AQA^*),\end{aligned}$$

from which we deduce

$$\begin{aligned}\frac{1}{t}\rho(|A^*|^2) + \nu(|\mathbb{1} - A|^2) = &\frac{1}{t}(\xi_\nu|L(A^*)\Delta_{\rho|\nu}L(A)\xi_\nu) + (\xi_\nu|L(|\mathbb{1}-A|^2)\xi_\nu) \\ &+ \frac{1}{t}\rho(AQA^*).\end{aligned}$$

With some elementary algebra, this identity leads to

$$\left(\xi_\nu|\Delta_{\rho|\nu}(\Delta_{\rho|\nu}+t)^{-1}\xi_\nu\right) = \frac{1}{t}\rho(|A^*|^2) + \nu(|\mathbb{1}-A|^2) - R_A,$$

where

$$R_A = \frac{1}{t}\rho(AQA^*) + \left\|(\mathbb{1}+\Delta_{\rho|\nu}/t)^{1/2}(L(A) - (\mathbb{1}+\Delta_{\rho|\nu}/t)^{-1})\xi_\nu\right\|^2.$$

Since $R_A \geq 0$, we get

$$\mathrm{tr}(\rho^\alpha\nu^{1-\alpha}) \leq \frac{\sin\pi\alpha}{\pi}\int_0^\infty t^{\alpha-1}\left[\frac{1}{t}\rho(|A(t)^*|^2) + \nu(|\mathbb{1} - A(t)|^2)\right]\mathrm{d}t,$$

for all $A \in C(\mathbb{R}_+, \mathcal{O})$, with equality iff $R_{A(t)} = 0$ for all $t > 0$. Since $\Delta_{\rho|\nu} \geq 0$, this happens iff $(\mathbb{1}+\Delta_{\rho|\nu}/t)L(A(t))\xi_\nu = \xi_\nu$ and $\rho^{1/2}A(t)Q = 0$ for all $t > 0$. The first condition is equivalent to

$$(\mathbb{1} - A(t))\nu = \frac{1}{t}\rho A(t)\mathrm{s}(\nu).$$

An integration by parts shows that the function

$$A_{\rm opt}(t) = t\int_0^\infty \mathrm{e}^{-s\rho}\nu\mathrm{e}^{-st\nu}\mathrm{d}s,$$

satisfies this condition as well as $A_{\rm opt}(t)Q = 0$ so that $R_{A_{\rm opt}(t)} = 0$. This proves Kosaki's variational principle.

Suppose that $B(t) \in C(\mathbb{R}_+, \mathcal{O})$ is such that $A(t) = A_{\rm opt}(t) + B(t)$ is also minimizer. It follows that $B(t)$ satisfies the two conditions

$$tB(t)\nu + \rho B(t)\mathrm{s}(\nu) = 0, \tag{2.38}$$

$$\rho^{1/2}B(t)(\mathbb{1} - \mathrm{s}(\nu)) = 0, \tag{2.39}$$

for all $t > 0$. Let ϕ be an eigenvector of ν to the eigenvalue $p > 0$. Condition (2.38) yields $(\rho + tp)B(t)\phi = 0$ which implies $B(t)\phi = 0$. We conclude that $B(t)\mathrm{s}(\nu) = 0$ and Condition 2.39 further yields $\rho^{1/2}B(t) = 0$. It follows that if either ν or ρ is faithful then $B(t) = 0$. □

As a second application of modular theory, we give an alternative proof of Uhlmann's monotonicity theorem.

Proof of Theorem 2.13. To simplify notation, we shall set $\hat\nu = \Phi^*(\nu)$ and $\hat\rho = \Phi^*(\rho)$. In terms of the extended modular operator, one has

$$S_\alpha(\rho|\nu) = \log\mathrm{tr}(\rho^\alpha\nu^{1-\alpha}) = \log(\xi_\nu|\Delta_{\rho|\nu}^\alpha\xi_\nu),$$

and we have to show that

$$(\xi_{\hat\nu}|\Delta_{\hat\rho|\hat\nu}^\alpha\xi_{\hat\nu}) \geq (\xi_\nu|\Delta_{\rho|\nu}^\alpha\xi_\nu), \tag{2.40}$$

for all $\alpha \in [0,1]$.

Consider the orthogonal decomposition $\mathcal{H}_{\mathcal{O}_\mathcal{K}} = \mathcal{O}_\mathcal{K}\xi_{\hat\nu} \oplus [\mathcal{O}_\mathcal{K}\xi_{\hat\nu}]^\perp$. For $A \in \mathcal{O}_\mathcal{K}$ and $\eta \in [\mathcal{O}_\mathcal{K}\xi_{\hat\nu}]^\perp$, the Schwarz inequality (2.14) yields

$$\begin{aligned}\|\Phi(A)\xi_\nu\|^2 &= (\xi_\nu|\Phi(A)^*\Phi(A)\xi_\nu)\\ &\leq (\xi_\nu|\Phi(A^*A)\xi_\nu) = \nu(\Phi(A^*A)) = \hat\nu(A^*A)\\ &= (\xi_{\hat\nu}|A^*A\xi_{\hat\nu}) = \|A\xi_{\hat\nu}\|^2\\ &\leq \|A\xi_{\hat\nu}\|^2 + \|\eta\|^2 = \|A\xi_{\hat\nu}\oplus\eta\|^2,\end{aligned}$$

which shows that the map $A\xi_{\hat\nu}\oplus\eta \mapsto \Phi(A)\xi_\nu$ is well defined as a linear contraction $T_\nu : \mathcal{H}_{\mathcal{O}_\mathcal{K}} \to \mathcal{H}_{\mathcal{O}_{\mathcal{K}'}}$. The map T_ρ is defined in a similar way.

For $A \in \mathcal{O}_\mathcal{K}$ and $\eta \in [\mathcal{O}_\mathcal{K}\xi_{\hat\nu}]^\perp$, one has

$$\begin{aligned}J\Delta_{\rho|\nu}^{1/2}T_\nu(A\xi_{\hat\nu}\oplus\eta) &= J\Delta_{\rho|\nu}^{1/2}T_\nu(A\mathrm{s}(\hat\nu)\xi_{\hat\nu}\oplus\eta)\\ &= J\Delta_{\rho|\nu}^{1/2}\Phi(A\mathrm{s}(\hat\nu))\xi_\nu\\ &= \mathrm{s}(\nu)\Phi(A\mathrm{s}(\hat\nu))^*\xi_\rho = \mathrm{s}(\nu)\Phi(\mathrm{s}(\hat\nu)A^*)\xi_\rho\\ &= \mathrm{s}(\nu)T_\rho\mathrm{s}(\hat\nu)A^*\xi_{\hat\rho}\\ &= \mathrm{s}(\nu)T_\rho J\Delta_{\hat\rho|\hat\nu}^{1/2}(A\xi_{\hat\nu}+\eta),\end{aligned}$$

from which we conclude that $\Delta_{\rho|\nu}^{1/2}T_\nu = K\Delta_{\hat\rho|\hat\nu}^{1/2}$ where $K = J\mathrm{s}(\nu)T_\rho J$ is a contraction. It follows that for $\varepsilon > 0$

$$\Delta_{\rho|\nu}^{1/2}T_\nu(\Delta_{\hat\rho|\hat\nu}^{1/2}+\varepsilon)^{-1} = K\Delta_{\hat\rho|\hat\nu}^{1/2}(\Delta_{\hat\rho|\hat\nu}^{1/2}+\varepsilon)^{-1},$$

and since $\sup_{x\geq0} x/(x+\varepsilon) = 1$ one has $\|\Delta_{\rho|\nu}^{1/2}T_\nu(\Delta_{\hat\rho|\hat\nu}^{1/2}+\varepsilon)^{-1}\| \leq 1$. The entire analytic function

$$F(z) = (\xi|(\Delta_{\hat\rho|\hat\nu}^{1/2}+\varepsilon)^{-z}T_\nu^*\Delta_{\rho|\nu}^z T_\nu(\Delta_{\hat\rho|\hat\nu}^{1/2}+\varepsilon)^{-z}\xi),$$

thus satisfies

$$|F(z)| \leq \frac{1}{\varepsilon^2}\|\Delta_{\rho|\nu}+\mathbb{1}\|\,\|\xi\|^2, \qquad |F(\mathrm{i}t)| \leq \|\xi\|^2, \qquad |F(1+\mathrm{i}t)| \leq \|\xi\|^2,$$

on the strip $0 \leq \operatorname{Re} z \leq 1$. By the three lines theorem $|F(z)| \leq \|\xi\|^2$ on this strip. Setting $z = \alpha \in [0,1]$, we conclude that

$$(T_\nu\xi|\Delta_{\rho|\nu}^{\alpha}T_\nu\xi) \leq (\xi|(\Delta_{\hat\rho|\hat\nu}^{1/2}+\varepsilon)^{2\alpha}\xi).$$

Letting $\varepsilon \downarrow 0$ we get

$$(T_\nu\xi|\Delta_{\rho|\nu}^{\alpha}T_\nu\xi) \leq (\xi|\Delta_{\hat\rho|\hat\nu}^{\alpha}\xi),$$

and (2.40) follows from the fact that $T_\nu\xi_{\hat\nu} = \Phi(\mathbb{1})\xi_\nu = \xi_\nu$. □

As a last illustration of the use of modular theory, we prove a lower bound for quantum hypothesis testing which complements Theorem 2.19. Our proof is an abstract version of similar results proven in [ANSV, HMO], where reader can find references for the previous works on the subject. The extension of our proof to the general von Neumann algebra setting can be found in [JOPS].

Let $D_p(\rho,\nu) = D_p(\rho,\nu,P_{\mathrm{opt}})$ be as in Section 1.3.7. Let $\Delta_{\rho|\nu}$ be the modular operator defined in the proof of Theorem 1.14, and let $\mu_{\rho|\nu}$ be the spectral measure for $\Delta_{\rho|\nu}$ and ξ_ν.

Proposition 2.26

$$D_p(\rho,\nu) \geq \frac{1}{2}\min(p,1-p)\mu_{\rho|\nu}([1,\infty[).$$

Proof. Let P be an orthogonal projection (a test). By Equ. (2.37), one has

$$\begin{aligned}
D_p(\rho,\nu,P) &= p\|(\mathbb{1}-P)\xi_\rho\|^2 + (1-p)\|P\xi_\nu\|^2 \\
&\geq p\|\mathrm{s}(\nu)(\mathbb{1}-P)\xi_\rho\|^2 + (1-p)\|P\xi_\nu\|^2 \\
&\geq p\|\Delta_{\rho|\nu}^{1/2}(\mathbb{1}-P)\xi_\nu\|^2 + (1-p)\|P\xi_\nu\|^2 \\
&\geq \min(p,1-p)\left(\|\Delta_{\rho|\nu}^{1/2}(\mathbb{1}-P)\xi_\nu\|^2 + \|P\xi_\nu\|^2\right) \\
&\geq \min(p,1-p)(\xi_\nu|((\mathbb{1}-P)\Delta_{\rho|\nu}(\mathbb{1}-P)+P\mathbb{1}P)\xi_\nu).
\end{aligned}$$

Let F be the characteristic function of the interval $[1,\infty[$. Since $\mathbb{1} \geq F(\Delta_{\rho|\nu})$ and $\Delta_{\rho|\nu} \geq F(\Delta_{\rho|\nu})$, we further have

$$D_p(\rho,\nu,P) \geq \min(p,1-p)(\xi_\nu|((\mathbb{1}-P)F(\Delta_{\rho|\nu})(\mathbb{1}-P)+PF(\Delta_{\rho|\nu})P)\xi_\nu).$$

From the identity

$$(\mathbb{1}-P)F(\Delta_{\rho|\nu})(\mathbb{1}-P)+PF(\Delta_{\rho|\nu})P - \frac{1}{2}F(\Delta_{\rho|\nu}) = (\mathbb{1}-2P)F(\Delta_{\rho|\nu})(\mathbb{1}-2P),$$

we deduce $(\mathbb{1}-P)F(\Delta_{\rho|\nu})(\mathbb{1}-P)+PF(\Delta_{\rho|\nu})P \geq \frac{1}{2}F(\Delta_{\rho|\nu})$ which allows us to conclude

$$D_p(\rho,\nu,P) \geq \frac{1}{2}\min(p,1-p)(\xi_\nu|F(\Delta_{\rho|\nu})\xi_\nu),$$

for all orthogonal projections $P \in \mathcal{O}$. Finally we note that

$$\begin{aligned}
D_p(\rho,\nu) = \min_P D_p(\rho,\nu,P) &\geq \frac{1}{2}\min(p,1-p)(\xi_\nu|F(\Delta_{\rho|\nu})\xi_\nu) \\
&= \frac{1}{2}\min(p,1-p)\mu_{\rho|\nu}([1,\infty[),
\end{aligned}$$

which concludes the proof. □

Exercise 2.19. Prove the following generalization of Kosaki's variational formula: for any $\rho, \nu \in \mathfrak{S}$, $B \in \mathcal{O}$ and $\alpha \in]0,1[$ one has

$$\operatorname{tr}\left(B^* \rho^\alpha B \nu^{1-\alpha}\right) = \inf_{A \in C(\mathbb{R}_+, \mathcal{O})} \frac{\sin \pi\alpha}{\pi} \int_0^\infty t^{\alpha-1} \left[\frac{1}{t}\rho(|A(t)^*|^2) + \nu(|B - A(t)|^2)\right] \mathrm{d}t.$$

Chapter 3

Entropic functionals and fluctuation relations of finite quantum systems

3.1 Quantum dynamical systems

Our starting point is a quantum dynamical system $(\mathcal{O}, \tau^t, \omega)$ on a finite dimensional Hilbert space $\mathcal{K}$, where $\mathbb{R} \ni t \mapsto \tau^t$ is a continuous group of $*$-automorphisms of $\mathcal{O}$, and ω a faithful state. We denote by δ the generator of τ^t and by H the corresponding Hamiltonian.

As in our discussion of the thermally driven harmonic chain in Chapter 1, time-reversal invariance (TRI) will play an important role in the sequel. An anti-linear $*$-automorphism Θ of $\mathcal{O}$ is called time-reversal of $(\mathcal{O}, \tau^t)$ if

$$\Theta \circ \Theta = \mathrm{id}, \qquad \tau^t \circ \Theta = \Theta \circ \tau^{-t}.$$

A state ω is called TRI iff $\omega(\Theta(A)) = \omega(A^*)$. The quantum dynamical system $(\mathcal{O}, \tau^t, \omega)$ is called TRI if there exists a time-reversal Θ of $(\mathcal{O}, \tau^t)$ such that ω is TRI.

Exercise 3.1. Suppose that Θ is a time-reversal of $(\mathcal{O}, \tau^t)$. Show that there exists an anti-unitary $U_\Theta : \mathcal{K} \to \mathcal{K}$, unique up to a phase, such that $\Theta(A) = U_\Theta A U_\Theta^{-1}$ and deduce that $\mathrm{tr}(\Theta(A)) = \mathrm{tr}(A^*)$. Show that $\Theta(H) = H$ and that a state ω is TRI iff $\Theta(\omega) = \omega$.
Hint: Recall Exercise 2.4.

3.2 Entropy balance

The relative Hamiltonian of ω_t w.r.t. ω, $\ell_{\omega_t|\omega} = \log \omega_t - \log \omega$, is easily seen to satisfy:

Proposition 3.1 (1) *For all $t, s \in \mathbb{R}$ the additive cocycle property*

$$\ell_{\omega_{t+s}|\omega} = \ell_{\omega_t|\omega} + \tau^{-t}(\ell_{\omega_s|\omega}), \tag{3.1}$$

holds.

(2) *If $(\mathcal{O}, \tau, \omega)$ is TRI, then*

$$\Theta(\ell_{\omega_t|\omega}) = -\tau^t(\ell_{\omega_t|\omega}), \tag{3.2}$$

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

Differentiating the cocycle relation (3.1) we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\ell_{\omega_t|\omega} = \tau^{-t}(\sigma),$$

where

$$\sigma = \frac{\mathrm{d}}{\mathrm{d}t}\ell_{\omega_t|\omega}\Big|_{t=0} = -\mathrm{i}[H, \log\omega] = \delta_\omega(H),$$

(recall that δ_ω denotes the generator of the modular group of ω). Thus, we can write

$$\ell_{\omega_t|\omega} = \int_0^t \sigma_{-s}\,\mathrm{d}s, \tag{3.3}$$

and the relation $S(\omega_t|\omega) = -\omega_t(\ell_{\omega_t|\omega})$ yields the quantum mechanical version of Equ. (1.5),

$$S(\omega_t|\omega) = -\int_0^t \omega(\sigma_s)\,\mathrm{d}s.$$

We shall refer to this identity as the *entropy balance equation* and call σ the *entropy production* observable.

Proposition 3.2 *$\omega(\sigma) = 0$ and if $(\mathcal{O}, \tau^t, \omega)$ is TRI then $\Theta(\sigma) = -\sigma$.*

Proof. $\omega(\sigma) = -\mathrm{i}\,\mathrm{tr}(\omega[H, \log\omega]) = \mathrm{i}\,\mathrm{tr}(H[\omega, \log\omega]) = 0$. Differentiating (3.2) at $t = 0$ one derives the second statement. □

An immediate consequence of the entropy balance equation is that the mean entropy production rate over the time interval $[0, t]$,

$$\Sigma^t = \frac{1}{t}\int_0^t \sigma_s\,\mathrm{d}s,$$

has a non-negative expectation

$$\omega(\Sigma^t) = \frac{1}{t}\int_0^t \omega(\sigma_s)\mathrm{d}s \geq 0. \tag{3.4}$$

Introducing the entropy observable $S = -\log\omega$ (so $S_t = \tau^t(S) = -\log\omega_{-t}$), we see that

$$\Sigma^t = \frac{1}{t}(S_t - S), \qquad \frac{\mathrm{d}}{\mathrm{d}t}S_t|_{t=0} = \sigma. \tag{3.5}$$

The observable S cannot survive the thermodynamic limit. However, the relative Hamiltonian and all other objects defined in this section do. All relations except (3.5) remain valid after the thermodynamic limit is taken.

Exercise 3.2. Assume that the quantum dynamical system $(\mathcal{O}, \tau^t, \omega)$ is in a steady state, $\omega(\tau^t(A)) = \omega(A)$ for all $A \in \mathcal{O}$ and $t \in \mathbb{R}$. Denote by K the standard Liouvillean of τ^t and by δ_ω the generator of the modular group of ω: $\varsigma_\omega^t = \mathrm{e}^{t\delta_\omega}$. Consider the perturbed dynamical system $(\mathcal{O}, \tau_V^t, \omega)$ associated to $V \in \mathcal{O}_{\mathrm{self}}$ (see Section 2.10).

1. Show that its entropy production observable is given by

$$\sigma = \delta_\omega(V).$$

2. Show that its standard Liouvillean is given by

$$K_V\xi = K\xi + V\xi - JVJ\xi.$$

3.3 Finite time Evans-Searles symmetry

At this point, looking back at Section 1.6, one may think that, for TRI quantum dynamical systems, the universal ES relation (1.13) holds between the spectral measure P^t of Σ^t associated to ω

$$\omega(f(\Sigma^t)) = P^t(f) = \int f(s)\,\mathrm{d}P^t(s),$$

and its reversal $\overline{P}^t(f) = \omega(f(-\Sigma^t))$. To check this point, we first note that, by Proposition 3.2,

$$\Theta(\Sigma^t) = \frac{1}{t}\int_0^t \Theta(\tau^s(\sigma))\,\mathrm{d}s = -\frac{1}{t}\int_0^t \tau^{-s}(\sigma)\,\mathrm{d}s = -\tau^{-t}(\Sigma^t),$$

which is the quantum counterpart of Equ. (1.10) and (1.12). Note that this relation implies that $s \in \mathrm{sp}(\Sigma^t)$ iff $-s \in \mathrm{sp}(\Sigma^t)$ and that the eigenvalues $\pm s$ have equal multiplicities. Furthermore,

$$\overline{P}^t(f) = \omega_t \circ \tau^{-t}(f(-\Sigma^t)) = \omega_t \circ \Theta(f(\Sigma^t)) = \omega_{-t}(f(\Sigma^t)) = \omega(f(\Sigma^t)\omega_{-t}\omega^{-1}),$$

which, using (3.3), can be rewritten as

$$\overline{P}^t(f) = \omega\left(f(\Sigma^t)\mathrm{e}^{\log\omega - t\Sigma^t}\mathrm{e}^{-\log\omega}\right).$$

If ω is not a steady state then $\log\omega$ and Σ^t do not commute and hence we can not conclude, as in the classical case, that $\overline{P}^t(f)$ equals $\omega\left(f(\Sigma^t)\mathrm{e}^{-t\Sigma^t}\right)$. Our naive attempt to generalize the ES relation (1.13) to quantum dynamical systems thus failed because quantum mechanical observables do not commute.

Exercise 3.3. Show that the ES-relation

$$\omega\left(\mathrm{e}^{-\alpha t\Sigma^t}\right) = \omega\left(\mathrm{e}^{-(1-\alpha)t\Sigma^t}\right).$$

holds for all t if and only if $[H,\omega] = 0$.
Hint: the relation implies $\omega(\mathrm{e}^{-t\Sigma^t}) = 1$. By Golden-Thompson inequality,

$$\omega(\mathrm{e}^{-t\Sigma^t}) = \mathrm{tr}(\mathrm{e}^{\log\omega}\mathrm{e}^{\log\omega_{-t} - \log\omega}) \geq \mathrm{tr}(\mathrm{e}^{\log\omega_{-t}}) = 1,$$

and equality holds iff ω and ω_{-t} commute (recall Exercise 2.8). Differentiating $\omega\omega_t = \omega_t\omega$ at $t = 0$ deduce that $H\omega^2 = \omega^2 H$.

As noticed in Section 1.6, the ES relation (1.13) is equivalent to the ES-symmetry (1.14) of the Laplace transform of the measure P^t. We recall also that this Laplace transform is related to the relative entropy through Equ. (1.9). It is therefore natural to check for the ES-symmetry of the function

$$\alpha \mapsto S_\alpha(\omega_t|\omega).$$

Assuming TRI, we have

$$\mathrm{tr}(\omega_t^\alpha\omega^{1-\alpha}) = \mathrm{tr}(\Theta(\omega^{1-\alpha}\omega_t^\alpha)) = \mathrm{tr}(\omega^{1-\alpha}\omega_{-t}^\alpha) = \mathrm{tr}(\omega_t^{1-\alpha}\omega^\alpha),$$

where we used that $\mathrm{tr}(\Theta(A)) = \mathrm{tr}(A^*)$ (Exercise 3.1). Thus,

$$S_\alpha(\omega_t|\omega) = \log\mathrm{tr}\,(\omega_t^\alpha\omega^{1-\alpha}) = \log\mathrm{tr}\,(\omega^{(1-\alpha)/2}\omega_t^\alpha\omega^{(1-\alpha)/2}),$$

satisfies the ES-symmetry.

In our non-commutative framework one may also define the entropy-like functional

$$\mathbb{R} \ni \alpha \mapsto e_{p,t}(\alpha) = \log \mathrm{tr} \left[\left(\omega^{(1-\alpha)/p} \omega_t^{2\alpha/p} \omega^{(1-\alpha)/p} \right)^{p/2} \right].$$

For reasons that will become clear later, we restrict the real parameter p to $p \geq 1$. Since $\log \omega_t = \log \omega + \ell_{\omega_t|\omega}$, Corollary 2.3 yields

$$e_{\infty,t}(\alpha) = \lim_{p\to\infty} e_{p,t}(\alpha) = \log \mathrm{tr}(\mathrm{e}^{(1-\alpha)\log\omega + \alpha \log \omega_t}) = \log \mathrm{tr}(\mathrm{e}^{\log\omega + \alpha \ell_{\omega_t|\omega}}).$$

We shall call the $e_{p,t}(\alpha)$ *entropic pressure functionals*. Their basic properties are:

Proposition 3.3 (1) *The function* $[1, \infty] \ni p \mapsto e_{p,t}(\alpha)$ *is continuous and monotonically decreasing.*

(2) *The function* $\mathbb{R} \ni \alpha \mapsto e_{p,t}(\alpha)$ *is real-analytic and convex. It satisfies* $e_{p,t}(0) = e_{p,t}(1) = 0$ *and*

$$e_{p,t}(\alpha) \begin{cases} \leq 0 & \text{for } \alpha \in [0,1], \\ \geq 0 & \text{otherwise}. \end{cases}$$

(3) $e_{p,t}(\alpha) = e_{p,-t}(1-\alpha)$.

(4) $\partial_\alpha e_{p,t}(\alpha)|_{\alpha=0} = \omega(\ell_{\omega_t|\omega}) = S(\omega|\omega_t)$ *and* $\partial_\alpha e_{p,t}(\alpha)|_{\alpha=1} = \omega_t(\ell_{\omega_t|\omega}) = -S(\omega_t|\omega)$.

(5) $\partial_\alpha^2 e_{\infty,t}(\alpha)|_{\alpha=0} = \langle \ell_{\omega_t|\omega} | \ell_{\omega_t|\omega} \rangle_\omega - \omega(\ell_{\omega_t|\omega})^2$.

(6) $\partial_\alpha^2 e_{2,t}(\alpha)|_{\alpha=0} = \omega(\ell_{\omega_t|\omega}^2) - \omega(\ell_{\omega_t|\omega})^2$.

(7) *If* $(\mathcal{O}, \tau^t, \omega)$ *is TRI, then the finite time quantum Evans-Searles* (ES) *symmetry holds,*

$$e_{p,t}(\alpha) = e_{p,t}(1-\alpha). \tag{3.6}$$

Proof. (1) Continuity is obvious. Writing

$$e_{p,t}(\alpha) = \log \|\omega_t^{\alpha/p} \omega^{(1-\alpha)/p}\|_p^p, \tag{3.7}$$

monotonicity follows from Corollary 2.3.

(2) Analyticity easily follows from the analytic functional calculus and convexity is a consequence of Corollary 2.4. The value taken by $e_{p,t}$ at $\alpha = 0$ and $\alpha = 1$ is evident and the remaining inequalities follow from convexity.

(3) Unitary invariance of the trace norms and Identity (2.11) give

$$\begin{aligned} \|\omega_t^{\alpha/p} \omega^{(1-\alpha)/p}\|_p &= \|\mathrm{e}^{-\mathrm{i}tH} \omega^{\alpha/p} \mathrm{e}^{\mathrm{i}tH} \omega^{(1-\alpha)/p}\|_p \\ &= \|\omega^{\alpha/p} \mathrm{e}^{\mathrm{i}tH} \omega^{(1-\alpha)/p} \mathrm{e}^{-\mathrm{i}tH}\|_p \\ &= \|\omega^{\alpha/p} \omega_{-t}^{(1-\alpha)/p}\|_p = \|\omega_{-t}^{(1-\alpha)/p} \omega^{\alpha/p}\|_p. \end{aligned}$$

(4) We consider only $p \in [1, \infty[$. The limiting case $p = \infty$ will be treated in the proof of Assertion (5). We set $T(\alpha) = \omega^{(1-\alpha)/p} \omega_t^{2\alpha/p} \omega^{(1-\alpha)/p}$ so that

$$\partial_\alpha e_{p,t}(\alpha)\Big|_{\alpha=0} = \partial_\alpha \mathrm{tr}\,(T(\alpha)^{p/2})\Big|_{\alpha=0}.$$

Let Γ be a closed contour on the right half-plane $\mathrm{Re}\, z > 0$ encircling the strictly positive spectrum of $T(0) = \omega^{2/p}$. Since $\alpha \mapsto T(\alpha)$ is continuous, Γ can be chosen in such a way that it encloses the spectrum of $T(\alpha)$ for α small enough. Hence, with $f(z) = z^{p/2}$, we can write

$$\mathrm{tr}\, T(\alpha)^{p/2} = \oint_\Gamma f(z) \mathrm{tr}\,((z - T(\alpha))^{-1}) \frac{\mathrm{d}z}{2\pi \mathrm{i}},$$

so that

$$\partial_\alpha \mathrm{tr}\,(T(\alpha)^{p/2})\Big|_{\alpha=0} = \oint_\Gamma f(z)\mathrm{tr}\left[(z-T(0))^{-1}T'(0)(z-T(0))^{-1}\right]\frac{\mathrm{d}z}{2\pi\mathrm{i}}.$$

An elementary calculation gives

$$T'(0) = \frac{2}{p}\,\omega^{1/p}\ell_{\omega_t|\omega}\,\omega^{1/p},$$

and the cyclicity of the trace allows us to write

$$\begin{aligned}\partial_\alpha \mathrm{tr}\,(T(\alpha)^{p/2})\Big|_{\alpha=0} &= \frac{2}{p}\oint_\Gamma f(z)\mathrm{tr}\left[(z-\omega^{2/p})^{-2}\omega^{2/p}\ell_{\omega_t|\omega}\right]\frac{\mathrm{d}z}{2\pi\mathrm{i}}\\ &= \frac{2}{p}\,\mathrm{tr}\left[f'(\omega^{2/p})\omega^{2/p}\ell_{\omega_t|\omega}\right] = \mathrm{tr}\,\omega\ell_{\omega_t|\omega} = S(\omega|\omega_t).\end{aligned}$$

The second statement also follows by taking (3) into account and observing that $S(\omega|\omega_{-t}) = S(\omega_t|\omega)$.

(5) Setting $T(\alpha) = \mathrm{e}^{\log\omega+\alpha\ell_{\omega_t|\omega}}$, we have $T(0)=\omega$ and

$$\begin{aligned}\partial_\alpha e_{\infty,t}(\alpha)\Big|_{\alpha=0} &= \mathrm{tr}\,(T'(0)),\\ \partial_\alpha^2 e_{\infty,t}(\alpha)\Big|_{\alpha=0} &= \mathrm{tr}\,(T''(0)) - (\mathrm{tr}\,(T'(0)))^2.\end{aligned}$$

Iterating Duhamel's formula (recall Exercise 2.3), we can write

$$T(\alpha) = \omega + \alpha\int_0^1 \omega^{1-s}\ell_{\omega_t|\omega}\omega^s\,\mathrm{d}s + \alpha^2\int_0^1\int_0^u \omega^{1-u}\ell_{\omega_t|\omega}\omega^s\ell_{\omega_t|\omega}\omega^{u-s}\,\mathrm{d}s\,\mathrm{d}u + O(\alpha^3),$$

so that

$$\mathrm{tr}\,(T'(0)) = \int_0^1 \mathrm{tr}\left[\omega^{1-s}\ell_{\omega_t|\omega}\omega^s\right]\,\mathrm{d}s = \omega(\ell_{\omega_t|\omega}) = S(\omega|\omega_t),$$

which proves (4) in the special case $p=\infty$, and

$$\begin{aligned}\mathrm{tr}\,(T''(0)) &= 2\int_0^1\int_0^u \mathrm{tr}\left[\omega^{1-s}\ell_{\omega_t|\omega}\omega^s\ell_{\omega_t|\omega}\right]\mathrm{d}s\,\mathrm{d}u\\ &= 2\int_0^1\int_s^1 \mathrm{tr}\left[\omega^{1-s}\ell_{\omega_t|\omega}\omega^s\ell_{\omega_t|\omega}\right]\mathrm{d}u\,\mathrm{d}s\\ &= 2\int_0^1 (1-s)\mathrm{tr}\left[\omega^{1-s}\ell_{\omega_t|\omega}\omega^s\ell_{\omega_t|\omega}\right]\mathrm{d}s\\ &= 2\int_0^1 s\,\mathrm{tr}\left[\omega^{s}\ell_{\omega_t|\omega}\omega^{1-s}\ell_{\omega_t|\omega}\right]\mathrm{d}s.\end{aligned}$$

Taking the mean of the last two expressions, we get

$$\begin{aligned}\mathrm{tr}\,(T''(0)) &= \int_0^1 \mathrm{tr}\left[\omega^{1-s}\ell_{\omega_t|\omega}\omega^s\ell_{\omega_t|\omega}\right]\mathrm{d}s\\ &= \int_0^1 \omega\left(\varsigma_\omega^{\mathrm{i}s}(\ell_{\omega_t|\omega})\ell_{\omega_t|\omega}\right)\mathrm{d}s,\end{aligned}$$

and hence

$$\partial_\alpha^2 e_{\infty,t}(\alpha)\Big|_{\alpha=0} = \int_0^1\left[\omega\left(\varsigma_\omega^{\mathrm{i}s}(\ell_{\omega_t|\omega})\ell_{\omega_t|\omega}\right) - \omega(\ell_{\omega_t|\omega})^2\right]\mathrm{d}s.$$

(6) Follows easily from the fact that $e_{2,t}(\alpha) = S_\alpha(\omega_t|\omega) = \log\mathrm{tr}\,(\omega_t^\alpha\omega^{1-\alpha})$.

(7) Under the TRI assumption one has $\Theta(\omega) = \omega$, $\Theta(\omega_t) = \omega_{-t}$,

$$\Theta\left(\left(\omega^{(1-\alpha)/p}\omega_t^{2\alpha/p}\omega^{(1-\alpha)/p}\right)^{p/2}\right) = \left(\omega^{(1-\alpha)/p}\omega_{-t}^{2\alpha/p}\omega^{(1-\alpha)/p}\right)^{p/2},$$

and hence $e_{p,t}(\alpha) = e_{p,-t}(\alpha)$. The result now follows from Assertion (3). □

According to our rule of thumb, we reformulate the definition of the functionals $e_{p,t}(\alpha)$ in terms which are susceptible to survive the thermodynamic limit. We first note that

$$e_{2,t}(\alpha) = S_\alpha(\omega_t|\omega) = \log(\xi_\omega|\Delta^\alpha_{\omega_t|\omega}\xi_\omega),$$

while Theorem 2.15 (2) yields the variational principle

$$e_{\infty,t}(\alpha) = \max_{\rho\in\mathfrak{S}} S(\rho|\omega) + \alpha\rho(\ell_{\omega_t|\omega}).$$

Moreover, Equ. (3.7) and Theorem 2.25 immediately lead to

$$e_{p,t}(\alpha) = \log\|\Delta^{\alpha/p}_{\omega_t|\omega}\xi_\omega\|^p_{\omega,p},$$

for $p \in [1,\infty[$.

Exercise 3.4. Show that

$$e_{\infty,t}(\alpha) = \log(\xi_\omega|\mathrm{e}^{\log\Delta_\omega+\alpha L(\ell_{\omega_t|\omega})}\xi_\omega).$$

Exercise 3.5. Show that the function $[1,\infty] \ni p \mapsto e_{p,t}(\alpha)$ is strictly decreasing unless H and ω commute.
Hint: recall Exercise 2.8.

3.4 Quantum transfer operators

For $p \in [1,\infty]$ we define a linear map $U_p(t) : \mathcal{H}_\mathcal{O} \to \mathcal{H}_\mathcal{O}$ by

$$U_p(t)\xi = \mathrm{e}^{-\mathrm{i}tH}\xi\omega^{-\frac{1}{2}+\frac{1}{p}}\mathrm{e}^{\mathrm{i}tH}\omega^{\frac{1}{2}-\frac{1}{p}}.$$

In terms of Connes cocycles and relative modular dynamics, one has

$$U_p(t)\xi = \mathrm{e}^{-\mathrm{i}tH}\xi\mathrm{e}^{\mathrm{i}tH}[D\omega_t : D\omega]^{\mathrm{i}(\frac{1}{2}-\frac{1}{p})} = \mathrm{e}^{-\mathrm{i}tH}\xi\mathrm{e}^{\mathrm{i}t\varsigma_\omega^{\mathrm{i}(\frac{1}{2}-\frac{1}{p})}(H)}. \tag{3.8}$$

One easily checks that $\mathbb{R} \ni t \mapsto U_p(t)$ is a group of operators on $\mathcal{H}_\mathcal{O}$ which satisfies

$$(\xi|U_p(t)\eta) = (U_q(-t)\xi|\eta), \tag{3.9}$$

for all $\xi,\eta \in \mathcal{H}_\mathcal{O}$ with $p^{-1}+q^{-1} = 1$. The following result elucidates the nature of this group: it is the unique isometric implementation of the dynamics on the Banach space $L^p(\mathcal{O},\omega)$ which preserves the positive cone $L^p_+(\mathcal{O},\omega)$.

Proposition 3.4 (1) *$t \mapsto U_p(t)$ is a group of isometries of $L^p(\mathcal{O},\omega)$.*
(2) *$U_p(t)L^p_+(\mathcal{O},\omega) \subset L^p_+(\mathcal{O},\omega)$.*

(3) $U_p(-t)L(A)U_p(t) = L(\tau^t(A))$ *for any* $A \in \mathcal{O}$.

(4) $U_p(t)$ *is uniquely characterized by Properties* (1)–(3).

The groups U_p are natural non-commutative generalizations of the classical Ruelle transfer operators. We call L^p*-Liouvillean* of the quantum dynamical system $(\mathcal{O}, \tau^t, \omega)$ the generator L_p of U_p,

$$U_p(t) = \mathrm{e}^{-\mathrm{i}tL_p}.$$

From Equ. (3.8) we immediately get

$$L_p\xi = H\xi - \xi\varsigma_\omega^{\mathrm{i}(\frac{1}{2}-\frac{1}{p})}(H).$$

Interpreting (3.9) in terms of the duality between $L^p(\mathcal{O},\omega)$ and $L^q(\mathcal{O},\omega)$, we can write

$$L_p^* = L_q.$$

Note that, in the special case $p = 2$, $L_2 = L_2^*$ coincide with the standard Liouvillean K of the dynamics τ^t.

Theorem 3.5 *For any* $p \in [1,\infty]$ *one has*

$$\mathrm{sp}(L_p) = \mathrm{sp}(K) = \{\lambda - \mu \,|\, \lambda, \mu \in \mathrm{sp}(H)\}.$$

Exercise 3.6. This is the continuation of Exercise 3.2. Show that the L^p-Liouvillean of the perturbed dynamical system $(\mathcal{O}, \tau_V^t, \omega)$ is given by

$$L_p\xi = K\xi + V\xi - J\varsigma_\omega^{-\mathrm{i}(\frac{1}{2}-\frac{1}{p})}(V)J\xi.$$

Interestingly enough, one can relate the groups U_p to the entropic pressure functionals introduced in the previous section. The resulting formulas are particularly well suited to investigate the large time limit of these functionals.

Theorem 3.6 *For* $\alpha \in [0,1]$,

$$e_{p,t}(\alpha) = \log \|\mathrm{e}^{-\mathrm{i}tL_{p/\alpha}}\xi_\omega\|_{\omega,p}^p,$$

holds provided $p \in [1,\infty[$. *In the special case* $p = 2$*, this reduces to*

$$e_{2,t}(\alpha) = \log\,(\xi_\omega|\mathrm{e}^{-\mathrm{i}tL_{1/\alpha}}\xi_\omega).$$

With the help of Theorem 2.25, the proof of the last theorem reduces to elementary calculations.

Proof of Proposition 3.4 and Theorem 3.5. Let K be the standard Liouvillean of $(\mathcal{O}, \tau^t, \omega)$. Since $\mathrm{e}^{-\mathrm{i}tK}\xi = \mathrm{e}^{-\mathrm{i}tH}\xi\mathrm{e}^{\mathrm{i}tH}$, it is obvious that $\mathrm{e}^{-\mathrm{i}tK}$ is a group of isometries of $L^p(\mathcal{O})$ which preserves the positive cone $L_+^p(\mathcal{O})$. Denote by $V_p : L^p(\mathcal{O}) \to L^p(\mathcal{O},\omega)$ the isometry defined in Theorem 2.25. Theorem 3.5 and Properties (1) and (2) of Proposition 3.4 follow from the facts that $U_p(t) = V_p\mathrm{e}^{-\mathrm{i}tK}V_p^{-1}$ and $L_+^p(\mathcal{O},\omega) = V_pL_+^p(\mathcal{O})$. To prove Property (3) we note that $V_p \in R(\mathcal{O}) = L(\mathcal{O})'$, so that

$$\begin{aligned}
U_p(-t)L(A)U_p(t) &= V_p\mathrm{e}^{\mathrm{i}tK}V_p^{-1}L(A)V_p\mathrm{e}^{-\mathrm{i}tK}V_p^{-1}\\
&= V_p\mathrm{e}^{\mathrm{i}tK}L(A)\mathrm{e}^{-\mathrm{i}tK}V_p^{-1}\\
&= V_pL(\tau^t(A))V_p^{-1} = L(\tau^t(A)).
\end{aligned}$$

(4) Let $\mathbb{R} \ni t \mapsto U^t$ be a group of linear operators on $\mathcal{H}_{\mathcal{O}}$ satisfying Properties (1)–(3) and set $V^t = L(\mathrm{e}^{\mathrm{i}tH})U^t$. The group property implies that

$$(V^t)^{-1} = (U^t)^{-1}L(\mathrm{e}^{\mathrm{i}tH})^{-1} = U^{-t}L(\mathrm{e}^{-\mathrm{i}tH}),$$

so that, by Property (3),

$$\begin{aligned} L(\tau^t(A)) = U^{-t}L(A)U^t &= (V^t)^{-1}L(\mathrm{e}^{\mathrm{i}tH})L(A)L(\mathrm{e}^{-\mathrm{i}tH})V^t \\ &= (V^t)^{-1}L(\mathrm{e}^{\mathrm{i}tH}A\mathrm{e}^{-\mathrm{i}tH})V^t = (V^t)^{-1}L(\tau^t(A))V^t, \end{aligned}$$

for all $A \in \mathcal{O}$. Setting $A = \tau^{-t}(B)$ we conclude that

$$V^tL(B) = L(B)V^t,$$

for all $B \in \mathcal{O}$, i.e., $V^t \in L(\mathcal{O})' = R(\mathcal{O})$. Using the group property of U^t one easily shows that $t \mapsto V^t$ is also a group. It follows that $V^t = R(\mathrm{e}^{\mathrm{i}t\widetilde{H}})$ for some $\widetilde{H} \in \mathcal{O}$. Thus, for any $A \in \mathcal{O}$, one has

$$U^tA\omega^{\frac{1}{2}-\frac{1}{p}} = \mathrm{e}^{\mathrm{i}tH}A\omega^{\frac{1}{2}-\frac{1}{p}}\mathrm{e}^{-\mathrm{i}t\widetilde{H}^*} = \mathrm{e}^{\mathrm{i}tH}A\mathrm{e}^{-\mathrm{i}tH^\#}\omega^{\frac{1}{2}-\frac{1}{p}},$$

where $H^\# = \varsigma_\omega^{-\mathrm{i}(\frac{1}{2}-\frac{1}{p})}(\widetilde{H}^*)$. Exercise 2.18 (1) and Property (2) imply that $\mathrm{e}^{\mathrm{i}tH}A\mathrm{e}^{-\mathrm{i}tH^\#} \in \mathcal{O}_+$ for any $A \in \mathcal{O}_+$. Since any self-adjoint element of $\mathcal{O}$ is a real linear combination of elements of $\mathcal{O}_+$, it follows that

$$\mathrm{e}^{\mathrm{i}tH}A\mathrm{e}^{-\mathrm{i}tH^\#} = \left(\mathrm{e}^{\mathrm{i}tH}A\mathrm{e}^{-\mathrm{i}tH^\#}\right)^* = \mathrm{e}^{\mathrm{i}tH^{\#*}}A\mathrm{e}^{-\mathrm{i}tH},$$

for any $A \in \mathcal{O}_{\mathrm{self}}$. This identity extends by linearity to arbitrary $A \in \mathcal{O}$. Differentiation at $t = 0$ yields

$$(H - H^{\#*})A = A(H^\# - H). \tag{3.10}$$

Setting $A = \mathbb{1}$, we deduce that $H^\# + H^{\#*} = 2H$, and hence that $H^\# = H + \mathrm{i}T$ with $T \in \mathcal{O}_{\mathrm{self}}$. Relation (3.10) now implies $TA = AT$ for all $A \in \mathcal{O}$ so that $T = \lambda\mathbb{1}$ for some $\lambda \in \mathbb{R}$. It follows that $H^\# = \varsigma_\omega^{\mathrm{i}(1/2-1/p)}(H)^* - \mathrm{i}\lambda$ and hence $U^t = \mathrm{e}^{\lambda t}U_p(t)$. Property (1) finally imposes $\lambda = 0$. □

3.5 Full counting statistics

The functional

$$e_{2,t}(\alpha) = S_\alpha(\omega_t|\omega) = \log(\xi_\omega|\Delta^\alpha_{\omega_t|\omega}\xi_\omega) = \log(\xi_\omega|\mathrm{e}^{\alpha\log\Delta_{\omega_t|\omega}}\xi_\omega),$$

can be interpreted in spectral terms. If we denote by Q^t the spectral measure of the self-adjoint operator

$$-\frac{1}{t}\log\Delta_{\omega_t|\omega} = -\frac{1}{t}\log\Delta_\omega - \frac{1}{t}L(\ell_{\omega_t|\omega}) = -\frac{1}{t}\log\Delta_\omega - L(\Sigma^{-t}),$$

for the vector ξ_ω then

$$e_{2,t}(\alpha) = \log\left[\int_{\mathbb{R}}\mathrm{e}^{-\alpha ts}\mathrm{d}Q^t(s)\right]. \tag{3.11}$$

As explained at the end of Section 1.6, the ES symmetry (3.6) can be expressed in terms of the measure Q^t in the following familiar form (see [TM]). Let $\mathfrak{r} : \mathbb{R} \to \mathbb{R}$ be the reflection $\mathfrak{r}(s) = -s$, and let $\overline{Q}^t = Q^t \circ \mathfrak{r}$ be the reflected spectral measure.

Proposition 3.7 *Suppose that $(\mathcal{O}, \tau^t, \omega)$ is TRI. Then the measures Q^t and $\overline{Q}^t$ are mutually absolutely continuous and*

$$\frac{\mathrm{d}\overline{Q}^t}{\mathrm{d}Q^t}(s) = \mathrm{e}^{-ts}.$$

The measure Q^t is not the spectral measure of any observable in $\mathcal{O}$ and on the first sight one may question its physical relevance. Its interpretation is somewhat striking and is linked to concept of *Full Counting Statistics* (FCS) of repeated quantum measurement of the entropy observable $S = -\log \omega$. To our knowledge, this interpretation goes back to Kurchan [Ku] (see also [DRM]).

At time $t = 0$, with the system in the state ω, we perform a measurement of S. The possible outcomes of the measurement are eigenvalues of S and $s \in \mathrm{sp}(S)$ is observed with probability $\omega(P_s)$, where P_s is the spectral projection of S onto its eigenvalue s. After the measurement, the state of the system reduces to

$$\frac{\omega P_s}{\omega(P_s)},$$

and this state now evolves according to

$$\frac{\mathrm{e}^{-\mathrm{i}tH}\omega P_s \mathrm{e}^{\mathrm{i}tH}}{\omega(P_s)}.$$

A second measurement of S at time t yields the result $s' \in \mathrm{sp}(S)$ with probability

$$\frac{\mathrm{tr}\left(\mathrm{e}^{-\mathrm{i}tH}\omega P_s \mathrm{e}^{\mathrm{i}tH} P_{s'}\right)}{\omega(P_s)}.$$

Thus, the joint probability distribution of the two measurement is given by

$$\mathrm{tr}\left(\mathrm{e}^{-\mathrm{i}tH}\omega P_s \mathrm{e}^{\mathrm{i}tH} P_{s'}\right),$$

and the probability distribution of the mean rate of change of entropy, $\phi = (s' - s)/t$, is given by

$$\mathbb{P}_t(\phi) = \sum_{s'-s=t\phi} \mathrm{tr}\left(\mathrm{e}^{-\mathrm{i}tH}\omega P_s \mathrm{e}^{\mathrm{i}tH} P_{s'}\right).$$

It follows that

$$\mathrm{tr}(\omega_t^{1-\alpha}\omega^\alpha) = \sum_{s,s'} \mathrm{e}^{-\alpha(s'-s)}\mathrm{tr}\left(\mathrm{e}^{-\mathrm{i}tH}\omega P_s \mathrm{e}^{\mathrm{i}tH} P_{s'}\right) = \sum_\phi \mathbb{P}_t(\phi)\mathrm{e}^{-t\alpha\phi}.$$

and we conclude that

$$e_{2,-t}(\alpha) = e_{2,t}(1-\alpha) = \log\left[\sum_\phi \mathbb{P}_t(\phi)\mathrm{e}^{-t\alpha\phi}\right].$$

Comparison with Equ. (3.11) allows us to conclude that the spectral measure Q^{-t} coincide with the distribution $\mathbb{P}_t(\phi)$. Consequently, applying Proposition 3.3, the expectation and variance of ϕ w.r.t. $\mathbb{P}_t$ are given by

$$\mathbb{E}_t(\phi) = -\frac{1}{t}\partial_\alpha e_{2,-t}(\alpha)\bigg|_{\alpha=0} = -\frac{1}{t}\omega(\ell_{\omega_{-t}|\omega}) = \omega(\Sigma^t),$$

$$\mathbb{E}_t(\phi^2) - \mathbb{E}_t(\phi)^2 = \frac{1}{t^2}\partial_\alpha^2 e_{2,-t}(\alpha)\bigg|_{\alpha=0} = \frac{1}{t^2}\left(\omega(\ell_{\omega_{-t}|\omega}^2) - \omega(\ell_{\omega_{-t}|\omega})^2\right) = \omega(\Sigma^{t\,2}) - \omega(\Sigma^t)^2.$$

They coincide with the expectation and variance of Σ^t w.r.t. ω. However, we warn the reader that such a relation does not hold true for higher order cumulants.

Note that time-reversal invariance played no role in the identification of $\overline{Q}^{-t}$ with $\mathbb{P}_t(\phi)$. However if $(\mathcal{O}, \tau, \omega)$ is TRI, then $\overline{Q}^{-t} = Q^t$ and Proposition 3.7 translates into the fluctuation relation

$$\frac{\mathbb{P}_t(-\phi)}{\mathbb{P}_t(\phi)} = \mathrm{e}^{-t\phi},$$

where $\phi \in (\mathrm{sp}(S) - \mathrm{sp}(S))/t$.

3.6 On the choice of reference state

Starting with entropy production, all the objects that we have introduced so far depend on the choice of the reference state ω. In this subsection we shall indicate by a subscript this dependence on ω (hence, σ_ω is the entropy production of $(\mathcal{O},\tau^t,\omega)$, etc.).

If ω and ρ are two faithful states on $\mathcal{O}$, then

$$\sigma_\omega-\sigma_\rho=\mathrm{i}[\ell_{\omega|\rho},H]=-\frac{\mathrm{d}}{\mathrm{d}t}\tau^t(\ell_{\omega|\rho})\bigg|_{t=0},$$

and hence

$$\Sigma_\omega^t-\Sigma_\rho^t=\frac{1}{t}\int_0^t\frac{\mathrm{d}}{\mathrm{d}s}\tau^s(\ell_{\omega|\rho})\,\mathrm{d}s=\frac{\tau^t(\ell_{\omega|\rho})-\ell_{\omega|\rho}}{t}.$$

Consequently,

$$\|\Sigma_\omega^t-\Sigma_\rho^t\|=\|\ell_{\omega|\rho}\|O(t^{-1}).$$

Thus, Σ_ω^t and Σ_ρ^t become indistinguishable for large t. A similar result holds for the properly normalized entropic functionals. For example:

Proposition 3.8 *For all $\alpha\in\mathbb{R}$ and $t\in\mathbb{R}$ one has the estimate*

$$\left|\frac{1}{t}e_{\infty,t,\omega}(\alpha)-\frac{1}{t}e_{\infty,t,\rho}(\alpha)\right|\le(|1-\alpha|+|\alpha|)\frac{\|\ell_{\omega|\rho}\|}{t}.$$

Proof. We have

$$\begin{aligned}\mathrm{tr}(\mathrm{e}^{\log\omega+\alpha\ell_{\omega_t|\omega}})&=\mathrm{tr}(\mathrm{e}^{\log\rho+\alpha\ell_{\rho_t|\rho}+(1-\alpha)\ell_{\omega|\rho}+\alpha\ell_{\omega_t|\rho_t}})\\&\le\mathrm{tr}(\mathrm{e}^{\log\rho+\alpha\ell_{\rho_t|\rho}}\mathrm{e}^{(1-\alpha)\ell_{\omega|\rho}+\alpha\ell_{\omega_t|\rho_t}})\\&\le\mathrm{e}^{(|1-\alpha|+|\alpha|)\|\ell_{\omega|\rho}\|}\mathrm{tr}(\mathrm{e}^{\log\rho+\alpha\ell_{\rho_t|\rho}}),\end{aligned}$$

where we have used the Golden-Thompson inequality (Corollary 2.3). Taking logarithms, we get

$$e_{\infty,t,\omega}(\alpha)-e_{\infty,t,\rho}(\alpha)\le(|1-\alpha|+|\alpha|)\|\ell_{\omega|\rho}\|.$$

Reversing the roles of ω and ρ and using that $\|\ell_{\omega|\rho}\|=\|\ell_{\rho|\omega}\|$ we deduce the statement. □

3.7 Compound systems

Consider the quantum dynamical system $(\mathcal{O},\tau^t,\omega)$ describing a compound system made of n subsystems. The underlying Hilbert space is given by a tensor product

$$\mathcal{K}=\bigotimes_{j=1}^n\mathcal{K}_j,$$

and

$$\mathcal{O}=\bigotimes_{j=1}^n\mathcal{O}_j,\tag{3.12}$$

where $\mathcal{O}_j=\mathcal{O}_{\mathcal{K}_j}$ is the algebra of observables of the j-th subsystem. We identify $A_j\in\mathcal{O}_j$ with $\mathbb{1}_{\otimes_{i=1}^{j-1}\mathcal{K}_i}\otimes A_j\otimes\mathbb{1}_{\otimes_{i=j+1}^n\mathcal{K}_i}\in\mathcal{O}$.

We assume that the reference state ω has the product structure

$$\omega(A_1\otimes\cdots\otimes A_n)=\prod_{j=1}^n\omega_j(A_j),\tag{3.13}$$

where ω_j is a faithful state on $\mathcal{O}_j$. According to the above convention, ω_j is identified with the positive operator $\mathbb{1}_{\otimes_{i=1}^{j-1}\mathcal{K}_i} \otimes \omega_j \otimes \mathbb{1}_{\otimes_{i=j+1}^{n}\mathcal{K}_i}$, so that $\log\omega_j$ is a self-adjoint element of $\mathcal{O}$ and

$$\log\omega = \sum_{j=1}^{n} \log\omega_j.$$

Accordingly, the entropy production observable of the system can be written as

$$\sigma = \mathrm{i}[\log\omega, H] = \sum_j \sigma_j,$$

where $\sigma_j = \mathrm{i}[\log\omega_j, H]$. Similarly, the relative Hamiltonian $\ell_{\omega_t|\omega}$ decomposes as

$$\ell_{\omega_t|\omega} = \sum_{j=1}^{n} \ell_{\omega_{jt}|\omega_j},$$

where

$$\ell_{\omega_{jt}|\omega_j} = \tau^{-t}(\log\omega_j) - \log\omega_j = \int_0^t \tau^{-s}(\sigma_j)\mathrm{d}s.$$

If the system $(\mathcal{O}, \tau^t, \omega)$ is TRI with time-reversal Θ, we shall always assume that

$$\Theta(\omega_j) = \omega_j.$$

This implies

$$\Theta(\sigma_j) = -\sigma_j.$$

For $\boldsymbol{\alpha} = (\alpha_1, \cdots, \alpha_n) \in \mathbb{R}^n$ we denote $\omega^{\boldsymbol{\alpha}} = \omega_1^{\alpha_1}\cdots\omega_n^{\alpha_n}$. Similarly,

$$\omega_t^{\boldsymbol{\alpha}} = \mathrm{e}^{-\mathrm{i}tH}\omega^{\boldsymbol{\alpha}}\mathrm{e}^{\mathrm{i}tH} = \prod_{j=1}^{n}\omega_{jt}^{\alpha_j}.$$

We also denote $\mathbf{1} = (1, \ldots, 1)$ and $\mathbf{0} = (0, \ldots, 0)$. The multi-parameter entropic pressure functionals are defined for $t \in \mathbb{R}$ and $\boldsymbol{\alpha} \in \mathbb{R}^n$ by

$$e_{p,t}(\boldsymbol{\alpha}) = \begin{cases} \log \mathrm{tr}\left[\left(\omega^{\frac{\mathbf{1}-\boldsymbol{\alpha}}{p}}\omega_t^{\frac{2\boldsymbol{\alpha}}{p}}\omega^{\frac{\mathbf{1}-\boldsymbol{\alpha}}{p}}\right)^{\frac{p}{2}}\right] & \text{for } 1 \le p < \infty, \\ \log \mathrm{tr}\left(\mathrm{e}^{\log\omega + \sum_j \alpha_j \ell_{\omega_{jt}|\omega_j}}\right) & \text{for } p = \infty. \end{cases}$$

These functionals are natural generalizations of the functionals introduced in Section 3.3 and have very similar properties:

Proposition 3.9 (1) *The function $[1,\infty] \ni p \mapsto e_{p,t}(\boldsymbol{\alpha})$ is continuous and monotonically increasing.*

(2) *The function $\mathbb{R}^n \ni \boldsymbol{\alpha} \mapsto e_{p,t}(\boldsymbol{\alpha})$ is real-analytic, convex, and $e_{p,t}(\mathbf{0}) = e_{p,t}(\mathbf{1}) = 0$.*

(3) $e_{p,t}(\boldsymbol{\alpha}) = e_{p,-t}(\mathbf{1}-\boldsymbol{\alpha})$.

(4) $\partial_{\alpha_j} e_{p,t}(\boldsymbol{\alpha})|_{\boldsymbol{\alpha}=\mathbf{0}} = \omega(\ell_{\omega_{jt}|\omega_j})$.

(5)
$$\partial_{\alpha_k}\partial_{\alpha_j} e_{\infty,t}(\boldsymbol{\alpha})|_{\boldsymbol{\alpha}=\mathbf{0}} = \langle \ell_{\omega_{kt}|\omega_k} | \ell_{\omega_{jt}|\omega_j}\rangle_\omega - \omega(\ell_{\omega_{kt}|\omega_k})\omega(\ell_{\omega_{jt}|\omega_j}).$$

(6)
$$\partial_{\alpha_k}\partial_{\alpha_j} e_{2,t}(\boldsymbol{\alpha})|_{\boldsymbol{\alpha}=\mathbf{0}} = \frac{1}{2}\int_0^t\int_0^t \omega\left((\sigma_{ks} - \omega(\sigma_{ks}))(\sigma_{ju} - \omega(\sigma_{ju}))\right)\mathrm{d}s\mathrm{d}u.$$

(7) *If* $(\mathcal{O}, \tau^t, \omega)$ *is TRI, then the finite time Evans-Searles* (ES) *symmetry holds:*

$$e_{p,t}(\boldsymbol{\alpha}) = e_{p,t}(\mathbf{1} - \boldsymbol{\alpha}).$$

The proof, which is similar to the proof of Proposition 3.3, is left as an exercise.

In order to express the multi-parameter entropic pressure functionals in terms of the modular structure of $(\mathcal{O}, \omega)$, we have to extend the definition of relative modular operator. Let us briefly indicate how to proceed. The main problem is that ω_j is not a state on $\mathcal{O}$ (it is not properly normalized, and cannot be normalized in the thermodynamic limit since the dimensions of the Hilbert spaces $\mathcal{K}_i$ diverge in this limit). However, as a state on $\mathcal{O}_j$, ω_j has a modular group ς_{ω_j} and a modular operator Δ_{ω_j} such that

$$\varsigma_{\omega_j}^s(A) = \Delta_{\omega_j}^{\mathrm{i}s} A \Delta_{\omega_j}^{-\mathrm{i}s}.$$

The formula

$$\mathbb{R}^n \ni \mathbf{s} = (s_1, \ldots, s_n) \mapsto \varsigma_\omega^{\mathbf{s}} = \bigotimes_{j=1}^n \varsigma_{\omega_j}^{s_j},$$

defines an abelian group of $*$-automorphisms of $\mathcal{O}$. With a slight abuse of language, we shall refer to the multi-parameter group $\varsigma_\omega^{\mathbf{s}}$ as the modular group of ω. We denote by

$$\Delta_\omega^{\mathrm{i}\mathbf{s}} = \bigotimes_{j=1}^n \Delta_{\omega_j}^{\mathrm{i}s_j}.$$

the corresponding abelian unitary group. Setting

$$\varsigma_{\omega_t}^{\mathbf{s}} = \tau^{-t} \circ \varsigma_\omega^{\mathbf{s}} \circ \tau^t,$$

we clearly have $\varsigma_\omega^{\mathbf{s}}(A) = \omega^{\mathrm{i}\mathbf{s}} A \omega^{-\mathrm{i}\mathbf{s}}$ and $\varsigma_{\omega_t}^{\mathbf{s}}(A) = \omega_t^{\mathrm{i}\mathbf{s}} A \omega_t^{-\mathrm{i}\mathbf{s}}$.

The two modular groups $\varsigma_\omega^{\mathbf{s}}$ and $\varsigma_{\omega_t}^{\mathbf{s}}$ are related by

$$\varsigma_{\omega_t}^{\mathbf{s}}(A) = [D\omega_t : D\omega]^{\mathbf{s}} \varsigma_\omega^{\mathbf{s}}(A) [D\omega : D\omega_t]^{\mathbf{s}},$$

where the unitary Connes cocycle

$$[D\omega_t : D\omega]^{\mathbf{s}} = \omega_t^{\mathrm{i}\mathbf{s}} \omega^{-\mathrm{i}\mathbf{s}} = \mathrm{e}^{\mathrm{i}\sum_j s_j \tau^{-t}(\log \omega_j)} \mathrm{e}^{-\mathrm{i}\sum_j s_j \log \omega_j} = \mathrm{e}^{-\mathrm{i}tH} \mathrm{e}^{\mathrm{i}t\varsigma_\omega^{\mathbf{s}}(H)}, \tag{3.14}$$

satisfies the two multiplicative cocycle relations

$$\begin{aligned} [D\omega_t : D\omega]^{\mathbf{s}} \varsigma_\omega^{\mathbf{s}}([D\omega_t : D\omega]^{\mathbf{s}'}) &= [D\omega_t : D\omega]^{\mathbf{s}+\mathbf{s}'}, \\ \tau^{-t}([D\omega_{t'} : D\omega]^{\mathbf{s}})[D\omega_t : D\omega]^{\mathbf{s}} &= [D\omega_{t+t'} : D\omega]^{\mathbf{s}}. \end{aligned} \tag{3.15}$$

Thanks to the first relation,

$$\mathbb{R}^n \ni \mathbf{s} \mapsto \Delta_{\omega_t|\omega}^{\mathrm{i}\mathbf{s}} = L([D\omega_t : D\omega]^{\mathbf{s}}) \Delta_\omega^{\mathrm{i}\mathbf{s}},$$

defines an abelian group of unitaries on $\mathcal{H}_{\mathcal{O}}$. One easily checks that $\Delta_{\omega_t|\omega}^{\mathrm{i}\mathbf{s}} \xi = \omega_t^{\mathrm{i}\mathbf{s}} \xi \omega^{-\mathrm{i}\mathbf{s}}$. The relative Hamiltonian $\ell_{\omega_{jt}|\omega_j} = \tau^{-t}(\log \omega_j) - \log \omega_j$ is given by

$$\ell_{\omega_{jt}|\omega_j} = \frac{1}{\mathrm{i}} \frac{\mathrm{d}}{\mathrm{d}s_j} [D\omega_t : D\omega]^{\mathbf{s}} \bigg|_{\mathbf{s}=\mathbf{0}}.$$

Using Theorem 2.25 and the fact that $\Delta_\omega^{\boldsymbol{\alpha}/p} \xi_\omega = \xi_\omega$ it is now easy to show that, for $p \in [1, \infty[$,

$$e_{p,t}(\boldsymbol{\alpha}) = \log \|\Delta_{\omega_t|\omega}^{\boldsymbol{\alpha}/p} \xi_\omega\|_{\omega,p}^p = \log \|[D\omega_t : D\omega]^{-\mathrm{i}\boldsymbol{\alpha}/p} \xi_\omega\|_{\omega,p}^p, \tag{3.16}$$

while Theorem 2.15 leads to

$$e_{\infty,t}(\boldsymbol{\alpha}) = \max_{\rho\in\mathfrak{S}}\left(S(\rho|\omega) + \sum_{j=1}^{n}\alpha_j\rho(\ell_{\omega_{jt}|\omega_j})\right).$$

In particular, one has

$$e_{2,t}(\boldsymbol{\alpha}) = \log(\xi_\omega|\Delta_{\omega_t|\omega}^{\boldsymbol{\alpha}}\xi_\omega) = \log\omega([D\omega_t : D\omega]^{-\mathrm{i}\boldsymbol{\alpha}}).$$

One can also generalize Theorem 3.6 to the present setup. To this end, let K be the standard Liouvillean of the dynamics τ^t. With $\mathbf{s}\in\mathbb{R}^n$, the second cocycle relation (3.15) allows us to construct the unitary group

$$\mathrm{e}^{-\mathrm{i}tK_{\mathbf{s}}} = R([D\omega_t : D\omega]^{\mathbf{s}})^*\mathrm{e}^{-\mathrm{i}tK},$$

on $\mathcal{H}_{\mathcal{O}}$. By (3.14), one has

$$\mathrm{e}^{-\mathrm{i}tK_{\mathbf{s}}}\xi = \mathrm{e}^{-\mathrm{i}tH}\xi\mathrm{e}^{\mathrm{i}tH}[D\omega_t : D\omega]^{\mathbf{s}} = \mathrm{e}^{-\mathrm{i}tH}\xi\mathrm{e}^{\mathrm{i}t\varsigma_\omega^{\mathbf{s}}(H)},$$

so that $K_{\mathbf{s}} = L(H) - R(\varsigma_\omega^{\mathbf{s}}(H))$. Analytic continuation of $\mathrm{e}^{-\mathrm{i}tK_{\mathbf{s}}}$ to $\mathbf{s} = \mathrm{i}(1/2 - 1/p)\mathbf{1}$ with $p\in[1,\infty]$ yields the group $U_p(t)$ of isometric implementation of the dynamics on the Araki-Masuda space $L^p(\mathcal{O},\omega)$ introduced in Section 3.4.

For $\boldsymbol{\alpha}\in[0,1]^n$ and $p\in[1,\infty]$, let us define

$$L_{\frac{p}{\boldsymbol{\alpha}}} = K_{\mathbf{s}}, \qquad \mathbf{s} = \mathrm{i}\left(\frac{\mathbf{1}}{2} - \frac{\boldsymbol{\alpha}}{p}\right).$$

From the identity

$$\mathrm{e}^{-\mathrm{i}tL_{\frac{p}{\boldsymbol{\alpha}}}}\xi_\omega = \omega_t^{\boldsymbol{\alpha}/p}\omega^{1/2-\boldsymbol{\alpha}/p} = [D\omega_t : D\omega]^{-\mathrm{i}\boldsymbol{\alpha}/p}\xi_\omega,$$

and Equ. (3.16) we deduce

$$e_{p,t}(\boldsymbol{\alpha}) = \log\|\mathrm{e}^{-\mathrm{i}tL_{\frac{p}{\boldsymbol{\alpha}}}}\xi_\omega\|_{\omega,p}^p.$$

In the special case $p=2$, this can be rewritten as

$$e_{2,t}(\boldsymbol{\alpha}) = \log(\xi_\omega|\mathrm{e}^{-\mathrm{i}tL_{\frac{1}{\boldsymbol{\alpha}}}}\xi_\omega).$$

Exercise 3.7. Show that the Connes cocycle $\Gamma(\mathbf{s},t) = [D\omega_t : D\omega]^{\mathbf{s}}$ satisfies the following differential equations,

$$-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\Gamma(\mathbf{s},t) = \tau^{-t}(\varsigma_\omega^{\mathbf{s}}(H) - H)\Gamma(\mathbf{s},t), \qquad \Gamma(\mathbf{s},0) = \mathbb{1},$$
$$-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}s_j}\Gamma(\mathbf{s},t) = \Gamma(\mathbf{s},t)\varsigma_\omega^{\mathbf{s}}(\tau^{-t}(\log\omega_j) - \log\omega_j), \qquad \Gamma(\mathbf{0},t) = \mathbb{1}.$$

Exercise 3.8. Assume that $H = H_0 + V$ with $[H_0,\omega] = 0$, *i.e.*, ω is a steady state for the dynamics τ_0^t generated by H_0. Show that

$$L_{\frac{1}{\boldsymbol{\alpha}}} = K_0 + L(V) - R(\varsigma_\omega^{\mathrm{i}(\boldsymbol{\alpha}-\mathbf{1}/2)}(V)),$$

where K_0 is the standard Liouvillean of τ_0^t.

3.8 Multi-parameter full counting statistics

We continue with the framework of the last section and extend to compound systems our discussion of full counting statistics started in Section 3.5.

With $\mathbf{1}_j = (0, \ldots, 1, \ldots, 0)$ (a single 1 at the j-th entry) we set

$$\Delta_{\omega_{jt}|\omega_j} = \Delta^{\mathbf{1}_j}_{\omega_t|\omega}.$$

In terms on the joint spectral measure Q^t of the commuting family of self-adjoint operators

$$-\frac{1}{t}\log\Delta_{\omega_{1t}|\omega_1}, \ldots, -\frac{1}{t}\log\Delta_{\omega_{nt}|\omega_n},$$

associated to the vector ξ_ω one has, for $\boldsymbol{\alpha} \in \mathbb{R}^n$,

$$(\xi_\omega|\Delta^{\boldsymbol{\alpha}}_{\omega_t|\omega}\xi_\omega) = (\xi_\omega|\mathrm{e}^{\sum_j \alpha_j \log \Delta_{\omega_{jt}|\omega_j}}\xi_\omega) = \int \mathrm{e}^{-t\boldsymbol{\alpha}\cdot\mathbf{s}}\,\mathrm{d}Q^t(\mathbf{s}).$$

Let $\mathfrak{r}$ denote the reflection $\mathfrak{r}(\mathbf{s}) = -\mathbf{s}$ on $\mathbb{R}^n$, and let $\overline{Q}^t = Q^t \circ \mathfrak{r}$ be the reflected spectral measure. The ES symmetry $e_{2,t}(\mathbf{1}-\boldsymbol{\alpha}) = e_{2,t}(\boldsymbol{\alpha})$ translates into

Proposition 3.10 *Suppose that $(\mathcal{O}, \tau^t, \omega)$ is TRI. Then the measures Q^t and $\overline{Q}^t$ are mutually absolutely continuous and*

$$\frac{\mathrm{d}\overline{Q}^t}{\mathrm{d}Q^t}(\mathbf{s}) = \mathrm{e}^{-t\mathbf{1}\cdot\mathbf{s}}.$$

To interpret this result, considered the vector observable

$$\mathbf{S} = (-\log\omega_1, \cdots, -\log\omega_n).$$

Since the ω_j's commute, the components of $\mathbf{S}$ can be simultaneously measured. Let $P_\mathbf{s}$ denote the joint spectral projection of $\mathbf{S}$ to the eigenvalue $\mathbf{s} \in \mathrm{sp}(\mathbf{S})$. The joint probability distribution of two measurements is

$$\mathrm{tr}\left(\mathrm{e}^{-\mathrm{i}tH}\omega P_\mathbf{s}\mathrm{e}^{\mathrm{i}tH}P_{\mathbf{s}'}\right).$$

Denote by $\mathbb{P}_t(\boldsymbol{\phi})$ the induced probability distribution of the vector $\boldsymbol{\phi} = (\mathbf{s}'-\mathbf{s})/t$ which describes the mean rate of change of $\mathbf{S}$ between the two measurements. For $\boldsymbol{\alpha} \in \mathbb{R}^n$ one has, by Proposition 3.9 (3),

$$\begin{aligned}(\xi_\omega|\Delta^{\boldsymbol{\alpha}}_{\omega_{-t}|\omega}\xi_\omega) = (\xi_\omega|\Delta^{\mathbf{1}-\boldsymbol{\alpha}}_{\omega_t|\omega}\xi_\omega) &= \mathrm{tr}(\omega_t^{\mathbf{1}-\boldsymbol{\alpha}}\omega^{\boldsymbol{\alpha}})\\ &= \sum_{\mathbf{s},\mathbf{s}'}\mathrm{e}^{-\sum_j \alpha_j(s'_j-s_j)}\mathrm{tr}(\mathrm{e}^{-\mathrm{i}tH}\omega P_\mathbf{s}\mathrm{e}^{\mathrm{i}tH}P_{\mathbf{s}'})\\ &= \sum_{\boldsymbol{\phi}}\mathrm{e}^{-\sum_j t\alpha_j\phi_j}\mathbb{P}_t(\boldsymbol{\phi}).\end{aligned}$$

As in Section 3.5, we can conclude that the spectral measure $\overline{Q}^{-t}$ coincide with the probability distribution $\mathbb{P}_t$. Assertion (4) and (6) of Proposition 3.9 yield the expectation and covariance of $\boldsymbol{\phi}$ w.r.t. $\mathbb{P}_t$,

$$\mathbb{E}_t(\phi_j) = -\frac{1}{t}\partial_{\alpha_j}e_{2,-t}(\boldsymbol{\alpha})\Big|_{\boldsymbol{\alpha}=0} = -\frac{1}{t}\omega(\ell_{\omega_{j(-t)}|\omega_j}) = \frac{1}{t}\int_0^t \omega(\sigma_{js})\mathrm{d}s,$$

$$\begin{aligned}\mathbb{E}_t(\phi_j\phi_k) - \mathbb{E}_t(\phi_j)\mathbb{E}_t(\phi_k) &= \frac{1}{t^2}\partial_{\alpha_j}\partial_{\alpha_k}e_{2,-t}(\boldsymbol{\alpha})\Big|_{\boldsymbol{\alpha}=0}\\ &= \frac{1}{2t^2}\int_0^t\int_0^t \omega\left((\sigma_{js}-\omega(\sigma_{js}))(\sigma_{ku}-\omega(\sigma_{ku}))\right)\mathrm{d}s\mathrm{d}u.\end{aligned}$$

If the system is TRI then $\overline{Q}^{-t} = Q^t$ and Theorem 3.10 yields the ES fluctuation relation

$$\frac{\mathbb{P}_t(-\boldsymbol{\phi})}{\mathbb{P}_t(\boldsymbol{\phi})} = \mathrm{e}^{-t\mathbf{1}\cdot\boldsymbol{\phi}}.$$

Exercise 3.9. The above formula for the covariance of the full counting statistics implies that

$$A_{jk} = \int_0^t \int_0^t \omega\left((\sigma_{js} - \omega(\sigma_{js}))(\sigma_{ku} - \omega(\sigma_{ku}))\right) \mathrm{d}s\mathrm{d}u,$$

is symmetric, $A_{jk} = A_{kj}$. Prove this directly, starting from the definition $\sigma_j = -\mathrm{i}[H, \log\omega_j]$.
Hint: show that

$$\begin{aligned}\int_0^t \int_0^t [\sigma_{js}, \sigma_{ku}]\mathrm{d}s\mathrm{d}u = [\log\omega_j, \log\omega_k] + \tau^t([\log\omega_j, \log\omega_k]) \\ - [\tau^t(\log\omega_j), \log\omega_k] - [\log\omega_j, \tau^t(\log\omega_k)].\end{aligned}$$

Exercise 3.10. Check that the tensor product structure (3.12) was never used in the last two sections. More precisely, replacing Assumption (3.13) with

$$\log\omega = \sum_{j=1}^n Q_j,$$

where $(Q_1, \ldots, Q_n)$ is a commuting family of self-adjoint elements of $\mathcal{O}$, and defining $\omega_j = \mathrm{e}^{Q_j}$ so that

$$\omega^{\boldsymbol{\alpha}} = \mathrm{e}^{\sum_{j=1}^n \alpha_j Q_j},$$

show that all the results of the two sections hold without modification.

3.9 Control parameters and fluxes

Suppose that our quantum dynamical system $(\mathcal{O}_X, \tau_X, \omega_X)$ depends on some control parameters $X = (X_1, \cdots, X_n) \in \mathbb{R}^n$. One can think of X_j's as mechanical or thermodynamical forces acting on the system. We denote by H_X the Hamiltonian generating the dynamics τ_X^t, by σ_X the entropy production observable, etc. We assume that ω_0 is τ_0^t invariant and refer to the value $X = 0$ as *equilibrium*. Note that this implies $\sigma_0 = 0$. We adopt the shorthands $\tau^t = \tau_0^t$, $\omega = \omega_0$.

Definition 3.11 *A vector-valued observable $\boldsymbol{\Phi}_X = (\Phi_X^{(1)}, \cdots, \Phi_X^{(n)}) \in \mathcal{O}_{\mathrm{self}}^n$, is called a flux relation if, for all X,*

$$\sigma_X = \sum_{j=1}^n X_j \Phi_X^{(j)}.$$

In what follows we will consider a family of quadruples $(\mathcal{O}, \tau_X^t, \omega_X, \boldsymbol{\Phi}_X)_{X\in\mathbb{R}^n}$, where $\boldsymbol{\Phi}_X$ is a given flux relation. Somewhat colloquially, we will refer to $\Phi_X^{(j)}$ as the flux (or current) observable associated to the force X_j. In concrete models, physical requirements typically select a unique flux relation $\boldsymbol{\Phi}_X$.

If $(\mathcal{O}_X, \tau_X^t, \omega_X)_{X\in\mathbb{R}^N}$ are time-reversal invariant (TRI), we shall always assume that

$$\Theta_X(\boldsymbol{\Phi}_X) = -\boldsymbol{\Phi}_X. \tag{3.17}$$

This assumption implies that $\omega_X(\mathbf{\Phi}_X) = 0$ for all X.

Notation. For $\nu \in \mathfrak{S}$, $\vartheta \in \mathrm{Aut}(\mathcal{O})$, $\mathbf{A} = (A_1, \ldots, A_n) \in \mathcal{O}^n$, and $Y = (Y_1, \ldots, Y_n) \in \mathbb{C}^n$ we shall use the shorthands

$$\nu(\mathbf{A}) = (\nu(A_1), \cdots, \nu(A_n)) \in \mathbb{C}^n,$$

$$\vartheta(\mathbf{A}) = (\vartheta(A_1), \cdots \vartheta(A_n)) \in \mathcal{O}^n,$$

$$\tau^t(\mathbf{A}) = \mathbf{A}_t = (\tau^t(A_1), \cdots, \tau^t(A_n)) \in \mathcal{O}^n,$$

$$Y \cdot \mathbf{A} = \sum_{j=1}^n Y_j A_j \in \mathcal{O}.$$

The relative Hamiltonian of ω_{Xt} w.r.t. ω_X is given by

$$\ell_{\omega_{Xt}|\omega_X} = \int_0^t \tau_X^{-s}(\sigma_X)\,\mathrm{d}s = X \cdot \int_0^t \mathbf{\Phi}_{X(-s)}\mathrm{d}s = \sum_{j=1}^n X_j \int_0^t \tau_X^{-s}(\Phi_X^{(j)})\mathrm{d}s.$$

We generalize the $p = \infty$ entropic pressure functional

$$e_{\infty,t}(\alpha) = \log \mathrm{tr}\left(\mathrm{e}^{\log \omega_X + \alpha \ell_{\omega_{Xt}|\omega_X}}\right),$$

by introducing

$$e_t(X, Y) = \log \mathrm{tr}\left(\mathrm{e}^{\log \omega_X + Y \cdot \int_0^t \mathbf{\Phi}_{X(-s)}\mathrm{d}s}\right), \tag{3.18}$$

where $Y \in \mathbb{R}^n$. The basic properties of $e_t(X, Y)$ are summarized in the next proposition.

Proposition 3.12 (1)

$$e_t(X, Y) = \sup_{\nu \in \mathfrak{S}} \left[S(\nu|\omega_X) + Y \cdot \int_0^t \nu(\mathbf{\Phi}_{X(-s)})\,\mathrm{d}s\right].$$

(2) *The function $\mathbb{R}^n \ni Y \mapsto e_t(X, Y)$ is convex and real analytic.*

(3) $e_{-t}(X, Y) = e_t(X, X - Y)$.

(4)

$$\partial_{Y_j} e_t(X, Y)\big|_{Y=0} = \int_0^t \omega_X(\Phi_{X(-s)}^{(j)})\mathrm{d}s, \tag{3.19}$$

$$\begin{aligned}\partial_{Y_k}\partial_{Y_j} e_t(X, Y)\big|_{Y=0} = \int_0^t \int_0^t \Big(&\langle \Phi_{X(-s_1)}^{(k)} | \Phi_{X(-s_2)}^{(j)} \rangle_{\omega_X} \\ &- \omega_X(\Phi_{X(-s_1)}^{(k)})\omega_X(\Phi_{X(-s_2)}^{(j)})\Big)\,\mathrm{d}s_2\mathrm{d}s_1.\end{aligned} \tag{3.20}$$

(5) *If $(\mathcal{O}_X, \tau_X^t, \omega_X)_{X \in \mathbb{R}^n}$ is TRI, then $e_{-t}(X, Y) = e_t(X, Y)$ and*

$$e_t(X, Y) = e_t(X, X - Y). \tag{3.21}$$

We shall refer to Relation (3.21) as the finite time Generalized Evans-Searles (GES) symmetry. Notice that

$$e_t(X, \alpha X) = \log \mathrm{tr}(\mathrm{e}^{\log \omega_X + \alpha \ell_{\omega_{Xt}|\omega_X}}) = e_{\infty,t}(\alpha),$$

which shows that the ES-symmetry of $e_{\infty,t}(\alpha) = e_{\infty,t}(1 - \alpha)$ is a special case of the GES-symmetry.

Proof. (1) follows from Theorem 2.15. (2) Convexity follows from (1) and analyticity is obvious. (3) is a consequence of the following elementary calculation:

$$
\begin{aligned}
\log\omega_X + (X-Y)\cdot\int_0^t \mathbf{\Phi}_{X(-s)}\mathrm{d}s &= \log\omega_X + \ell_{\omega_{Xt}|\omega_X} - Y\cdot\int_0^t \mathbf{\Phi}_{X(-s)}\mathrm{d}s \\
&= \log\omega_{Xt} - Y\cdot\int_0^t \mathbf{\Phi}_{X(-s)}\mathrm{d}s \\
&= \mathrm{e}^{-\mathrm{i}tH_X}\left(\log\omega_X - Y\cdot\int_0^t \mathbf{\Phi}_{X(t-s)}\mathrm{d}s\right)\mathrm{e}^{\mathrm{i}tH_X} \\
&= \mathrm{e}^{-\mathrm{i}tH_X}\left(\log\omega_X - Y\cdot\int_0^t \mathbf{\Phi}_{Xs}\mathrm{d}s\right)\mathrm{e}^{\mathrm{i}tH_X} \\
&= \mathrm{e}^{-\mathrm{i}tH_X}\left(\log\omega_X + Y\cdot\int_0^{-t} \mathbf{\Phi}_{X(-s)}\mathrm{d}s\right)\mathrm{e}^{\mathrm{i}tH_X}.
\end{aligned}
$$

To prove (4) invoke Duhamel formula to differentiate (3.18) (see the proof of Assertion (5) of Proposition 3.3). (5) follows from (2) and Assumption (3.17) which implies that $\Theta_X(\mathbf{\Phi}_{X(-s)}) = -\mathbf{\Phi}_{Xs}$, so that

$$
\begin{aligned}
\Theta_X\left(\log\omega_X + Y\cdot\int_0^t \mathbf{\Phi}_{X(-s)}\mathrm{d}s\right) &= \log\omega_X - Y\cdot\int_0^t \mathbf{\Phi}_{Xs}\mathrm{d}s \\
&= \log\omega_X + Y\cdot\int_0^{-t} \mathbf{\Phi}_{X(-s)}\mathrm{d}s.
\end{aligned}
$$

□

3.10 Finite time linear response theory

Finite time linear response theory is concerned with the first order perturbation theory (w.r.t. X) of the expectation values

$$\langle\mathbf{\Phi}_X\rangle_t = \frac{1}{t}\int_0^t \omega_X(\mathbf{\Phi}_{Xs})\mathrm{d}s.$$

In the discussion of linear response theory we shall always assume that functions

$$X\mapsto H_X, \qquad X\mapsto\omega_X, \qquad X\mapsto\mathbf{\Phi}_X,$$

are continuously differentiable. This implies that the function $X\mapsto\langle\mathbf{\Phi}_X\rangle_t$ is continuously differentiable for all t.

The finite time kinetic transport coefficients are defined by

$$L_{jkt} = \partial_{X_k}\langle\Phi_X^{(j)}\rangle_t\big|_{X=0}.$$

Since

$$\langle\sigma_X\rangle_t = \sum_j X_j\langle\Phi_X^{(j)}\rangle_t = \sum_{j,k} L_{jkt}X_jX_k + o(|X|^2) \geq 0, \tag{3.22}$$

the *real* quadratic form determined by the finite time Onsager matrix $[L_{jkt}]$ is positive definite. This fact does not depend on the TRI assumption and *does not* imply that $L_{jkt} = L_{kjt}$. We shall call the relations

$$L_{jkt} = L_{kjt},$$

the finite time Onsager reciprocity relations (ORR). As a general structural relations, they can hold only for TRI systems.

Another direct consequence of (3.22) is:

Proposition 3.13 *Let $\mathbf{\Phi}_X, \widetilde{\mathbf{\Phi}}_X$ be two flux relations. Then the corresponding finite time transport coefficients satisfy*

$$L_{jkt} + L_{kjt} = \widetilde{L}_{jkt} + \widetilde{L}_{kjt}.$$

If the finite time ORR hold, then $L_{jkt} = \widetilde{L}_{jkt}$.

The next proposition shows that the finite time ORR and Green-Kubo formula follow from the finite time GES symmetry. Recall our notational convention $\tau^t_{X=0} = \tau^t$, $\omega_{X=0} = \omega$, $\Phi^{(j)}_{X=0} = \Phi^{(j)}$, etc.

Proposition 3.14 *If $(\mathcal{O}_X, \tau^t_X, \omega_X)_{X\in\mathbb{R}^n}$ is TRI, then*

(1)
$$L_{jkt} = \frac{1}{2}\int_{-t}^{t} \langle \Phi^{(k)} | \tau^s(\Phi^{(j)})\rangle_\omega \left(1 - \frac{|s|}{t}\right) \mathrm{d}s,$$

(2) $L_{jkt} = L_{kjt}$.

Proof. By Relation (3.19) and the TRI property one has

$$\langle \Phi^{(j)}_X \rangle_t = -\partial_{Y_j} \frac{1}{t} e_t(X,Y)\big|_{Y=0},$$

so that

$$L_{jkt} = -\partial_{X_k}\partial_{Y_j} \frac{1}{t} e_t(X,Y)\big|_{X=Y=0}.$$

The GES-symmetry implies that

$$-\partial_{X_k}\partial_{Y_j} \frac{1}{t} e_t(X,Y)\big|_{X=Y=0} = \frac{1}{2t}\partial_{Y_k Y_j} e_t(0,Y)\big|_{Y=0},$$

(recall the derivation of (1.37)). Since $\omega(\mathbf{\Phi}) = 0$ and ω is τ^t invariant, Relation (3.20) yields

$$L_{jkt} = \frac{1}{2t}\int_0^t\int_0^t \langle \Phi^{(k)}_{-s_1} | \Phi^{(j)}_{-s_2}\rangle_\omega \mathrm{d}s_1\mathrm{d}s_2 = \frac{1}{2t}\int_0^t\int_0^t \langle \Phi^{(k)} | \Phi^{(j)}_{s_1-s_2}\rangle_\omega \mathrm{d}s_1\mathrm{d}s_2.$$

A simple change of integration variable leads to (1). (2) follows from the equality of the mixed partial derivatives $\partial_{Y_k}\partial_{Y_j} e_t(0,Y) = \partial_{Y_j}\partial_{Y_k} e_t(0,Y)$. □

Chapter 4

Open quantum systems

4.1 Coupling to reservoirs

Let $\mathcal{R}_j$, $j = 1, \cdots, n$, be finite quantum systems with Hilbert spaces $\mathcal{K}_j$. Each $\mathcal{R}_j$ is described by a quantum dynamical system $(\mathcal{O}_j, \tau_j^t, \omega_j)$. Besides the Hamiltonian H_j which generates τ_j, we assume the existence of a "conserved charge" N_j, a self-adjoint element of $\mathcal{O}_j$ such that $[H_j, N_j] = 0$. It follows that N_j is invariant under the dynamics τ_j^t and that the gauge group $\vartheta_j^t(A) = \mathrm{e}^{\mathrm{i}tN_j} A \mathrm{e}^{-\mathrm{i}tN_j}$ commutes with τ_j^t. We suppose that $\mathcal{R}_j$ is in thermal equilibrium at inverse temperature β_j and chemical potential μ_j, *i.e.*, that

$$\omega_j = \frac{\mathrm{e}^{-\beta_j(H_j - \mu_j N_j)}}{\mathrm{tr}(\mathrm{e}^{-\beta_j(H_j - \mu_j N_j)})}.$$

The modular group of this state is given by

$$\varsigma_{\omega_j}^t = \tau_j^{-\beta_j t} \circ \vartheta_j^{\beta_j \mu_j t}.$$

Thus, denoting by $\delta_j = \mathrm{i}[H_j, \cdot\,]$ the generator of τ_j^t and by $\xi_j = \mathrm{i}[N_j, \cdot\,]$ the generator of ϑ_j^t, one has

$$\delta_{\omega_j} = -\beta_j(\delta_j - \mu_j \xi_j).$$

Note that in cases where there is no conserved charge, one may simply set $N_j = \mathbb{1}_{\mathcal{K}_j}$ so that the gauge group becomes trivial, $\xi_j = 0$, and the states ω_j independent of the chemical potential μ_j. In such cases, one can simply set $\mu_j = 0$.

The joint system $\mathcal{R} = \mathcal{R}_1 + \cdots + \mathcal{R}_n$ is described by

$$(\mathcal{O}_\mathcal{R}, \tau_\mathcal{R}^t, \omega_\mathcal{R}) = \bigotimes_{j=1}^n (\mathcal{O}_j, \tau_j^t, \omega_j).$$

The generators of the dynamics $\tau_\mathcal{R}^t$, the gauge group $\vartheta_\mathcal{R}^t = \otimes_{j=1}^n \vartheta_j^t$ and the modular group $\varsigma_{\omega_\mathcal{R}}^t = \otimes_{j=1}^n \varsigma_{\omega_j}^t$ are given by

$$\begin{array}{rclclcrcl}
\delta_\mathcal{R} & = & \sum_{j=1}^n \delta_j & = & \mathrm{i}[H_\mathcal{R}, \cdot\,], & \qquad & H_\mathcal{R} & = & \sum_{j=1}^n H_j, \\
\xi_\mathcal{R} & = & \sum_{j=1}^n \xi_j & = & \mathrm{i}[N_\mathcal{R}, \cdot\,], & & N_\mathcal{R} & = & \sum_{j=1}^n N_j, \\
\delta_{\omega_\mathcal{R}} & = & \sum_{j=1}^n \delta_{\omega_j} & = & \mathrm{i}[\log \omega_\mathcal{R}, \cdot\,], & & \log \omega_\mathcal{R} & = & -\sum_{j=1}^n \beta_j (H_j - \mu_j N_j),
\end{array}$$

with the notational convention of Section 3.7.

Let $\mathcal{S}$ be a finite quantum system described by $(\mathcal{O}_\mathcal{S}, \tau_\mathcal{S}^t, \omega_\mathcal{S})$, the dynamics $\tau_\mathcal{S}^t$ being generated by the Hamiltonian $H_\mathcal{S}$. We assume the existence of a conserved charge $N_\mathcal{S}$ such that $\mathrm{i}[H_\mathcal{S}, N_\mathcal{S}] = 0$ and denote $\vartheta_\mathcal{S}^t$ the corresponding gauge group on $\mathcal{O}_\mathcal{S}$.

A gauge invariant coupling of $\mathcal{S}$ to the system of reservoirs $\mathcal{R}$ is a collection of self-adjoint elements $V_j \in \mathcal{O}_\mathcal{S} \otimes \mathcal{O}_j$ such that $[N_j + N_\mathcal{S}, V_j] = 0$. Denoting $V = \sum_j V_j$, the Hamiltonian

$$H_V = H_\mathcal{R} + H_\mathcal{S} + V,$$

generates a perturbation τ_V^t of the dynamics $\tau^t = \tau_\mathcal{S}^t \otimes \tau_\mathcal{R}^t$ on $\mathcal{O} = \mathcal{O}_\mathcal{S} \otimes \mathcal{O}_\mathcal{R}$. Moreover, τ_V^t preserves the total charge $N = N_\mathcal{R} + N_\mathcal{S}$ and hence commutes with the gauge group $\vartheta^t = \vartheta_\mathcal{S}^t \otimes \vartheta_\mathcal{R}^t$.

The quantum dynamical system $(\mathcal{O}, \tau_V^t, \omega)$, where $\omega = \omega_\mathcal{S} \otimes \omega_\mathcal{R}$, is called *open quantum system*. Open quantum systems are examples of compound systems considered in Sections 3.7–3.8.

The definition of open quantum system requires some minor modifications if the particle statistics (bosons/fermions) is taken into account. These modifications are straightforward (see Section 6.6 for an example) and for simplicity of exposition we shall not discuss them in abstract form.

The entropy production observable of $(\mathcal{O}, \tau_V^t, \omega)$ is

$$\sigma = \delta_\omega(H_V).$$

Since

$$\delta_\omega = \delta_{\omega_\mathcal{R}} + \delta_{\omega_\mathcal{S}} = -\sum_j \beta_j(\delta_j - \mu_j \xi_j) - \mathrm{i}[Q, \cdot\,],$$

where $Q = -\log \omega_\mathcal{S}$, we have

$$\sigma = -\sum_j \beta_j(\Phi_j - \mu_j \mathcal{J}_j) + \sigma_\mathcal{S}, \tag{4.1}$$

where

$$\Phi_j = \delta_j(V), \qquad \mathcal{J}_j = \xi_j(V), \qquad \sigma_\mathcal{S} = \mathrm{i}[H_V, Q].$$

Observing that

$$\Phi_j = -\mathrm{i}[H_V, H_j], \qquad \mathcal{J}_j = -\mathrm{i}[H_V, N_j], \tag{4.2}$$

we derive

$$H_{jt} - H_j = -\int_0^t \Phi_{js} \mathrm{d}s, \qquad N_{jt} - N_j = -\int_0^t \mathcal{J}_{js} \mathrm{d}s. \tag{4.3}$$

The observables Φ_j and $\mathcal{J}_j$ describe the energy and charge fluxes out of the j-th reservoir $\mathcal{R}_j$. The observable $\beta_j(\Phi_j - \mu_j \mathcal{J}_j)$ describes entropy flux out of $\mathcal{R}_j$.

The entropy balance equation (more precisely Inequality (3.4)) implies

$$\begin{aligned}\rho_t(Q) - \rho(Q) &\geq \sum_j \beta_j \int_0^t \rho_s(\Phi_j - \mu_j \mathcal{J}_j)\mathrm{d}s \\ &= \sum_j \beta_j \left[(\rho(H_j) - \rho_t(H_j)) - \mu_j(\rho(N_j) - \rho_t(N_j))\right],\end{aligned} \tag{4.4}$$

for any state ρ on $\mathcal{O}$. We note in particular that if ρ is a steady state for the dynamics τ_V^t then both sides of this inequality vanish as long as the joint system remains finite. However, if the reservoirs become infinitely extended while the system $\mathcal{S}$ remains confined then the observable Q remains well defined while H_j and N_j loose their meaning. A very important feature of the proper mathematical formulation of (4.4) in the thermodynamic limit is that the left hand side still vanishes while the right hand side is typically non-zero.

Note also that

$$\omega_t = Z^{-1} \mathrm{e}^{-Q_{-t} - \sum_j \beta_j [(H_j - \mu_j N_j) + \int_0^t (\Phi_{j(-s)} - \mu_j \mathcal{J}_{j(-s)})\mathrm{d}s]}, \tag{4.5}$$

where

$$Z = \mathrm{tr}(\mathrm{e}^{-\sum_j \beta_j (H_j - \mu_j N_j)}).$$

The density matrix ω_t expressed in the form (4.5) is known as McLennan-Zubarev dynamical ensemble.

4.2 Full counting statistics

We continue with the framework of the previous subsection and adapt our discussion of full counting statistics from Section 3.8 to the open quantum system $(\mathcal{O}, \tau_V^t, \omega)$. We note that the reference state ω factorizes into a product of commuting self-adjoint operators

$$\omega = Z^{-1}\mathrm{e}^{-Q-\sum_{j=1}^n \beta_j H_j + \sum_{j=1}^n \beta_j\mu_j N_j} = Z^{-1}\mathrm{e}^{-Q}\left(\prod_{j=1}^n \mathrm{e}^{-\beta_j H_j}\right)\left(\prod_{j=1}^n \mathrm{e}^{\beta_j\mu_j N_j}\right).$$

Defining, according to Exercise 3.10,

$$\omega^{\boldsymbol{\alpha}} = Z^{-\gamma_0}\mathrm{e}^{-\gamma_0 Q}\left(\prod_{j=1}^n \mathrm{e}^{-\gamma_j\beta_j H_j}\right)\left(\prod_{j=1}^n \mathrm{e}^{\gamma_j'\beta_j\mu_j N_j}\right),$$

for $\boldsymbol{\alpha} = (\gamma_0, \boldsymbol{\gamma}, \boldsymbol{\gamma}') \in \mathbb{R}\times\mathbb{R}^n\times\mathbb{R}^n$ we have,

$$\operatorname{tr}(\omega_t^{\mathbf{1}-\boldsymbol{\alpha}}\omega^{\boldsymbol{\alpha}}) = \sum_{q,\boldsymbol{\varepsilon},\boldsymbol{\nu}} \mathrm{e}^{-t(\gamma_0 q + \boldsymbol{\gamma}\cdot\boldsymbol{\varepsilon} + \boldsymbol{\gamma}'\cdot\boldsymbol{\nu})}\mathbb{P}_t(q, \boldsymbol{\varepsilon}, \boldsymbol{\nu}), \tag{4.6}$$

where $\mathbb{P}_t(q, \boldsymbol{\varepsilon}, \boldsymbol{\nu})$ is the joint probability distribution for the mean rates of change of the commuting set of observables

$$\mathbf{S} = (Q, \beta_1 H_1, \ldots, \beta_n H_n, -\beta_1\mu_1 N_1, \ldots, -\beta_n\mu_n N_n),$$

between two successive joint measurements at time 0 and t. The sum in (4.6) extends over all $(q, \boldsymbol{\varepsilon}, \boldsymbol{\nu}) \in (\mathrm{sp}(\mathbf{S}) - \mathrm{sp}(\mathbf{S}))/t$. As shown in Section 3.8, the distribution $\mathbb{P}_t$ coincide with the joint spectral measure of a family of commuting relative modular operators.

Expectation and covariance of $(\boldsymbol{\varepsilon}, \boldsymbol{\nu})$ w.r.t. $\mathbb{P}_t$ are given by

$$\begin{aligned}\mathbb{E}_t(\varepsilon_j) &= -\frac{\beta_j}{t}\int_0^t \omega_s(\Phi_j)\mathrm{d}s,\\ \mathbb{E}_t(\nu_j) &= \frac{\beta_j\mu_j}{t}\int_0^t \omega_s(\mathcal{J}_j)\mathrm{d}s,\end{aligned} \tag{4.7}$$

and,

$$\begin{aligned}\mathbb{E}_t(\varepsilon_j\varepsilon_k) - \mathbb{E}_t(\varepsilon_j)\mathbb{E}_t(\varepsilon_k) &= \frac{\beta_j\beta_k}{t^2}\int_0^t\int_0^t \omega\left((\Phi_{js} - \omega(\Phi_{js}))(\Phi_{ku} - \omega(\Phi_{ku}))\right)\mathrm{d}s\mathrm{d}u,\\ \mathbb{E}_t(\nu_j\nu_k) - \mathbb{E}_t(\nu_j)\mathbb{E}_t(\nu_k) &= \frac{\beta_j\mu_j\beta_k\mu_k}{t^2}\int_0^t\int_0^t \omega\left((\mathcal{J}_{js} - \omega(\mathcal{J}_{js}))(\mathcal{J}_{ku} - \omega(\mathcal{J}_{ku}))\right)\mathrm{d}s\mathrm{d}u,\\ \mathbb{E}_t(\varepsilon_j\nu_k) - \mathbb{E}_t(\varepsilon_j)\mathbb{E}_t(\nu_k) &= -\frac{\beta_j\beta_k\mu_k}{t^2}\int_0^t\int_0^t \omega\left((\Phi_{js} - \omega(\Phi_{js}))(\mathcal{J}_{ku} - \omega(\mathcal{J}_{ku}))\right)\mathrm{d}s\mathrm{d}u.\end{aligned} \tag{4.8}$$

In terms of Liouvillean, the moment generating function (4.6) reads

$$\operatorname{tr}(\omega_t^{\mathbf{1}-\boldsymbol{\alpha}}\omega^{\boldsymbol{\alpha}}) = (\xi_\omega|\mathrm{e}^{\mathrm{i}tL_{\frac{1}{\boldsymbol{\alpha}}}}\xi_\omega), \tag{4.9}$$

with (as derived in Exercise 3.8)

$$L_{\frac{1}{\boldsymbol{\alpha}}} = K_0 + L(V) - R(W_{\boldsymbol{\alpha}}), \tag{4.10}$$

where K_0 denotes the standard Liouvillean of the decoupled dynamics τ^t,

$$W_{\boldsymbol{\alpha}} = \varsigma_\omega^{\mathrm{i}(\boldsymbol{\alpha}-\mathbf{1}/2)}(V) = \sum_{j=1}^n T_j(\boldsymbol{\alpha})V_jT_j(\boldsymbol{\alpha})^{-1},$$

and

$$T_j(\boldsymbol{\alpha}) = \mathrm{e}^{-(1/2-\gamma_0)Q-\beta_j[(1/2-\gamma_j)H_j-\mu_j(1/2-\gamma_j')N_j]}.$$

If $(\mathcal{O}, \tau_V^t, \omega)$ is TRI, then the fluctuation relation

$$\frac{\mathbb{P}_t(-q,-\boldsymbol{\varepsilon},-\boldsymbol{\nu})}{\mathbb{P}_t(q,\boldsymbol{\varepsilon},\boldsymbol{\nu})} = \mathrm{e}^{-t(q+\mathbf{1}\cdot\boldsymbol{\varepsilon}+\mathbf{1}\cdot\boldsymbol{\nu})},$$

holds.

4.3 Linear response theory

We continue our discussion of open quantum systems. We now adopt the point of view of Section 3.9 and describe finite time linear response theory. Let $\beta_{\rm eq}$ and $\mu_{\rm eq}$ be given equilibrium values of the inverse temperature and chemical potential. The thermodynamical forces $X = (X_1, \cdots, X_{2n})$ are

$$X_j = \beta_{\rm eq} - \beta_j, \quad X_{n+j} = -\beta_{\rm eq}\mu_{\rm eq} + \beta_j\mu_j, \quad (j = 1, \ldots, n).$$

The reference state of the system is taken to be

$$\omega_X = Z_X^{-1}\mathrm{e}^{-\beta_{\rm eq}(H_V-\mu_{\rm eq}N)+\sum_{j=1}^n(X_jH_j+X_{n+j}N_j)},$$

where $N = N_{\mathcal{R}} + N_{\mathcal{S}}$ and $Z_X = \mathrm{tr}(\mathrm{e}^{-\beta_{\rm eq}(H_V-\mu_{\rm eq}N)+\sum_{j=1}^n(X_jH_j+X_{n+j}N_j)})$. Clearly,

$$\omega_0 = Z_0^{-1}\mathrm{e}^{-\beta_{\rm eq}(H_V-\mu_{\rm eq}N)},$$

is the thermal equilibrium state of $(\mathcal{O}, \tau_V^t)$ at inverse temperature $\beta_{\rm eq}$ and chemical potential $\mu_{\rm eq}$. Hence, we shall use the notation $\omega_0 = \omega_{\rm eq}$. The dynamical system $(\mathcal{O}, \tau_V^t, \omega_X)$ fits into the framework of Section 3.9 (with $\tau_X^t = \tau_V^t$ independent of X).

Note that the family of states ω_X is distinct from the one used in the previous section: it contains the coupling V. In particular, ω_X is not a product state. This is however in complete parallel with our discussion of linear response theory in classical harmonic chain. If the perturbation V remains local in the thermodynamic limit, the product state ω and the state ω_X describe the same thermodynamics. We shall discuss this issue in more details in Section 5.9.

The entropy production observable of the dynamical system $(\mathcal{O}, \tau_V^t, \omega_X)$ is

$$\sigma_X = \mathrm{i}[\log\omega_X, H_V] = \sum_{j=1}^n X_j\Phi_j + X_{n+j}\mathcal{J}_j, \tag{4.11}$$

where the observables

$$\Phi_j = -\mathrm{i}[H_V, H_j], \qquad \mathcal{J}_j = -\mathrm{i}[H_V, N_j],$$

describe the energy and charge flux out of the j-th reservoir. Clearly, (4.11) is a natural (and X-independent) flux relation. Φ_j is the flux associated to the thermodynamical force $\beta_{\rm eq} - \beta_j$ and $\mathcal{J}_j$ is the flux associated to the thermodynamical force $-\beta_{\rm eq}\mu_{\rm eq} + \beta_j\mu_j$.

The generalized entropic pressure is given by

$$e_t(X,Y) = \log\mathrm{tr}\left(\mathrm{e}^{\log\omega_X+\sum_{j=1}^n(Y_j\int_0^t\Phi_{j(-s)}\mathrm{d}s+Y_{n+k}\int_0^t\mathcal{J}_{j(-s)}\mathrm{d}s)}\right).$$

Recall that the equilibrium canonical correlation is

$$\langle A|B\rangle_{\rm eq} = \int_0^1 \omega_{\rm eq}(A^*\tau_V^{\mathrm{i}\beta s}(B))\mathrm{d}s.$$

Proposition 3.14 implies the finite Green-Kubo formulas and finite time Onsager reciprocity relations for energy and charge fluxes.

Proposition 4.1 *Suppose that $(\mathcal{O}, \tau_V^t, \omega_{\rm eq})$ is TRI with time reversal Θ satisfying $\Theta(V_j) = V_j$, $\Theta(H_j) = H_j$ and $\Theta(N_j) = N_j$ for all j. Then*

$$\begin{aligned}
L^{\rm ee}_{jkt} &= \partial_{X_k} \quad \left.\left(\frac{1}{t}\int_0^t \omega_X(\Phi_{js}){\rm d}s\right)\right|_{X=0} = \frac{1}{2}\int_{-t}^t \langle \Phi_k|\Phi_{js}\rangle_{\rm eq}\left(1-\frac{|s|}{t}\right){\rm d}s,\\
L^{\rm ec}_{jkt} &= \partial_{X_{n+k}} \left.\left(\frac{1}{t}\int_0^t \omega_X(\Phi_{js}){\rm d}s\right)\right|_{X=0} = \frac{1}{2}\int_{-t}^t \langle \mathcal{J}_k|\Phi_{js}\rangle_{\rm eq}\left(1-\frac{|s|}{t}\right){\rm d}s,\\
L^{\rm ce}_{jkt} &= \partial_{X_k} \quad \left.\left(\frac{1}{t}\int_0^t \omega_X(\mathcal{J}_{js}){\rm d}s\right)\right|_{X=0} = \frac{1}{2}\int_{-t}^t \langle \Phi_k|\mathcal{J}_{js}\rangle_{\rm eq}\left(1-\frac{|s|}{t}\right){\rm d}s,\\
L^{\rm cc}_{jkt} &= \partial_{X_{n+k}} \left.\left(\frac{1}{t}\int_0^t \omega_X(\mathcal{J}_{js}){\rm d}s\right)\right|_{X=0} = \frac{1}{2}\int_{-t}^t \langle \mathcal{J}_k|\mathcal{J}_{js}\rangle_{\rm eq}\left(1-\frac{|s|}{t}\right){\rm d}s,
\end{aligned} \tag{4.12}$$

(the indices e/c *stand for energy/charge) and*

$$\begin{aligned}
L^{\rm ee}_{jkt} &= L^{\rm ee}_{kjt},\\
L^{\rm cc}_{jkt} &= L^{\rm cc}_{kjt},\\
L^{\rm ec}_{jkt} &= L^{\rm ce}_{kjt}.
\end{aligned}$$

The special structure of open quantum systems allows for a further insight into linear response theory. Consider the auxiliary Hamiltonian

$$H_X = H_V - \mu_{\rm eq} N - \frac{1}{\beta_{\rm eq}}\sum_{j=1}^n (X_j H_j + X_{n+j} N_j),$$

and note that

$$\omega_X = \frac{1}{Z_X}{\rm e}^{-\beta_{\rm eq} H_X},$$

where $Z_X = {\rm tr}({\rm e}^{-\beta_{\rm eq} H_X})$. Hence, ω_X is the $\beta_{\rm eq}$-KMS state of the dynamics τ_X^t generated by the Hamiltonian H_X. By Equ. (4.3) one has

$$\omega_{Xt} = {\rm e}^{-{\rm i}tH_V}\omega_X {\rm e}^{{\rm i}tH_V} = \frac{1}{Z_X}{\rm e}^{-\beta_{\rm eq}(H_X+P_t)},$$

where

$$P_t = -\frac{1}{\beta_{\rm eq}}\sum_j \left(X_j\int_0^t \Phi_{j(-s)}{\rm d}s + X_{n+j}\int_0^t \mathcal{J}_{j(-s)}{\rm d}s\right).$$

We conclude that ω_{Xt} is the KMS state at inverse temperature $\beta_{\rm eq}$ of the perturbed dynamics generated by $H_X + P_t$. Moreover, the perturbation satisfies $P_t = O(X)$ as $X \to 0$. Applying the perturbation expansion (2.32) and the formula for the coefficient $b_1(A)$ derived in Exercise 2.14, we obtain

$$\omega_{Xt}(A) = \omega_X(A) - \beta_{\rm eq}\int_0^1 \omega_X\left(P_t(\tau_X^{{\rm i}s\beta_{\rm eq}}(A) - \omega_X(A))\right){\rm d}s + O(|X|^2).$$

Since $\omega_X = \omega_{\rm eq} + O(X)$ and $P_t = O(X)$, one has

$$\begin{aligned}
\omega_X\left(P_t(\tau_X^{{\rm i}s\beta_{\rm eq}}(A) - \omega_X(A))\right) &= \omega_{\rm eq}\left(P_t(\tau_X^{{\rm i}s\beta_{\rm eq}}(A) - \omega_{\rm eq}(A))\right) + O(|X|^2)\\
&= \omega_{\rm eq}\left(P_t\tau_X^{{\rm i}s\beta_{\rm eq}}(A)\right) - \omega_{\rm eq}(P_t)\omega_{\rm eq}(A) + O(|X|^2).
\end{aligned}$$

From the fact that $\omega_{\rm eq}(\Phi_{js}) = \omega_{\rm eq}(\Phi_j) = 0$ and $\omega_{\rm eq}(\mathcal{J}_{js}) = \omega_{\rm eq}(\mathcal{J}_j) = 0$ we deduce $\omega_{\rm eq}(P_t) = 0$. Since

$$\tau_X^{{\rm i}s\beta_{\rm eq}}(A) = {\rm e}^{-s\beta_{\rm eq}(H_V - \mu_{\rm eq}N)} A {\rm e}^{s\beta_{\rm eq}(H_V - \mu_{\rm eq}N)} + O(X),$$

and $[P_t, N] = 0$, we can further write,

$$\omega_{Xt}(A) = \omega_X(A) - \beta_{\rm eq} \int_0^1 \omega_{\rm eq}\left(P_t \tau_V^{{\rm i}s\beta_{\rm eq}}(A)\right) \,{\rm d}s + O(|X|^2). \tag{4.13}$$

By Duhamel's formula one has

$$\partial_{X_k} {\rm e}^{-\beta_{\rm eq} H_X}|_{X=0} = \int_0^{\beta_{\rm eq}} {\rm e}^{-s(H_V - \mu_{\rm eq}N)} \left.\frac{\partial H_X}{\partial X_k}\right|_{X=0} {\rm e}^{-(\beta_{\rm eq}-s)(H_V - \mu_{\rm eq}N)} \,{\rm d}s,$$

from which one easily derives

$$\partial_{X_k}\omega_X(A)|_{X=0} = \left\{ \begin{array}{ll} \langle H_k | A - \omega_{\rm eq}(A)\rangle_{\rm eq} & \text{for } 1 \le k \le n, \\ \langle N_k | A - \omega_{\rm eq}(A)\rangle_{\rm eq} & \text{for } n+1 \le k \le 2n. \end{array} \right.$$

Finally, (4.13) yields that for $1 \le k \le n$,

$$\begin{aligned} \partial_{X_k}\omega_X(A_t)|_{X=0} &= \langle H_k | A - \omega_{\rm eq}(A)\rangle_{\rm eq} + \int_0^t \langle \Phi_k | A_s\rangle_{\rm eq} {\rm d}s, \\ \partial_{X_{n+k}}\omega_X(A_t)|_{X=0} &= \langle N_k | A - \omega_{\rm eq}(A)\rangle_{\rm eq} + \int_0^t \langle \mathcal{J}_k | A_s\rangle_{\rm eq} {\rm d}s. \end{aligned} \tag{4.14}$$

These linear response formulas hold without time reversal assumption and for any observable $A \in \mathcal{O}$. Under the assumptions of Proposition 4.1, ω_X is TRI. If $A = \Phi_j$ or $A = \mathcal{J}_j$ then $\omega_X(A) = 0$. This implies $\partial_{X_k}\omega_X(A)|_{X=0} = 0$ for $k = 1, \ldots, 2n$, and (4.14) reduces to the Green-Kubo formulas (4.12). Using (4.14) it is easy to exhibit examples of open quantum systems for which finite time Onsager reciprocity relations fail in the absence of time reversal.

Chapter 5

The thermodynamic limit and the large time limit

Apart from Section 5.1 and the first part of Section 5.6 which should be accessible to all readers, this section is intended for more advanced readers and may be skipped on first reading.

We shall describe, typically without proofs, the thermodynamic limit procedure and how one extends the results of the last two sections to general quantum systems. We shall also discuss the large time limit for infinitely extended quantum system.

5.1 Overview

From a mathematical point of view, the dynamics of a finite quantum system $(\mathcal{O},\tau^t,\omega)$ and that of the finite classical harmonic chain of Chapter 1 are very similar: both are described by a linear quasi-periodic propagator. In particular, the limit

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

does not exist, except in trivial cases. However, the Cesàro limit

$$\omega_+(A)=\lim_{T\to\infty}\frac{1}{T}\int_0^T\omega(\tau^t(A))\,\mathrm{d}t, \tag{5.1}$$

exists for all $A\in\mathcal{O}$ and defines a steady state ω_+ of the system.

Exercise 5.1.

1. Show that for a finite quantum system $(\mathcal{O},\tau^t,\omega)$ with Hamiltonian H, the limit (5.1) exists and that the limiting state ω_+ is described by the density matrix

$$\omega_+=\sum_{\lambda\in\mathrm{sp}(H)}P_\lambda(H)\omega P_\lambda(H).$$

2. For $A\in\mathcal{O}_{\rm self}$, set $\Phi_A=\mathrm{i}[H,A]$. Show that

$$\omega_+(\Phi_A)=0,$$

for any A. Conclude that, in particular, the mean entropy production rate vanishes,

$$\omega_+(\sigma)=\lim_{t\to\infty}\omega(\Sigma^t)=0.$$

3. Show that the same conclusions hold if the system is infinite (*i.e.*, the Hilbert space $\mathcal{K}$ is infinite dimensional) but confined in the sense that its Hamiltonian H has purely discrete spectrum.

Thus, in order to obtain a thermodynamically non-trivial steady state – with non-vanishing currents and strictly positive entropy production rate – we need to perform a thermodynamic (TD) limit before taking the large time limit (5.1). In other words, some parts of the system, *e.g.*, the reservoirs of an open system, have to be infinitely extended.

There are two difficulties associated with the TD limit: the first one is to describe the reference state of the extended system, the second one is to define its dynamics. These problems have been extensively studied in the 70' and have led to the algebraic approach to quantum statistical mechanics and quantum field theory. Algebraic quantum statistical mechanics provides a very attractive mathematical framework for the description of infinitely extended quantum systems.

In algebraic quantum statistical mechanics an extended system is described by a triple $(\mathcal{O}, \tau^t, \omega)$, where $\mathcal{O}$ is a C^*-algebra with identity $\mathbb{1}$ (recall Exercise 2.1), ω is a state (*i.e.*, positive normalized linear functional on $\mathcal{O}$) and τ^t is a C^*-dynamics, that is, a norm continuous group of $*$-automorphisms of $\mathcal{O}$. The triple $(\mathcal{O}, \tau^t, \omega)$ is often called *quantum dynamical system*[1]. The observables are elements of $\mathcal{O}$, ω describes the initial thermodynamical state of our system and the group τ^t describes its time evolution. The observables evolve in time as $A_t = \tau^t(A)$ and the states as $\omega_t = \omega \circ \tau^t$.

Infinitely extended systems of physical interest arise as TD limit of finite dimensional systems. There is a number of different ways the TD limit can be realized in practice. In the next section we describe one of them that is suitable for spin systems and quasi-free or locally interacting fermionic systems.

5.2 Thermodynamic limit: Setup

One starts with a family $\{\mathcal{Q}_M\}_{M\in\mathbb{N}}$ of finite quantum systems described by a sequence of finite dimensional Hilbert spaces $\mathcal{K}_M$, algebras $\mathcal{O}_{\mathcal{K}_M}$, Hamiltonians H_M and faithful states ω_M. σ_M is the entropy production observable of $\mathcal{Q}_M$. In the presence of control parameters $X \in \mathbb{R}^n$ ($H_{M,X}$ and $\omega_{M,X}$ depend on X), $\mathbf{\Phi}_{M,X}$ denotes a chosen flux relation. The number M typically corresponds to the "size" of $\mathcal{Q}_M$. For example, $\mathcal{Q}_M$ could be a spin system or Fermi gas confined to a box $[-M, M]^d$ of the lattice $\mathbb{Z}^d$.[2] The limiting infinitely extended system is described by a quantum dynamical system $(\mathcal{O}, \tau^t, \omega)$ satisfying the following:

(A1) For all M there is a faithful representation $\pi_M : \mathcal{O}_{\mathcal{K}_M} \to \mathcal{O}$ such that

$$\pi_M(\mathcal{O}_{\mathcal{K}_M}) \subset \pi_{M+1}(\mathcal{O}_{\mathcal{K}_{M+1}}).$$

(A2) $\mathcal{O}_{\rm loc} = \cup_M \pi_M(\mathcal{O}_{\mathcal{K}_M})$ is dense in $\mathcal{O}$. The elements of $\mathcal{O}_{\rm loc}$ are sometimes called *local observables* of $\mathcal{O}$.

(A3) For $A \in \mathcal{O}_{\rm loc}$, $\lim_{M\to\infty} \omega_M \circ \pi_M^{-1}(A) = \omega(A)$ and

$$\lim_{M\to\infty} \pi_M \circ \tau_M^t \circ \pi_M^{-1}(A) = \tau^t(A),$$

where the convergence is uniform for t in compact intervals of $\mathbb{R}$.

(A4) $\lim_{M\to\infty} \pi_M(\sigma_M) = \sigma$, exists in the norm of $\mathcal{O}$. σ is the entropy production observable of $(\mathcal{O}, \tau^t, \omega)$.

(A5) In the presence of control parameters X, $\lim_{M\to\infty} \pi_M(\mathbf{\Phi}_{M,X}) = \mathbf{\Phi}_X$ exists in the norm of $\mathcal{O}$. $\mathbf{\Phi}_X$ is a flux relation of $(\mathcal{O}, \tau_X^t, \omega_X)$,

$$\sigma_X = \sum_{j=1}^n X_j \Phi_X^{(j)}.$$

[1] Such quantum dynamical systems are suitable for the description of spin systems or fermionic systems. In the case of bosonic system, $\mathcal{O}$ is a W^*-algebra, ω is a normal state, and τ^t is weakly continuous. We shall not discuss such systems in these lecture notes (see, *e.g.*, [Pi]).

[2] For continuous models one may need to slightly modify this setup. For example, in the case of a free Fermi gas on $\mathbb{R}$, $M = (L, \mathcal{E})$, where L is the spatial cut-off, $\mathcal{E}$ is the energy cut-off, and $M \to \infty$ stands for the ordered limit $\lim_{L\to\infty} \lim_{\mathcal{E}\to\infty}$, see Exercise 6.4. The extension of our axiomatic scheme to this more general setup is straightforward.

(A6) For $p \in [1,\infty]$ and $\alpha, t \in \mathbb{R}$ the limit

$$e_{t,p}(\alpha) = \lim_{M\to\infty} e_{M,t,p}(\alpha),$$

exists and is finite. In the presence of control parameters, the limit

$$e_t(X,Y) = \lim_{M\to\infty} e_{M,t}(X,Y),$$

exists and is finitefor all $t \in \mathbb{R}$ and $X, Y \in \mathbb{R}^n$.

The verification of (A1)–(A5) in the context of spin systems and Fermi gases is discussed in virtually any mathematically oriented monograph on statistical mechanics (see, *e.g.*, [BR2]). For such systems, the proof of (A6) is typically an easy exercise in the techniques developed in 70's (see Exercise 6.9 below). In some models $e_{t,p}(\alpha)/e_t(X,Y)$ may be defined/finite only for a restricted range of the parameter $\alpha/(X,Y)$ and in this case the fluctuation theorems need to be suitable modified (this was the case in our introductory example of a thermally driven harmonic chain!).

In what follows we assume that (A1)–(A6) hold. For reasons of space and notational simplicity *we shall assume from the onset that all quantum systems $\mathcal{Q}_M$ are* TRI. Also, we shall discuss only the TD/large time limit of the functionals $e_{M,2,t}(\alpha)$ and $e_{M,t}(X,Y)$.

5.3 Thermodynamic limit: Full counting statistics

The reader should recall the notation and results of Section 3.5 where we introduced full counting statistics. We have

$$e_{M,2,t}(\alpha) = e_{M,2,t}(1-\alpha) = \log \int_{\mathbb{R}} \mathrm{e}^{-t\alpha\phi} \mathrm{d}\mathbb{P}_{M,t}(\phi),$$

where $\mathbb{P}_{M,t}$ is the probability distribution of the mean rate of entropy change associated to the repeated measurement process described in Section 3.5.

By (A6),

$$e_{2,t}(\alpha) = \lim_{M\to\infty} e_{M,2,t}(\alpha),$$

exists for all t and α. The implications are:

Proposition 5.1 (1) *The sequence of Borel probability measures $\{\mathbb{P}_{M,t}\}$ converges weakly to a Borel probability measure $\mathbb{P}_t$, i.e., for any bounded continuous function $f : \mathbb{R} \to \mathbb{R}$,*

$$\lim_{M\to\infty} \int_{\mathbb{R}} f \mathrm{d}\mathbb{P}_{M,t} = \int_{\mathbb{R}} f \mathrm{d}\mathbb{P}_t.$$

(2) *For all $\alpha \in \mathbb{R}$,*

$$e_{2,t}(\alpha) = \log \int_{\mathbb{R}} \mathrm{e}^{-t\alpha\phi} \mathrm{d}\mathbb{P}_t(\phi).$$

(3) *$e_{2,t}(\alpha)$ is real-analytic and*

$$e_{2,t}(\alpha) = e_{2,t}(1-\alpha). \tag{5.2}$$

(4) *All the cumulants of $\mathbb{P}_{M,t}$ converge to corresponding cumulants of $\mathbb{P}_t$. In particular,*

$$\partial_\alpha e_{2,t}(\alpha)|_{\alpha=0} = -\int_0^t \omega(\sigma_s)\mathrm{d}s \le 0.$$

(5) *Let $\mathfrak{r} : \mathbb{R} \to \mathbb{R}$ be the reflection $\mathfrak{r}(\phi) = -\phi$ and $\overline{\mathbb{P}}_t = \mathbb{P}_t \circ \mathfrak{r}$ the reflected measure. The measures $\overline{\mathbb{P}}_t$ and $\mathbb{P}_t$ are equivalent and*

$$\frac{\mathrm{d}\overline{\mathbb{P}}_t(\phi)}{\mathrm{d}\mathbb{P}_t(\phi)} = \mathrm{e}^{-t\phi}. \tag{5.3}$$

The limiting probability measure $\mathbb{P}_t$ is called full counting statistics of the infinitely extended system $(\mathcal{O}, \tau^t, \omega)$. Relations (5.2) and (5.3) are finite time Evans-Searles symmetries.

Recall that $\mathbb{P}_{M,t}$ is related to the modular structure of $\mathcal{Q}_M$: $\mathbb{P}_{M,t} = Q_M^t$, where Q_M^t is the spectral measure for

$$-\frac{1}{t}\log \Delta_{\omega_{M,t}|\omega_M},$$

and the vector ξ_{ω_M}. Our next goal is to relate $\mathbb{P}_t$ to the modular structure of the infinitely extended systems $(\mathcal{O}, \tau^t, \omega)$. We start with a brief description of this structure assuming that the reader is familiar with the topic.

(1) Let $(\mathcal{H}_\omega, \pi_\omega, \xi_\omega)$ be the GNS-representation of $\mathcal{O}$ associated to ω. $\mathfrak{M}_\omega = \pi_\omega(\mathcal{O})''$ denotes the *enveloping von Neumann algebra.* A vector $\xi \in \mathcal{H}_\omega$ is called cyclic if $\mathfrak{M}_\omega \xi$ is dense in $\mathcal{H}_\omega$ and separating if $A\xi = 0$ for $A \in \mathfrak{M}_\omega$ implies $A = 0$. ξ_ω is automatically cyclic. The state ω is called *modular* if ξ_ω is also separating. We assume ω to be modular.

(2) The anti-linear operator $S_\omega : A\xi_\omega \mapsto A^*\xi_\omega$ with domain $\mathfrak{M}_\omega\xi_\omega$ is closable. We denote by the same letter its closure. Let $S_\omega = J\Delta_\omega^{1/2}$ be the polar decomposition of S_ω. J is the *modular conjugation,* an anti-unitary involution on $\mathcal{H}_\omega$, and Δ_ω is the *modular operator* of ω. Δ_ω has a trivial kernel and $\varsigma_\omega^t(A) = \Delta_\omega^{\mathrm{i}t} A \Delta_\omega^{-\mathrm{i}t}$ is a group of $*$-automorphism of $\mathfrak{M}_\omega$, the *modular group* of ω.

(3) The set $\mathcal{H}_+ = \{AJA\xi_\omega \mid A \in \mathfrak{M}_\omega\}^{\mathrm{cl}}$ (cl denotes the closure in $\mathcal{H}_\omega$) is the *natural cone.* It is a self-dual cone in $\mathcal{H}_\omega$. A state ν on $\mathcal{O}$ is called normal (or, more precisely, ω-normal) if there exists a density matrix ρ on $\mathcal{H}_\omega$ such that $\nu(A) = \mathrm{tr}(\rho\pi_\omega(A))$. $\mathcal{N}_\omega$ denotes the collection of all ω-normal states. $\mathcal{N}_\omega$ is a norm closed subset of the dual $\mathcal{O}^*$. Any state $\nu \in \mathcal{N}_\omega$ has a unique *vector representative* $\xi_\nu \in \mathcal{H}_+$ such that $\nu(A) = (\xi_\nu|\pi_\omega(A)\xi_\nu)$. ξ_ν is cyclic iff it is separating, *i.e.*, iff ν is modular.

(4) Let $\nu \in \mathcal{N}_\omega$ be a modular state. The anti-linear operator $S_{\nu|\omega} : A\xi_\omega \mapsto A^*\xi_\nu$ is closable on $\mathfrak{M}_\omega\xi_\omega$ and we denote by the same letter its closure. This operator has the polar decomposition $S_{\nu|\omega} = J\Delta_{\nu|\omega}^{1/2}$, where J is the modular conjugation introduced in (2) and $\Delta_{\nu|\omega} > 0$ is the relative modular operator of ν w.r.t. ω.

(5) The Rényi relative entropy of order $\alpha \in \mathbb{R}$ of a state ν w.r.t. ω is defined by

$$S_\alpha(\nu|\omega) = \begin{cases} \log(\xi_\omega|\Delta_{\nu|\omega}^\alpha\xi_\omega) & \text{if } \nu \in \mathcal{N}_\omega, \\ -\infty & \text{otherwise.} \end{cases}$$

Its relative entropy w.r.t. ω is defined by

$$S(\nu|\omega) = \begin{cases} (\xi_\nu|\log \Delta_{\nu|\omega}\xi_\nu) & \text{if } \nu \in \mathcal{N}_\omega, \\ -\infty & \text{otherwise.} \end{cases}$$

To link the modular structure of the finite quantum systems $\mathcal{Q}_M$ to that of $(\mathcal{O}, \tau^t, \omega)$, in addition to (A1)–(A6) we assume:

(A7) Let $\varsigma_{\omega_M}^t$ be the modular group of ω_M. Then for all $A \in \mathcal{O}_{\mathrm{loc}}$,

$$\lim_{M\to\infty} \pi_\omega \circ \pi_M \circ \varsigma_{\omega_M}^t \circ \pi_M^{-1}(A) = \varsigma_\omega^t \circ \pi_\omega(A),$$

and the convergence is uniform for t in compact intervals of $\mathbb{R}$.

Again, the verification of (A7) for spin/fermionic systems is typically an easy exercise. Given (A1)–(A7), we have:

Proposition 5.2 (1) *Let Q^t be the spectral measure for $-\frac{1}{t}\log \Delta_{\omega_t|\omega}$ and ξ_ω. Then $Q^t = \mathbb{P}_t$.*

(2) $\lim_{M\to\infty} S_\alpha(\omega_{M,t}|\omega_M) = S_\alpha(\omega_t|\omega)$ *and* $\lim_{M\to\infty} S(\omega_{M,t}|\omega_M) = S(\omega_t|\omega)$. *In particular,*

$$S(\omega_t|\omega) = -\int_0^t \omega(\sigma_s)\mathrm{d}s.$$

The proof of the last proposition is somewhat technical and can be found in [JOPP].

Finally, we link $e_{2,t}(\alpha)$ and the full counting statistics $\mathbb{P}_t$ to quantum transfer operators. To avoid introduction of the full machinery of the Araki-Masuda L^p-spaces we shall focus here on the special case described in Exercise 3.8 (this special case covers open quantum systems). Suppose that the finite quantum systems $\mathcal{Q}_M$ have the following additional structure:

(A8) $H_M = H_{M,0} + V_M$, where $[H_{M,0}, \omega_M] = 0$ and

$$\lim_{M\to\infty} \pi_M(V_M) = V,$$

in the norm of $\mathcal{O}$. Moreover, for any $a > 0$,

$$\sup_{|\alpha|<a, M} \|\varsigma_{\omega_M}^{\mathrm{i}\alpha}(V_M)\| < \infty. \tag{5.4}$$

(A8) is essentially an assumption on the structure of the model and is easily verifiable in practice. (A3), (A8) and perturbation theory imply that the dynamics $\tau_{M,0}^t$ generated by $H_{M,0}$ converges to the C^*-dynamics τ_0^t, *i.e.*, that for $A \in \mathcal{O}_{\rm loc}$ and uniformly for t in compact intervals,

$$\lim_{M\to\infty} \pi_M \circ \tau_{M,0}^t \circ \pi_M^{-1}(A) = \tau_0^t(A).$$

Clearly, $\omega \circ \tau_0^t = \omega$. The assumption (5.4) and Vitali's theorem ensure that the map

$$\mathbb{R} \ni t \mapsto \varsigma_\omega^{\mathrm{i}t}(\pi_\omega(V)) \in \mathfrak{M}_\omega,$$

has an analytic continuation to the entire complex plane and that for $z \in \mathbb{C}$,

$$\lim_{M\to\infty} \pi_\omega \circ \pi_M \circ \varsigma_{\omega_M}^z(V_M) = \varsigma_\omega^z \circ \pi_\omega(V).$$

Let K_0 be the standard Liouvillean of $(\mathcal{O}, \tau_0, \omega)$. K_0 is the unique self-adjoint operator on $\mathcal{H}_\omega$ satisfying

$$\pi_\omega(\tau_0^t(A)) = \mathrm{e}^{\mathrm{i}tK_0}\pi_\omega(A)\mathrm{e}^{-\mathrm{i}tK_0}, \qquad \mathrm{e}^{\mathrm{i}tK_0}\mathcal{H}_+ = \mathcal{H}_+,$$

for all $t \in \mathbb{R}$ and $A \in \mathcal{O}$. For $\alpha \in \mathbb{R}$ we set

$$L_{\frac{1}{\alpha}} = K_0 + \pi_\omega(V) - J\varsigma_\omega^{\mathrm{i}(\alpha-\frac{1}{2})}(\pi_\omega(V))J.$$

$L_{\frac{1}{\alpha}}$ is a closed operator with the same domain as K_0. Except in trivial cases, $L_{\frac{1}{\alpha}}$ is not self-adjoint unless $\alpha = 1/2$. $L_2 = K$ is the standard Liouvillean of $(\mathcal{O}, \tau^t, \omega)$, *i.e.*, the unique self-adjoint operator on $\mathcal{H}_\omega$ such that

$$\pi_\omega(\tau^t(A)) = \mathrm{e}^{\mathrm{i}tK}(A)\mathrm{e}^{-\mathrm{i}tK}, \qquad \mathrm{e}^{\mathrm{i}tK}\mathcal{H}_+ = \mathcal{H}_+,$$

for all $t \in \mathbb{R}$ and $A \in \mathcal{O}$.

The following result, which is of considerable conceptual and computational importance, is the extension of Exercise 3.8 to the setting of infinitely extended systems.

Proposition 5.3 *For all t and α,*

$$e_{2,t}(\alpha) = (\xi_\omega|\mathrm{e}^{-\mathrm{i}tL_{\frac{1}{\alpha}}}\xi_\omega).$$

The extension of the results of this section to the multi-parameter/open quantum system full counting statistics is straightforward.

5.4 Thermodynamic limit: Control parameters

By (A6), the limit

$$e_t(X,Y) = \lim_{M\to\infty} e_{M,t}(X,Y),$$

exists for all t and $X, Y \in \mathbb{R}^n$. The basic properties of $e_t(X,Y)$ are summarized in:

Proposition 5.4 (1)

$$e_t(X,Y) = \sup_{\nu\in\mathcal{N}_{\omega_X}} \left[S(\nu|\omega_X) + Y\cdot\int_0^t \nu(\mathbf{\Phi}_{Xs})\,\mathrm{d}s \right].$$

(2) *The function* $\mathbb{R}^n \ni Y \mapsto e_t(X,Y)$ *is convex and real analytic.*

(3) $e_t(X,Y) = e_t(X, X-Y)$.

(4)

$$\partial_{Y_j} e_t(X,Y)\big|_{Y=0} = \int_0^t \omega_X(\Phi_{Xs}^{(j)})\mathrm{d}s,$$

$$\partial_{Y_k}\partial_{Y_j} e_t(X,Y)\big|_{Y=0} = \int_0^t\int_0^t \left(\langle \Phi_{Xs_1}^{(k)} | \Phi_{Xs_2}^{(j)} \rangle_{\omega_X} - \omega_X(\Phi_{Xs_1}^{(k)})\omega_X(\Phi_{Xs_2}^{(j)}) \right) \mathrm{d}s_2\mathrm{d}s_1.$$

These results are the extension of Proposition 3.12 to the setting of infinitely extended systems. The only difference is that, for simplicity of the exposition, we have exploited the time reversal in the formulation of the results.

The proof of Proposition 5.4 can be found in [JOPP] and we restrict ourselves to several comments. Part (3), the generalized finite time Evans-Searles symmetry, is of course an immediate consequences of the same property of the functionals $e_{M,t}(X,Y)$. The convexity of $Y \mapsto e_t(X,Y)$ follows in the same way (note that convexity also follows from (1)). The most natural way to prove the remaining parts is to use Araki's perturbation theory of the KMS/modular structure (this theory is, in part, an extension of the results of Section 2.10 to general von Neumann algebras). The Kubo-Mari inner product $\langle \Phi_{Xs_1}^{(k)} | \Phi_{Xs_2}^{(j)} \rangle_{\omega_X}$ in Part (4) is formally similar to its finite-dimensional counterpart. It is a part of the modular structure that for all $A, B \in \mathfrak{M}_{\omega_X}$, the function $t \mapsto (\xi_{\omega_X} | A^* \varsigma_{\omega_X}^t(B)\xi_{\omega_X})$ has an analytic continuation to the strip $-1 < \operatorname{Im} z < 0$ which is bounded on continuous on its closure. Then

$$\langle \Phi_{Xs_1}^{(k)} | \Phi_{Xs_2}^{(j)} \rangle_{\omega_X} = \int_0^1 (\xi_{\omega_X} | \pi_{\omega_X}(\Phi_{Xs_1}^{(k)}) \varsigma_{\omega_X}^{-\mathrm{i}u}(\pi_{\omega_X}(\Phi_{Xs_2}^{(j)}))\xi_{\omega_X})\mathrm{d}u.$$

The finite time linear response theory for family of infinitely extended systems $(\mathcal{O}, \tau_X^t, \omega_X)$ can be developed along two complementary routes. We shall use the same notational conventions as in Section 3.10: $\omega_0 = \omega$, $\tau_0 = \tau$, $\mathbf{\Phi}_0 = \mathbf{\Phi}$. Since

$$\langle \mathbf{\Phi}_X \rangle_t = \frac{1}{t}\int_0^t \omega_X(\mathbf{\Phi}_{Xs})\mathrm{d}s = \frac{1}{t}\nabla_Y e_t(X,Y)|_{Y=0},$$

we have the following:

Proposition 5.5 *Suppose that the map* $(X,Y) \mapsto e_t(X,Y)$ *is* C^2 *in an open set containing* $(0,0)$. *Then the finite time kinetic transport coefficients*

$$L_{jkt} = \partial_{X_k} \langle \Phi_X^{(j)} \rangle_t |_{X=0} = \partial_{X_k}\partial_{Y_j} e_t(X,Y)_{X=Y=0},$$

satisfy :

(1)

$$L_{jkt} = \frac{1}{2}\int_{-t}^t \langle \Phi^{(k)} | \Phi_s^{(j)} \rangle_\omega \left(1 - \frac{|s|}{t} \right) \mathrm{d}s.$$

(2) *$L_{jkt} = L_{kjt}$ and the quadratic form determined by $[L_{jkt}]$ is positive definite.*

Given Proposition 5.4, the proof of Proposition 5.5 is exactly the same as the proof of its finite dimensional counterpart (Proposition 3.14 in Section 3.10).

A complementary route is based on the thermodynamical limit of the finite time finite volume linear response theory. This route is both technically and conceptually less satisfactory and we shall not discuss it here.

5.5 Large time limit: Full counting statistics

To describe fluctuations of $\mathbb{P}_t$ as $t \to \infty$ we need to assume:

(A9) The limit

$$e_{2,+}(\alpha) = \lim_{t\to\infty} \frac{1}{t} e_{2,t}(\alpha),$$

exists for α in some open interval $\mathcal{I}$ containing $[0,1]$. Moreover, the limiting entropic functional $e_{2,+}(\alpha)$ is differentiable on $\mathcal{I}$.

The verification of (A9) (and (A10) below) is the central step of the program. Unlike (A1)–(A8), which are typically easily verifiable structural/thermodynamical limit properties of a given model, the verification of (A9) is usually a difficult analytical problem.

The quantum Evans-Searles fluctuation theorem for the full counting statistics follows from (A9) and the Gärtner-Ellis theorem. We describe its conclusions. Without loss of generality we may assume that $\mathcal{I}$ is centered at $\alpha = 1/2$ (recall that we assume the system to be TRI).

Proposition 5.6 (1) *$e_{2,+}(\alpha)$ is convex on $\mathcal{I}$, the Evans-Searles symmetry*

$$e_{2,+}(\alpha) = e_{2,+}(1-\alpha),$$

holds, and

$$e'_{2,+}(0) = -\lim_{t\to\infty} \mathbb{E}_t(\phi) = -\lim_{t\to\infty} \frac{1}{t} S(\omega_t|\omega) = -\lim_{t\to\infty} \frac{1}{t}\int_0^t \omega(\sigma_s)\mathrm{d}s.$$

The non-negative number $\langle\sigma\rangle_+ = -e'_{2,+}(0)$ is called the entropy production of $(\mathcal{O}, \tau^t, \omega)$. Notice that $\langle\sigma\rangle_+ = 0$ iff the function $e_{2,+}(\alpha) = 0$ for $\alpha \in [0,1]$.

(2) *Let*

$$\theta = \sup_{\alpha\in\mathcal{I}} e'_{2,+}(\alpha) = -\inf_{\alpha\in\mathcal{I}} e'_{2,+}(\alpha).$$

The function

$$I(s) = -\inf_{\alpha\in\mathcal{I}} \left(\alpha s + e_{2,+}(\alpha)\right),$$

is non-negative, convex and differentiable on $]-\theta,\theta[$. [3] *$I(s) = 0$ iff $s = -\langle\sigma\rangle_+$ and the Evans-Searles symmetry implies*

$$I(-s) = s + I(s).$$

The last relation is sometimes called the Evans-Searles symmetry for the rate function.

(3) *For any open set $J \subset]-\theta,\theta[$,*

$$\lim_{t\to\infty} \frac{1}{t}\log \mathbb{P}_t(J) = -\inf_{s\in J} I(s).$$

[3] If $\theta < \infty$, then $I(s)$ is linear on $]-\infty,-\theta]$ and $[\theta,\infty[$.

The interpretation of the quantum ES theorem for the full counting statistics is similar to the classical case. The full counting statistics concerns the operationally defined “mean entropy flow" across the system. Its expectation value converges, as $t \to \infty$, to the entropy production $\langle\sigma\rangle_+$ of the model. Its fluctuations of order 1 are described by the theory of large deviations. The specific aspect of the ES theorem is that the time reversal invariance implies the universal symmetry of the rate function which in turn implies that the “mean entropy flow" is exponentially more likely to be positive then negative, *i.e.*, the probability of violating the second law of thermodynamics is exceedingly small for large t.

We now describe schematically how Proposition 5.3 can be used to verify the key Assumption (A9).

(i) In typical situations where spectral techniques are applicable the standard Liouvillean K_0 has purely absolutely continuous spectrum filling the real line except for finitely many embedded eigenvalues of finite multiplicity. This is precisely what happens in the study of open quantum systems describing a finite quantum system $\mathcal{S}$ coupled to an infinitely extended reservoir $\mathcal{R}$. Typically, $\mathcal{R}$ will consists of several independent sub-reservoirs $\mathcal{R}_j$ which are in thermal equilibrium at inverse temperatures β_j and chemical potentials μ_j, but we do not need at this point to specify further the structure of $\mathcal{R}$. The reservoir system is described by C^*-dynamical system $(\mathcal{O}_\mathcal{R}, \tau_\mathcal{R}^t, \omega_\mathcal{R})$ where $\omega_\mathcal{R}$ is stationary for the dynamics $\tau_\mathcal{R}^t$ and assumed to be modular. Let $(\mathcal{H}_\mathcal{R}, \pi_\mathcal{R}, \xi_\mathcal{R})$ be the corresponding GNS representation and let $K_\mathcal{R}$ be the corresponding standard Liouvillean. Since $\omega_\mathcal{R}$ is steady, $K_\mathcal{R}\xi_\mathcal{R} = 0$. We assume that apart from a simple eigenvalue at 0, $K_\mathcal{R}$ has purely absolutely continuous spectrum filling the entire real line. This assumption ensures that $\mathcal{R}$ has strong ergodic properties and in particular that $(\mathcal{O}_\mathcal{R}, \tau_\mathcal{R}^t, \omega_\mathcal{R})$ is mixing, *i.e.*, that

$$\lim_{|t|\to\infty} \omega_\mathcal{R}(A\tau_\mathcal{R}^t(B)) = \omega_\mathcal{R}(A)\omega_\mathcal{R}(B),$$

for $A, B \in \mathcal{O}_\mathcal{R}$. In the simplest nontrivial case, $\mathcal{S}$ is a 2-level system, described by the Hilbert space $\mathbb{C}^2$ and the Hamiltonian $\sigma^{(3)}$ (the third Pauli matrix). Then the standard Liouvillean of the joint but decoupled system $\mathcal{S} + \mathcal{R}$ acts on the Hilbert space $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathcal{H}_\mathcal{R}$ and has the form

$$K_0 = (\sigma^{(3)} \otimes \mathbb{1} - \mathbb{1} \otimes \sigma^{(3)}) \otimes \mathbb{1} + \mathbb{1} \otimes K_\mathcal{R}.$$

This will be precisely the case in the Spin-Fermion model which we will discuss in Section 6.5. For simplicity of exposition, we assume in the following that the point spectrum of K_0 is $\{-2, 0, 2\}$, where the eigenvalues ± 2 are simple and 0 is doubly degenerate. The rest of the spectrum of K_0 is purely absolutely continuous and fills the real line, see Fig. 5.1.

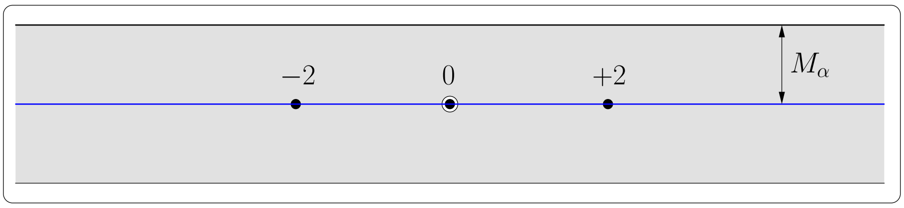

Figure 5.1: The point spectrum of the uncoupled standard Liouvillean K_0. The spectrum of the transfer operator $L_{\frac{1}{\alpha}}$ is contained in the grey strip.

(ii) An application of the numerical range theorem yields that the spectrum of $L_{\frac{1}{\alpha}}$ is contained in the strip $\{z \,|\, |\mathrm{Im}\, z| \le M_\alpha\}$, where

$$M_\alpha = \|\varsigma_\omega^{\mathrm{i}(\alpha-\frac{1}{2})}(\pi_\omega(V))\| + \|\pi_\omega(V)\|.$$

Thus, the resolvent $(z - L_{\frac{1}{\alpha}})^{-1}$ is an analytic function of z on the half-plane $\mathrm{Im}\, z > M_\alpha$.

(iii) By using complex deformation techniques one proves that for some $\mu > 0$ and all vectors ξ, η in some dense subspace of $\mathcal{H}$ the functions

$$z \mapsto (\xi|(z - L_{\frac{1}{\alpha}})^{-1}\eta),$$

have a meromorphic continuation from the half-plane $\operatorname{Im} z > M_\alpha$ to the half-plane $\operatorname{Im} z > -\mu$. This extension has four simple poles located at the points $e_\pm(\alpha)$, $e(\alpha)$, $e_1(\alpha)$, where $e(\alpha)$ is the pole closest to the real axis, see Fig. 5.2. For symmetry reasons $e(\alpha)$ is purely imaginary. These poles are resonances of $L_{\frac{1}{\alpha}}$, or in other words, eigenvalues of a complex deformation of $L_{\frac{1}{\alpha}}$. They can be computed by an application of analytic perturbation theory. For this purpose it is convenient to introduce a control parameter $\lambda \in \mathbb{R}$ and replace the interaction term V with λV. The parameter λ controls the strength of the coupling and analytic perturbation theory applies for small values of λ. One proves that given $\alpha_0 > 1/2$ one can find $\Lambda > 0$ such that for $|\alpha - \frac{1}{2}| < \alpha_0$ and $|\lambda| < \Lambda$, μ can be chosen independently of α and λ and that the poles are analytic functions of α. In particular, for α small enough,

$$e(\alpha) = \mathrm{i}\sum_{n=1}^{\infty} E_n(\lambda)\alpha^n,$$

where each coefficient $E_n(\lambda)$ is real-analytic function of λ.

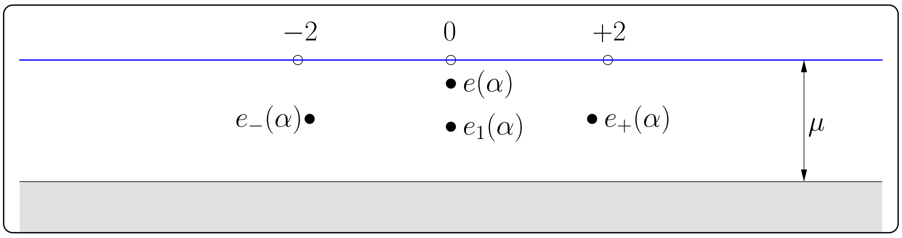

Figure 5.2: The resonances of the transfer operator $L_{\frac{1}{\alpha}}$.

(iv) One now starts with the expression

$$(\xi_\omega|\mathrm{e}^{-\mathrm{i}tL_{\frac{1}{\alpha}}}\xi_\omega) = \int_{\operatorname{Re} z = a} \mathrm{e}^{-\mathrm{i}tz}(\xi_\omega|(z - L_{\frac{1}{\alpha}})^{-1}\xi_\omega)\frac{\mathrm{d}z}{2\pi\mathrm{i}}, \tag{5.5}$$

where $a > M_\alpha$. Moving the line of integration to $\operatorname{Re} z = -\mu'$, where $\mu' \in]0, \mu[$ is such that the poles of the integrand are contained in $\{z \,|\, \operatorname{Im} z > -\mu'\}$ for $|\lambda| < \Lambda$ and $|\alpha - \frac{1}{2}| < \alpha_0$, and picking the contribution from theses poles one derives

$$(\xi_\omega|\mathrm{e}^{-\mathrm{i}tL_{\frac{1}{\alpha}}}\xi_\omega) = \mathrm{e}^{-\mathrm{i}te(\alpha)}(1 + R(t, \alpha)), \tag{5.6}$$

where $R(t, \alpha)$ decays exponentially in t as $t \to \infty$. It then follows that

$$e_{2,+}(\alpha) = \lim_{t\to\infty} \frac{1}{t} e_{2,t}(\alpha) = -\mathrm{i}e(\alpha).$$

A proper mathematical justification of (5.5) and (5.6) is typically the technically most demanding part of the argument.

(v) Recall that

$$\partial_\alpha e_{2,+}(\alpha)|_{\alpha=0} = E_1 = -\langle\sigma\rangle_+ = -\lim_{t\to\infty} \mathbb{E}_t(\phi).$$

Given (iv), an application of Vitali's theorem yields

$$\begin{aligned}\partial_\alpha^2 e_{2,+}(\alpha)_{\alpha=0} = E_2 &= \lim_{t\to\infty} \frac{1}{t}\int_0^t \int_0^t (\omega(\sigma_s\sigma_u) - \omega(\sigma_s)\omega(\sigma_u))\mathrm{d}s\mathrm{d}u \\ &= \lim_{t\to\infty} t(\mathbb{E}_t(\phi^2) - (\mathbb{E}_t(\phi))^2).\end{aligned}$$

(vi) The arguments/estimates in (iv) extend to complex α's satisfying $|\alpha - \frac{1}{2}| < \alpha_0$ and one shows that for α real,

$$\lim_{t\to\infty}\int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}\alpha\sqrt{t}(\phi-\langle\sigma\rangle_+)}\mathrm{d}\mathbb{P}_t(\phi) = \lim_{t\to\infty} \mathrm{e}^{\mathrm{i}\alpha\sqrt{t}\langle\sigma\rangle_+}(\xi_\omega|\mathrm{e}^{-\mathrm{i}tL_{\frac{\sqrt{t}}{\mathrm{i}\alpha}}}\xi_\omega) = \mathrm{e}^{-E_2\alpha^2}.$$

Hence, the central limit theorem holds for the full counting statistics $\mathbb{P}_t$, that is, for any interval $[a,b]$,

$$\lim_{t\to\infty}\mathbb{P}_t\left(\langle\sigma\rangle_+ + \frac{1}{\sqrt{tE_2}}[a,b]\right) = \frac{1}{\sqrt{2\pi}}\int_a^b \mathrm{e}^{-\frac{x^2}{2}}\mathrm{d}x.$$

The above spectral scheme is technically delicate and its implementation requires a number of regularity assumptions on the structure of reservoirs and the interaction V. On the positive side, when applicable the spectral scheme provides a wealth of information and a very satisfactory conceptual picture. In the classical case, the quantum transfer operators reduce to Ruelle-Perron-Frobenius operators and the above spectral scheme is a well-known chapter in the theory of classical dynamical systems, see Section 5.4 in [JPR] and [Ba].

5.6 Hypothesis testing of the arrow of time

Theorem 2.19 clearly links the $p = 2$ entropic functional to quantum hypothesis testing. This link, somewhat surprisingly, can be interpreted as quantum hypothesis testing of the second law of thermodynamics and arrow of time: how well can we distinguish the state $\omega_t = \omega\circ\tau^t$, from the same initial state evolved backward in time $\omega_{-t} = \omega\circ\tau^{-t}$? More precisely, we shall investigate the asymptotic behavior of the minimal error probability for the hypothesis testing associated to the pair (ω_{-t},ω_t) as $t\to\infty$.

We start with the family of pairs $\{(\omega_{M,-t},\omega_{M,t})\,|\,t>0\}$. Again, the thermodynamic limit $M\to\infty$ has to be taken prior to the limit $t\to\infty$.

Given their a priori probabilities, $1-p$ and p, the minimal error probability in distinguishing the states $\omega_{M,-t/2}$ and $\omega_{M,t/2}$ is given by Theorem 2.19,

$$D_{M,p}(t) = \frac{1}{2}\left(1 - \mathrm{tr}\,|(1-p)\,\omega_{M,-t/2} - p\,\omega_{M,t/2}|\right).$$

We set

$$\underline{D}_p(t) = \liminf_{M\to\infty} D_{M,p}(t), \qquad \overline{D}_p(t) = \limsup_{M\to\infty} D_{M,p}(t),$$

and define the Chernoff error exponents by

$$\underline{d}_p = \liminf_{t\to\infty}\frac{1}{t}\log\underline{D}_p(t), \qquad \overline{d}_p = \limsup_{t\to\infty}\frac{1}{t}\log\overline{D}_p(t).$$

Theorem 5.7 *For any $p\in]0,1[$,*

$$\underline{d}_p = \overline{d}_p = \inf_{\alpha\in[0,1]} e_{2,+}(\alpha).$$

Moreover, since the system is TRI the infimum is achieved at $\alpha = 1/2$.

Proof. We first notice that

$$D_{M,p}(t) = \frac{1}{2}\left(1 - \mathrm{tr}\,|(1-p)\,\omega_{M,0} - p\,\omega_{M,t}|\right).$$

Theorem 2.19 (3) and the existence of the limiting functional $e_{2,t}(\alpha)$ (for $M\to\infty$) yield the inequality

$$\log\overline{D}_p(t) \le e_{2,2t}(\alpha) + (1-\alpha)\log(1-p) + \alpha\log p,$$

for all $\alpha \in [0,1]$. Dividing by t and letting $t \to \infty$ we obtain the upper bound

$$\overline{d}_p \leq \inf_{\alpha \in [0,1]} e_{2,+}(\alpha).$$

For finite M, a lower bound is provided by Proposition 2.26,

$$D_{M,p}(t) \geq \frac{1}{2} \min(p, 1-p)\, \mathbb{P}_{M,t}(]0,\infty[),$$

where $\mathbb{P}_{M,t}$ is the full counting statistics of $\mathcal{Q}_M$. As we have already discussed, the convergence of $e_{M,2,t}(\alpha)$ to $e_{2,t}(\alpha)$ as $M \to \infty$ implies that $\mathbb{P}_{M,t}$ converges weakly to the full counting statistics $\mathbb{P}_t$ of the extended system. The Portmanteau theorem ([Bi1], Theorem 2.1) implies

$$\liminf_{M\to\infty} \mathbb{P}_{M,t}(]0,\infty[) \geq \mathbb{P}_t(]0,\infty[),$$

and hence

$$\underline{D}_p(t) \geq \frac{1}{2} \min(p, 1-p)\, \mathbb{P}_t(]0,\infty[) \geq \frac{1}{2} \min(p, 1-p)\, \mathbb{P}_t(]0,1[).$$

Assumption (A9) and the Gärtner-Ellis theorem (or more specifically Proposition A.4 in Appendix A.2) imply

$$\liminf_{t\to\infty} \frac{1}{t} \log \mathbb{P}_t(]0,1[) \geq -\varphi(0),$$

where

$$\varphi(s) = \sup_{\alpha\in\mathbb{R}} (s\alpha - e_{2,+}(\alpha)).$$

Since

$$\varphi(0) = -\inf_{\alpha\in\mathbb{R}} e_{2,+}(\alpha) = -\inf_{\alpha\in[0,1]} e_{2,+}(\alpha),$$

(recall that, by Proposition 3.3, $e_{2,+}(\alpha) \leq 0$ for $\alpha \in [0,1]$ and $e_{2,+}(\alpha) \geq 0$ otherwise) we have

$$\underline{d}_p \geq \liminf_{t\to\infty} \frac{1}{t} \left(-\log 2 + \min(\log p, \log(1-p)) + \log(\mathrm{P}_t(]0,1[))\right) \geq \inf_{\alpha\in[0,1]} e_{2,+}(\alpha).$$

The convexity and the symmetry $e_{2,+}(1-\alpha) = e_{2,+}(\alpha)$ imply that the infimum is achieved at $\alpha = 1/2$. □

Note that the above result and its proof link the fluctuations of the full counting statistics $\mathbb{P}_t$ as $t \to \infty$ to Chernoff error exponents in quantum hypothesis testing of the arrow of time. The TD limit plays an important role in the discussion of full counting statistics since its physical interpretation in terms of repeated quantum measurement is possible only for finite quantum systems. However, apart from the above mentioned connection with full counting statistics, quantum hypothesis testing can be formulated in the framework of extended quantum systems without reference to the TD limit. In fact, by considering directly an infinitely extended system, one can considerably refine the quantum hypothesis testing of the arrow of time. In the remaining part of this section we indicate how this can be done, referring the reader to [JOPS] for proofs and additional information.

(i) We start with an infinitely extended system $\mathcal{Q}$ described by the C^*-dynamical system $(\mathcal{O}, \tau^t, \omega)$. The GNS-representation of $\mathcal{O}$ associated to the state ω is denoted $(\mathcal{H}_\omega, \pi_\omega, \xi_\omega)$, and the enveloping von Neumann algebra is $\mathfrak{M}_\omega = \pi_\omega(\mathcal{O})''$. We assume that ω is modular. The group $\pi_\omega \circ \tau^t$ extends to a weakly continuous group τ_ω^t of $*$-automorphisms of $\mathfrak{M}_\omega$. With a slight abuse of notation we denote the vector state $(\xi_\omega | \cdot\, \xi_\omega)$ on $\mathfrak{M}_\omega$ again by ω. The triple $(\mathfrak{M}_\omega, \tau_\omega^t, \omega)$ is the W^*-quantum dynamical system induced by $(\mathcal{O}, \tau^t, \omega)$. We denote $\omega_t = \omega \circ \tau_\omega^t$. The quantum hypothesis testing of the arrow of time concerns the family of pairs $\{(\omega_{-t}, \omega_t) \,|\, t > 0\}$.

(ii) Consider the following competing hypothesis:

Hypothesis I : $\mathcal{Q}$ is in the state $\omega_{t/2}$;

Hypothesis II : $\mathcal{Q}$ is in the state $\omega_{-t/2}$;

We know *a priori* that Hypothesis I is realized with probability p and II with probability $1-p$. A *test* is a self-adjoint projection $P \in \mathfrak{M}_\omega$ and a result of a measurement of the corresponding observable is a number in $\mathrm{sp}(P) = \{0,1\}$. If the outcome is 1, one accepts I, otherwise one accepts II. The error probability of the test P is

$$D_p(\omega_{t/2}, \omega_{-t/2}, P) = p\,\omega_{t/2}(\mathbb{1} - P) + (1-p)\,\omega_{-t/2}(P),$$

and

$$D_p(\omega_{t/2}, \omega_{-t/2}) = \inf_P D_p(\omega_{t/2}, \omega_{-t/2}, P),$$

is the minimal error probability.

(iii) The quantum Neyman-Pearson lemma holds:

$$\begin{aligned} D_p(\omega_{t/2}, \omega_{-t/2}) = D_p(\omega_{t/2}, \omega_{-t/2}, P_{\mathrm{opt}}) &= \frac{1}{2}(1 - \|(1-p)\omega_{-t/2} - p\omega_{t/2}\|) \\ &= \frac{1}{2}(1 - \|(1-p)\omega - p\omega_t\|), \end{aligned}$$

where P_{opt} is the support projection of the linear functional $((1-p)\omega_{-t/2} - p\omega_{t/2})_+$ (the positive part of $(1-p)\omega_{-t/2} - p\omega_{t/2}$). Just like in the classical case, the proof of the quantum Neyman-Pearson lemma is straightforward.

(iv) Let $\mu_{\omega_t|\omega}$ be the spectral measure for $\Delta_{\omega_t|\omega}$ and ξ_ω. Then

$$\frac{1}{2}\min(p, 1-p)\mu_{\omega_t|\omega}([1,\infty[) \le D_p(\omega_{t/2}, \omega_{-t/2}) \le p^\alpha(1-p)^{1-\alpha}(\xi_\omega|\Delta^\alpha_{\omega_t|\omega}\xi_\omega).$$

The proof of the lower bound in exactly the same as in finite case (recall Proposition 2.26). The proof of the upper bound is based on an extension of Ozawa's argument (see the proof of Part (3) of Theorem 2.19) to the modular setting and is more subtle, see [Og].

(v) Assuming (A9), *i.e.*, that

$$e_{2,+}(\alpha) = \lim_{t\to\infty} \frac{1}{t}\log(\xi_\omega|\Delta^\alpha_{\omega_t|\omega}\xi_\omega),$$

exist and is differentiable for α is some interval containing $[0,1]$, then a straightforward application of the Gärtner-Ellis theorem yields

$$\lim_{t\to\infty} \frac{1}{t}\log D_p(\omega_t, \omega_{-t}) = \inf_{\alpha\in[0,1]} e_{2,+}(\alpha). \tag{5.7}$$

Results of this type are often called quantum Chernoff bounds. Our TRI assumption implies that the infimum is achieved for $\alpha = 1/2$.

The Chernoff bound (5.7) quantifies the separation between the past and the future as time $t \uparrow \infty$. Taking $p = 1/2$ and noticing that

$$\frac{1}{2}(2 - \|\omega_{t/2} - \omega_{-t/2}\|) = \omega_{t/2}(\mathrm{s}_-(t/2)) + \omega_{-t/2}(\mathrm{s}_+(t/2)),$$

where $\mathrm{s}_\pm(t)$ is the support projection of the positive linear functional $(\omega_t - \omega_{-t})_\pm$ on $\mathfrak{M}_\omega$, we see that the Chernoff bound implies

$$\begin{aligned} \limsup_{t\to\infty} \frac{1}{t}\log\omega_t(\mathrm{s}_-(t)) &\le 2\inf_{s\in[0,1]} e_{2,+}(s), \\ \limsup_{t\to\infty} \frac{1}{t}\log\omega_{-t}(\mathrm{s}_+(t)) &\le 2\inf_{s\in[0,1]} e_{2,+}(s). \end{aligned}$$

Therefore, as $t \uparrow \infty$, the state ω_t concentrates exponentially fast on $\mathrm{s}_+(t)\mathfrak{M}_\omega$ while the state ω_{-t} concentrates exponentially fast on $\mathrm{s}_-(t)\mathfrak{M}_\omega$.

(vi) In the infinite dimensional setting one can introduce other error exponents. For $r \in \mathbb{R}$ the Hoeffding exponents are defined by

$$\overline{B}(r) = \inf_{\{P_t\}} \left\{ \limsup_{t\to\infty} \frac{1}{t} \log \omega_{t/2}(\mathbb{1} - P_t) \,\middle|\, \limsup_{t\to\infty} \frac{1}{t} \log \omega_{-t/2}(P_t) < -r \right\},$$

$$\underline{B}(r) = \inf_{\{P_t\}} \left\{ \liminf_{t\to\infty} \frac{1}{t} \log \omega_{t/2}(\mathbb{1} - P_t) \,\middle|\, \limsup_{t\to\infty} \frac{1}{t} \log \omega_{-t/2}(P_t) < -r \right\},$$

$$B(r) = \inf_{\{P_t\}} \left\{ \lim_{t\to\infty} \frac{1}{t} \log \omega_{t/2}(\mathbb{1} - P_t) \,\middle|\, \limsup_{t\to\infty} \frac{1}{t} \log \omega_{-t/2}(P_t) < -r \right\},$$

where the infimum are taken over families $\{P_t\}_{t>0}$ of orthogonal projections in $\mathfrak{M}_\omega$ subject, in the last case, to the constraint that $\lim_{t\to\infty} t^{-1} \log \omega_{t/2}(\mathbb{1} - P_t)$ exists.

The Hoeffding exponents are increasing functions of r, $\underline{B}(r) \le \overline{B}(r) \le B(r) \le 0$, and $\underline{B}(r) = \overline{B}(r) = B(r) = -\infty$ if $r < 0$. The functions $\underline{B}(r), \overline{B}(r), B(r)$ are left continuous and upper semi-continuous. If (A9) holds and $\langle \sigma \rangle_+ > 0$, then for all $r \in \mathbb{R}$,

$$\underline{B}(r) = \overline{B}(r) = B(r) = b(r) = -\sup_{0\le s<1} \frac{-sr - e_{2,+}(s)}{1-s},$$

see [JOPS]. Results of this type are called quantum Hoeffding bounds.

Let $r > 0$ and let P_t be projections in $\mathfrak{M}_\omega$ such that

$$\limsup_{t\to\infty} \frac{1}{t} \log \omega_{-t/2}(P_t) < -r.$$

The Hoeffding bound asserts

$$\liminf_{t\to\infty} \frac{1}{t} \log \omega_{t/2}(\mathbb{1} - P_t) \ge b(r).$$

Moreover, one can show that for a suitable choice of P_t,

$$\lim_{t\to\infty} \frac{1}{t} \log \omega_{t/2}(\mathbb{1} - P_t) = b(r).$$

Hence, if $\omega_{-t/2}$ is concentrating exponentially fast on $(\mathbb{1} - P_t)\mathfrak{M}_\omega$ with an exponential rate $< -r$, then $\omega_{t/2}$ is concentrating on $P_t\mathfrak{M}_\omega$ with the optimal exponential rate $b(r)$.

(vii) For $\epsilon \in]0,1[$ set

$$\begin{aligned} \overline{B}_\epsilon &= \inf_{\{P_t\}} \left\{ \limsup_{t\to\infty} \frac{1}{t} \log \omega_{t/2}(\mathbb{1} - P_t) \,\middle|\, \omega_{-t/2}(P_t) \le \epsilon \right\}, \\ \underline{B}_\epsilon &= \inf_{\{P_t\}} \left\{ \liminf_{t\to\infty} \frac{1}{t} \log \omega_{t/2}(\mathbb{1} - P_t) \,\middle|\, \omega_{-t/2}(P_t) \le \epsilon \right\}, \\ B_\epsilon &= \inf_{\{P_t\}} \left\{ \lim_{t\to\infty} \frac{1}{t} \log \omega_{t/2}(\mathbb{1} - P_t) \,\middle|\, \omega_{-t/2}(P_t) \le \epsilon \right\}, \end{aligned} \tag{5.8}$$

where the infimum is taken over families of tests $\{P_t\}_{t>0}$ subject, in the last case, to the constraint that $\lim_{t\to\infty} t^{-1} \log \omega_{t/2}(\mathbb{1} - P_t)$ exists. Note that if

$$\beta_t(\epsilon) = \inf_P \{\omega_{t/2}(\mathbb{1} - P) \,|\, \omega_{-t/2}(P) \le \epsilon\},$$

then

$$\liminf_{t\to\infty} \frac{1}{t} \log \beta_t(\epsilon) = \underline{B}_\epsilon, \qquad \limsup_{t\to\infty} \frac{1}{t} \log \beta_t(\epsilon) = \overline{B}_\epsilon.$$

We also define

$$\overline{B} = \inf_{\{P_t\}} \left\{ \limsup_{t\to\infty} \frac{1}{t} \log \omega_{t/2}(\mathbb{1} - P_t) \,\middle|\, \lim_{t\to\infty} \omega_{-t/2}(P_t) = 0 \right\},$$

$$\underline{B} = \inf_{\{P_t\}} \left\{ \liminf_{t\to\infty} \frac{1}{t} \log \omega_{t/2}(\mathbb{1} - P_t) \,\middle|\, \lim_{t\to\infty} \omega_{-t/2}(P_t) = 0 \right\}, \tag{5.9}$$

$$B = \inf_{\{P_t\}} \left\{ \lim_{t\to\infty} \frac{1}{t} \log \omega_{t/2}(\mathbb{1} - P_t) \,\middle|\, \lim_{t\to\infty} \omega_{-t/2}(P_t) = 0 \right\},$$

where again in the last case the infimum is taken over all families of tests $\{P_t\}_{t>0}$ for which the limit $\lim_{t\to\infty} t^{-1} \log \omega_t(\mathbb{1} - P_t)$ exists.

We shall call the numbers defined in (5.8) and (5.9) the Stein exponents. Clearly, $\underline{B}_\epsilon \leq \overline{B}_\epsilon \leq B_\epsilon$, $\underline{B} \leq \overline{B} \leq B$, $\underline{B}_\epsilon \leq \underline{B}$, $\overline{B}_\epsilon \leq \overline{B}$, $B_\epsilon \leq B$. If (A9) holds, then for any $\epsilon \in]0,1[$,

$$\underline{B} = \overline{B} = B = \underline{B}_\epsilon = \overline{B}_\epsilon = B_\epsilon = -\langle\sigma\rangle_+,$$

see [JOPS]. Results of this type are called quantum Stein Lemma.

Stein's Lemma asserts that for any family of projections P_t such that

$$\sup_{t>0} \omega_{-t}(P_t) < 1, \tag{5.10}$$

one has

$$\liminf_{t\to\infty} \frac{1}{t} \log \omega_t(\mathbb{1} - P_t) \geq -2\langle\sigma\rangle_+,$$

and that for any $\delta > 0$ one can find a sequence of projections $P_t^{(\delta)}$ satisfying (5.10) and

$$\lim_{t\to\infty} \frac{1}{t} \log \omega_t(\mathbb{1} - P_t^{(\delta)}) \leq -2\langle\sigma\rangle_+ + \delta.$$

Hence, if no restrictions are made on P_t w.r.t. ω_{-t} except (5.10) (which is needed to avoid trivial result), the optimal exponential rate of concentration of ω_t as $t \uparrow \infty$ is precisely twice the negative entropy production.

5.7 Large time limit: Control parameters

We continue with the framework of Section 5.4. The infinitely extended systems $(\mathcal{O}, \tau_X, \omega_X)$ are parameterized by control parameters $X \in \mathbb{R}^n$. Recall the shorthands $\omega = \omega_0$, $\tau = \tau_0$, $\mathbf{\Phi} = \mathbf{\Phi}_0$, etc. We assume

(A10) For all $t > 0$ the functional $(X,Y) \mapsto e_t(X,Y)$ has an analytic continuation to the polydisk $D_{\delta,\epsilon} = \{(X,Y) \in \mathbb{C}^n \times \mathbb{C}^n \mid \max_j |X_j| < \delta, \max_j |Y_j| < \epsilon\}$ satisfying

$$\sup_{\substack{(X,Y)\in D_{\delta,\epsilon} \\ t>0}} \left| \frac{1}{t} e_t(X,Y) \right| < \infty.$$

In addition, the limit

$$e_+(X,Y) = \lim_{t\to\infty} \frac{1}{t} e_t(X,Y),$$

exists for all $(X,Y) \in D_{\delta,\epsilon} \cap (\mathbb{R}^n \times \mathbb{R}^n)$.

As in the case of (A9), establishing (A10) for physically interesting models is typically a very difficult analytical problem. Although (A10) is certainly not a minimal assumption under which the results of this section hold (for the minimal axiomatic scheme see [JOPP]), it can be verified in interesting examples and allows for a transparent exposition of the material of this section.

A consequence of the first part of (A10) is that finite time linear response theory holds for $(\mathcal{O}, \tau_X^t, \omega_X)$. By Vitali's theorem, $e_+(X, Y)$ is analytic on $D_{\delta,\epsilon}$ and we have:

Proposition 5.8 (1) *For any $X \in \mathbb{R}^n$ such that $\max_j |X_j| < \delta$,*

$$\langle \mathbf{\Phi}_X \rangle_+ = \lim_{t\to\infty} \frac{1}{t} \int_0^t \omega_X \left(\mathbf{\Phi}_{Xs} \right) \mathrm{d}s = \mathbf{\nabla}_Y e_+(X, Y)|_{Y=0}.$$

(2) *The kinetic transport coefficients defined by*

$$L_{jk} = \partial_{X_k} \langle \Phi_X^{(j)} \rangle_+ |_{X=0},$$

satisfy

$$L_{jk} = \lim_{t\to\infty} L_{jkt} = \lim_{t\to\infty} \frac{1}{2} \int_{-t}^t \langle \Phi^{(k)} | \Phi_s^{(j)} \rangle_\omega \left(1 - \frac{|s|}{t} \right) \mathrm{d}s.$$

(3) *The Onsager matrix $[L_{jk}]$ is symmetric and positive semi-definite.*

(4) *Suppose that ω is a (τ, β)-KMS state for some $\beta > 0$ and that $(\mathcal{O}, \tau, \omega)$ is mixing, i.e., that*

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

for all $A, B \in \mathcal{O}$. Then

$$L_{jk} = \lim_{t\to\infty} \frac{1}{2} \int_{-t}^t \omega(\Phi^{(j)} \Phi_s^{(k)}) \mathrm{d}s.$$

Parts (1)–(3) are an immediate consequence of Vitali's theorem (see Proposition B.1 in Appendix B). Part (4) recovers the familiar form of the Green-Kubo formula under the assumption that for vanishing control parameters the infinitely extended system is in thermal equilibrium (and is strongly ergodic). For the proof of (4) see [JOPP] or the proof of Theorem 2.3 in [JOP2].

5.8 Large time limit: Non-equilibrium steady states (NESS)

Consider our infinitely extended system $(\mathcal{O}, \tau^t, \omega)$ and suppose

(A11) The limit

$$\lim_{t\to\infty} \omega_t(A) = \omega_+(A),$$

exists for all $A \in \mathcal{O}$. ω_+ is a stationary state called the NESS of $(\mathcal{O}, \tau^t, \omega)$.

Albeit a hard ergodic-type problem, the verification of (A11) is typically easier then the proof of (A9) or (A10). In fact, in all known non-trivial models satisfying (A9)/(A10), the proof of (A11) is a consequence of the proof of (A9)/(A10).

The structural theory of NESS was one of the central topics of the lecture notes [AJPP1] and we will not discuss it here. In relation with entropic fluctuations, the NESS plays a central role in the Gallavotti-Cohen fluctuation theorem. We will not enter into this subject in these lecture notes.

5.9 Stability with respect to the reference state

In addition to (A11), one expects that under normal conditions any normal state $\nu \in \mathcal{N}_\omega$ is in the basin of attraction of the NESS ω_+, *i.e.*, that the following holds:

(A12)

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

for all $\nu \in \mathcal{N}_\omega$ and $A \in \mathcal{O}$.

As for (A11), in all known non-trivial models, (A12) follows from the proofs of (A9)/(A10).

(A12) is a mathematical formulation of the fact that under normal conditions the NESS and more generally the large time thermodynamics do not depend on local perturbations of the initial state ω. More specifically, in the context of open quantum systems, if the coupling V is well localized in the reservoirs, then in the TD limit (the $\mathcal{R}_j$'s becoming infinitely extended and the system $\mathcal{S}$ remaining finite), the effect of including V in the reference state becomes negligible for large times. In other words, the product state ω used in Sections 4.1–4.2 and the state ω_X of Section 4.3 become equivalent for large times. More generally, the system loses memory of any localized perturbation of its initial state.

In a similar vein one expects that, under normal conditions, the limiting entropic functionals do not depend on local perturbations of the initial state. To illustrate this point, we consider the functional $e_{\infty,+}(\alpha)$ (and assume that the reader is familiar with Araki's perturbation theory of the KMS structure). ω has a modular group ς_ω^t and if ω_W is the KMS state (at temperature -1) of the perturbed group $\varsigma_{\omega W}^t$ for some $W \in \mathcal{O}_{\rm self}$ (which, for finite systems, amounts to set $\omega_W = \mathrm{e}^{\log\omega + W}/\mathrm{tr}(\mathrm{e}^{\log\omega+W})$), then

$$\omega_W(A) = \frac{\omega(A\mathrm{E}_W(-\mathrm{i}))}{\omega(\mathrm{E}_W(-\mathrm{i}))},$$

where the cocycle E_W is given by (2.28). The set of states $\{\omega_W \,|\, W \in \mathcal{O}_{\rm self}\}$ is norm dense in the (norm closed) set $\mathcal{N}_\omega$ of all normal state on $\mathcal{O}$. Since $\ell_{\omega_W|\omega} = W$, one has $\ell_{\omega_{Wt}|\omega_W} = \ell_{\omega_t|\omega} + \tau^{-t}(W) - W$ and hence

$$\omega_+(\sigma_\omega) = \omega_+(\sigma_{\omega_W}).$$

Similarly, for $\alpha \in]0,1[$, Proposition 3.8 holds for infinitely extended systems (this can be proven either via a TD limit argument or by direct application of modular theory), and so

$$\lim_{t\to\infty} \frac{1}{t}(e_{\infty,t,\omega}(\alpha) - e_{\infty,t,\omega_W}(\alpha)) = 0.$$

Hence,

$$e_{\infty,+,\omega}(\alpha) = \lim_{t\to\infty} \frac{1}{t} e_{\infty,t,\omega}(\alpha),$$

exists iff

$$e_{\infty,+,\omega_W}(\alpha) = \lim_{t\to\infty} \frac{1}{t} e_{\infty,t,\omega_W}(\alpha),$$

exists and the limiting entropic functionals are equal. Similar stability results for other entropic functionals can be established under additional regularity assumptions [JOPP].

5.10 Full counting statistics and quantum fluxes: a comparison

In this section we shall focus on open quantum systems described in Chapter 4. For simplicity of notation we set the chemical potentials μ_j of the reservoirs $\mathcal{R}_j$ to zero and deal only with energy fluxes Φ_j.

Full counting statistics deals with the mean entropy/energy flow operationally defined by a repeated quantum measurement. It does not refer to the measurement of a single quantum observable. In fact, surprisingly, it gives a physical interpretation to quantities which are considered unobservable from the traditional point of view: the spectral projections of a relative modular operator. Full counting statistics is of purely quantum origin and has no counterpart in classical statistical mechanics. In contrast, the energy flux observables Φ_j introduced in Chapter 4 arise by direct operator quantization of the corresponding classical observables. In this section, we take a closer look at the relation between full counting statistics and energy flux observables.

For open quantum systems, the TD limit concerns only the reservoirs $\mathcal{R}_j$, the finite quantum system $\mathcal{S}$ remaining fixed. As discussed in the previous section, if we are not interested in transient properties then we may assume, without loss of generality, that $\omega_{\mathcal{S}}$ is the chaotic state (2.15). After the TD limit is taken, the infinitely extended reservoir $\mathcal{R}_j$ is described by the quantum dynamical system $(\mathcal{O}_j, \tau_j^t, \omega_j)$, where ω_j is a (τ_j, β_j)-KMS state on $\mathcal{O}_j$. The joint system $\mathcal{R} = \mathcal{R}_1 + \cdots + \mathcal{R}_n$ is described by

$$(\mathcal{O}_{\mathcal{R}}, \tau_{\mathcal{R}}^t, \omega_{\mathcal{R}}) = \bigotimes_{j=1}^{n} (\mathcal{O}_j, \tau_j^t, \omega_j).$$

The joint but decoupled system $\mathcal{S} + \mathcal{R}$ is described by $(\mathcal{O}, \tau^t, \omega)$ where

$$\mathcal{O} = \mathcal{O}_{\mathcal{S}} \otimes \mathcal{O}_{\mathcal{R}}, \qquad \tau^t = \tau_{\mathcal{S}}^t \otimes \tau_{\mathcal{R}}^t, \qquad \omega = \omega_{\mathcal{S}} \otimes \omega_{\mathcal{R}}.$$

The interaction of $\mathcal{S}$ with $\mathcal{R}_j$ is described by a self-adjoint element $V_j \in \mathcal{O}_{\mathcal{S}} \otimes \mathcal{O}_j$. The full interaction $V = \sum_j V_j$ and the corresponding perturbed C^*-dynamics τ_V^t finally yield the quantum dynamical system $(\mathcal{O}, \tau_V^t, \omega)$ which describes the infinitely extended open quantum system. Without further saying, we shall always assume that all relevant quantities are realized as TD limit of the corresponding quantities of a sequence $\{\mathcal{Q}_M\}$ of finite, TRI open quantum systems. In particular, that is so for the energy flux observables

$$\Phi_j = \delta_j(V_j),$$

where δ_j is the generator of τ_j ($\tau_j^t = \mathrm{e}^{t\delta_j}$), and the entropy production observable

$$\sigma = -\sum_j \beta_j \Phi_j,$$

of the infinitely extended open quantum system $(\mathcal{O}, \tau_V^t, \omega)$.

Recall Section 4.2. Let $\mathbb{P}_t$ be the full counting statistics of the infinitely extended open systems $(\mathcal{O}, \tau_V^t, \omega)$. The probability measure $\mathbb{P}_t$ arises as the weak limit of the full counting statistics $\mathbb{P}_{M,t}$ of $\mathcal{Q}_M$ (this realization is essential for the physical interpretation of $\mathbb{P}_t$). Thus, it follows from Relations (4.7), (4.8), that

$$\langle \varepsilon_j \rangle_+ = \lim_{t\to\infty} \mathbb{E}_t(\varepsilon_j) = -\beta_j \omega_+(\Phi_j), \tag{5.11}$$

$$\begin{aligned} D_{\mathrm{fcs},jk} &= \lim_{t\to\infty} t\left(\mathbb{E}_t(\varepsilon_j\varepsilon_k) - \mathbb{E}_t(\varepsilon_j)\mathbb{E}_t(\varepsilon_k)\right) \\ &= \beta_j\beta_k \int_{-\infty}^{\infty} \omega_+\left((\Phi_j - \omega_+(\Phi_j))(\Phi_{kt} - \omega_+(\Phi_k))\right) \mathrm{d}t. \end{aligned} \tag{5.12}$$

Here, ω_+ is the NESS of $(\mathcal{O}, \tau_V^t, \omega)$ and we have assumed that the correlation function

$$t \mapsto \omega_+\left((\Phi_j - \omega_+(\Phi_j))(\Phi_{kt} - \omega_+(\Phi_k))\right),$$

is integrable on $\mathbb{R}$.

The fluctuations of $\mathbb{P}_t$ as $t \to \infty$ are described by a central limit theorem and a large deviation principle. The central limit theorem holds if for all $\boldsymbol{\alpha} \in \mathbb{R}^n$,

$$\lim_{t\to\infty} \int_{\mathbb{R}^n} \mathrm{e}^{\mathrm{i}\sqrt{t}\boldsymbol{\alpha}\cdot(\boldsymbol{\varepsilon} - \langle\boldsymbol{\varepsilon}\rangle_+)} \mathrm{d}\mathbb{P}_t(\boldsymbol{\varepsilon}) = \int_{\mathbb{R}^n} \mathrm{e}^{\mathrm{i}\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}} \mathrm{d}\mu_{\mathbf{D}_{\mathrm{fcs}}}(\boldsymbol{\varepsilon}),$$

where $\mu_{\mathbf{D}_{\rm fcs}}$ is the centered Gaussian measure on $\mathbb{R}^n$ with covariance $\mathbf{D}_{\rm fcs} = [D_{{\rm fcs},jk}]$. To discuss the large deviation principle, recall that

$$e_{2,t}(\boldsymbol{\alpha}) = \log \int_{\mathbb{R}^n} {\rm e}^{-t\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}} {\rm d}\mathbb{P}_t(\boldsymbol{\varepsilon}).$$

Suppose that

$$e_{2,+}(\boldsymbol{\alpha}) = \lim_{t\to\infty} \frac{1}{t} e_t(\boldsymbol{\alpha}),$$

exists for $\boldsymbol{\alpha} \in \mathbb{R}^n$ and satisfies the conditions of Gärtner-Ellis theorem (Theorem A.6 in Appendix A.3). Then for any Borel set $G \subset \mathbb{R}^d$,

$$-\inf_{\mathbf{s}\in{\rm int}(G)} I(\mathbf{s}) \le \liminf_{t\to\infty} \frac{1}{t} \log \mathbb{P}_t(G) \le \limsup_{t\to\infty} \frac{1}{t} \log \mathbb{P}_t(G) \le -\inf_{\mathbf{s}\in{\rm cl}(G)} I(\mathbf{s}),$$

where

$$I(\mathbf{s}) = -\inf_{\boldsymbol{\alpha}\in\mathbb{R}^n} \left(\mathbf{s}\cdot\boldsymbol{\alpha} + e_{2,+}(\boldsymbol{\alpha})\right).$$

Note that $I(\mathbf{s})$ satisfies the Evans-Searles symmetry

$$I(-\mathbf{s}) = \mathbf{1}\cdot\mathbf{s} + I(\mathbf{s}).$$

For some models the central limit theorem and the large deviation principle can be proven following the spectral scheme outlined in Section 5.5 (for example, this is the case for Spin-Fermion model, see Section 6.5). For other models, scattering techniques are effective (see Section 6.6). In general, however, verifications of the central limit theorem and the large deviation principle are difficult problems.

Let now

$$X_j = \beta_{\rm eq} - \beta_j,$$

be the thermodynamic forces. The new reference state ω_X is the TD limit of the states $\omega_{M,X}$ of the finite open quantum systems $\mathcal{Q}_M$. Alternatively, ω_X can be described directly in terms of the modular structure, see [JOP1]. ω_X is modular and normal w.r.t. ω. The entropy production observables of $(\mathcal{O}, \tau_V^t, \omega_X)$ is

$$\sigma_X = \sum_{j=1}^n X_j \Phi_j.$$

The NESS ω_{X+} also depends on X and, for $X = 0$, reduces to a $(\tau_V, \beta_{\rm eq})$-KMS state $\omega_{\beta_{\rm eq}}$. Let $e_t(X, Y)$ be the entropic functional of the infinitely extended system $(\mathcal{O}, \tau_V^t, \omega_X)$ and suppose that (A10) holds. Then Proposition 5.8 implies that the transport coefficients

$$L_{jk} = \partial_{X_k} \omega_{X+}(\Phi_j)|_{X=0},$$

are defined, satisfy the Onsager reciprocity relations

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

and the Green-Kubo formulas

$$L_{jk} = \frac{1}{2} \int_{-\infty}^{\infty} \omega_{\beta_{\rm eq}}(\Phi_j \Phi_{kt}) {\rm d}t.$$

Here we have assumed that the quantum dynamical system $(\mathcal{O}, \tau_V^t, \omega_{\beta_{\rm eq}})$ is mixing and that the correlation function $t \mapsto \omega_{\beta_{\rm eq}}(\Phi_j \Phi_{kt})$ is integrable.

The linear response theory derived for quantum fluxes Φ_j immediately yields the linear response theory for the full counting statistics. Indeed, it follows from the formulas (5.11) and (5.12) that

$$L_{{\rm fcs},kj} = \partial_{X_k} \langle \varepsilon_j \rangle_+|_{X=0} = -\beta_{\rm eq} L_{kj} = -\frac{1}{\beta_{\rm eq}} D_{{\rm fcs},kj}|_{X=0}.$$

The last relation also yields the Fluctuation-Dissipation Theorem for the full counting statistics. The Einstein relation takes the form

$$L_{\mathrm{fcs},kj} = -\frac{1}{2\beta_{\mathrm{eq}}} D_{\mathrm{fcs},kj}|_{X=0}.$$

and relates the kinetic transport coefficients of the full counting statistics to its fluctuations in thermal equilibrium. The factor $-\beta_{\mathrm{eq}}^{-1}$ is due to our choice to keep the entropic form of the full counting statistics in the discussion of energy transport. In the energy form of the full counting statistics one considers $\mathbb{E}_t(-\varepsilon_j/\beta_j)$ and then the Einstein relation hold in the usual form $L_{\mathrm{fcs},kj} = \frac{1}{2} D_{\mathrm{fcs},kj}|_{X=0}$. The disadvantage of the energy form is that the Evans-Searles symmetry has to be scaled. The choice between scaling Einstein relations or scaling symmetries is of course of no substance.

At this point let us introduce a “naive" cumulant generating function

$$e_{\mathrm{naive},t}(\boldsymbol{\alpha}) = \log \omega \left(\mathrm{e}^{-\sum_{j=1}^{n} \alpha_j \beta_j \int_0^t \Phi_{js} \mathrm{d}s} \right), \tag{5.13}$$

and the “naive" cumulants

$$\chi_t(k_1, \ldots, k_n) = \partial_{\alpha_1}^{k_1} \cdots \partial_{\alpha_n}^{k_n} e_{\mathrm{naive},t}(\boldsymbol{\alpha})|_{\boldsymbol{\alpha}=0}.$$

The function $e_{\mathrm{naive},t}(\boldsymbol{\alpha})$ is just the direct quantization of the classical cumulant generating function for the entropy transfer

$$\mathbf{S^t} = (S_1^t, \ldots, S_n^t) = \int_0^t (-\beta_1 \Phi_{1s}, \ldots, -\beta_n \Phi_{ns}) \mathrm{d}s,$$

in the state ω. Except in the special case $\boldsymbol{\alpha} = \alpha \mathbf{1}$, $e_{\mathrm{naive},t}(\boldsymbol{\alpha})$ cannot be described in terms of classical probability, *i.e.*, $e_{\mathrm{naive},t}(\boldsymbol{\alpha})$ *is not* the cumulant generating function of a probability measure on $\mathbb{R}^n$. If $\boldsymbol{\alpha} = \alpha \mathbf{1}$, then

$$e_{\mathrm{naive},t}(\alpha \mathbf{1}) = \log \omega \left(\mathrm{e}^{\alpha \int_0^t \sigma_s \mathrm{d}s} \right) = \log \int_{\mathbb{R}} \mathrm{e}^{t\alpha s} \mathrm{d}\mu_{\omega,t}(s),$$

where, in the GNS-representation of $\mathcal{O}$ associated to ω, $\mu_{\omega,t}$ is the spectral measure for $t^{-1}\int_0^t \pi_\omega(\sigma_s)\mathrm{d}s$ and ξ_ω.

In general the functional $e_{\mathrm{naive},t}(\boldsymbol{\alpha})$ will not satisfy the Evans-Searles symmetry, *i.e.*, $e_{\mathrm{naive},t}(\mathbf{1}-\boldsymbol{\alpha}) \neq e_{\mathrm{naive},t}(\boldsymbol{\alpha})$, and the same remark applies to the limiting functional

$$e_{\mathrm{naive},+}(\boldsymbol{\alpha}) = \lim_{t\to\infty} \frac{1}{t} e_{\mathrm{naive},t}(\boldsymbol{\alpha}),$$

which, we assume, exists and is differentiable on some open set containing $\mathbf{0}$. One easily checks that the first and second order cumulants satisfy

$$\partial_{\alpha_j} e_{\mathrm{naive},t}(\boldsymbol{\alpha})|_{\boldsymbol{\alpha}=\mathbf{0}} = \partial_{\alpha_j} e_{2,t}(\boldsymbol{\alpha})|_{\boldsymbol{\alpha}=\mathbf{0}},$$

$$\partial_{\alpha_k}\partial_{\alpha_j} e_{\mathrm{naive},t}(\boldsymbol{\alpha})|_{\boldsymbol{\alpha}=\mathbf{0}} = \partial_{\alpha_k}\partial_{\alpha_j} e_{2,t}(\boldsymbol{\alpha})|_{\boldsymbol{\alpha}=\mathbf{0}},$$

and if the limits and derivatives could be exchanged,

$$\partial_{\alpha_j} e_{\mathrm{naive},+}(\boldsymbol{\alpha})|_{\boldsymbol{\alpha}=\mathbf{0}} = \partial_{\alpha_j} e_{2,+}(\boldsymbol{\alpha})|_{\boldsymbol{\alpha}=\mathbf{0}},$$

$$\partial_{\alpha_k}\partial_{\alpha_j} e_{\mathrm{naive},+}(\boldsymbol{\alpha})|_{\boldsymbol{\alpha}=\mathbf{0}} = \partial_{\alpha_k}\partial_{\alpha_j} e_{2,+}(\boldsymbol{\alpha})|_{\boldsymbol{\alpha}=\mathbf{0}}.$$

We summarize our observations:

(i) The first and second order cumulants of the full counting statistics are the same as the corresponding “naive" quantum energy flux cumulants, *i.e.*, the direct quantization of the classical energy flux cumulants. In general, higher order “naive” cumulants do not coincide with the corresponding cumulants of the full counting statistics.

(ii) The limiting expectation $\langle \varepsilon \rangle_+$ and covariance $\mathbf{D}_{\rm fcs}$ of the full counting statistics are expressed in terms of the NESS ω_+ and quantized fluxes Φ_j. They are direct quantization of the corresponding classical expressions. The same remark applies to the central limit theorem, linear response theory and fluctuation-dissipation theorem. If the full counting statistics is restricted to the entropy production observable, then its limiting expectation, covariance and central limit theorem coincide with those of the spectral measure for $t^{-1}\int_0^t \sigma_s {\rm d}s$ and ω.

(iii) We emphasize: to detect the difference between full counting statistics and the “naive" cumulant generating function one needs to consider cumulants of at least third order. In Chapter 6 we shall illustrate this point on some examples of physical interest.

Chapter 6

Fermionic systems

In this section we discuss non-equilibrium statistical mechanics of fermionic systems and describe several physically relevant models to which the structural theory developed in these lecture notes applies.

6.1 Second quantization

We start with some notation. Let $\mathcal{Q}$ be a finite set. $\ell^2(\mathcal{Q})$ denotes the Hilbert space of all function $f : \mathcal{Q} \to \mathbb{C}$ equipped with the inner product

$$\langle f|g\rangle = \sum_{q\in\mathcal{Q}} \overline{f(q)}g(q).$$

The functions $\{\delta_q \,|\, q \in \mathcal{Q}\}$, where $\delta_q(x) = 1$ if $x = q$ and 0 otherwise, form an orthonormal basis for $\ell^2(\mathcal{Q})$. Any Hilbert space of dimension $|\mathcal{Q}|$ is isomorphic to $\ell^2(\mathcal{Q})$.

Let the configuration space of a single particle be the finite set $\mathcal{Q}$. Typically, $\mathcal{Q}$ will be a subset of some lattice, but at this point we do not need to specify its structure further. The Hilbert space of a single particle is $\mathcal{K} = \ell^2(\mathcal{Q})$. If $\psi \in \mathcal{K}$ is a normalized wave function, then $|\psi(q)|^2$ is probability that the particle is located at $q \in \mathcal{Q}$. The configuration space of a system of n distinguishable particles is $\mathcal{Q}^n$ and $\ell^2(\mathcal{Q}^n)$ is its Hilbert space. For $q = (q_1, \ldots, q_n) \in \mathcal{Q}^n$ we set $\delta_q(x_1, \ldots, x_n) = \delta_{q_1}(x_1)\cdots\delta_{q_n}(x_n)$. $\{\delta_q \,|\, q \in \mathcal{Q}^n\}$ is an orthonormal basis of $\ell^2(\mathcal{Q}^n)$. Let $\mathcal{K}^{\otimes n}$ be the n-fold tensor product of $\mathcal{K}$ with itself. Identifying δ_q with $\delta_{q_1} \otimes \cdots \otimes \delta_{q_n}$ we obtain an isomorphism between $\ell^2(\mathcal{Q}^n)$ and $\mathcal{K}^{\otimes n}$. In the following we shall identify these two spaces.

If $\psi \in \mathcal{K}^{\otimes n}$ is the normalized wave function of the system of n particles and $\psi_1, \ldots, \psi_n \in \mathcal{K}$ are normalized one-particle wave functions, then $|\langle\psi|\psi_1 \otimes \cdots \otimes \psi_n\rangle|^2$ is the probability for the j-th particle to be in the state ψ_j, $j = 1, \ldots, n$. According to Pauli's principle, if the particles are identical fermions, then this probability must vanish if at least two of the ψ_j's are equal. It follows that the multilinear functional $F(\psi_1, \ldots, \psi_n) = \langle\psi|\psi_1 \otimes \cdots \otimes \psi_n\rangle$ has to vanish if at least two of its arguments coincide. Hence, for $j \neq k$,

$$F(\psi_1, \ldots, \psi_j + \psi_k, \ldots, \psi_k + \psi_j, \ldots, \psi_n) = 0,$$

for any $\psi_1, \ldots, \psi_n \in \mathcal{K}$. By multilinearity, this is equivalent to

$$\begin{aligned} 0 &= F(\psi_1, \ldots, \psi_j, \ldots, \psi_k, \ldots, \psi_n) + F(\psi_1, \ldots, \psi_j, \ldots, \psi_j, \ldots, \psi_n) \\ &\quad + F(\psi_1, \ldots, \psi_k, \ldots, \psi_k, \ldots, \psi_n) + F(\psi_1, \ldots, \psi_k, \ldots, \psi_j, \ldots, \psi_n) \\ &= F(\psi_1, \ldots, \psi_j, \ldots, \psi_k, \ldots, \psi_n) + F(\psi_1, \ldots, \psi_k, \ldots, \psi_j, \ldots, \psi_n), \end{aligned}$$

and we conclude that F must be alternating, *i.e.*, , changing sign under transposition of two of its arguments,

$$F(\psi_1, \ldots, \psi_j, \ldots, \psi_k, \ldots, \psi_n) = -F(\psi_1, \ldots, \psi_k, \ldots, \psi_j, \ldots, \psi_n). \tag{6.1}$$

Let S_n be the group of permutations of the set $\{1, \ldots, n\}$. For $\pi \in S_n$ we set

$$\pi\psi_1 \otimes \cdots \otimes \psi_n = \psi_{\pi(1)} \otimes \cdots \otimes \psi_{\pi(n)},$$

and extend this definition to $\mathcal{K}^{\otimes n}$ by linearity. One easily checks that this action of S_n on $\mathcal{K}^{\otimes n}$ is unitary. If $\pi = (jk) = \pi^{-1}$ is the transposition whose only effect is to interchange j and k, then (6.1) is equivalent to

$$\langle \pi\psi|\psi_1 \otimes \cdots \otimes \psi_n\rangle = \langle \psi|\pi\psi_1 \otimes \cdots \otimes \psi_n\rangle = -\langle \psi|\psi_1 \otimes \cdots \otimes \psi_n\rangle,$$

and so $\pi\psi = -\psi$. More generally, if π is the composition of m transpositions, $\pi = (j_1k_1)\cdots(j_mk_m)$, then we must have $\pi\psi = (-1)^m\psi$. Any permutation $\pi \in S_n$ can be decomposed into a product of transpositions and the corresponding number $(-1)^m$, the signature of π, is denoted by $\mathrm{sign}(\pi)$ (one can show that $\mathrm{sign}(\pi) = (-1)^t$ where t is the number of pairs $(j,k) \in \{1,\ldots n\}$ such that $j < k$ and $\pi(j) > \pi(k)$). We conclude that the wave function ψ of a system of n identical fermions must satisfy

$$\pi\psi = \mathrm{sign}(\pi)\psi,$$

for all $\pi \in S_n$. More explicitly, for $\pi \in S_n$ the wave function ψ satisfies

$$\psi(x_{\pi(1)},\ldots,x_{\pi(n)}) = \mathrm{sign}(\pi)\psi(x_1,\ldots,x_n). \tag{6.2}$$

Functions satisfying (6.2) are called completely antisymmetric. The set of all completely antisymmetric functions on $\mathcal{Q}^n$ is a subspace of $\ell^2(\mathcal{Q}^n)$ which we denote by $\ell^2_-(\mathcal{Q}^n)$.

Exercise 6.1.

1. Show that the orthogonal projection P_- on $\ell^2_-(\mathcal{Q}^n)$ is given by

$$P_-\psi = \frac{1}{n!}\sum_{\pi\in S_n}\mathrm{sign}(\pi)\pi\psi.$$

Hint: use the morphism property of the signature, $\mathrm{sign}(\pi\circ\pi') = \mathrm{sign}(\pi)\mathrm{sign}(\pi')$, to show that $\pi P_- = \mathrm{sign}(\pi)P_-$.

2. Define the wedge product of $\psi_1,\ldots,\psi_n \in \mathcal{K}$ by

$$\psi_1\wedge\cdots\wedge\psi_n = \sqrt{n!}\,P_-\psi_1\otimes\cdots\otimes\psi_n,$$

and show that

$$\langle\psi_1\wedge\cdots\wedge\psi_n|\phi_1\wedge\cdots\wedge\phi_n\rangle = \det[\langle\psi_i|\phi_j\rangle]_{1\le i,j\le n}. \tag{6.3}$$

Hint: use Leibnitz formula

$$\det A = \sum_{\pi\in S_n}\mathrm{sign}(\pi)A_{1\pi(1)}\cdots A_{n\pi(n)},$$

for the determinant of the $n\times n$ matrix $A = [A_{jk}]$.

3. Denote by $\mathcal{K}^{\wedge n}$ the linear span of the set $\{\psi_1\wedge\cdots\wedge\psi_n\,|\,\psi_1,\ldots,\psi_n\in\mathcal{K}\}$. Suppose that $n \le d = |\mathcal{Q}| = \dim\mathcal{K}$ and let $\{\phi_1,\ldots,\phi_d\}$ be an orthonormal basis of $\mathcal{K}$. Prove that

$$\{\phi_{j_1}\wedge\cdots\wedge\phi_{j_n}\,|\,1\le j_1<\cdots<j_n\le d\},$$

is an orthonormal basis of $\mathcal{K}^{\wedge n}$ and deduce that

$$\dim\mathcal{K}^{\wedge n} = \binom{\dim\mathcal{K}}{n}.$$

In particular, the vector space $\mathcal{K}^{\wedge\dim\mathcal{K}}$ is one dimensional. For $n > \dim\mathcal{K}$ the vector spaces $\mathcal{K}^{\wedge n}$ are trivial, that is, consist only of the zero vector.

According to our identification of $\mathcal{K}^{\otimes n}$ with $\ell^2(\mathcal{Q}^n)$, the subspaces $\ell_-(\mathcal{Q}^n)$ and $\mathcal{K}^{\wedge n}$ coincide (they are both the range of the projection P_-). We denote by

$$\Gamma_n(\mathcal{K}) = \mathcal{K}^{\wedge n},$$

the Hilbert space of a system of n fermions with the single particle Hilbert space $\mathcal{K}$. By definition, $\Gamma_0(\mathcal{K}) = \mathbb{C}$ is the vacuum sector.

For $A \in \mathcal{O}_\mathcal{K}$ and $n \geq 1$, let $\Gamma_n(A)$ and $\mathrm{d}\Gamma_n(A)$ be the elements of $\mathcal{O}_{\Gamma_n(\mathcal{K})}$ defined by

$$\Gamma_n(A)(\psi_1 \wedge \cdots \wedge \psi_n) = A\psi_1 \wedge \cdots \wedge A\psi_n,$$

$$\mathrm{d}\Gamma_n(A)(\psi_1 \wedge \cdots \wedge \psi_n) = A\psi_1 \wedge \cdots \wedge \psi_n + \cdots + \psi_1 \wedge \cdots \wedge A\psi_n.$$

For $n = 0$, we define $\Gamma_0(A)$ to be the identity map on $\Gamma_0(\mathcal{K})$ and set $\mathrm{d}\Gamma_0(A) = 0$. One easily checks the relations

$$\begin{aligned} \Gamma_n(A^*) &= \Gamma_n(A)^*, & \mathrm{d}\Gamma_n(A^*) &= \mathrm{d}\Gamma_n(A)^*, \\ \Gamma_n(AB) &= \Gamma_n(A)\Gamma_n(B), & \mathrm{d}\Gamma_n(A + \lambda B) &= \mathrm{d}\Gamma_n(A) + \lambda \mathrm{d}\Gamma_n(B), \\ \mathrm{d}\Gamma_n(A) &= \left.\frac{\mathrm{d}}{\mathrm{d}t}\Gamma_n(\mathrm{e}^{tA})\right|_{t=0}, & \Gamma_n(\mathrm{e}^A) &= \mathrm{e}^{\mathrm{d}\Gamma_n(A)}, \end{aligned} \tag{6.4}$$

for $A, B \in \mathcal{O}_\mathcal{K}$ and $\lambda \in \mathbb{C}$. The Fermionic Fock space over $\mathcal{K}$ is defined by

$$\Gamma(\mathcal{K}) = \bigoplus_{n=0}^{\dim \mathcal{K}} \Gamma_n(\mathcal{K}),$$

i.e., as the set of vectors $\Psi = (\psi_0, \psi_1, \ldots)$ with $\psi_n \in \Gamma_n(\mathcal{K})$ and the inner product

$$\langle \Psi | \Phi \rangle = \sum_{n=0}^{\dim \mathcal{K}} \langle \psi_n | \phi_n \rangle.$$

Clearly,

$$\dim \Gamma(\mathcal{K}) = \sum_{n=0}^{\dim \mathcal{K}} \dim \Gamma_n(\mathcal{K}) = \sum_{n=0}^{\dim \mathcal{K}} \binom{\dim \mathcal{K}}{n} = 2^{\dim \mathcal{K}}.$$

A normalized vector $\Psi = (\psi_0, \psi_1, \ldots) \in \Gamma(\mathcal{K})$ is interpreted as a state of a gas of identical fermions with one particle Hilbert space $\mathcal{K}$ in the following way. Setting $p_n = \|\psi_n\|^2$, $\phi_n = \psi_n / \|\psi_n\|$ and $\Phi^{(n)} = (0, \ldots, \phi_n, \ldots, 0)$ one can write Ψ as

$$\Psi = \sum_{n=0}^{\dim \mathcal{K}} \sqrt{p_n}\, \Phi^{(n)},$$

a coherent superposition of:

- a state $\Phi^{(0)}$ with no particle. Up to a phase factor, $\Phi^{(0)}$ is the so called vacuum vector

$$\Omega = (1, 0, \ldots, 0),$$

- a state $\Phi^{(1)}$ with 1 particle in the state $\phi_1 \in \mathcal{K}$;
- a state $\Phi^{(2)}$ with 2 particles in the state $\phi_2 \in \Gamma_2(\mathcal{K})$, etc.

Since the vectors $\Phi^{(n)}$ are mutually orthogonal, p_n is the probability for n particles to be present in the system. Pauli's principle forbid more than $\dim \mathcal{K}$ particles. With a slight abuse of notation, we shall identify the n-particle wave function $\phi \in \Gamma_n(\mathcal{K})$ with the vector $\Phi = (0, \ldots, \phi, \ldots, 0) \in \Gamma(\mathcal{K})$.

For $A \in \mathcal{O}_{\mathcal{K}}$ one defines $\Gamma(A)$ and $\mathrm{d}\Gamma(A)$ in $\mathcal{O}_{\Gamma(\mathcal{K})}$ by

$$\Gamma(A) = \bigoplus_{n=0}^{\dim \mathcal{K}} \Gamma_n(A), \qquad \mathrm{d}\Gamma(A) = \bigoplus_{n=0}^{\dim \mathcal{K}} \mathrm{d}\Gamma_n(A).$$

Relations (6.4) yield

$$\begin{aligned} \Gamma(A^*) &= \Gamma(A)^*, & \mathrm{d}\Gamma(A^*) &= \mathrm{d}\Gamma(A)^*, \\ \Gamma(AB) &= \Gamma(A)\Gamma(B), & \mathrm{d}\Gamma(A+\lambda B) &= \mathrm{d}\Gamma(A) + \lambda \mathrm{d}\Gamma(B), \\ \mathrm{d}\Gamma(A) &= \frac{\mathrm{d}}{\mathrm{d}t}\Gamma(\mathrm{e}^{tA})\bigg|_{t=0}, & \Gamma(\mathrm{e}^A) &= \mathrm{e}^{\mathrm{d}\Gamma(A)}. \end{aligned} \tag{6.5}$$

Note that $\Gamma(A)$ is invertible iff A is invertible and in this case $\Gamma(A)^{-1} = \Gamma(A^{-1})$. Moreover, one easily checks that

$$\Gamma(A)\mathrm{d}\Gamma(B)\Gamma(A^{-1}) = \mathrm{d}\Gamma(ABA^{-1}). \tag{6.6}$$

In particular, one has

$$\mathrm{e}^{t\mathrm{d}\Gamma(A)}\mathrm{d}\Gamma(B)\mathrm{e}^{-t\mathrm{d}\Gamma(A)} = \Gamma(\mathrm{e}^{tA})\mathrm{d}\Gamma(B)\Gamma(\mathrm{e}^{-tA}) = \mathrm{d}\Gamma(\mathrm{e}^{tA}B\mathrm{e}^{-tA}).$$

which, upon differentiation at $t = 0$, yields

$$[\mathrm{d}\Gamma(A), \mathrm{d}\Gamma(B)] = \mathrm{d}\Gamma([A, B]). \tag{6.7}$$

The reader familiar with Lie groups will recognize $A \mapsto \Gamma(A)$ as a representation of the linear group $\mathrm{GL}(\mathcal{K})$ in $\Gamma(\mathcal{K})$ and $B \mapsto \mathrm{d}\Gamma(B)$ as the induced representation of its Lie algebra $\mathcal{O}_{\mathcal{K}}$.

Example 6.1 $N = \mathrm{d}\Gamma(\mathbb{1})$ is called the number operator. Since

$$N|_{\Gamma_n(\mathcal{K})} = n\mathbb{1}_{\Gamma_n(\mathcal{K})},$$

N is the observable describing the number of particles in the system.

We finish this section with a result which will be important in Section 6.3.

Lemma 6.1 *For any $A \in \mathcal{O}_{\mathcal{K}}$, one has*

$$\mathrm{tr}(\Gamma(A)) = \det(\mathbb{1} + A).$$

Proof. We first prove the result for self-adjoint A. Let $\{\psi_1, \ldots, \psi_d\}$ be an eigenbasis of A such that $A\psi_j = \lambda_j\psi_j$. Since

$$\begin{aligned} \det(\mathbb{1} + A) &= \prod_{j=1}^{d}(1+\lambda_j) = \sum_{J \subset \{1,\ldots,d\}} \prod_{k\in J} \lambda_k \\ &= \sum_{n=0}^{d} \sum_{\substack{J\subset\{1,\ldots,d\} \\ |J|=n}} \prod_{k\in J}\lambda_k = \sum_{n=0}^{d} \sum_{1\le j_1<\cdots<j_n\le d} \lambda_{j_1}\cdots\lambda_{j_n}, \end{aligned}$$

and $\lambda_{j_1}\cdots\lambda_{j_n} = \langle \psi_{j_1}\wedge\cdots\wedge\psi_{j_n}|\Gamma_n(A)\psi_{j_1}\wedge\cdots\wedge\psi_{j_n}\rangle$, it follows from Part 3 of Exercise 6.1 that

$$\sum_{1\le j_1<\cdots<j_n\le d} \lambda_{j_1}\cdots\lambda_{j_n} = \mathrm{tr}_{\Gamma_n(\mathcal{K})}(\Gamma_n(A)).$$

Hence,

$$\det(\mathbb{1}+A) = \sum_{n=0}^{d} \mathrm{tr}_{\Gamma_n(\mathcal{K})}(\Gamma_n(A)) = \mathrm{tr}(\Gamma(A)),$$

holds for self-adjoint A. If A is not self-adjoint, we set

$$A(\lambda)=\frac{A+A^*}{2}+\lambda\frac{A-A^*}{2\mathrm{i}}.$$

Clearly, $A(\lambda)$ is self-adjoint for $\lambda\in\mathbb{R}$ and so $\det(\mathbb{1}+A(\lambda))=\mathrm{tr}(\Gamma(A(\lambda)))$. Since both sides of this identity are analytic functions of λ (in fact, polynomials), the identity extends to the value $\lambda=\mathrm{i}$ for which $A(\mathrm{i})=A$. □

6.2 The canonical anticommutation relations (CAR)

For $\psi,\psi_1,\ldots,\psi_n\in\mathcal{K}$ we set

$$a^*(\psi)\Omega=\psi,$$
$$a^*(\psi)(\psi_1\wedge\cdots\wedge\psi_n)=\psi\wedge\psi_1\wedge\cdots\wedge\psi_n.$$

By linearity, $a^*(\psi)$ extends to an element of $\mathcal{O}_{\Gamma(\mathcal{K})}$ which maps $\Gamma_n(\mathcal{K})$ into $\Gamma_{n+1}(\mathcal{K})$ and in particular $\Gamma_{\dim\mathcal{K}}(\mathcal{K})$ to $\{0\}$. Since $a^*(\psi)$ acts on a state Ψ by adding to it a particle in the state ψ, it is called creation operator. We note that

$$\psi_1\wedge\cdots\wedge\psi_n=a^*(\psi_1)\cdots a^*(\psi_n)\Omega.$$

Similarly, one defines an element $a(\psi)$ of $\mathcal{O}_{\Gamma(\mathcal{K})}$ by

$$a(\psi)\Omega=0,$$
$$a(\psi)\psi_1=\langle\psi|\psi_1\rangle\Omega,$$
$$a(\psi)(\psi_1\wedge\cdots\wedge\psi_n)=\sum_{j=1}^n(-1)^{1+j}\langle\psi|\psi_j\rangle\,\psi_1\wedge\cdots\wedge\cancel{\psi_j}\wedge\cdots\wedge\psi_n.$$

$a(\psi)$ maps $\Gamma_n(\mathcal{K})$ into $\Gamma_{n-1}(\mathcal{K})$ and in particular $\Gamma_0(\mathcal{K})$ to $\{0\}$. Since it acts on a state Ψ by removing from it a particle in the state ψ, it is called annihilation operator. In the sequel, $a^\#(\psi)$ denotes either $a^*(\psi)$ or $a(\psi)$. The basic properties of creation and annihilation operators are summarized in

Proposition 6.2 (1) *The map $\psi\mapsto a^*(\psi)$ is linear and the map $\psi\mapsto a(\psi)$ is anti-linear.*

(2) $a(\psi)^*=a^*(\psi)$.

(3) *The Canonical Anticommutation Relations* (CAR) *hold:*

$$\{a(\psi),a(\phi)\}=\{a^*(\psi),a^*(\phi)\}=0,\qquad\{a(\psi),a^*(\phi)\}=\langle\psi|\phi\rangle\mathbb{1},$$

where $\{A,B\}=AB+BA$ denotes the anticommutator of A and B.

(4) *The family of operators $\mathfrak{A}=\{a^\#(\psi)\,|\,\psi\in\mathcal{K}\}$ is irreducible in $\mathcal{O}_{\Gamma(\mathcal{K})}$, that is,*

$$\mathfrak{A}'=\{B\in\mathcal{O}_{\Gamma(\mathcal{K})}\,|\,[A,B]=0\,\textit{for all}\,A\in\mathfrak{A}\}=\mathbb{C}\mathbb{1}_{\Gamma(\mathcal{K})}.$$

(5) $\|a^*(\psi)\|=\|a(\psi)\|=\|\psi\|$.

(6) *For any $A\in\mathcal{O}_{\mathcal{K}}$,*

$$\Gamma(A)a^*(\psi)=a^*(A\psi)\Gamma(A),\qquad\Gamma(A^*)a(A\psi)=a(\psi)\Gamma(A^*).$$

In particular, if U is unitary,

$$\Gamma(U)a^\#(\psi)\Gamma(U^*)=a^\#(U\psi).$$

(7) *For any* $A \in \mathcal{O}_{\mathcal{K}}$*,*

$$[\mathrm{d}\Gamma(A), a^*(\psi)] = a^*(A\psi), \qquad [\mathrm{d}\Gamma(A), a(\psi)] = -a(A^*\psi).$$

In particular, if A *is self-adjoint,*

$$\mathrm{i}[\mathrm{d}\Gamma(A), a^\#(\psi)] = a^\#(\mathrm{i}A\psi).$$

(8) $a^*(\phi)a(\psi) = \mathrm{d}\Gamma(|\phi\rangle\langle\psi|)$.

(9) *For any* $A \in \mathcal{O}_{\mathcal{K}}$ *and any orthonormal basis* $\{\psi_1, \ldots, \psi_d\}$ *of* $\mathcal{K}$ *one has*

$$\mathrm{d}\Gamma(A) = \sum_{j,k=1}^{d} \langle\psi_j|A\psi_k\rangle a^*(\psi_j)a(\psi_k).$$

Proof. (1) is obvious from the definitions of the creation/annihilation operators.

(2) follows from Laplace formula for developing the determinant of a $n \times n$ matrix A along one of its row,

$$\det A = \sum_{j=1}^{n} (-1)^{i+j} A_{ij} \det A_{(ij)}, \tag{6.8}$$

where $A_{(ij)}$ denotes the matrix obtained from A be removing its i-th row and j-th column. Indeed, by (6.3)

$$\begin{aligned}
\langle\phi_1 \wedge \cdots \wedge \phi_{n-1}|a^*(\psi)^*\psi_1 \wedge \cdots \wedge \psi_n\rangle &= \langle a^*(\psi)\phi_1 \wedge \cdots \wedge \phi_{n-1}|\psi_1 \wedge \cdots \wedge \psi_n\rangle \\
&= \langle\psi \wedge \phi_1 \wedge \cdots \wedge \phi_{n-1}|\psi_1 \wedge \cdots \wedge \psi_n\rangle \\
&= \det A,
\end{aligned}$$

where

$$A = \begin{bmatrix}
\langle\psi|\psi_1\rangle & \langle\psi|\psi_2\rangle & \cdots & \langle\psi|\psi_n\rangle \\
\langle\phi_1|\psi_1\rangle & \langle\phi_1|\psi_2\rangle & \cdots & \langle\phi_1|\psi_n\rangle \\
\vdots & \vdots & \ddots & \vdots \\
\langle\phi_{n-1}|\psi_1\rangle & \langle\phi_{n-1}|\psi_2\rangle & \cdots & \langle\phi_{n-1}|\psi_n\rangle
\end{bmatrix}.$$

Developing the determinant of A along its first row and using the fact that

$$\det A_{(1j)} = \langle\phi_1 \wedge \cdots \wedge \phi_{n-1}|\psi_1 \wedge \cdots \wedge \cancel{\psi_j} \wedge \cdots \wedge \psi_n\rangle,$$

we obtain

$$\det A = \sum_{j=1}^{n} (-1)^{1+j} \langle\psi|\psi_j\rangle\langle\phi_1 \wedge \cdots \wedge \phi_{n-1}|\psi_1 \wedge \cdots \wedge \cancel{\psi_j} \wedge \cdots \wedge \psi_n\rangle.$$

Hence,

$$a^*(\psi)^*\psi_1 \wedge \cdots \wedge \psi_n = \sum_{j=1}^{n} (-1)^{1+j} \langle\psi|\psi_j\rangle\psi_1 \wedge \cdots \wedge \cancel{\psi_j} \wedge \cdots \wedge \psi_n,$$

and we conclude that $a(\psi)^* = a^*(\psi)$.

(3) The relation $\{a^*(\psi), a^*(\phi)\} = 0$ follows from the fact that $\psi \wedge \phi \wedge \psi_1 \cdots \wedge \psi_n$ changes sign when ψ and ϕ are exchanged. The relation $\{a(\psi), a(\phi)\} = 0$ is obtained by conjugating the previous relation. Finally, adding the two formulas

$$\begin{aligned}
a^*(\phi)a(\psi)\psi_1 \wedge \cdots \wedge \psi_n &= \sum_{j=1}^{n} (-1)^{j+1} \langle\psi|\psi_j\rangle\phi \wedge \psi_1 \wedge \cdots \wedge \cancel{\psi_j} \wedge \cdots \wedge \psi_n, \\
a(\psi)a^*(\phi)\psi_1 \wedge \cdots \wedge \psi_n &= (-1)^{1+1} \langle\psi|\phi\rangle\psi_1 \wedge \cdots \wedge \psi_n \\
&\quad + \sum_{j=1}^{n} (-1)^{j+2} \langle\psi|\psi_j\rangle\phi \wedge \psi_1 \wedge \cdots \wedge \cancel{\psi_j} \wedge \cdots \wedge \psi_n,
\end{aligned}$$

yields the last relation $\{a^*(\phi), a(\psi)\} = \langle\psi|\psi_j\rangle\mathbb{1}$.

(4) We first notice that if $\Psi \in \Gamma(\mathcal{K})$ is such that $a(\psi)\Psi = 0$ for all $\psi \in \mathcal{K}$, then

$$\langle\psi_n \wedge \cdots \wedge \psi_1|\Psi\rangle = \langle a^*(\psi_n)\psi_{n-1} \wedge \cdots \wedge \psi_1|\Psi\rangle = \langle\psi_{n-1} \wedge \cdots \wedge \psi_1|a(\psi_n)\Psi\rangle = 0,$$

from which we conclude that $\Psi \perp \Gamma_n(\mathcal{K})$ for $n \geq 1$. Hence, $\Psi \in \Gamma_0(\mathcal{K})$, *i.e.*, $\Psi = \lambda\Omega$ for some $\lambda \in \mathbb{C}$. Let $B \in \mathcal{O}_{\Gamma(\mathcal{K})}$ commute with all creation/annihilation operators. It follows that $a(\psi)B\Omega = Ba(\psi)\Omega = 0$ for all $\psi \in \mathcal{K}$. From the previous remark, we conclude that $B\Omega = \lambda\Omega$ for some $\lambda \in \mathbb{C}$. Then, we can write

$$\begin{aligned} B\psi_1 \wedge \cdots \wedge \psi_n &= Ba^*(\psi_1) \cdots a^*(\psi_n)\Omega \\ &= a^*(\psi_1) \cdots a^*(\psi_n)B\Omega \\ &= \lambda a^*(\psi_1) \cdots a^*(\psi_n)\Omega = \lambda\psi_1 \wedge \cdots \wedge \psi_n, \end{aligned}$$

which shows that $B|_{\Gamma_n(\mathcal{K})} = \lambda\mathbb{1}_{\Gamma_n(\mathcal{K})}$ and that $B = \lambda\mathbb{1}_{\Gamma(\mathcal{K})}$.

(5) is obvious if $\psi = 0$. The CAR imply

$$\begin{aligned} (a^*(\psi)a(\psi))^2 &= a^*(\psi)(\{a(\psi), a^*(\psi)\} - a^*(\psi)a(\psi))a(\psi) \\ &= \langle\psi|\psi\rangle a^*(\psi)a(\psi) - a^*(\psi)^2a(\psi)^2 \\ &= \|\psi\|^2a^*(\psi)a(\psi), \end{aligned}$$

from which we deduce $\|a^*(\psi)a(\psi)\|^2 = \|(a^*(\psi)a(\psi))^2\| = \|\psi\|^2\|a^*(\psi)a(\psi)\|$. If $\psi \neq 0$ then $a(\psi) \neq 0$ and hence $\|a^*(\psi)a(\psi)\| \neq 0$ so that we can conclude

$$\|a(\psi)\|^2 = \|a^*(\psi)\|^2 = \|a^*(\psi)a(\psi)\| = \|\psi\|^2.$$

(6) It follows from the definitions that $\Gamma(A)a^*(\psi)\Omega = \Gamma(A)\psi = A\psi = a^*(A\psi)\Gamma(A)\Omega$ and

$$\begin{aligned} \Gamma(A)a^*(\psi)\psi_1 \wedge \cdots \wedge \psi_n &= \Gamma(A)\psi \wedge \psi_1 \wedge \cdots \wedge \psi_n \\ &= A\psi \wedge A\psi_1 \wedge \cdots \wedge A\psi_n \\ &= a^*(A\psi)\Gamma(A)\psi_1 \wedge \cdots \wedge \psi_n. \end{aligned}$$

Thus, one has $\Gamma(A)a^*(\psi) = a^*(A\psi)\Gamma(A)$. By conjugation, we also get $\Gamma(A^*)a(A\psi) = a(\psi)\Gamma(A^*)$.

(7) It follows from (6) that

$$\mathrm{e}^{t\mathrm{d}\Gamma(A)}a^*(\psi) = a^*(\mathrm{e}^{tA}\psi)\mathrm{e}^{t\mathrm{d}\Gamma(A)}.$$

Differentiation at $t = 0$ yields the first relation in (7). The second is obtained by conjugation.

(8) The CAR imply

$$\begin{aligned} [a^*(\phi)a(\psi), a^*(\chi)] &= a^*(\phi)a(\psi)a^*(\chi) - a^*(\chi)a^*(\phi)a(\psi) \\ &= a^*(\phi)a(\psi)a^*(\chi) + a^*(\phi)a^*(\chi)a(\psi) \\ &= a^*(\phi)\{a(\psi), a^*(\chi)\} = \langle\psi|\chi\rangle a^*(\phi). \end{aligned}$$

On the other hand, (7) implies that $[\mathrm{d}\Gamma(|\phi\rangle\langle\psi|), a^*(\chi)] = \langle\psi|\chi\rangle a^*(\phi)$. Thus, setting $B = a^*(\phi)a(\psi) - \mathrm{d}\Gamma(|\phi\rangle\langle\psi|)$ we get $[B, a^*(\chi)] = 0$ for all $\chi \in \mathcal{K}$. Interchanging ϕ and ψ, we obtain in the same way $[B, a(\chi)]^* = -[B^*, a^*(\chi)] = 0$, and so $[B, a(\chi)] = 0$. Hence $B \in \mathfrak{A}'$ and (4) implies that $B = \lambda\mathbb{1}$ for some $\lambda \in \mathbb{C}$. Since $B\Omega = 0$ we conclude that $B = 0$.

(9) Follows from (8) and the representation $A = \sum_{j,k=1}^{d}\langle\psi_j|A\psi_k\rangle|\psi_j\rangle\langle\psi_k|$. □

Given a Hilbert space $\mathcal{K}$, a representation of the CAR over $\mathcal{K}$ on a Hilbert space $\mathcal{H}$ is a pair of maps

$$\psi \mapsto b(\psi), \qquad \psi \mapsto b^*(\psi),$$

from $\mathcal{K}$ to $\mathcal{O}_{\mathcal{H}}$ satisfying Properties (1)–(3) of Proposition (6.2). Such a representation is called irreducible if it also satisfies Property (4) with $\mathcal{O}_{\Gamma(\mathcal{K})}$ replaced by $\mathcal{O}_{\mathcal{H}}$. The particular irreducible representation $\psi \mapsto a^{\#}(\psi)$ on $\Gamma(\mathcal{K})$ is called the Fock representation. We will construct another important representation of the CAR in Sections 6.4 and 6.7.2.

Proposition 6.3 *Let $\mathcal{K}$ be a finite dimensional Hilbert space and $\psi \mapsto b^{\#}(\psi)$ an irreducible representation of the CAR over $\mathcal{K}$ on $\mathcal{H}$. Then, there exists a unitary operator $U : \Gamma(\mathcal{K}) \to \mathcal{H}$ such that $Ua^{\#}(\psi)U^* = b^{\#}(\psi)$ for all $\psi \in \mathcal{K}$. Moreover, U is unique up to a phase factor.*

In other words, any two irreducible representations of the CAR over a finite dimensional Hilbert space are unitarily equivalent. A proof of Proposition 6.3 is sketched in the next exercise.

Exercise 6.2. Let $\mathcal{K} \ni \psi \mapsto b(\psi) \in \mathcal{O}_{\mathcal{H}}$ be an irreducible representation of CAR over the d-dimensional Hilbert space $\mathcal{K}$ in the Hilbert space $\mathcal{H}$. Denote by $\{\chi_1, \ldots, \chi_d\}$ an orthonormal basis of $\mathcal{K}$ an set

$$\widetilde{N} = \sum_{n=1}^{d} b^*(\chi_n)b(\chi_n).$$

1. Show that $0 \le \widetilde{N} \le d\mathbb{1}$ and $\widetilde{N}b(\psi) = b(\psi)(\widetilde{N} - \mathbb{1})$ for any $\psi \in \mathcal{K}$.

2. Let $\phi \in \mathcal{H}$ be a normalized eigenvector to the smallest eigenvalue of $\widetilde{N}$. Show that $b(\psi)\phi = 0$ for all $\psi \in \mathcal{K}$.

3. Set $\mathcal{H}_0 = \mathbb{C}\phi$ and denote by $\mathcal{H}_n$ the linear span of $\{b^*(\psi_1)\cdots b^*(\psi_n)\phi \,|\, \psi_1, \ldots, \psi_n \in \mathcal{K}\}$. Show that $\mathcal{H}_n \perp \mathcal{H}_m$ for $n \neq m$ and $\mathcal{H}_n = \{0\}$ for $n > d$.
Hint: show that $\widetilde{N}|_{\mathcal{H}_n} = n\mathbb{1}_{\mathcal{H}_n}$.

4. Show that

$$\langle b^*(\psi_1)\cdots b^*(\psi_n)\phi | b^*(\psi_1')\cdots b^*(\psi_n')\phi\rangle = \det[\langle\psi_i|\psi_j'\rangle]_{1\le i,j\le n},$$

and conclude that the map $\psi_1\wedge\cdots\wedge\psi_n \mapsto b^*(\psi_1)\cdots b^*(\psi_n)\phi$ extends to an isometry $U : \Gamma(\mathcal{K}) \to \mathcal{H}$.

5. Show that $Ua^{\#}(\psi)U^* = b^{\#}(\psi)$.

6. Show that $[UU^*, b(\psi)] = 0$ for all $\psi \in \mathcal{K}$ and conclude that U is unitary.

One can hardly overestimate the importance of the CAR. Indeed, as we shall see, they characterize completely the algebra of observables of a Fermi gas with a given finite-dimensional one-particle Hilbert space $\mathcal{K}$.

Proposition 6.4 *A representation $\psi \mapsto b^{\#}(\psi)$ of the CAR over the finite dimensional Hilbert space $\mathcal{K}$ in $\mathcal{H}$ is irreducible iff the smallest $*$-subalgebra of $\mathcal{O}_{\mathcal{H}}$ containing the set $\mathfrak{B} = \{b^{\#}(\psi) \,|\, \psi \in \mathcal{K}\}$ is $\mathcal{O}_{\mathcal{H}}$.*

Note that the smallest $*$-subalgebra of $\mathcal{O}_{\mathcal{H}}$ containing $\mathfrak{B}$ must contain all polynomials in the operators $b^{\#}(\psi)$, *i.e.*, all linear combinations of monomials of the form $b^{\#}(\psi_1)\cdots b^{\#}(\psi_k)$. But the set of all these polynomials is obviously a $*$-algebra. Hence, a representation $\psi \mapsto b^{\#}(\psi)$ is irreducible iff any operator on $\mathcal{H}$ can be written as a polynomial in the operators $b^{\#}$. We can draw important conclusions from this fact:

1. Since the Fock representation $\psi \mapsto a^{\#}(\psi)$ is irreducible, any operator on the Fock space $\Gamma(\mathcal{K})$ is a polynomial in the creation/annihilation operators $a^{\#}$.
2. Any representation of the CAR over $\mathcal{K}$ on a Hilbert space $\mathcal{H}$ extends to a representation of the $*$-algebra $\mathcal{O}_{\Gamma(\mathcal{K})}$ on $\mathcal{H}$, *i.e.*, to a $*$-morphism $\pi : \mathcal{O}_{\Gamma(\mathcal{K})} \to \mathcal{O}_{\mathcal{H}}$.
3. If the representation is irreducible, this morphism is an isomorphism.

To prove Proposition 6.4, we shall need the following result, von Neumann's bicommutant theorem. A subset $\mathfrak{A} \subset \mathcal{O}_{\mathcal{K}}$ is called self-adjoint if $A \in \mathfrak{A}$ implies $A^* \in \mathfrak{A}$ and unital if $\mathbb{1} \in \mathfrak{A}$.

Theorem 6.5 *Let $\mathcal{K}$ be a finite dimensional Hilbert space and $\mathfrak{A}$ a unital self-adjoint subset of $\mathcal{O}_{\mathcal{K}}$. Then its bicommutant $\mathfrak{A}''$ is the smallest $*$-subalgebra of $\mathcal{O}_{\mathcal{K}}$ containing $\mathfrak{A}$.*

Proof. Denote by $\mathcal{A}$ the smallest $*$-subalgebra of $\mathcal{O}_{\mathcal{K}}$ containing $\mathfrak{A}$, *i.e.*, the set of polynomials in elements of $\mathfrak{A}$. One clearly has $\mathcal{A}' = \mathfrak{A}'$ and hence $\mathcal{A}'' = \mathfrak{A}''$. Thus, it suffices to show that $\mathcal{A} = \mathcal{A}''$ (a $*$-algebra satisfying this condition is a von Neumann algebra, and we are about to show that any finite dimensional unital $*$-algebra is a von Neumann algebra).

Since any element of $\mathcal{A}$ commutes with all elements of $\mathcal{A}'$ one obviously have $\mathcal{A} \subset \mathcal{A}''$. We must prove the reverse inclusion. Let $\{\psi_1, \ldots, \psi_n\}$ be a basis of $\mathcal{K}$, $\{e_1, \ldots, e_n\}$ a basis of $\mathbb{C}^n$ and set

$$\Psi = \sum_{j=1}^{n} \psi_j \otimes e_j \in \mathcal{H} = \mathcal{K} \otimes \mathbb{C}^n.$$

To any $A \in \mathcal{O}_{\mathcal{K}}$ we associate the linear operator $\widehat{A} = A \otimes \mathbb{1} \in \mathcal{O}_{\mathcal{H}}$. It follows that $\widehat{\mathcal{A}} = \{\widehat{A} \,|\, A \in \mathcal{A}\}$ is a $*$-subalgebra of $\mathcal{O}_{\mathcal{H}}$ and $\widehat{\mathcal{A}}\Psi = \{\widehat{A}\Psi \,|\, A \in \mathcal{A}\}$ a subspace of $\mathcal{H}$. Denote by P the orthogonal projection of $\mathcal{H}$ onto this subspace. We claim that $P \in \widehat{\mathcal{A}}'$. Indeed, for any $\widehat{A} \in \widehat{\mathcal{A}}$ and $\Phi \in \mathcal{H}$, one has $\widehat{A}P\Phi \in \widehat{\mathcal{A}}\Psi$, and hence

$$\widehat{A}P\Phi = P\widehat{A}P\Phi.$$

We deduce that $\widehat{A}P = P\widehat{A}P$ for all $\widehat{A} \in \widehat{\mathcal{A}}$ and since $\widehat{\mathcal{A}}$ is self-adjoint, one also has

$$P\widehat{A} = (\widehat{A}^* P)^* = (P\widehat{A}^* P)^* = P\widehat{A}P = \widehat{A}P.$$

Since $\mathcal{A}$ is unital, so is $\widehat{\mathcal{A}}$. It follows that $\Psi \in \widehat{\mathcal{A}}\Psi$ and hence $P\Psi = \Psi$. Recall that $X \in \mathcal{O}_{\mathcal{H}}$ is described by a $n \times n$ matrix $[X_{jk}]$ of elements of $\mathcal{O}_{\mathcal{K}}$ (see Section 2.3) via the formula

$$X(\psi \otimes e_k) = \sum_{j=1}^{n} (X_{jk}\psi) \otimes e_j.$$

Consequently, one has $\widehat{\mathcal{A}}' = \{X = [X_{jk}] \,|\, X_{jk} \in \mathcal{A}'\}$. Let $B \in \mathcal{A}''$. By the previous formula, $\widehat{B} \in \widehat{\mathcal{A}}''$, and so $\widehat{B}$ commutes with P. We conclude that

$$\widehat{B}\Psi = \widehat{B}P\Psi = P\widehat{B}\Psi \in \widehat{\mathcal{A}}\Psi,$$

and so there exists $A \in \mathcal{A}$ such that $\widehat{B}\Psi = \widehat{A}\Psi$, *i.e.*,

$$B\psi_j = A\psi_j,$$

for $j = 1, \ldots, n$. We conclude that $B = A \in \mathcal{A}$. □

Proof of Proposition 6.4. Note that $\{b^*(\psi), b(\psi)\} = \|\psi\|^2 \mathbb{1}$, so that any $*$-subalgebra of $\mathcal{O}_{\mathcal{H}}$ containing

$$\mathfrak{B} = \{b^{\#}(\psi) \,|\, \psi \in \mathcal{K}\},$$

also contains the unital self-adjoint subset $\widetilde{\mathfrak{B}} = \mathfrak{B} \cup \{\mathbb{1}\}$. It follows that the smallest $*$-subalgebra of $\mathcal{O}_{\mathcal{H}}$ containing $\mathfrak{B}$ coincide with the smallest $*$-subalgebra of $\mathcal{O}_{\mathcal{H}}$ containing $\widetilde{\mathfrak{B}}$. Moreover, one clearly has $\widetilde{\mathfrak{B}}' = \mathfrak{B}'$ and hence $\widetilde{\mathfrak{B}}'' = \mathfrak{B}''$. By the von Neumann bicommutant theorem, $\mathfrak{B}''$ is the smallest $*$-subalgebra of $\mathcal{O}_{\mathcal{H}}$ containing $\mathfrak{B}$. Now the representation $\psi \mapsto b^{\#}(\psi)$ is irreducible iff $\mathfrak{B}' = \mathbb{C}\mathbb{1}$, *i.e.*, iff $\mathfrak{B}'' = \mathcal{O}_{\mathcal{H}}$. □

Exercise 6.3. Let $\mathcal{K}_1$ and $\mathcal{K}_2$ be two finite dimensional Hilbert spaces. Show that there exists a unitary map $U : \Gamma(\mathcal{K}_1 \oplus \mathcal{K}_2) \to \Gamma(\mathcal{K}_1) \otimes \Gamma(\mathcal{K}_2)$ such that $U\Omega = \Omega \otimes \Omega$ and

$$Ua(\psi \oplus \phi)U^* = a(\psi) \otimes \mathbb{1} + \mathrm{e}^{\mathrm{i}\pi N} \otimes a(\phi).$$

Hint: try to apply Proposition 6.3.

Remark. Apart from a few important exceptions, the material of this and the previous section extends with minor changes to the case where $\mathcal{K}$ is an infinite dimensional Hilbert space. For example:

1. The definition of the Fock space $\Gamma(\mathcal{K})$ has to be complemented with the obvious topological condition that $\Psi = (\psi_0, \psi_1, \ldots) \in \Gamma(\mathcal{K})$ iff $\|\Psi\|^2 = \sum_{n\in\mathbb{N}} \|\psi_n\|^2 < \infty$.

2. The definition of $\Gamma_n(A)$ carries over to bounded operators A on $\mathcal{K}$ and $\|\Gamma_n(A)\| \le \|A\|^n$. Thus, $\Gamma(A) = \oplus_{n\ge0}\Gamma_n(A)$ is well defined if:

   - $\|A\| \le 1$, and then $\|\Gamma(A)\| = \sup_{n\ge0} \|\Gamma_n(A)\| = 1$. In particular, if U is unitary, so is $\Gamma(U)$.
   - A has finite rank m so that $\Gamma_n(A) = 0$ for $n > m$ and then $\|\Gamma(A)\| = \sup_{n\ge0} \|\Gamma_n(A)\| \le \max(1, \|A\|^m)$. In fact, using the polar decomposition $A = U|A|$ together with Lemma 6.1, one sees that $\Gamma(A)$ is trace class with $\|\Gamma(A)\|_1 = \mathrm{tr}\,\Gamma(|A|) = \det(\mathbb{1} + |A|)$. By a simple approximation argument, one can then show that $\Gamma(A)$ is well defined and trace class provided A is trace class, and Lemma 6.1 carries over.

3. If A generates a strongly continuous contraction semi-group e^{tA} on $\mathcal{K}$, then $\mathrm{d}\Gamma(A)$ is defined as the generator of the strongly continuous contraction semi-group $\Gamma(\mathrm{e}^{tA})$ on $\Gamma(\mathcal{K})$. In particular, if A is self-adjoint, so is $\mathrm{d}\Gamma(A)$. However, some care is required since $\mathrm{d}\Gamma(A)$ is unbounded unless $A = 0$. If A is bounded, the dense subspace $\Gamma_{\mathrm{fin}}(\mathcal{K}) = \cup_{n\ge0}(\oplus_{k\le n}\Gamma_k(\mathcal{K}))$ of $\Gamma(\mathcal{K})$ is a core of $\mathrm{d}\Gamma(A)$ and on this subspace, $\mathrm{d}\Gamma(A)$ acts as in the finite dimensional case.

4. The definition of the creation/annihilation operators carries over without change. Parts (1)–(5) of Proposition 6.2 hold with the same proofs while Parts (6)–(8) are easily adapted. Part (9) still holds if A is trace class and it follows that $\|\mathrm{d}\Gamma(A)\| \le \|A\|_1$.

5. The unitary equivalence described in Exercise 6.3 still holds for infinite dimensional $\mathcal{K}_1$ and $\mathcal{K}_2$ (prove it!).

Proposition 6.3 does not hold for infinite dimensional $\mathcal{K}$. In fact, there are many unitarily inequivalent irreducible representations of the CAR over $\mathcal{K}$. Also Proposition 6.4 and Theorem 6.5 do not hold for infinite dimensional $\mathcal{K}$. In the latter, one has to replace "smallest $*$-subalgebra of $\mathcal{O}_\mathcal{K}$" by "smallest weakly closed $*$-subalgebra of $\mathcal{O}_\mathcal{K}$" (see, *e.g.*, Theorem 2.4.11 in [BR1]). Proposition 6.4 has to be modified accordingly: The representation $\psi \mapsto b^\#(\psi)$ in $\mathcal{H}$ is irreducible iff any bounded operator on $\mathcal{H}$ is a weak limit of a net of polynomials in the elements of $\mathfrak{B}$.

6.3 Quasi-free states of the CAR algebra

We now turn to states of a free Fermi gas. Let $T \in \mathcal{O}_\mathcal{K}$ be a non-zero operator satisfying $0 \le T < \mathbb{1}$. In our context, we shall refer to T as *density operator* or just *density*. To such T we associate density matrix on $\Gamma(\mathcal{K})$ by

$$\omega_T = \frac{1}{Z_T}\Gamma\left(\frac{T}{\mathbb{1} - T}\right),$$

where

$$Z_T = \mathrm{tr}\left(\Gamma\left(\frac{T}{\mathbb{1} - T}\right)\right).$$

As usual, we denote by the same letter the corresponding state on $\mathcal{O}_{\Gamma(\mathcal{K})}$. ω_T is called quasi-free state associated to the density T. Its properties are summarized in

Proposition 6.6 (1) *If $\phi_1, \ldots, \phi_n, \psi_1, \ldots, \psi_m \in \mathcal{K}$, then*

$$\omega_T(a^*(\phi_n)\cdots a^*(\phi_1)a(\psi_1)\cdots a(\psi_m)) = \delta_{nm}\det[\langle\psi_i|T\phi_j\rangle].$$

In particular, $\omega_T(a^*(\phi)a(\psi)) = \langle\psi|T\phi\rangle$.

(2) $\log Z_T = -\log\det(\mathbb{1} - T) = -\mathrm{tr}(\log(\mathbb{1} - T))$.

(3) $\omega_T(\Gamma(A)) = \det(\mathbb{1} + T(A - \mathbb{1}))$.

(4) $\omega_T(\mathrm{d}\Gamma(A)) = \mathrm{tr}(TA)$.

(5) $S(\omega_T) = -\mathrm{tr}(T\log T + (\mathbb{1}-T)\log(\mathbb{1}-T))$.

(6) $\omega_{T_1} \ll \omega_{T_2}$ *iff* $\mathrm{Ker}\, T_1 \subset \mathrm{Ker}\, T_2$, *and then*

$$S(\omega_{T_1}|\omega_{T_2}) = \mathrm{tr}\left(T_1(\log(T_2)-\log(T_1)) + (\mathbb{1}-T_1)(\log(\mathbb{1}-T_2)-\log(\mathbb{1}-T_1))\right).$$

Proof. (1) We set $Q = T(\mathbb{1}-T)^{-1}$, $A = a^*(\phi_n)\cdots a^*(\phi_1)a(\psi_1)\cdots a(\psi_m)$ and note that

$$\mathrm{e}^{-\mathrm{i}tN}\omega_T\,\mathrm{e}^{\mathrm{i}tN} = \frac{1}{Z_T}\Gamma(\mathrm{e}^{-\mathrm{i}t})\Gamma(Q)\Gamma(\mathrm{e}^{\mathrm{i}t}) = \frac{1}{Z_T}\Gamma(\mathrm{e}^{-\mathrm{i}t}Q\mathrm{e}^{\mathrm{i}t}) = \frac{1}{Z_T}\Gamma(Q) = \omega_T,$$

so that

$$\omega_T(\mathrm{e}^{\mathrm{i}tN}A\mathrm{e}^{-\mathrm{i}tN}) = \omega_T(A).$$

By Proposition 6.2 (6), we have

$$\mathrm{e}^{\mathrm{i}tN}a^*(\phi_j)\,\mathrm{e}^{-\mathrm{i}tN} = a^*(\mathrm{e}^{\mathrm{i}t}\phi_j) = \mathrm{e}^{\mathrm{i}t}a^*(\phi_j), \qquad \mathrm{e}^{\mathrm{i}tN}a(\psi_k)\,\mathrm{e}^{-\mathrm{i}tN} = a(\mathrm{e}^{\mathrm{i}t}\psi_k) = \mathrm{e}^{-\mathrm{i}t}a(\psi_k),$$

from which we deduce that $\mathrm{e}^{\mathrm{i}tN}A\,\mathrm{e}^{-\mathrm{i}tN} = \mathrm{e}^{\mathrm{i}t(n-m)}A$, and hence that $\omega_T(A) = 0$ if $n \neq m$. We shall handle the case $n = m$ by induction on n. For $n = 1$, one has

$$\begin{aligned}
\omega_T(a^*(\phi)a(\psi)) &= Z_T^{-1}\mathrm{tr}(\Gamma(Q)a^*(\phi)a(\psi))\\
&= Z_T^{-1}\mathrm{tr}(a^*(Q\phi)\Gamma(Q)a(\psi))\\
&= Z_T^{-1}\mathrm{tr}(\Gamma(Q)a(\psi)a^*(Q\phi))\\
&= Z_T^{-1}\mathrm{tr}(\Gamma(Q)(\{a(\psi),a^*(Q\phi)\} - a^*(Q\phi)a(\psi)))\\
&= \langle\psi|Q\phi\rangle - \omega_T(a^*(Q\phi)a(\psi)),
\end{aligned}$$

from which we deduce that $\omega_T(a^*((\mathbb{1}+Q)\phi)a(\psi)) = \langle\psi|Q\phi\rangle$. Since $(\mathbb{1}+Q) = (\mathbb{1}-T)^{-1}$, we finally get

$$\omega_T(a^*(\phi)a(\psi)) = \langle\psi|Q(\mathbb{1}-T)\phi\rangle = \langle\psi|T\phi\rangle.$$

Assuming now that the result holds for $n-1$, we write

$$\begin{aligned}
&\omega_T(a^*(\phi_n)\cdots a^*(\phi_1)a(\psi_1)\cdots a(\psi_n))\\
&\quad= Z_T^{-1}\mathrm{tr}(\Gamma(Q)a^*(\phi_n)\cdots a^*(\phi_1)a(\psi_1)\cdots a(\psi_n))\\
&\quad= Z_T^{-1}\mathrm{tr}(a^*(Q\phi_n)\Gamma(Q)a^*(\phi_{n-1})\cdots a^*(\phi_1)a(\psi_1)\cdots a(\psi_n))\\
&\quad= \omega_T(a^*(\phi_{n-1})\cdots a^*(\phi_1)a(\psi_1)\cdots a(\psi_n)a^*(Q\phi_n)).
\end{aligned}$$

Making repeated use of the CAR,

$$a(\psi_j)a^*(Q\phi_n) = \langle\psi_j|Q\phi_n\rangle - a^*(Q\phi_n)a(\psi_j), \qquad a^*(\phi_j)a^*(Q\phi_n) = -a^*(Q\phi_n)a^*(\phi_j),$$

we move the last factor $a^*(Q\phi_n)$ back to its original position to get

$$\begin{aligned}
\omega_T(a^*(\phi_n)\cdots a^*(\phi_1)a(\psi_1)\cdots a(\psi_n)) &= -\omega_T(a^*(Q\phi_n)\cdots a^*(\phi_1)a(\psi_1)\cdots a(\psi_n))\\
&+ \sum_{j=1}^n(-1)^{n+j}\langle\psi_j|Q\phi_n\rangle\omega_T(a^*(\phi_{n-1})\cdots a^*(\phi_1)a(\psi_1)\cdots \cancel{a(\psi_j)}\cdots a(\psi_n)).
\end{aligned}$$

By the same argument as in the $n = 1$ case, we deduce

$$\begin{aligned}
&\omega_T(a^*(\phi_n)\cdots a^*(\phi_1)a(\psi_1)\cdots a(\psi_n))\\
&\quad= \sum_{j=1}^n(-1)^{n+j}\langle\psi_j|T\phi_n\rangle\omega_T(a^*(\phi_{n-1})\cdots a^*(\phi_1)a(\psi_1)\cdots \cancel{a(\psi_j)}\cdots a(\psi_n)),
\end{aligned}$$

and the induction step is achieved by Laplace formula (6.8).

(2) and (3) are immediate consequences of Lemma 6.1, (4) follows from (1) and Proposition 6.2 (9).
(5) We again set $Q = T(\mathbb{1} - T)^{-1}$ and notice that

$$\log \Gamma(Q) = \mathrm{d}\Gamma(\log Q),$$

so that, by (4),

$$S(\omega_T) = -\omega_T \left(\log \left(Z_T^{-1}\Gamma(Q)\right)\right) = -\omega_T(\mathrm{d}\Gamma(\log Q) - \log Z_T) = \log Z_T - \mathrm{tr}\,(T \log Q)\,.$$

Using (2), we conclude that

$$S(\omega_T) = -\mathrm{tr}(\log(\mathbb{1} - T)) - \mathrm{tr}(T(\log(T) - \log(\mathbb{1} - T))),$$

from which the desired formula immediately follows.
(6) We set $Q_j = T_j(\mathbb{1} - T_j)^{-1}$ and notice that $\mathrm{Ker}\, Q_j = \mathrm{Ker}\, T_j$. It easily follows from $\mathrm{Ker}\, T_1 \subset \mathrm{Ker}\, T_2$ that $\mathrm{Ker}\,\Gamma(Q_1) \subset \mathrm{Ker}\,\Gamma(Q_2)$ and hence $\omega_{T_1} \ll \omega_{T_2}$. The remaining statement is proved in a similar way as (5). □

Let $h = h^* \in \mathcal{O}_\mathcal{K}$ be the one-particle Hamiltonian – the total energy observable of a single fermion. The Hamiltonian of the free Fermi gas is

$$H = \mathrm{d}\Gamma(h).$$

Indeed, if $\{\psi_1, \ldots, \psi_d\}$ denotes an eigenbasis of h such that $h\psi_j = \varepsilon_j \psi_j$, then the state

$$\Psi = a^*(\psi_{j_1}) \cdots a^*(\psi_{j_n})\Omega,$$

describes n fermions with energies $\varepsilon_{j_1}, \ldots, \varepsilon_{j_n}$, and one has

$$H\Psi = \mathrm{d}\Gamma_n(h)\psi_{j_1} \wedge \cdots \wedge \psi_{j_n} = \left(\sum_{i=1}^{n} \varepsilon_{j_i}\right)\Psi.$$

The thermal equilibrium state at inverse temperature $\beta \in \mathbb{R}$ and chemical potential $\mu \in \mathbb{R}$ is described by the Gibbs grand canonical ensemble

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

Since

$$\mathrm{e}^{-\beta(H-\mu N)} = \mathrm{e}^{-\mathrm{d}\Gamma(\beta(h - \mu \mathbb{1}))} = \Gamma(\mathrm{e}^{-\beta(h-\mu\mathbb{1})}),$$

solving the equation

$$\mathrm{e}^{-\beta(h-\mu\mathbb{1})} = \frac{T}{\mathbb{1} - T},$$

for T we see that the density operator of a free Fermi gas in thermal equilibrium at inverse temperature β and chemical potential μ is given by

$$T_{\beta,\mu} = (\mathbb{1} + \mathrm{e}^{\beta(h-\mu\mathbb{1})})^{-1}.$$

$T_{\beta,\mu}$ is commonly called the Fermi-Dirac distribution. Following the notation introduced in Section 2.9, one has

$$\begin{aligned}
E &= \rho_{\beta,\mu}(H) = \mathrm{tr}(hT_{\beta,\mu}),\\
\varrho &= \rho_{\beta,\mu}(N) = \mathrm{tr}(T_{\beta,\mu}),\\
P(\beta,\mu) &= \log \mathrm{tr}(\mathrm{e}^{-\beta(H-\mu N)}) = \mathrm{tr}\left(\log(\mathbb{1} + \mathrm{e}^{-\beta(h-\mu\mathbb{1})})\right),\\
S(\beta,\mu) &= S(\rho_{\beta,\mu}) = \beta(E - \mu\varrho) + P(\beta,\mu).
\end{aligned} \tag{6.9}$$

Exercise 6.4. The purpose of this exercise is to provide a complete discussion of the thermodynamic limit of a 1D free Fermi gas starting from the description of a finite Fermi gas. The target system is the ideal Fermi gas with one particle Hamiltonian $h = k^2/2$ on the one-particle Hilbert space $\mathcal{K} = L^2(\mathbb{R}, \mathrm{d}k/2\pi)$ in the thermal equilibrium state at inverse temperature β and chemical potential μ.

To describe the finite approximation, consider the operator

$$(h_L\psi)(x) = -\frac{1}{2}\psi''(x),$$

on $L^2([-L/2, L/2], \mathrm{d}x)$ with periodic boundary conditions $\psi(x+L) = \psi(x)$. h_L is self-adjoint with a purely discrete spectrum consisting of simple eigenvalues $\varepsilon(k) = k^2/2$ with eigenfunctions $\psi_k(x) = L^{-1/2}\mathrm{e}^{\mathrm{i}kx}$, $k \in \mathcal{Q}_L = \{2\pi j/L \,|\, j \in \mathbb{Z}\}$. The Fourier transform

$$\hat{\psi}(k) = \langle \psi_k|\psi\rangle = \frac{1}{\sqrt{L}}\int_{-L/2}^{L/2} \psi(x)\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x,$$

provides a unitary map from the position representation $L^2([-L/2, L/2])$ to the "momentum" representation $\ell^2(\mathcal{Q}_L)$ such that $\widehat{h_L\psi}(k) = \varepsilon(k)\hat{\psi}(k)$. In what follows, we work in the momentum representation and set $\mathcal{K}_L = \ell^2(\mathcal{Q}_L)$ and $(h_L\psi)(k) = \varepsilon(k)\psi(k)$. Let $\mathcal{E} > 0$ be an energy cut-off, set $\mathcal{Q}_{L,\mathcal{E}} = \{k \in \mathcal{Q}_L \,|\, \varepsilon(k) \leq \mathcal{E}\}$ and consider the free Fermi gas with single particle Hilbert space $\mathcal{K}_{L,\mathcal{E}} = \ell^2(\mathcal{Q}_{L,\mathcal{E}})$, and one-particle Hamiltonian $(h_{L,\mathcal{E}}\psi)(k) = \varepsilon(k)\psi(k)$. Let $E_{L,\mathcal{E}}$, $\varrho_{L,\mathcal{E}}$, $P_{L,\mathcal{E}}(\beta,\mu)$ be defined by (6.9).

1. Prove that

$$\lim_{L\to\infty}\lim_{\mathcal{E}\to\infty}\frac{E_{L,\mathcal{E}}}{L} = \int_{-\infty}^{\infty}\frac{\varepsilon(k)}{1+\mathrm{e}^{\beta(\varepsilon(k)-\mu)}}\frac{\mathrm{d}k}{2\pi},$$

$$\lim_{L\to\infty}\lim_{\mathcal{E}\to\infty}\frac{\varrho_{L,\mathcal{E}}}{L} = \int_{-\infty}^{\infty}\frac{1}{1+\mathrm{e}^{\beta(\varepsilon(k)-\mu)}}\frac{\mathrm{d}k}{2\pi},$$

$$\lim_{L\to\infty}\lim_{\mathcal{E}\to\infty}\frac{P_{L,\mathcal{E}}(\beta,\mu)}{L} = \int_{-\infty}^{\infty}\log(1+\mathrm{e}^{-\beta(\varepsilon(k)-\mu)})\frac{\mathrm{d}k}{2\pi}.$$

2. A wave function $\psi \in \mathcal{K}_{L,\mathcal{E}}$ can be isometrically extended to an element of $\mathcal{K}$ by setting

$$\widetilde{\psi}(k) = \sqrt{L}\sum_{\xi\in\mathcal{Q}_{L,\mathcal{E}}}\psi(\xi)\chi_{[\xi-\pi/L,\xi+\pi/L[}(k),$$

where χ_I denotes the indicator function of the interval I. Thus, we can identify $\mathcal{K}_{L,\mathcal{E}}$ with a finite dimensional subspace of the Hilbert space $\mathcal{K}$. Denote by $\mathbb{1}_{L,\mathcal{E}}$ the orthogonal projection on this subspace. Then $\Gamma(\mathbb{1}_{L,\mathcal{E}})$ is an orthogonal projection in $\Gamma(\mathcal{K})$ whose range can be identified with $\Gamma(\mathcal{K}_{L,\mathcal{E}})$. Show that we can identify the equilibrium density matrix

$$\rho_{\beta,\mu,L,\mathcal{E}} = \frac{\Gamma(\mathrm{e}^{-\beta(h_{L,\mathcal{E}}-\mu\mathbb{1})})}{\mathrm{tr}(\Gamma(\mathrm{e}^{-\beta(h_{L,\mathcal{E}}-\mu\mathbb{1})}))};$$

of the finite Fermi gas on $\Gamma(\mathcal{K}_{L,\mathcal{E}})$ with the density matrix

$$\widetilde{\rho}_{\beta,\mu,L,\mathcal{E}} = \frac{\Gamma(\mathrm{e}^{-\beta(h-\mu\mathbb{1})}\mathbb{1}_{L,\mathcal{E}})}{\mathrm{tr}(\Gamma(\mathrm{e}^{-\beta(h-\mu\mathbb{1})}\mathbb{1}_{L,\mathcal{E}}))},$$

on $\Gamma(\mathcal{K})$ in the sense that

$$\mathrm{tr}\left(\rho_{\beta,\mu,L,\mathcal{E}}a^*(\psi_1)\cdots a^*(\psi_n)a(\phi_m)\cdots a(\phi_1)\right) = \mathrm{tr}\left(\widetilde{\rho}_{\beta,\mu,L,\mathcal{E}}a^*(\widetilde{\psi}_1)\cdots a^*(\widetilde{\psi}_n)a(\widetilde{\phi}_m)\cdots a(\widetilde{\phi}_1)\right),$$

for all $\psi_1, \ldots, \psi_n, \phi_1, \ldots, \phi_m \in \mathcal{K}_{L,\mathcal{E}}$.

3. Show that, in $\Gamma(\mathcal{K})$, the limit

$$\widetilde{\rho}_{\beta,\mu,L} = \lim_{\mathcal{E}\to\infty} \widetilde{\rho}_{\beta,\mu,L,\mathcal{E}},$$

exists in the trace norm and that $\widetilde{\rho}_{\beta,\mu,L}$ is a density matrix that can be identified with

$$\rho_{\beta,\mu,L} = \frac{\Gamma(\mathrm{e}^{-\beta(h_L-\mu\mathbb{1})})}{\mathrm{tr}(\Gamma(\mathrm{e}^{-\beta(h_L-\mu\mathbb{1})}))},$$

on $\Gamma(\mathcal{K}_L)$. Show that

$$\mathrm{s}-\lim_{L\to\infty} \widetilde{\rho}_{\beta,\mu,L} = 0,$$

i.e., the equilibrium density matrix disappears in the thermodynamic limit $L \to \infty$.

4. Show that,

$$\mathcal{D} = \bigcup_{L>0,\mathcal{E}>0} \mathcal{K}_{L,\mathcal{E}},$$

is a dense subspace of $\mathcal{K}$ and that for $\phi, \psi \in \mathcal{D}$ one has

$$\lim_{L\to\infty}\lim_{\mathcal{E}\to\infty} \mathrm{tr}\,(\widetilde{\rho}_{\beta,\mu,L,\mathcal{E}} a^*(\phi)a(\psi)) = \int_{-\infty}^{\infty} \frac{\overline{\psi(k)}\phi(k)}{1+\mathrm{e}^{\beta(\varepsilon(k)-\mu)}}\frac{\mathrm{d}k}{2\pi} = \langle\psi|T\phi\rangle,$$

where $T = (\mathbb{1} + \mathrm{e}^{\beta(h-\mu)})^{-1}$.

5. Since we have identified $\mathcal{K}_{L,\mathcal{E}}$ with a subspace of $\mathcal{K}$, we can also identify the $*$-algebra $\mathcal{O}_{\mathcal{K}_{L,\mathcal{E}}}$ with a subalgebra of the $*$-algebra $\mathcal{O}_{\mathcal{K}}$ of all bounded linear operators on $\mathcal{K}$. This identification is isometric and

$$\mathcal{O}_\infty = \bigcup_{L>0,\mathcal{E}>0} \mathcal{O}_{\mathcal{K}_{L,\mathcal{E}}},$$

is the $*$-algebra of all polynomials in the creation/annihilation operators $a^\#(\psi)$, $\psi \in \mathcal{D}$. Show that the limit

$$\rho_{\beta,\mu}(A) = \lim_{L\to\infty}\lim_{\mathcal{E}\to\infty} \mathrm{tr}\,(\widetilde{\rho}_{\beta,\mu,L,\mathcal{E}} A)\,,$$

exists for all $A \in \mathcal{O}_\infty$.

Hint: show that

$$\lim_{L\to\infty}\lim_{\mathcal{E}\to\infty} \mathrm{tr}\,(\widetilde{\rho}_{\beta,\mu,L,\mathcal{E}} a^*(\psi_1)\cdots a^*(\psi_n)a(\phi_m)\cdots a(\phi_1)) = \delta_{n,m}\det[\langle\phi_j|T\psi_k\rangle],$$

for all $\psi_1, \ldots, \psi_n, \phi_1, \ldots, \phi_m \in \mathcal{D}$.

6. Denote by $\mathcal{O}_\infty^{\mathrm{cl}}$ the norm closure of $\mathcal{O}_\infty$ in $\mathcal{O}_{\mathcal{K}}$ ($\mathcal{O}_\infty^{\mathrm{cl}}$ is the C^*-algebra generated by $\mathcal{O}_\infty$). Show that for any $A \in \mathcal{O}_\infty^{\mathrm{cl}}$ and any sequence $A_n \in \mathcal{O}_\infty$ which converges to A the limit

$$\rho_{\beta,\mu}(A) = \lim_{n\to\infty} \rho_{\beta,\mu}(A_n),$$

exists and is independent of the approximating sequence A_n. The C^*-algebra $\mathcal{O}_\infty^{\mathrm{cl}}$ is the algebra of observables of the infinitely extended ideal Fermi gas and $\rho_{\beta,\mu}$ is its thermal equilibrium state.

6.4 The Araki-Wyss representation

Araki and Wyss [AWy] have discovered a specific cyclic representation of $\mathcal{O}_{\Gamma(\mathcal{K})}$ associated to the quasi-free state ω_T which is of considerable conceptual and computational importance. Although any two cyclic representations of $\mathcal{O}_{\Gamma(\mathcal{K})}$ associated to the state ω_T are unitarily equivalent, the specific structure inherent to the Araki-Wyss (AW) representation has played a central role in many developments in non-equilibrium quantum statistical mechanics over the last decade.

For the purpose of this section we may assume that $T > 0$ (otherwise, replace $\mathcal{K}$ with $\mathrm{Ran}\, T$). Then the quasi-free state ω_T on $\mathcal{O}_{\Gamma(\mathcal{K})}$ is faithful. Set

$$\mathcal{H}_{\mathrm{AW}} = \Gamma(\mathcal{K}) \otimes \Gamma(\mathcal{K}),$$

$$\Omega_{\mathrm{AW}} = \Omega \otimes \Omega,$$

$$b^*_{\mathrm{AW}}(\psi) = a^*((\mathbb{1} - T)^{1/2}\psi) \otimes \mathbb{1} + \mathrm{e}^{\mathrm{i}\pi N} \otimes a(\overline{T^{1/2}\psi}),$$

$$b_{\mathrm{AW}}(\psi) = a((\mathbb{1} - T)^{1/2}\psi) \otimes \mathbb{1} + \mathrm{e}^{\mathrm{i}\pi N} \otimes a^*(\overline{T^{1/2}\psi}),$$

where $\overline{\psi}$ denotes the complex conjugate of $\psi \in \mathcal{K} = \ell^2(\mathcal{Q})$. For $\Psi \in \Gamma(\mathcal{K})$, $\overline{\Psi}$ denotes the complex conjugate of Ψ (defined in the obvious way). If A is a linear operator, we define the linear operator $\overline{A}$ by $\overline{A}\,\overline{\psi} = \overline{A\psi}$.

Proposition 6.7 (1) *The maps $\psi \mapsto b^{\#}_{\mathrm{AW}}(\psi)$ define a representation of the CAR over $\mathcal{K}$ on the Hilbert space $\mathcal{H}_{\mathrm{AW}}$.*

(2) *Let π_{AW} be the induced representation of $\mathcal{O}_{\Gamma(\mathcal{K})}$ on $\mathcal{H}_{\mathrm{AW}}$. Ω_{AW} is a cyclic vector for this representation and*

$$\omega_T(A) = (\Omega_{AW}|\pi_{\mathrm{AW}}(A)\Omega_{\mathrm{AW}}), \tag{6.10}$$

for all $A \in \mathcal{O}_{\Gamma(\mathcal{K})}$. In other words, π_{AW} is a cyclic representation of $\mathcal{O}_{\Gamma(\mathcal{K})}$ associated to the faithful state ω_T.

Proof. The verification of (1) is simple and we leave it as an exercise for the reader. To check that Ω_{AW} is cyclic, we shall show by induction on $n+m$ that each subspace $D_{n,m} = \Gamma_n(\mathcal{K}) \otimes \Gamma_m(\mathcal{K})$ belongs to $\pi_{\mathrm{AW}}(\mathcal{O}_{\Gamma(\mathcal{K})})\Omega_{\mathrm{AW}}$. For $n+m=1$, we deduce from $\mathrm{Ran}\,(\mathbb{1}-T)^{1/2} = \mathrm{Ran}\,\overline{T}^{1/2} = \mathcal{K}$ that

$$D_{1,0} = \{b^*_{\mathrm{AW}}(\psi)\Omega_{\mathrm{AW}} \,|\, \psi \in \mathcal{K}\}, \qquad D_{0,1} = \{b_{\mathrm{AW}}(\psi)\Omega_{\mathrm{AW}} \,|\, \psi \in \mathcal{K}\}.$$

Assuming $D_{n,m} \subset \pi_{\mathrm{AW}}(\mathcal{O}_{\Gamma(\mathcal{K})})\Omega_{\mathrm{AW}}$ for $n+m \le k$, we observe that $\Psi \in D_{n+1,m}$ can be written as

$$\Psi = a^*((\mathbb{1}-T)^{1/2}\psi) \otimes \mathbb{1}\Phi,$$

for some $\psi \in \mathcal{K}$ and $\Phi \in D_{n,m}$. Equivalently, we can write

$$\Psi = b^*_{\mathrm{AW}}((\mathbb{1}-T)^{1/2}\psi)\Phi - \Phi'$$

where $\Phi' = (-\mathbb{1})^N \otimes a(\overline{T^{1/2}\psi})\Phi \in D_{n,m-1}$. It follows that $\Psi \in \pi_{\mathrm{AW}}(\mathcal{O}_{\Gamma(\mathcal{K})})\Omega_{\mathrm{AW}}$. A similar argument shows that $D_{n,m+1} \subset \pi_{\mathrm{AW}}(\mathcal{O}_{\Gamma(\mathcal{K})})\Omega_{\mathrm{AW}}$. Hence, the induction property is verified for $n+m \le k+1$. Finally, (6.10) follows from an elementary calculation based on Equ. (6.3). □

The triple $(\mathcal{H}_{\mathrm{AW}}, \pi_{\mathrm{AW}}, \Omega_{\mathrm{AW}})$ is called the Araki-Wyss representation of the CAR over $\mathcal{K}$ associated to the quasi-free state ω_T. Since ω_T is faithful, it follows from Part (2) of Proposition 6.7 and Part 4 of Exercise 2.15 that this representation is unitarily equivalent to the standard representation and hence carries the entire modular structure. The modular structure in the Araki-Wyss representation takes the following form.

Proposition 6.8 (1) *The modular conjugation is given by*

$$J(\Psi_1 \otimes \Psi_2) = u\overline{\Psi}_2 \otimes u\overline{\Psi}_1,$$

where $u = \mathrm{e}^{\mathrm{i}\pi N(N-1)/2}$.

(2) *The modular operator of ω_T is*

$$\Delta_{\omega_T} = \Gamma(\mathrm{e}^{k_T}) \otimes \Gamma(\mathrm{e}^{-\overline{k_T}}),$$

where $k_T = \log(T(\mathbb{1}-T)^{-1})$. In particular

$$\log \Delta_{\omega_T} = \mathrm{d}\Gamma(k_T) \otimes \mathbb{1} - \mathbb{1} \otimes \mathrm{d}\Gamma(\overline{k_T}).$$

(3) *If ω_{T_1} is the quasi-free state of density $T_1 > 0$, then its relative Hamiltonian w.r.t. ω_T is*

$$\ell_{\omega_{T_1}|\omega_T} = \log\det\left((\mathbb{1}-T_1)(\mathbb{1}-T)^{-1}\right) + \mathrm{d}\Gamma(k_{T_1} - k_T),$$

and its relative modular operator is determined by

$$\log \Delta_{\omega_{T_1}|\omega_T} = \log \Delta_{\omega_T} + \pi_{\mathrm{AW}}(\ell_{\omega_{T_1}|\omega_T}).$$

(4) *Suppose that the self-adjoint operator h commutes with T. Then the quasi-free state ω_T is invariant under the dynamics τ^t generated by $H = \mathrm{d}\Gamma(h)$. Moreover, the operator*

$$K = \mathrm{d}\Gamma(h) \otimes \mathbb{1} - \mathbb{1} \otimes \mathrm{d}\Gamma(\overline{h}),$$

is the standard Liouvillean of this dynamics.

Remark. Since the $*$-subalgebra $\mathcal{O}_{\mathrm{AW}} = \pi_{\mathrm{AW}}(\mathcal{O}_{\Gamma(\mathcal{K})})$ is the set of polynomials in the $b_{\mathrm{AW}}^{\#}$, the dual $*$-subalgebra $\mathcal{O}'_{\mathrm{AW}} = J\mathcal{O}_{\mathrm{AW}}J$ is the set of polynomials in the $b'^{\#}_{\mathrm{AW}} = Jb^{\#}_{\mathrm{AW}}J$. By Propositions 2.23 and 2.24, one has

$$\begin{aligned}\mathcal{O}_{\mathrm{AW}} \cap \mathcal{O}'_{\mathrm{AW}} &= \mathbb{C}\mathbb{1},\\ \mathcal{O}_{\mathrm{AW}} \vee \mathcal{O}'_{\mathrm{AW}} &= \mathcal{O}_{\mathcal{H}_{\mathrm{AW}}}.\end{aligned}$$

Proof. We set $\Delta = \Gamma(\mathrm{e}^{k_T}) \otimes \Gamma(\mathrm{e}^{-\overline{k_T}})$ and $s = \mathrm{e}^{\mathrm{i}\pi N}$. Since J is clearly an anti-unitary involution and $\Delta > 0$, we deduce from the observation following Equ. (2.34) that in order to prove (1) and (2) it suffices to show that $J\Delta^{1/2}A\Omega_{\mathrm{AW}} = A^*\Omega_{\mathrm{AW}}$ for any monomial $A = b^{\#}_{\mathrm{AW}}(\psi_n)\cdots b^{\#}_{\mathrm{AW}}(\psi_1)$. We shall do that by induction on the degree n.

We first compute

$$b'_{\mathrm{AW}}(\psi) = Jb_{\mathrm{AW}}(\psi)J = a^*(T^{1/2}\psi)s \otimes s + \mathbb{1} \otimes sa(\overline{(\mathbb{1}-T)^{1/2}\psi}),$$

$$b'^{*}_{\mathrm{AW}}(\psi) = Jb^{*}_{\mathrm{AW}}(\psi)J = sa(T^{1/2}\psi) \otimes s + \mathbb{1} \otimes a^*(\overline{(\mathbb{1}-T)^{1/2}\psi})s,$$

and check that $[b'_{\mathrm{AW}}(\psi), b^{\#}_{\mathrm{AW}}(\phi)] = [b'^{*}_{\mathrm{AW}}(\psi), b^{\#}_{\mathrm{AW}}(\phi)] = 0$ for all $\psi, \phi \in \mathcal{K}$. We thus conclude that $b'^{\#}_{\mathrm{AW}}(\psi) \in \mathcal{O}'_{\mathrm{AW}}$. Next, we observe that

$$\Delta^{1/2}b_{\mathrm{AW}}(\psi)\Delta^{-1/2} = b_{\mathrm{AW}}(\mathrm{e}^{-k_T/2}\psi), \qquad \Delta^{1/2}b^{*}_{\mathrm{AW}}(\psi)\Delta^{-1/2} = b^{*}_{\mathrm{AW}}(\mathrm{e}^{k_T/2}\psi).$$

For $n = 1$, the claim follows from the fact that

$$\begin{aligned}J\Delta^{1/2}b_{\mathrm{AW}}(\psi)\Omega_{\mathrm{AW}} &= J\Delta^{1/2}b_{\mathrm{AW}}(\psi)\Delta^{-1/2}J\Omega_{\mathrm{AW}}\\ &= b'_{\mathrm{AW}}(\mathrm{e}^{-k_T/2}\psi)\Omega_{\mathrm{AW}}\\ &= a^*(\mathrm{e}^{-k_T}T^{1/2}\psi) \otimes \mathbb{1}\Omega_{\mathrm{AW}}\\ &= b^{*}_{\mathrm{AW}}(\psi)\Omega_{\mathrm{AW}}.\end{aligned}$$

To deal with the induction step, let A be a monomial of degree less than n in the $b_{\mathrm{AW}}^{\#}$ and assume that $J\Delta^{1/2}A\Omega_{\mathrm{AW}} = A^*\Omega_{\mathrm{AW}}$ for all such monomials. Then, we can write

$$\begin{aligned}
J\Delta^{1/2}b_{\mathrm{AW}}^{\#}(\psi)A\Omega_{\mathrm{AW}} &= (J\Delta^{1/2}b_{\mathrm{AW}}^{\#}(\psi)\Delta^{-1/2}J)J\Delta^{1/2}A\Omega_{\mathrm{AW}}\\
&= (Jb_{\mathrm{AW}}^{\#}(\mathrm{e}^{\mp k_T/2}\psi)J)A^*\Omega_{\mathrm{AW}}\\
&= b_{\mathrm{AW}}^{\prime\#}(\mathrm{e}^{\mp k_T/2}\psi)A^*\Omega_{\mathrm{AW}}\\
&= A^*b_{\mathrm{AW}}^{\prime\#}(\mathrm{e}^{\mp k_T/2}\psi)\Omega_{\mathrm{AW}}\\
&= A^*J\Delta^{1/2}b_{\mathrm{AW}}^{\#}(\psi)\Delta^{-1/2}J\Omega_{\mathrm{AW}}\\
&= A^*J\Delta^{1/2}b_{\mathrm{AW}}^{\#}(\psi)\Omega_{\mathrm{AW}}\\
&= A^*b_{\mathrm{AW}}^{\#}(\psi)^*\Omega_{\mathrm{AW}},
\end{aligned}$$

which shows that the induction property holds for all monomials of degree less than $n+1$.

(3) The first claim is an immediate consequence of the definition (2.36) of the relative Hamiltonian. Since, by Part (4) of Exercise 2.15, the Araki-Wyss representation is unitarily equivalent to the standard representation on $\mathcal{H}_{\mathcal{O}}$, the second claim follows from Property (3) of the relative Hamiltonian given on page 64.

(4) The fact that ω_T is invariant under the dynamics τ^t is evident. Recall from Exercise 2.16 that the standard Liouvillean is the unique self-adjoint operator K on $\mathcal{H}_{\mathrm{AW}}$ (the Hilbert space carrying the standard representation) such that the unitary group $\mathrm{e}^{\mathrm{i}tK}$ implements the dynamics and preserves the natural cone. These two conditions can be formulated as

$$\mathrm{e}^{\mathrm{i}tK}b_{\mathrm{AW}}(\psi)\mathrm{e}^{-\mathrm{i}tK} = b_{\mathrm{AW}}(\mathrm{e}^{\mathrm{i}th}\psi), \qquad JK+KJ=0,$$

and are easily verified by $K = \mathrm{d}\Gamma(h)\otimes\mathbb{1} - \mathbb{1}\otimes\mathrm{d}\Gamma(\bar{h})$. □

Remark. The Araki-Wyss representation of the CAR over $\mathcal{K}$ immediately extends to infinite dimensional $\mathcal{K}$ and the proof of Proposition 6.7 carries over without modification. The same is true for Proposition 6.8 provided one assumes, in Part (3), that $\log(T_1)-\log(T)$ and $\log(\mathbb{1}-T_1)-\log(\mathbb{1}-T)$ are both trace class.

6.5 Spin-Fermion model

The Spin-Fermion (SF) model describes a two level atom (or a spin $1/2$), denoted $\mathcal{S}$, interacting with $n\geq 2$ independent free Fermi gas reservoirs $\mathcal{R}_j$. The Hilbert space of $\mathcal{S}$ is $\mathcal{H}_{\mathcal{S}} = \mathbb{C}^2$ and its Hamiltonian is the third Pauli matrix

$$H_{\mathcal{S}} = \sigma^{(3)} = \begin{bmatrix} 1 & 0\\ 0 & -1\end{bmatrix}.$$

Its initial state is $\omega_{\mathcal{S}} = \mathbb{1}/2$. The reservoir $\mathcal{R}_j$ is described by the single particle Hilbert space $\mathcal{K}_j = \ell^2(\mathcal{Q}_j)$ and single particle Hamiltonian h_j. The Hamiltonian and the number operator of $\mathcal{R}_j$ are denoted by $H_j = \mathrm{d}\Gamma(h_j)$ and N_j. The creation/annihilation operators on the Fock space $\Gamma(\mathcal{K}_j)$ are denoted by $a_j^{\#}$. We assume that $\mathcal{R}_j$ is in the state

$$\omega_{\beta_j,\mu_j} = \frac{\mathrm{e}^{-\beta_j(H_j-\mu_j N_j)}}{\mathrm{tr}(\mathrm{e}^{-\beta_j(H_j-\mu_j N_j)})},$$

that is, that $\mathcal{R}_j$ is in thermal equilibrium at inverse temperature β_j and chemical potential μ_j. The complete reservoir system $\mathcal{R} = \sum_j \mathcal{R}_j$ is described by the Hilbert space

$$\mathcal{H}_{\mathcal{R}} = \bigotimes_{j=1}^{n}\Gamma(\mathcal{K}_j),$$

its Hamiltonian is

$$H_{\mathcal{R}} = \sum_{j=1}^{n} H_j,$$

and its initial state is

$$\omega_{\mathcal{R}} = \otimes_{j=1}^{n} \omega_{\beta_j,\mu_j} = \frac{1}{Z} \mathrm{e}^{-\sum_{j=1}^{n} \beta_j (H_j - \mu_j N_j)},$$

where $Z = \mathrm{tr}(\mathrm{e}^{-\sum_j \beta_j (H_j - \mu_j N_j)})$. The Hilbert space of the joint system $\mathcal{S} + \mathcal{R}$ is

$$\mathcal{H} = \mathcal{H}_{\mathcal{S}} \otimes \mathcal{H}_{\mathcal{R}},$$

its initial state is $\omega = \omega_{\mathcal{S}} \otimes \omega_{\mathcal{R}}$, and in the absence of interaction its Hamiltonian is

$$H_0 = H_{\mathcal{S}} + H_{\mathcal{R}}.$$

The interaction of $\mathcal{S}$ with $\mathcal{R}_j$ is described by

$$V_j = \sigma^{(1)} \otimes P_j,$$

where $\sigma^{(1)}$ is the first Pauli matrix and P_j is a self-adjoint polynomial in the field operators

$$\varphi_j(\psi) = \frac{1}{\sqrt{2}}(a_j(\psi) + a_j^*(\psi)) \in \mathcal{O}_{\Gamma(\mathcal{K}_j)}.$$

For example $P_j = \varphi_j(\psi_j)$ or $P_j = \mathrm{i}\varphi_j(\psi_j)\varphi_j(\phi_j)$ with $\psi_j \perp \phi_j$. The complete interaction is $V = \sum_{j=1}^{n} V_j$ and the full (interacting) Hamiltonian of the SF model is

$$H_\lambda = H_0 + \lambda V,$$

where $\lambda \in \mathbb{R}$ is a coupling constant.

Exercise 6.5. Check that the SF model is an example of open quantum system as defined in Section 4.1. Warning: gauge invariance is broken in the SF model.

Exercise 6.6.

1. Denote by $\{e_1, e_2\}$ the standard basis of $\mathcal{H}_{\mathcal{S}} = \mathbb{C}^2$. Show that the triple $(\mathcal{H}_{\mathcal{S}} \otimes \mathcal{H}_{\mathcal{S}}, \pi_{\mathcal{S}}, \Omega_{\mathcal{S}})$, where $\pi_{\mathcal{S}}(A) = A \otimes \mathbb{1}$ and

$$\Omega_{\mathcal{S}} = \frac{1}{\sqrt{2}}(e_1 \otimes e_1 + e_2 \otimes e_2),$$

is a GNS representation of $\mathcal{O}_{\mathcal{H}_{\mathcal{S}}}$ associated to $\rho_{\mathcal{S}}$. Since $\rho_{\mathcal{S}}$ is faithful, this representation carries the modular structure of $\mathcal{O}_{\mathcal{S}}$. Show that the modular conjugation and the modular operator are given by $J_{\mathcal{S}} : f \otimes g \mapsto \overline{g} \otimes \overline{f}$ and $\Delta_{\omega_{\mathcal{S}}} = \mathbb{1}$.
Note that this part of the exercise is the simplest non-trivial example of Exercise 2.15 (5).

2. Let $(\mathcal{H}_{\mathrm{AW},j}, \pi_{\mathrm{AW},j}, \Omega_{\mathrm{AW},j})$ be the Araki-Wyss representation of the j-th reservoir associated to the quasi-free state ω_{β_j,μ_j}. Show that $\pi_{\mathrm{SF}} = \pi_{\mathcal{S}} \otimes \pi_{\mathrm{AW},1} \otimes \cdots \otimes \pi_{\mathrm{AW},n}$ is the standard representation of $\mathcal{O}_{\mathcal{H}}$ on the Hilbert space

$$\mathcal{H}_{\mathrm{SF}} = (\mathcal{H}_{\mathcal{S}} \otimes \mathcal{H}_{\mathcal{S}}) \otimes \mathcal{H}_{\mathrm{AW},1} \otimes \cdots \mathcal{H}_{\mathrm{AW},n},$$

with the cyclic vector

$$\Omega_{\mathrm{SF}} = \Omega_{\mathcal{S}} \otimes \Omega_{\mathrm{AW},1} \otimes \cdots \otimes \Omega_{\mathrm{AW},n}.$$

3. Consider the SF model with interaction $P_j = \varphi_j(\psi_j)$. Show that in the above standard representation the operator $L_{\frac{1}{\alpha}}$, defined by (4.10), takes the form

$$
\begin{aligned}
L_{\frac{1}{\alpha}} &= (H_{\mathcal{S}} \otimes \mathbb{1}_{\mathcal{H}_{\mathcal{S}}} - \mathbb{1}_{\mathcal{H}_{\mathcal{S}}} \otimes H_{\mathcal{S}}) \otimes \mathbb{1}_{\mathcal{H}_{\mathrm{AW},1}} \otimes \cdots \otimes \mathbb{1}_{\mathcal{H}_{\mathrm{AW},n}} \\
&+ \sum_{j=1}^{n} (\mathbb{1}_{\mathcal{H}_{\mathcal{S}}} \otimes \mathbb{1}_{\mathcal{H}_{\mathcal{S}}}) \otimes \mathbb{1}_{\mathcal{H}_{\mathrm{AW},1}} \otimes \cdots \otimes (\mathrm{d}\Gamma(h_j) \otimes \mathbb{1} - \mathbb{1} \otimes \mathrm{d}\Gamma(\overline{h}_j)) \otimes \cdots \otimes \mathbb{1}_{\mathcal{H}_{\mathrm{AW},n}} \\
&+ \lambda \sum_{j=1}^{n} (\sigma^{(1)} \otimes \mathbb{1}_{\mathcal{H}_{\mathcal{S}}}) \otimes \mathbb{1}_{\mathcal{H}_{\mathrm{AW},1}} \otimes \cdots \otimes \frac{1}{\sqrt{2}} \left(b_{\mathrm{AW},j}(\psi_j) + b^*_{\mathrm{AW},j}(\psi_j) \right) \otimes \cdots \otimes \mathbb{1}_{\mathcal{H}_{\mathrm{AW},n}} \\
&- \lambda \sum_{j=1}^{M} (\mathbb{1}_{\mathcal{H}_{\mathcal{S}}} \otimes \sigma^{(1)}) \otimes \mathbb{1}_{\mathcal{H}_{\mathrm{AW},1}} \otimes \cdots \otimes \frac{1}{\sqrt{2}} \left(b'_{\mathrm{AW},j}(\psi_j^+) + b'^*_{\mathrm{AW},j}(\psi_j^-) \right) \otimes \cdots \otimes \mathbb{1}_{\mathcal{H}_{\mathrm{AW},n}},
\end{aligned}
\tag{6.11}
$$

where $\boldsymbol{\alpha} = (0, \boldsymbol{\gamma}, \boldsymbol{\gamma}')$ and

$$\psi_j^{\pm} = \mathrm{e}^{\pm \beta_j [(1/2 - \gamma_j) h_j - \mu_j (1/2 - \gamma_j')]} \psi_j.$$

Starting with the seminal papers of Davies [Dav], Lebowitz-Spohn [LS2] and Davies-Spohn [DS], the SF model (together with the closely related Spin-Boson model) became a paradigm in mathematically rigorous studies of non-equilibrium quantum statistical mechanics. Despite the number of new results obtained in the last decade many basic questions about this model are still open.

The study of the SF model requires sophisticated analytical tools and for reasons of space we shall not make a detailed exposition of specific results in these lecture notes. Instead, we will restrict ourselves to a brief description on the main new conceptual ideas that made the proofs of these results possible. We refer the reader to the original articles for more details.

The key new idea, which goes back to Jakšić-Pillet [JP3], is to use modular theory and quantum transfer operators to study large time limits. As we have repeatedly emphasized, before taking the limit $t \to \infty$ one must take reservoirs to their thermodynamic limit. The advantage of the modular structure is that it remains intact in the thermodynamic limit. In other words, the basic objects and relations of the theory remain valid for infinitely extended systems.

In the thermodynamic limit the Hilbert spaces $\mathcal{K}_j$ become infinite dimensional. Under very general conditions the operator $L_{\frac{1}{\alpha}}$ converges to a limiting operator. In the example of Exercise 6.6, this limit has exactly the same form (6.11) on the limiting Hilbert space $\mathcal{H}_{\mathrm{SF}}$ which carries representations $\psi \mapsto b_j^{\#}(\psi)$ of the CAR over the infinite dimensional $\mathcal{K}_j$. Moreover, the limiting moment generating function for the full counting statistics (4.6) is related to this operator as in (4.9). Under suitable technical assumptions on the ψ_j's one then can prove a large deviation principle for full counting statistics by a careful study of the spectral resonances of $L_{\frac{1}{\alpha}}$. It is precisely this last step that is technically most demanding and requires a number of additional assumptions. The existing proofs are based on perturbation arguments that require small λ and, for technical reasons, vanishing chemical potentials μ_j. We remark that the proofs follow line by line the spectral scheme outlined in Section 5.5 and we refer the interested reader to [JOPP] for details and additional information.

For $\boldsymbol{\alpha} = (0, \mathbf{1}/2, \mathbf{1}/2)$, the operators $L_{\frac{1}{\alpha}}$ is the standard Liouvillean K. The spectral analysis of this operator is a key ingredient in the proof of return to equilibrium when all reservoirs are at the same temperature. For related results, see [JP1, BFS, DJ, FM]. More generally, the spectrum of K provides information about the normal invariant states of the system, *i.e.*, the density matrices on the space $\mathcal{H}_{\mathrm{SF}}$ which correspond to steady states. In particular, if K has no point spectrum then the system has no normal invariant state and hence its steady states have to be singular w.r.t. the reference state ρ (see, *e.g.*, [AJPP1, Pi] for details).

In the case $\boldsymbol{\alpha} = (0, \mathbf{0}, \mathbf{0})$, the operator $L_{\frac{1}{\alpha}}$ reduces to the L^∞-Liouvillean (or C-Liouvillean) L_∞ introduced in [JP3]. In this work the relaxation to a non-equilibrium steady state was proven by using the identity

$$\omega_t(A) = \langle \Omega_{\rm SF} | \mathrm{e}^{\mathrm{i}tL_\infty} \pi_{\rm SF}(A) \Omega_{\rm SF} \rangle,$$

and by a careful study of resonances and resonance eigenfunctions of the operator L_∞. This approach was adapted to the Spin-Boson model in [MMS2].

For a different approach to the large deviation principle for the spin-fermion and the spin-boson model we refer the reader to [DR].

6.6 Electronic black box model

6.6.1 Model

Let $\mathcal{S}$ be a finite set and $h_\mathcal{S}$ a one-particle Hamiltonian on $\mathcal{K}_\mathcal{S} = \ell^2(\mathcal{S})$. We think of $\mathcal{S}$ as a "black box" representing some electronic device (*e.g.*, a quantum dot). To feed this device, we connect it to several, say n, reservoirs $\mathcal{R}_1, \ldots, \mathcal{R}_n$. For simplicity, each reservoir $\mathcal{R}_j$ is a finite lead described, in the tight binding approximation, by a box $\Lambda = [0, M]$ in $\mathbb{Z}$ (see Figure 6.1). The one-particle Hilbert space of a finite lead is $\mathcal{K}_j = \ell^2(\Lambda)$ and its one-particle Hamiltonian is $h_j = -\frac{1}{2}\Delta_\Lambda$, where Δ_Λ denotes the discrete Laplacian on Λ with Dirichlet boundary conditions (see Section 1.1). The Electronic Black Box (EBB) model is a free Fermi gas with single particle Hilbert space

$$\mathcal{K} = \mathcal{K}_\mathcal{S} \oplus \left(\oplus_{j=1}^n \mathcal{K}_j \right).$$

In the following, we identify $\mathcal{K}_\mathcal{S}$ and $\mathcal{K}_j$ with the corresponding subspaces of $\mathcal{K}$ and we denote by $\mathbb{1}_\mathcal{S}$ and $\mathbb{1}_j$ the orthogonal projections of $\mathcal{K}$ on these subspaces. In the absence of coupling between $\mathcal{S}$ and the reservoirs, the Hamiltonian of the EBB model is

$$H_0 = \mathrm{d}\Gamma(h_0),$$

where

$$h_0 = h_\mathcal{S} \oplus \left(\oplus_{j=1}^n h_j \right).$$

The reference state of the system, denoted ω_0, is the quasi-free state associated to the density

$$T_0 = T_\mathcal{S} \oplus \left(\oplus_{j=1}^n T_j \right),$$

where $T_\mathcal{S} > 0$ is a density operator on $\mathcal{K}_\mathcal{S}$ which commutes with $h_\mathcal{S}$ and

$$T_j = (\mathbb{1} + \mathrm{e}^{\beta_j (h_j - \mu_j \mathbb{1})})^{-1},$$

is the Fermi-Dirac density describing the thermal equilibrium of the j-th reservoir at inverse temperature β_j and chemical potential μ_j.

The coupling of the black box $\mathcal{S}$ to the j-th reservoir is described as follows. Let $\chi_j \in \mathcal{K}_\mathcal{S}$ be a unit vector and let $\delta_0^{(j)} \in \mathcal{K}_j$ be the Dirac delta function at site $0 \in \Lambda$, both identified with elements of $\mathcal{K}$. Set $v_j = |\chi_j\rangle\langle\delta_0^{(j)}| + |\delta_0^{(j)}\rangle\langle\chi_j|$. The single particle Hamiltonian of the coupled EBB model is

$$h_\lambda = h_0 + \lambda \sum_{j=1}^n v_j,$$

where $\lambda \in \mathbb{R}$ is a coupling constant. Denoting by $a^\#$ the creation/annihilation operators on $\Gamma(\mathcal{K})$ and using Part (8) of Proposition 6.2 we see that the full Hamiltonian of the coupled EBB model is

$$H_\lambda = \mathrm{d}\Gamma(h_\lambda) = H_0 + \lambda \sum_{j=1}^n \left[a^*(\chi_j) a(\delta_0^{(j)}) + a^*(\delta_0^{(j)}) a(\chi_j) \right],$$

and that the induced dynamics on the CAR algebra over $\mathcal{K}$ is completely determined by

$$\tau_\lambda^t(a^\#(\psi)) = \mathrm{e}^{\mathrm{i}tH_\lambda} a^\#(\psi) \mathrm{e}^{-\mathrm{i}tH_\lambda} = a^\#(\mathrm{e}^{\mathrm{i}th_\lambda}\psi).$$

Assume that the black box $\mathcal{S}$ is TRI, *i.e.*, that there exists an anti-unitary involution $\theta_\mathcal{S}$ on $\mathcal{K}_\mathcal{S}$ such that $\theta_\mathcal{S} h_\mathcal{S} \theta_\mathcal{S}^* = h_\mathcal{S}$ and $\theta_\mathcal{S} T_\mathcal{S} \theta_\mathcal{S}^* = T_\mathcal{S}$. If $\theta_\mathcal{S}\chi_j = \chi_j$ for $j = 1, \dots, n$, then one easily shows that the EBB model is TRI, with the time reversal

$$\Theta = \Gamma(\theta), \qquad \theta = \theta_\mathcal{S} \oplus (\oplus_{j=1}^n \theta_j),$$

where θ_j denotes the complex conjugation on $\mathcal{K}_j = \ell^2(\Lambda)$.

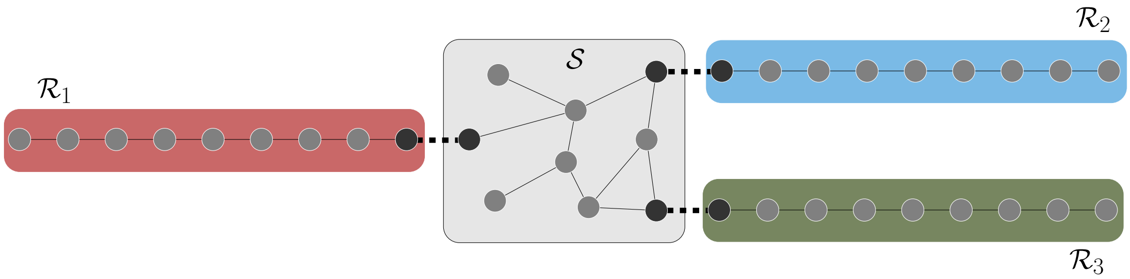

Figure 6.1: The EBB model with three leads.

6.6.2 Fluxes

The energy operator of the j-th reservoir is $H_j = \mathrm{d}\Gamma(h_j)$. Applying Equ. (4.2), using Relation (6.7) and Part (8) of Proposition 6.2, we see that the energy flux observables are given by

$$\begin{aligned}\Phi_j &= -\mathrm{i}[H_\lambda, H_j] = -\mathrm{d}\Gamma(\mathrm{i}[h_\lambda, h_j]) = \lambda\, \mathrm{d}\Gamma(\mathrm{i}[h_j, v_j]) \\ &= \mathrm{i}\lambda \left(a^*(h_j \delta_0^{(j)}) a(\chi_j) - a^*(\chi_j) a(h_j \delta_0^{(j)}) \right).\end{aligned} \tag{6.12}$$

The charge operator of $\mathcal{S}$ is $N_\mathcal{S} = \mathrm{d}\Gamma(\mathbb{1}_\mathcal{S})$ and $N_j = \mathrm{d}\Gamma(\mathbb{1}_j)$ is the charge operator of $\mathcal{R}_j$. Note that the total charge $N = N_\mathcal{S} + \sum_{j=1}^n N_j = \mathrm{d}\Gamma(\mathbb{1})$ commutes with H. The charge flux observables are

$$\begin{aligned}\mathcal{J}_j &= -\mathrm{i}[H_\lambda, N_j] = -\mathrm{d}\Gamma(\mathrm{i}[h_\lambda, \mathbb{1}_j]) = \lambda\, \mathrm{d}\Gamma(\mathrm{i}[\mathbb{1}_j, v_j]) \\ &= \mathrm{i}\lambda \left(a^*(\delta_0^{(j)}) a(\chi_j) - a^*(\chi_j) a(\delta_0^{(j)}) \right).\end{aligned} \tag{6.13}$$

It follows from Part (6) of Proposition 6.2 and Part (1) of Proposition 6.6 that the heat and charge fluxes at time t are

$$\begin{aligned}\omega_0(\tau_\lambda^t(\Phi_j)) &= 2\lambda\, \mathrm{Im}\, \langle \mathrm{e}^{\mathrm{i}th_\lambda} h_j \delta_0^{(j)} | T_0 \mathrm{e}^{\mathrm{i}th_\lambda} \chi_j \rangle, \\ \omega_0(\tau_\lambda^t(\mathcal{J}_j)) &= 2\lambda\, \mathrm{Im}\, \langle \mathrm{e}^{\mathrm{i}th_\lambda} \delta_0^{(j)} | T_0 \mathrm{e}^{\mathrm{i}th_\lambda} \chi_j \rangle.\end{aligned}$$

6.6.3 Entropy production

One easily concludes from Part (1) of proposition 6.6 that $\omega_t = \omega_0 \circ \tau_\lambda^t$ is the quasi-free state with density $T_t = \mathrm{e}^{-\mathrm{i}th_\lambda} T_0 \mathrm{e}^{\mathrm{i}th_\lambda}$. We set

$$k_0 = \log\left(T_0(\mathbb{1} - T_0)^{-1}\right) = \log\left(T_\mathcal{S}(\mathbb{1}_\mathcal{S} - T_\mathcal{S})^{-1}\right) \oplus \left(\oplus_{j=1}^n [-\beta_j(h_j - \mu_j \mathbb{1}_j)]\right),$$

so that

$$k_t = \log\left(T_t(\mathbb{1} - T_t)^{-1}\right) = \mathrm{e}^{-\mathrm{i}th_\lambda} k_0 \mathrm{e}^{\mathrm{i}th_\lambda}.$$

Proposition 6.8 allows us to write the relative Hamiltonian of ω_t w.r.t. ω_0 as

$$\ell_{\omega_t|\omega_0} = \mathrm{d}\Gamma(k_t - k_0).$$

It follows that the entropy production observable is

$$\sigma = \frac{\mathrm{d}}{\mathrm{d}t}\ell_{\omega_t|\omega_0}\bigg|_{t=0} = \mathrm{d}\Gamma(-\mathrm{i}[h_\lambda, k_0]) = -\mathrm{i}[H_\lambda, Q_{\mathcal{S}}] - \sum_{j=1}^{n}\beta_j(\Phi_j - \mu_j\mathcal{J}_j), \tag{6.14}$$

where $Q_{\mathcal{S}} = \mathrm{d}\Gamma(\log(T_{\mathcal{S}}(\mathbb{1}_{\mathcal{S}} - T_{\mathcal{S}})^{-1}))$ (compare this expression with Equ. (4.1)). The entropy balance equation thus reads

$$S(\omega_t|\omega_0) = \omega_0(\tau_\lambda^t(Q_{\mathcal{S}}) - Q_{\mathcal{S}}) + \sum_{j=1}^{n}\beta_j\int_0^t \omega_s(\Phi_j - \mu_j\mathcal{J}_j)\,\mathrm{d}s. \tag{6.15}$$

6.6.4 Entropic pressure functionals

Not surprisingly, these functionals can be expressed in terms of one-particle quantities. For $p \in [1, \infty[$ one has, by Lemma 6.1,

$$\begin{aligned}
e_{p,t}(\alpha) &= \log\mathrm{tr}\left[\left(\omega_0^{(1-\alpha)/p}\omega_t^{2\alpha/p}\omega_0^{(1-\alpha)/p}\right)^{p/2}\right] \\
&= \log\mathrm{tr}\left[\frac{1}{Z_{T_0}}\Gamma\left(\left(\mathrm{e}^{k_0(1-\alpha)/p}\mathrm{e}^{k_t 2\alpha/p}\mathrm{e}^{k_0(1-\alpha)/p}\right)^{p/2}\right)\right] \\
&= -\log Z_{T_0} + \log\det\left(\mathbb{1} + \left(\mathrm{e}^{k_0(1-\alpha)/p}\mathrm{e}^{k_t 2\alpha/p}\mathrm{e}^{k_0(1-\alpha)/p}\right)^{p/2}\right) \\
&= \log\left[\frac{\det\left(\mathbb{1} + \left(\mathrm{e}^{k_0(1-\alpha)/p}\mathrm{e}^{k_t 2\alpha/p}\mathrm{e}^{k_0(1-\alpha)/p}\right)^{p/2}\right)}{\det\left(\mathbb{1} + \mathrm{e}^{k_0}\right)}\right].
\end{aligned} \tag{6.16}$$

After some elementary algebra, one gets

$$e_{p,t}(\alpha) = \log\det\left[\mathbb{1} + T_0\left(\mathrm{e}^{-k_0}\left(\mathrm{e}^{k_0(1-\alpha)/p}\mathrm{e}^{k_t 2\alpha/p}\mathrm{e}^{k_0(1-\alpha)/p}\right)^{p/2} - \mathbb{1}\right)\right].$$

In particular, for $p = 2$,

$$e_{2,t}(\alpha) = \log\det\left(\mathbb{1} + T_0(\mathrm{e}^{-\alpha k_0}\mathrm{e}^{\alpha k_t} - \mathbb{1})\right),$$

and for $p = \infty$ we obtain

$$e_{\infty,t}(\alpha) = \lim_{p\to\infty} e_{p,t}(\alpha) = \log\det\left(\mathbb{1} + T_0(\mathrm{e}^{-k_0}\mathrm{e}^{(1-\alpha)k_0 + \alpha k_t} - \mathbb{1})\right).$$

Exercise 6.7. The multi-parameter formalism of Section 3.7 is easily adapted to the EBB model. Indeed, one has

$$\log\omega_0 = (Q_{\mathcal{S}} - \log Z_{T_0}) - \sum_{j=1}^{n}\beta_j H_j + \sum_{j=1}^{n}\beta_j\mu_j N_j,$$

and the $n+1$ terms in this sum form a commuting family (the scalar term $-\log Z_T$ plays no role in the following, we can pack it with the $Q_{\mathcal{S}}$ term which will turn out to become irrelevant in the large time limit). Following Exercise 3.10, define

$$\omega_0^{\boldsymbol{\alpha}} = \mathrm{e}^{\alpha_{\mathcal{S}}(Q_{\mathcal{S}} - \log Z_{T_0}) - \sum_{j=1}^{n}\alpha_j\beta_j H_j + \sum_{j=1}^{n}\alpha_{n+j}\beta_j\mu_j N_j}, \qquad \omega_t^{\boldsymbol{\alpha}} = \mathrm{e}^{-\mathrm{i}tH_\lambda}\omega_0^{\boldsymbol{\alpha}}\mathrm{e}^{\mathrm{i}tH_\lambda},$$

for $\boldsymbol{\alpha} = (\alpha_{\mathcal{S}}, \alpha_1, \ldots, \alpha_{2n}) \in \mathbb{R}^{2n+1}$.

1. Show that the generating functional for multi-parameter full counting statistics is given by

$$e_{2,t}(\boldsymbol{\alpha}) = \log \operatorname{tr}\left(\omega_0^{\mathbf{1}-\boldsymbol{\alpha}}\omega_t^{\boldsymbol{\alpha}}\right) = \log \det\left(\mathbb{1} + T_0(\mathrm{e}^{-k(\boldsymbol{\alpha})}\mathrm{e}^{k_t(\boldsymbol{\alpha})} - \mathbb{1})\right)$$

where

$$k(\boldsymbol{\alpha}) = \alpha_{\mathcal{S}} \log(T_{\mathcal{S}}(\mathbb{1} - T_{\mathcal{S}})^{-1}) - \sum_{j=1}^{n} \alpha_j \beta_j h_j + \sum_{j=1}^{n} \alpha_{n+j}\beta_j\mu_j \mathbb{1}_j,$$

and $k_t(\boldsymbol{\alpha}) = \mathrm{e}^{-\mathrm{i}th_\lambda}k(\boldsymbol{\alpha})\mathrm{e}^{\mathrm{i}th_\lambda}$.

2. Show that the "naive" generating function (5.13) is given by

$$e_{\mathrm{naive},t}(\boldsymbol{\alpha}) = \log\det\left(\mathbb{1} + T_0(\mathrm{e}^{k_{-t}(\boldsymbol{\alpha})-k(\boldsymbol{\alpha})} - \mathbb{1})\right).$$

Exercise 6.8. Following Section 4.3, introduce the control parameters $X_j = \beta_{\mathrm{eq}} - \beta_j$ and $X_{n+j} = \beta_{\mathrm{eq}}\mu_{\mathrm{eq}} - \beta_j\mu_j$, where β_{eq} and μ_{eq} are some equilibrium values of the inverse temperature and chemical potential. Denote by ω_X the quasi-free state on the CAR algebra over $\mathcal{K}$ with density

$$T_X = \left(\mathbb{1} + \mathrm{e}^{\beta_{\mathrm{eq}}(h_\lambda - \mu_{\mathrm{eq}}\mathbb{1}) - \sum_{j=1}^{n}(X_j h_j + X_{n+j}\mathbb{1}_j)}\right)^{-1},$$

and set $k_X = \log\left(T_X(\mathbb{1} - T_X)^{-1}\right) = -\beta_{\mathrm{eq}}(h_\lambda - \mu_{\mathrm{eq}}\mathbb{1}) + \sum_{j=1}^{n}(X_j h_j + X_{n+j}\mathbb{1}_j)$.

1. Show that

$$\sigma_X = \mathrm{d}\Gamma(-\mathrm{i}[h_\lambda, k_X]) = \sum_{j=1}^{n} X_j\Phi_j + X_{n+j}\mathcal{J}_j,$$

where the individual fluxes are given by (6.12) and (6.13).

2. Show that the generalized entropic pressure is given by

$$e_t(X,Y) = \log\det\left(\mathbb{1} + T_X\left(\mathrm{e}^{-k_X}\mathrm{e}^{k_{X-Y}+k_{Y,t}-k_0} - \mathbb{1}\right)\right),$$

where $k_{Y,t} = \mathrm{e}^{-\mathrm{i}th_\lambda}k_Y\mathrm{e}^{\mathrm{i}th_\lambda}$.

3. Develop the finite time linear response theory of the EBB model.

6.6.5 Thermodynamic limit

The thermodynamic limit of the EBB model is achieved by letting $M \to \infty$, keeping the system $\mathcal{S}$ untouched. We shall not enter into a detailed description of this step which is completely analogous to the thermodynamic limit of the classical harmonic chain discussed in Section 1.8 (see Exercise 6.9 below). The one particle Hilbert space of the reservoir $\mathcal{R}_j$ becomes $\mathcal{K}_j = \ell^2(\mathbb{N})$ and its one particle Hamiltonian $h_j = -\frac{1}{2}\Delta$, where Δ is the discrete Laplacian on $\mathbb{N}$ with Dirichlet boundary condition. Using the discrete Fourier transform

$$\widehat{\psi}(\xi) = \sqrt{\frac{2}{\pi}}\sum_{x\in\mathbb{N}}\psi(x)\sin(\xi(x+1)),$$

we can identify $\mathcal{K}_j$ with $L^2([0,\pi],\mathrm{d}\xi)$ and h_j becomes the operator of multiplication by $\varepsilon(\xi) = 1 - \cos\xi$. In particular, the spectrum of h_j is purely absolutely continuous and fills the interval $[0,2]$ with constant multiplicity one. Thus, the spectrum of the decoupled Hamiltonian h_0 consists of an absolutely continuous part filling the same interval with constant multiplicity n and of a discrete part given by the eigenvalues of

$h_{\mathcal{S}}$. We denote by $\mathbb{1}_{\mathcal{R}} = \mathbb{1} - \mathbb{1}_{\mathcal{S}} = \sum_{j=1}^{n} \mathbb{1}_j$ the projection on the absolutely continuous part of h_0. In the momentum representation one has $\mathcal{K}_{\mathcal{R}} = \mathrm{Ran}\, \mathbb{1}_{\mathcal{R}} = L^2([0,\pi]) \otimes \mathbb{C}^n$. Denoting by $1_j = |e_j\rangle\langle e_j|$ the orthogonal projection of $\mathbb{C}^n$ onto the subspace generated by the j-th vector of its standard basis, we have $\mathbb{1}_j = \mathbb{1} \otimes 1_j$ and $h_j = \varepsilon(\xi) \otimes 1_j$.

Exercise 6.9. Denote by the subscript $(\cdot)_M$ the dependence on the parameter M of the various objects associated to the EBB model, *e.g.*, $\omega_{M,0}$ is the reference state with density $T_{M,0} = T_{\mathcal{S}} \oplus (\oplus_{j=1}^{n} T_{M,j})$, etc.

1. Show that

$$\lim_{M\to\infty} T_{M,0}(\mathrm{e}^{-\alpha k_{M,0}} \mathrm{e}^{\alpha k_{M,t}} - \mathbb{1}) = T_0(\mathrm{e}^{-\alpha k_0} \mathrm{e}^{\alpha k_t} - \mathbb{1}),$$

holds in trace norm, where $T_0 = \mathrm{s} - \lim\limits_{M\to\infty} T_{M,0}$, $k_0 = \log(T_0(\mathbb{1} - T_0))$, $k_t = \mathrm{e}^{-\mathrm{i}th_\lambda} k_0 \mathrm{e}^{\mathrm{i}th_\lambda}$ and $h_\lambda = \mathrm{s} - \lim\limits_{M\to\infty} h_{M,\lambda}$.

Hint: write $\mathrm{e}^{-\alpha k_{M,0}} \mathrm{e}^{\alpha k_{M,t}} - \mathbb{1}$ as the integral of its derivative w.r.t. t and observe that $[h_{M,\lambda}, k_{M,0}]$ is a finite rank operator that does not depend on M.

2. Show that, for any $\alpha, t \in \mathbb{R}$,

$$\lim_{M\to\infty} e_{M,2,t}(\alpha) = \log\det\left(\mathbb{1} + T_0(\mathrm{e}^{-\alpha k_0} \mathrm{e}^{\alpha k_t} - \mathbb{1})\right).$$

Hint: recall that $\det(\mathbb{1} + T_{M,0}(\mathrm{e}^{-\alpha k_{M,0}} \mathrm{e}^{\alpha k_{M,t}} - \mathbb{1})) = \omega_{M,0}(\Gamma(\mathrm{e}^{-\alpha k_{M,0}/2} \mathrm{e}^{\alpha k_{M,t}} \mathrm{e}^{-\alpha k_{M,0}/2})) > 0$.

Remark. The implications of this exercise are described in Proposition 5.1.

Exercise 6.10. Let $\mathrm{P}_{M,t}$ denote the spectral measure of $\log(\Delta_{\omega_{M,t}|\omega_{M,0}})$ and $\xi_{\omega_{M,0}}$. Through the following steps, show that the spectral measure P_t of $\log(\Delta_{\omega_t|\omega_0})$ and ξ_{ω_0} is the weak limit of the sequence $\{\mathrm{P}_{M,t}\}$. (Up to a rescaling, $\mathrm{P}_{M,t}$ is the full counting statistics of the finite EBB model.)

1. Show that, for all $\alpha \in \mathbb{R}$, the characteristic function of $\mathrm{P}_{M,t}$,

$$\begin{aligned}
\chi_{M,t}(\alpha) = \int \mathrm{e}^{\mathrm{i}\alpha x} \mathrm{d}\mathrm{P}_{M,t}(x) &= (\xi_{\omega_{M,0}} | \Delta^{\mathrm{i}\alpha}_{\omega_{M,t}|\omega_{M,0}} \xi_{\omega_{M,0}}) \\
&= \mathrm{tr}\left(\omega_{M,0}^{1-\mathrm{i}\alpha}\, \omega_{M,t}^{\mathrm{i}\alpha}\right) \\
&= \det\left(\mathbb{1} + T_{M,0}(\mathrm{e}^{\mathrm{i}\alpha k_{M,t}} \mathrm{e}^{-\mathrm{i}\alpha k_{M,0}} - \mathbb{1})\right),
\end{aligned}$$

converges, as $M \to \infty$, towards

$$\chi_t(\alpha) = \det\left(\mathbb{1} + T_0(\mathrm{e}^{\mathrm{i}\alpha k_t} \mathrm{e}^{-\mathrm{i}\alpha k_0} - \mathbb{1})\right) = \omega_0\left(\Gamma(\mathrm{e}^{\mathrm{i}\alpha k_t} \mathrm{e}^{-\mathrm{i}\alpha k_0})\right).$$

2. In the Araki-Wyss representation associated to the state ω_0, show that

$$(\xi_{\omega_0} | \Delta^{\mathrm{i}\alpha}_{\omega_t|\omega_0} \xi_{\omega_0}) = (\xi_{\omega_0} | \Gamma_t(\alpha) \xi_{\omega_0}),$$

where the cocycle $\Gamma_t(\alpha) = \Delta^{\mathrm{i}\alpha}_{\omega_t|\omega_0} \Delta^{-\mathrm{i}\alpha}_{\omega_0}$ satisfies the Cauchy problem

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\Gamma_t(\alpha) = \mathrm{i}\,\Gamma_t(\alpha)\left(\Delta^{\mathrm{i}\alpha}_{\omega_0} \pi_{\mathrm{AW}}(\ell_{\omega_t|\omega_0}) \Delta^{-\mathrm{i}\alpha}_{\omega_0}\right), \qquad \Gamma_t(0) = \mathbb{1}.$$

3. Show that $\Gamma_t(\alpha) = \pi_{\mathrm{AW}}(\gamma_t(\alpha))$ where

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\gamma_t(\alpha) = \mathrm{i}\,\gamma_t(\alpha)\left(\mathrm{e}^{\mathrm{i}\alpha \mathrm{d}\Gamma(k_0)} \ell_{\omega_t|\omega_0} \mathrm{e}^{-\mathrm{i}\alpha \mathrm{d}\Gamma(k_0)}\right), \qquad \gamma_t(0) = \mathbb{1}.$$

Conclude that $(\xi_{\omega_0}|\Delta^{i\alpha}_{\omega_t|\omega}\xi_{\omega_0}) = \omega_0(\gamma_t(\alpha))$.

4. Show that

$$\gamma_t(\alpha) = [D\omega_t : D\omega_0]^\alpha = \mathrm{e}^{\mathrm{i}\alpha \mathrm{d}\Gamma(k_t)}\mathrm{e}^{-\mathrm{i}\alpha \mathrm{d}\Gamma(k_0)} = \Gamma(\mathrm{e}^{\mathrm{i}\alpha k_t}\mathrm{e}^{-\mathrm{i}\alpha k_0}),$$

and conclude that

$$\chi_t(\alpha) = \int \mathrm{e}^{\mathrm{i}\alpha x}\mathrm{dP}_t(x).$$

5. Invoke the Lévy-Cramér continuity theorem (Theorem 7.6 in [Bi1]) to conclude that $\mathrm{P}_{M,t}$ converges weakly towards P_t.

6.6.6 Large time limit

Let us briefly discuss the limit $t \to \infty$. For simplicity, we shall assume that the one particle Hamiltonian h_λ has purely absolutely continuous spectrum. This is the generic situation for small coupling λ in the fully resonant case where $\mathrm{sp}(h_{\mathcal{S}}) \subset]0, 2[$. Since $h_\lambda - h_0 = v = \sum_{j=1}^n v_j$ is finite rank, the wave operators

$$w_\pm = \mathrm{s} - \lim_{t\to\pm\infty} \mathrm{e}^{ith_\lambda}\mathrm{e}^{-ith_0}\mathbb{1}_{\mathcal{R}},$$

exist and are complete, $w_\pm w_\pm^* = \mathbb{1}$, $w_\pm^* w_\pm = \mathbb{1}_{\mathcal{R}}$. The scattering matrix $s = w_+^* w_-$ is unitary on $\mathcal{K}_{\mathcal{R}}$. It acts as the operator of multiplication by a unitary $n \times n$ matrix $s(\xi) = [s_{jk}(\xi)]$. Since $[h_0, T_0] = 0$, one has

$$\begin{aligned}\lim_{t\to\infty}\langle\psi|T_t\phi\rangle &= \lim_{t\to\infty}\langle \mathrm{e}^{ith_\lambda}\psi|T_0\mathrm{e}^{ith_\lambda}\phi\rangle\\ &= \lim_{t\to\infty}\langle \mathrm{e}^{-ith_0}\mathrm{e}^{ith_\lambda}\psi|T_0\mathrm{e}^{-ith_0}\mathrm{e}^{ith_\lambda}\phi\rangle\\ &= \langle w_-^*\psi|T_0 w_-^*\phi\rangle = \langle\psi|T_+\phi\rangle,\end{aligned}$$

whith $T_+ = w_- T_0 w_-^*$. It follows that for any polynomial A in the creation/annihilation operators on $\Gamma(\mathcal{K})$, one has

$$\lim_{t\to\infty}\omega_0\circ\tau_\lambda^t(A) = \omega_+(A),$$

where ω_+ is the quasi-free state with density T_+. We conclude that the NESS ω_+ of the EBB model is the quasi-free state with density

$$T_+ = w_- T_0 w_-^*. \tag{6.17}$$

The large time asymptotics of the entropic pressure functionals can be obtained along the same line as in Section 1.11. We shall only consider the case $p = 2$ and leave the general case as an exercise.

Starting with (6.16) and using the result of Exercise 1.8, we can write

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\alpha}e_{2,t}(\alpha) &= \frac{\mathrm{d}}{\mathrm{d}\alpha}\operatorname{tr}\log\left(\mathbb{1} + \mathrm{e}^{(1-\alpha)k_0}\mathrm{e}^{\alpha k_t}\right)\\ &= \operatorname{tr}\left((\mathbb{1} + \mathrm{e}^{(1-\alpha)k_0}\mathrm{e}^{\alpha k_t})^{-1}\mathrm{e}^{(1-\alpha)k_0}(k_t - k_0)\mathrm{e}^{\alpha k_t}\right)\\ &= \operatorname{tr}\left((\mathbb{1} + \mathrm{e}^{-(1-\alpha)k_0}\mathrm{e}^{-\alpha k_t})^{-1}(k_t - k_0)\right)\\ &= -t\int_0^1 \operatorname{tr}\left((\mathbb{1} + \mathrm{e}^{-(1-\alpha)k_0}\mathrm{e}^{-\alpha k_t})^{-1}\mathrm{e}^{-ituh_\lambda}\mathrm{i}[h_\lambda, k_0]\mathrm{e}^{ituh_\lambda}\right)\mathrm{d}u\\ &= -t\int_0^1 \operatorname{tr}\left(\mathrm{e}^{ituh_\lambda}(\mathbb{1} + \mathrm{e}^{-(1-\alpha)k_0}\mathrm{e}^{-\alpha k_t})^{-1}\mathrm{e}^{-ituh_\lambda}\mathrm{i}[h_\lambda, k_0]\right)\mathrm{d}u\\ &= -t\int_0^1 \operatorname{tr}\left((\mathbb{1} + \mathrm{e}^{-(1-\alpha)k_{-tu}}\mathrm{e}^{-\alpha k_{t(1-u)}})^{-1}\mathrm{i}[h_\lambda, k_0]\right)\mathrm{d}u.\end{aligned}$$

The final relation

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\, e_{2,t}(\alpha) = -t \int_0^1 \mathrm{tr}\left((\mathbb{1} + \mathrm{e}^{-(1-\alpha)k_{-tu}} \mathrm{e}^{-\alpha k_{t(1-u)}})^{-1} \mathrm{i}[h_\lambda, k_0] \right) \mathrm{d}u$$

remains valid after the thermodynamic limit is taken. Since k_0 is a bounded operator commuting with h_0, one easily shows that

$$\mathrm{s}-\lim_{t\to\pm\infty} k_t = k_\pm = w_\mp k_0 w_\mp^*,$$

which leads to

$$\begin{aligned}
\mathrm{s}-\lim_{t\to\infty} (\mathbb{1} + \mathrm{e}^{-(1-\alpha)k_{-ts}} \mathrm{e}^{-\alpha k_{t(1-s)}})^{-1} &= (\mathbb{1} + \mathrm{e}^{-(1-\alpha)k_-} \mathrm{e}^{-\alpha k_+})^{-1} \\
&= (\mathbb{1} + w_+ \mathrm{e}^{-(1-\alpha)k_0} w_+^* w_- \mathrm{e}^{-\alpha k_0} w_-^*)^{-1} \\
&= (\mathbb{1} + w_- s^* \mathrm{e}^{-(1-\alpha)k_0} s \mathrm{e}^{-\alpha k_0} w_-^*)^{-1} \\
&= w_- (\mathbb{1} + s^* \mathrm{e}^{-(1-\alpha)k_0} s \mathrm{e}^{-\alpha k_0})^{-1} w_-^*.
\end{aligned}$$

Since $\mathrm{i}[h_\lambda, k_0]$ is finite rank, it follows that

$$\begin{aligned}
&\lim_{t\to\infty} \mathrm{tr}_{\mathcal{K}} \left((\mathbb{1} + \mathrm{e}^{-(1-\alpha)k_{-tu}} \mathrm{e}^{-\alpha k_{t(1-u)}})^{-1} \mathrm{i}[h_\lambda, k_0] \right) \\
&\qquad = \mathrm{tr}_{\mathcal{K}_\mathcal{R}} \left((\mathbb{1} + s^* \mathrm{e}^{-(1-\alpha)k_0} s \mathrm{e}^{-\alpha k_0})^{-1} \mathcal{T} \right),
\end{aligned}$$

where $\mathcal{T} = w_-^* \mathrm{i}[h_\lambda, k_0] w_-$. Since $e_{2,t}(0) = 0$, we can write

$$e_{2,+}(\alpha) = \lim_{t\to\infty} \frac{1}{t}\, e_{2,t}(\alpha) = \lim_{t\to\infty} \frac{1}{t} \int_0^\alpha \frac{\mathrm{d}}{\mathrm{d}\gamma}\, e_{2,t}(\gamma)\, \mathrm{d}\gamma,$$

and the dominated convergence theorem yields

$$\begin{aligned}
e_{2,+}(\alpha) &= -\int_0^\alpha \int_0^1 \mathrm{tr}\left((\mathbb{1} + s^* \mathrm{e}^{-(1-\gamma)k_0} s \mathrm{e}^{-\gamma k_0})^{-1} \mathcal{T} \right) \mathrm{d}u\mathrm{d}\gamma \\
&= -\int_0^\alpha \mathrm{tr}\left((\mathbb{1} + s^* \mathrm{e}^{-(1-\gamma)k_0} s \mathrm{e}^{-\gamma k_0})^{-1} \mathcal{T} \right) \mathrm{d}\gamma.
\end{aligned}$$

The trace class operator $\mathcal{T}$ on $\mathcal{K}_\mathcal{R}$ has an integral kernel $\mathcal{T}(\xi, \xi')$ in the momentum representation. Following the argument leading to (1.28), one shows that its diagonal is given by

$$\mathcal{T}(\xi, \xi) = \frac{\varepsilon'(\xi)}{2\pi} \left(s^*(\xi) k(\xi) s(\xi) - k(\xi) \right), \tag{6.18}$$

where $k(\xi)$ is the operator on $\mathbb{C}^n$ defined by

$$k(\xi) = -\sum_{j=1}^n \beta_j (\varepsilon(\xi) - \mu_j) 1_j.$$

Thus, one has

$$\begin{aligned}
&\mathrm{tr}_{\mathcal{K}_\mathcal{R}} \left((\mathbb{1} + s^* \mathrm{e}^{-(1-\alpha)k_0} s \mathrm{e}^{-\alpha k_0})^{-1} \mathcal{T} \right) \\
&= -\int_0^\pi \mathrm{tr}_{\mathbb{C}^n} \left((\mathbb{1} + s^*(\xi) \mathrm{e}^{-(1-\alpha)k(\xi)} s(\xi) \mathrm{e}^{-\alpha k(\xi)})^{-1} \left(k(\xi) - s^*(\xi) k(\xi) s(\xi) \right) \right) \varepsilon'(\xi) \frac{\mathrm{d}\xi}{2\pi} \\
&= -\frac{\mathrm{d}}{\mathrm{d}\alpha} \int_0^\pi \mathrm{tr}_{\mathbb{C}^n} \left(\log(\mathbb{1} + s^*(\xi) \mathrm{e}^{(1-\alpha)k(\xi)} s(\xi) \mathrm{e}^{\alpha k(\xi)}) \right) \varepsilon'(\xi) \frac{\mathrm{d}\xi}{2\pi},
\end{aligned}$$

and we conclude that

$$e_{2,+}(\alpha)=\int_0^\pi \log\left[\frac{\det\left(\mathbb{1}+\mathrm{e}^{(1-\alpha)k(\xi)}s(\xi)\mathrm{e}^{\alpha k(\xi)}s^*(\xi)\right)}{\det\left(\mathbb{1}+\mathrm{e}^{k(\xi)}\right)}\right]\frac{\mathrm{d}\varepsilon(\xi)}{2\pi}.$$

After a simple algebraic manipulation, this can be rewritten as

$$e_{2,+}(\alpha)=\int_0^\pi \log\det\left(\mathbb{1}+T(\xi)(\mathrm{e}^{-\alpha k(\xi)}s(\xi)\mathrm{e}^{\alpha k(\xi)}s^*(\xi)-\mathbb{1})\right)\frac{\mathrm{d}\varepsilon(\xi)}{2\pi}, \tag{6.19}$$

where $T(\xi)=(\mathbb{1}+\mathrm{e}^{-k(\xi)})^{-1}$. In the following exercise, this calculation is extended to various other entropic functionals.

Exercise 6.11.

1. Show that for $p\in[1,\infty[$ one has

$$\begin{aligned}e_{p,+}(\alpha)&=\lim_{t\to\infty}\frac{1}{t}\,e_{p,t}(\alpha)\\&=\int_0^\pi \log\det\left[\mathbb{1}+T(\xi)\left(\mathrm{e}^{-k(\xi)}\left(\mathrm{e}^{k(\xi)(1-\alpha)/p}s(\xi)\mathrm{e}^{k(\xi)2\alpha/p}s^*(\xi)\mathrm{e}^{k(\xi)(1-\alpha)/p}\right)^{p/2}-\mathbb{1}\right)\right]\frac{\mathrm{d}\varepsilon(\xi)}{2\pi}.\end{aligned}$$

2. Show that

$$\begin{aligned}e_{\infty,+}(\alpha)&=\lim_{t\to\infty}\frac{1}{t}\,e_{\infty,t}(\alpha)\\&=\int_0^\pi \log\det\left(\mathbb{1}+T(\xi)(\mathrm{e}^{-k(\xi)}\mathrm{e}^{(1-\alpha)k(\xi)+\alpha s(\xi)k(\xi)s(\xi)^*}-\mathbb{1})\right)\frac{\mathrm{d}\varepsilon(\xi)}{2\pi}.\end{aligned}$$

3. Compute

$$e_{\mathrm{naive},+}(\alpha)=\lim_{t\to\infty}\frac{1}{t}e_{\mathrm{naive},t}(\alpha).$$

4. Show that the large time asymptotics of the multi-parameter functional of Exercise 6.7 is given by

$$\begin{aligned}e_{2,+}(\boldsymbol{\alpha})&=\lim_{t\to\infty}\frac{1}{t}\,e_{2,t}(\boldsymbol{\alpha})\\&=\int_0^\pi \log\det\left(\mathbb{1}+T(\xi)(\mathrm{e}^{-k(\boldsymbol{\alpha},\xi)}s(\xi)\mathrm{e}^{k(\boldsymbol{\alpha},\xi)}s^*(\xi)-\mathbb{1})\right)\frac{\mathrm{d}\varepsilon(\xi)}{2\pi},\end{aligned}$$

where

$$k(\boldsymbol{\alpha},\xi)=-\sum_{j=1}^n\beta_j\left(\alpha_j\varepsilon(\xi)-\alpha_{n+j}\mu_j\right)1_j.$$

Note in particular that $e_{2,+}(\boldsymbol{\alpha})$ does not depend on the first component $\alpha_{\mathcal{S}}$ of $\boldsymbol{\alpha}$.

5. Show that the large time asymptotics of the generalized functional of Exercise 6.8 is given by

$$\begin{aligned}e_{+}(X,Y)&=\lim_{t\to\infty}\frac{1}{t}\,e_{t}(X,Y)\\&=\int_0^\pi \log\det\left(\mathbb{1}+T_X(\xi)(\mathrm{e}^{-k_X(\xi)}\mathrm{e}^{k_{X-Y}(\xi)+s(\xi)k_Y(\xi)s^*(\xi)-k_0(\xi)}-\mathbb{1})\right)\frac{\mathrm{d}\varepsilon(\xi)}{2\pi},\end{aligned}$$

where $k_X(\xi)$ is the diagonal $n\times n$ matrix with entries $-(\beta_{\mathrm{eq}}-X_j)\varepsilon(\xi)+(\beta_{\mathrm{eq}}\mu_{\mathrm{eq}}+X_{n+j})$ and $T_X(\xi)=(\mathbb{1}+\mathrm{e}^{-k_X(\xi)})^{-1}$.

6. Develop the linear response theory of the EBB model.

For $\xi \in [0, \pi]$, denote by ω_ξ the density matrix

$$\omega_\xi = \frac{\Gamma(\mathrm{e}^{k(\xi)})}{\mathrm{tr}_{\Gamma(\mathbb{C}^n)}(\Gamma(\mathrm{e}^{k(\xi)}))},$$

on $\Gamma(\mathbb{C}^n)$. Clearly, ω_ξ defines a state on $\Gamma(\mathbb{C}^n)$ which is quasi-free with density $T(\xi)$. By Part (3) of Proposition 6.6, the Rényi relative entropy of the state $\Gamma(s(\xi))\omega_\xi\Gamma(s(\xi))^*$ w.r.t. ω_ξ is given by

$$\begin{aligned}
S_\alpha(\Gamma(s(\xi))\omega_\xi\Gamma(s(\xi))^*|\omega_\xi) &= \log \mathrm{tr}\left(\omega_\xi^{1-\alpha}\Gamma(s(\xi))\omega_\xi^\alpha\Gamma(s(\xi))^*\right) \\
&= \log \omega_\xi\left(\Gamma(\mathrm{e}^{-\alpha k(\xi)}s(\xi)\mathrm{e}^{\alpha k(\xi)}s^*(\xi))\right) \\
&= \log\det\left(\mathbb{1} + T(\xi)(\mathrm{e}^{-\alpha k(\xi)}s(\xi)\mathrm{e}^{\alpha k(\xi)}s^*(\xi) - \mathbb{1})\right).
\end{aligned}$$

Thus, we can rewrite Formula (6.19) as

$$e_{2,+}(\alpha) = \int_0^\pi S_\alpha(\Gamma(s(\xi))\omega_\xi\Gamma(s(\xi))^*|\omega_\xi)\frac{\mathrm{d}\varepsilon(\xi)}{2\pi}.$$

Using the second identity in (2.19), we deduce

$$\left.\frac{\mathrm{d}}{\mathrm{d}\alpha}e_{2,+}(\alpha)\right|_{\alpha=1} = -\int_0^\pi S(\Gamma(s(\xi))\omega_\xi\Gamma(s(\xi))^*|\omega_\xi)\frac{\mathrm{d}\varepsilon(\xi)}{2\pi}.$$

Since $\log\omega_\xi = \mathrm{d}\Gamma(k(\xi)) - \log\det(\mathbb{1} + \mathrm{e}^{k(\xi)})$, Relation (6.6) and Part (4) of Proposition 6.6 yield

$$\begin{aligned}
S(\Gamma(s(\xi))\omega_\xi\Gamma(s(\xi))^*|\omega_\xi) &= \mathrm{tr}\left[\Gamma(s(\xi))\omega_\xi\Gamma(s(\xi))^*\left(\log\omega_\xi - \Gamma(s(\xi))\log\omega_\xi\Gamma(s(\xi))^*\right)\right] \\
&= \mathrm{tr}\left[\omega_\xi(\Gamma(s(\xi))^*\log\omega_\xi\Gamma(s(\xi)) - \log\omega_\xi)\right] \\
&= \omega_\xi\left(\mathrm{d}\Gamma(s^*(\xi)k(\xi)s(\xi) - k(\xi))\right) \\
&= \mathrm{tr}\left(T(\xi)(s^*(\xi)k(\xi)s(\xi) - k(\xi))\right).
\end{aligned}$$

Hence, it follows from (6.18)and (6.17) that

$$\begin{aligned}
\int_0^\pi S(\Gamma(s(\xi))\omega_\xi\Gamma(s(\xi))^*|\omega_\xi)\frac{\mathrm{d}\varepsilon(\xi)}{2\pi} &= -\int_0^\pi \mathrm{tr}\left(T(\xi)\mathcal{T}(\xi,\xi)\right)\mathrm{d}\xi \\
&= -\mathrm{tr}(T_0\mathcal{T}) \\
&= -\mathrm{tr}(T_0 w_-^*\mathrm{i}[h_\lambda, k_0]w_-) \\
&= -\mathrm{tr}(T_+\mathrm{i}[h_\lambda, k_0]).
\end{aligned}$$

Finally, (6.14) allows us to write

$$-\mathrm{tr}\left(T_+\mathrm{i}[h_\lambda, k_0]\right) = \omega_+\left(\mathrm{d}\Gamma(-\mathrm{i}[h_\lambda, k_0])\right) = \omega_+(\sigma).$$

Thus, we have shown that

$$\left.\frac{\mathrm{d}}{\mathrm{d}\alpha}e_{2,+}(\alpha)\right|_{\alpha=1} = \omega_+(\sigma) = -\int_0^\pi S(\Gamma(s(\xi))\omega_\xi\Gamma(s(\xi))^*|\omega_\xi)\frac{\mathrm{d}\varepsilon(\xi)}{2\pi}.$$

Invoking Part (1) of Proposition 2.17 we observe that if $\omega_+(\sigma) = 0$ then we must have

$$S(\Gamma(s(\xi))\omega_\xi\Gamma(s(\xi))^*|\omega_\xi) = 0,$$

for almost all $\xi \in [0, \pi]$ which in turn implies that $\Gamma(s(\xi))\omega_\xi\Gamma(s(\xi))^* = \omega_\xi$, *i.e.*, that $[k(\xi), s(\xi)] = 0$ for almost all $\xi \in [0, \pi]$. The last condition can be written as

$$[(\beta_k - \beta_j)\varepsilon(\xi) - (\beta_k\mu_k - \beta_j\mu_j)]\, s_{jk}(\xi) = 0,$$

for all $j, k \in \{1, \ldots, n\}$, and we conclude that if there exists $j, k \in \{1, \ldots, n\}$ and a set $\Omega \subset [0, \pi]$ of positive Lebesgue measure such that $j \neq k$, $s_{jk}(\xi) \neq 0$ for $\xi \in \Omega$ and $(\beta_j, \mu_j) \neq (\beta_k, \mu_k)$, then $\omega_+(\sigma) > 0$. In more physical terms, if there is an open scattering channel between two leads $\mathcal{R}_j$ and $\mathcal{R}_k$ which are not in mutual thermal equilibrium, then entropy production in the NESS is strictly positive.

Note that since (6.14) implies

$$\omega_+(\sigma) = -\sum_{j=1}^{n} \beta_j \left(\omega_+(\Phi_j) - \mu_j \omega_+(\mathcal{J}_j)\right),$$

the expected currents $\omega_+(\Phi_j)$, $\omega_+(\mathcal{J}_j)$ can not all vanish if entropy production is strictly positive.

Exercise 6.12. Deduce from Relation (6.15) that

$$-\lim_{t\to\infty} \frac{1}{t} S(\omega_t|\omega_0) = \omega_+(\sigma).$$

Thus, if $\omega_+(\sigma) > 0$ then the entropy of ω_t w.r.t. ω_0 diverges as $t \to \infty$.

Exercise 6.13. Derive the Landauer-Büttiker formulas for the expected energy and charge currents in the steady state ω_+,

$$\omega_+(\Phi_j) = \sum_{k=1}^{n} \int_0^{\pi} t_{jk}(\xi)(\varrho_j(\xi) - \varrho_k(\xi))\varepsilon(\xi) \frac{\mathrm{d}\varepsilon(\xi)}{2\pi},$$
$$\omega_+(\mathcal{J}_j) = \sum_{k=1}^{n} \int_0^{\pi} t_{jk}(\xi)(\varrho_j(\xi) - \varrho_k(\xi)) \frac{\mathrm{d}\varepsilon(\xi)}{2\pi},$$

where $\varrho_j(\xi) = (1 + \mathrm{e}^{\beta_j(\varepsilon(\xi)-\mu_j)})^{-1}$ is the Fermi-Dirac density of the j-th reservoir and

$$t_{jk}(\xi) = |s_{jk}(\xi) - \delta_{jk}|^2.$$

Hint: start with $\omega_+(\Phi_j) = -\mathrm{tr}\,(T_+ \mathrm{i}[h_\lambda, h_j]) = -\mathrm{tr}\,(T_0 \mathcal{T}_j)$ where $\mathcal{T}_j = w_-^* \mathrm{i}[h_\lambda, h_j] w_-$, and deduce from (6.18) that the diagonal part of the integral kernel of $\mathcal{T}_j$ is given by

$$\mathcal{T}_j(\xi, \xi) = \frac{\varepsilon'(\xi)}{2\pi} \varepsilon(\xi) \left(s^*(\xi) 1_j s(\xi) - 1_j\right).$$

Proceed in a similar way for the charge currents. (For more information on the Landauer-Büttiker formalism, see [Da, Im]. More general mathematical derivations can be found in [AJPP2, Ne, BS].

Exercise 6.14. Starting with the Landauer-Büttiker formulas develop the linear response theory of the EBB model.

Exercise 6.15. Consider the full counting statistics of charge transport in the framework of Section 3.8. Let $\mathbb{P}_t^c(\mathbf{q})$, $\mathbf{q} = (q_1, \ldots, q_n)$, denote the probability for the results, $\mathbf{n}$ and $\mathbf{n}'$, of two successive joint measurements of $\mathbf{N} = (N_1, \ldots, N_n)$, at time 0 and t, to be such that $\mathbf{n}' - \mathbf{n} = t\mathbf{q}$. Loosely speaking, $\mathbb{P}_t^c(q_1, \ldots, q_n)$ is the probability for the charge (number of fermions) of the reservoir $\mathcal{R}_j$ to increase by tq_j $(j = 1, \ldots, n)$ during the time interval $[0, t]$. Denote by

$$\chi_t(\boldsymbol{\nu}) = \sum_{\mathbf{q}} \mathbb{P}_t^c(\mathbf{q}) \mathrm{e}^{-t\boldsymbol{\nu}\cdot\mathbf{q}},$$

the Laplace transform of this distribution (that is, the moment generating function of $\mathbb{P}_t^c$).

1. Show that the logarithm of $\chi_t(\boldsymbol{\nu})$ is related to the functional $e_{2,t}(\boldsymbol{\alpha})$ of Exercise 6.7 by

$$\log \chi_t(\boldsymbol{\nu}) = e_{2,t}(\mathbf{1} - \boldsymbol{\alpha}),$$

provided $\boldsymbol{\nu} = (\nu_1, \dots, \nu_n)$ is related to $\boldsymbol{\alpha} = (\alpha_{\mathcal{S}}, \alpha_1, \dots, \alpha_{2n})$ according to

$$\alpha_j = \alpha_{\mathcal{S}} = 0, \quad \nu_j = -\alpha_{n+j}\beta_j\mu_j, \qquad (j = 1, \dots, n).$$

2. Show that in the thermodynamic limit

$$\chi_t(\boldsymbol{\nu}) = \det\left(\mathbb{1} + T_0(\mathrm{e}^{q_t(\boldsymbol{\nu})}\mathrm{e}^{-q(\boldsymbol{\nu})} - \mathbb{1})\right),$$

where

$$q(\boldsymbol{\nu}) = \sum_{j=1}^{n} \nu_j \mathbb{1}_j,$$

and $q_t(\boldsymbol{\nu}) = \mathrm{e}^{-\mathrm{i}th_\lambda} q(\boldsymbol{\nu}) \mathrm{e}^{\mathrm{i}th_\lambda}$.
Hint: combine Part 1 with the result of Exercise 6.7.

3. Derive the Levitov-Lesovik formula

$$\lim_{t\to\infty} \frac{1}{t} \log \chi_t(\boldsymbol{\nu}) = \int_0^\pi \log\det\left(\mathbb{1} + T(\xi)(s^*(\xi)s^{\boldsymbol{\nu}}(\xi) - \mathbb{1})\right) \frac{\mathrm{d}\varepsilon(\xi)}{2\pi},$$

where the matrix $s^{\boldsymbol{\nu}}(\xi) = [s^{\boldsymbol{\nu}}_{jk}(\xi)]$ is defined by

$$s^{\boldsymbol{\nu}}_{jk}(\xi) = s_{jk}(\xi)\mathrm{e}^{\nu_k - \nu_j}.$$

(See [LL], where the Fourier transform of the probability distribution $\mathbb{P}_t^c$ is considered instead of its Laplace transform. See also [ABGK].)

Exercise 6.16. Consider EBB model with two reservoirs. Prove that the following statements are equivalent.

1. $e_{p,+}(\alpha)$ does not depend on p.
2. $s_{11}(\xi) = s_{22}(\xi) = 0$ for Lebesgue a.e. $\xi \in [0, \pi]$.
3. The fluctuation relation $e_{\mathrm{naive},+}(\alpha) = e_{\mathrm{naive},+}(1 - \alpha)$ holds.
4. $e_{\mathrm{naive},+}(\alpha) = e_{\infty,+}(\alpha)$.

Exercise 6.17. Consider the following variant of the EBB model. $\mathcal{S}$ is a box $\Lambda = [-l, l]$ in $\mathbb{Z}$ and $h_{\mathcal{S}} = -\frac{1}{2}\Delta_\Lambda$ is the discrete Laplacian on Λ with Dirichlet boundary condition. The box $\mathcal{S}$ is connected to the left and right lead which, before the thermodynamical limit is taken, are described by the boxes $\Lambda_L =]-M, -l-1]$, $\Lambda_R = [l+1, M[$, where $l \ll M$, and after the thermodynamic limit is taken, by the boxes $\Lambda_L =]-\infty, -l-1]$, $\Lambda_R = [l+1, \infty[$. The one particle Hamiltonians are $h_L = -\frac{1}{2}\Delta_{\Lambda_L}$, $h_R = -\frac{1}{2}\Delta_{\Lambda_R}$, where, as usual, Δ_{Λ_L} and Δ_{Λ_R} are the discrete Laplacians on Λ_L and Λ_R with Dirichlet boundary condition. The corresponding EBB model is a free Fermi gas with single particle Hilbert space

$$\ell^2(\Lambda_L) \oplus \ell^2(\Lambda) \oplus \ell^2(\Lambda_R) = \ell^2(\Lambda_L \cup \Lambda \cup \Lambda_R).$$

In the absence of coupling its Hamiltonian is $H_0 = \mathrm{d}\Gamma(h_0)$, where $h_0 = h_L \oplus h_\mathcal{S} \oplus h_R$. The Hamiltonian of the joint system is $H = \mathrm{d}\Gamma(h)$, where $h = -\frac{1}{2}\Delta_{\Lambda_L \cup \Lambda \cup \Lambda_R}$ and $\Delta_{\Lambda_L \cup \Lambda \cup \Lambda_R}$ is the discrete Laplacian on $\Lambda_L \cup \Lambda \cup \Lambda_R$ with Dirichlet boundary condition. The reference state of the system is a quasi free state with density

$$T_0 = T_L \oplus T_\mathcal{S} \oplus T_R,$$

where $T_\mathcal{S} > 0$ is a density operator on $\ell^2(\Lambda)$ that commutes with $h_\mathcal{S}$ and

$$T_L = (\mathbb{1} + \mathrm{e}^{\beta_L(h_L - \mu_L \mathbb{1})})^{-1}, \qquad T_R = (\mathbb{1} + \mathrm{e}^{\beta_R(h_R - \mu_R \mathbb{1})})^{-1},$$

are the Fermi-Dirac densities of the left and right reservoir.

1. Discuss in detail the thermodynamic limit $M \to \infty$ and compare the model with the classical harmonic chain discussed in Section 1.

The remaining parts of this exercise concern the infinitely extended model.

2. Using the discrete Fourier transform

$$\ell^2(\Lambda_L) \oplus \ell^2(\Lambda_R) \ni \psi_L \oplus \psi_R \mapsto \widehat{\psi}_L \oplus \widehat{\psi}_R \in L^2([0,\pi], \mathrm{d}\xi) \oplus L^2([0,\pi], \mathrm{d}\xi),$$

$$\widehat{\psi}_L(\xi) = \sqrt{\frac{2}{\pi}} \sum_{x \in \Lambda_L} \psi_L(x) \sin(\xi(x-1)), \qquad \widehat{\psi}_R(\xi) = \sqrt{\frac{2}{\pi}} \sum_{x \in \Lambda_R} \psi_R(x) \sin(\xi(x+1)),$$

identify $h_L \oplus h_R$ with the operator of multiplication by $(1-\cos\xi) \oplus (1-\cos\xi)$ on $L^2([0,\pi], \mathrm{d}\xi) \oplus L^2([0,\pi], \mathrm{d}\xi)$. The wave operators

$$w_\pm = \mathrm{s} - \lim_{t \to \pm\infty} \mathrm{e}^{ith} \mathrm{e}^{-ith_0} \mathbb{1}_\mathcal{R},$$

exist and are complete ($\mathbb{1}_\mathcal{R}$ is the orthogonal projection onto $\ell^2(\Lambda_L) \oplus \ell^2(\Lambda_R)$). The scattering matrix

$$s = w_+^* w_- : \ell^2(\Lambda_L) \oplus \ell^2(\Lambda_R) \to \ell^2(\Lambda_L) \oplus \ell^2(\Lambda_R),$$

is a unitary operator commuting with $h_L \oplus h_R$. Following computations in Section 1.9 verify that in the Fourier representation s acts as the operator of multiplication by the unitary matrix

$$s(\xi) = \mathrm{e}^{2il\xi} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

3. Show that for $p \in [1, \infty]$,

$$e_{p,+}(\alpha) = \frac{1}{2\pi} \int_0^2 \log\left(1 - \frac{\sinh \frac{\alpha(\beta_R(\varepsilon-\mu_R) - \beta_L(\varepsilon-\mu_L))}{2} \sinh \frac{(1-\alpha)(\beta_R(\varepsilon-\mu_R) - \beta_L(\varepsilon-\mu_L))}{2}}{\cosh \frac{\beta_L(\varepsilon-\mu_L)}{2} \cosh \frac{\beta_R(\varepsilon-\mu_R)}{2}}\right) \mathrm{d}\varepsilon. \tag{6.20}$$

Note that, in accordance with Exercise 6.16, $e_{p,+}(\alpha)$ does not depend on p. The function (6.20) can be expressed in terms of Euler dilogarithm, see the end of Section 6.7.3.

4. Verify directly that $e_{\mathrm{naive},+}(\alpha) = e_{p,+}(\alpha)$.

5. (Recall Exercise 6.11). Show that

$$e_{2,+}(\boldsymbol{\alpha}) = \frac{1}{2\pi} \int_0^2 \log\left(1 + \mathcal{D}(\varepsilon)\right) \mathrm{d}\varepsilon, \tag{6.21}$$

where

$$\mathcal{D}(\varepsilon) = \frac{\sinh \frac{\beta_L(\alpha_1\varepsilon - \alpha_3\mu_L) - \beta_R(\alpha_2\varepsilon - \alpha_4\mu_L)}{2} \sinh \frac{\beta_R((1-\alpha_2)\varepsilon - (1-\alpha_4)\mu_R) - \beta_L((1-\alpha_1)\varepsilon - (1-\alpha_3)\mu_L)}{2}}{\cosh \frac{\beta_L(\varepsilon-\mu_L)}{2} \cosh \frac{\beta_R(\varepsilon-\mu_R)}{2}}.$$

6. Using (6.21) show that the steady state charge and heat fluxes out of the left reservoir are

$$\omega_+(\mathcal{J}_L) = \frac{1}{2\pi}\int_0^2 \left[\frac{1}{1+\mathrm{e}^{\beta_L(\varepsilon-\mu_L)}} - \frac{1}{1+\mathrm{e}^{\beta_R(\varepsilon-\mu_R)}}\right]\mathrm{d}\varepsilon,$$

$$\omega_+(\Phi_L) = \frac{1}{2\pi}\int_0^2 \varepsilon\left[\frac{1}{1+\mathrm{e}^{\beta_L(\varepsilon-\mu_L)}} - \frac{1}{1+\mathrm{e}^{\beta_R(\varepsilon-\mu_R)}}\right]\mathrm{d}\varepsilon,$$

and that $\omega_+(\mathcal{J}_R) = -\omega_+(\mathcal{J}_L)$, $\omega_+(\Phi_R) = -\omega_+(\Phi_L)$.

Exercise 6.18. This exercise is intended for technically advanced reader. Consider an infinitely extended EBB model with two reservoirs except that now we keep the single particle Hilbert spaces $\mathcal{K}_j$ and Hamiltonians h_j general. The coupling is defined in the same way as previously except that now $\delta_0^{(j)}$ is just a given vector in $\mathcal{K}_j$. We absorb λ in $\delta_0^{(j)}$ and denote by h the single particle Hamiltonian of the joint system. We shall suppose that the spectral measure ν_j for h_j and $\delta_0^{(j)}$ is purely absolutely continuous and denote by $\mathrm{d}\nu_j(\varepsilon)/\mathrm{d}\varepsilon$ its Radon-Nikodym derivative w.r.t. the Lebesgue measure. We also suppose that h has purely absolutely continuous spectrum. Since h preserves the cyclic subspace spanned by $\{\mathcal{K}_\mathcal{S}, \delta_0^{(1)}, \delta_0^{(2)}\}$ and h_0, without loss of generality we may assume that $\mathcal{K}_j = L^2(\mathbb{R}, \mathrm{d}\nu_j)$ and that h_j is the operator of multiplication by ε.

1. Show that the scattering matrix is given by

$$s(\varepsilon) = \mathbb{1} + 2\mathrm{i}\pi\left[\begin{array}{cc} \langle\chi_1|(h-\varepsilon+\mathrm{i}0)^{-1}\chi_1\rangle\frac{\mathrm{d}\nu_1(\varepsilon)}{\mathrm{d}\varepsilon} & \langle\chi_1|(h-\varepsilon+\mathrm{i}0)^{-1}\chi_2\rangle\sqrt{\frac{\mathrm{d}\nu_1(\varepsilon)}{\mathrm{d}\varepsilon}\frac{\mathrm{d}\nu_2(\varepsilon)}{\mathrm{d}\varepsilon}} \\ \langle\chi_2|(h-\varepsilon+\mathrm{i}0)^{-1}\chi_1\rangle\sqrt{\frac{\mathrm{d}\nu_1(\varepsilon)}{\mathrm{d}\varepsilon}\frac{\mathrm{d}\nu_2(\varepsilon)}{\mathrm{d}\varepsilon}} & \langle\chi_2|(h-\varepsilon+\mathrm{i}0)^{-1}\chi_2\rangle\frac{\mathrm{d}\nu_2(\varepsilon)}{\mathrm{d}\varepsilon} \end{array}\right].$$

2. Compute $e_{p,+}(\alpha)$ for $p\in[1,\infty]$.

3. Verify that Exercise 6.16 applies to this more general model. Classify the examples for which $e_{p,+}(\alpha)$ does not depend on p.

4. Compute $e_{\mathrm{naive},+}(\alpha)$.

5. Compute $e_{2,+}(\boldsymbol{\alpha})$ and derive the formulas for the steady state charge and heat fluxes.

6. Verify the results by comparing them with Exercise 6.17.

Remark. For more information about the Exercises 6.16, 6.17, and 6.18 we refer the reader to [BJP].

6.6.7 Local interactions

One can easily modify the EBB model to allow for interactions between fermions in the device $\mathcal{S}$. For example, let q be a pair interaction on $\mathcal{S}$, *i.e.*, a self-adjoint operator on $\Gamma_2(\mathcal{K})$ acting like

$$(q\psi)(x_1,x_2) = \begin{cases} q(x_1,x_2)\psi(x_1,x_2) & \text{if } x_1,x_2\in\mathcal{S}, \\ 0 & \text{otherwise.}\end{cases}$$

Then the operator

$$Q = \frac{1}{2}\sum_{x,y\in\mathcal{S}} q(x,y)a^*(\delta_x)a^*(\delta_y)a(\delta_y)a(\delta_x),$$

is self-adjoint on $\Gamma(\mathcal{K})$ and leaves all the $\Gamma_k(\mathcal{K})$ invariant. It vanishes on $\Gamma_0(\mathcal{K})$ and $\Gamma_1(\mathcal{K})$ and acts like

$$(Q\psi)(x_1,\ldots,x_k)=\left(\frac{1}{2}\sum_{\substack{x,y\in\{x_1,\ldots,x_k\}\cap\mathcal{S}\\ x\neq y}}q(x,y)\right)\psi(x_1,\ldots,x_k),$$

on $\Gamma_k(\mathcal{K})$ for $k\geq 2$. For $\kappa\in\mathbb{R}$, the Hamiltonian

$$H_{\lambda,\kappa}=H_\lambda+\kappa Q,$$

is self-adjoint on $\Gamma(\mathcal{K})$ and defines a dynamics $\tau^t_{\lambda,\kappa}$ on the CAR algebra over $\mathcal{K}$. It is easy to perform the thermodynamic limit of this locally interacting EBB model, the interaction term Q being confined to the finite sample $\mathcal{S}$. The large time limit is a more delicate problem. Hilbert space scattering techniques are no more adapted to this problem and one has to deal with the much harder C^*-scattering theory, *e.g.*, the existence of the limit

$$\gamma_\pm(A)=\lim_{t\to\pm\infty}\tau_\lambda^{-t}\circ\tau^t_{\lambda,\kappa}(A).$$

Such problems first appeared in the works of Hepp [He] and Robinson [Ro]. In the specific context of non-equilibrium statistical mechanics, the scattering approach was advocated by Ruelle [Ru1] (see also [Ru2, Ru3]). A systematic approach to the scattering problem for local perturbations of free Fermi gases has been developed by Botvich and Malyshev [BM], Aizenstadt and Malyshev [AMa] and Malyshev [Ma]. It relies on the well known Cook argument and a uniform (in t) control of the Dyson expansion

$$\begin{aligned}\tau^t_{\lambda,\kappa}(A)&=\tau^t_\lambda(A)\\ &+\sum_{k\geq1}(\mathrm{i}\kappa)^k\int_{0\leq s_k\leq\cdots\leq s_1\leq t}[\tau_\lambda^{s_k}(Q),[\cdots[\tau_\lambda^{s_1}(Q),\tau^t_\lambda(A)]\cdots]]\mathrm{d}s_1\cdots\mathrm{d}s_k.\end{aligned}$$

Optimal bounds for the uniform convergence of such expansions have been obtained by Maassen and Botvich [MB]. The interested reader should consult [FMU, JOP2, JPP] and references therein.

6.7 The XY-spin chain

In this section, we describe a simple example of extended quantum spin system on a 1D-lattice. We shall follow closely the approach of Chapter 1, starting from the standard quantum mechanical description of a finite sub-lattice.

6.7.1 Finite spin systems

Let Λ be a finite set. A spin $\frac{1}{2}$ system on Λ is a finite quantum system obtained by attaching to each site $x\in\Lambda$ a spin $\frac{1}{2}$. Thus, the Hilbert space of such a spin system is given by

$$\mathcal{H}_\Lambda=\bigotimes_{x\in\Lambda}\mathcal{H}_x,$$

where each $\mathcal{H}_x$ is a copy of $\mathbb{C}^2$. The corresponding $*$-algebra is

$$\mathcal{O}_\Lambda=\bigotimes_{x\in\Lambda}\mathcal{O}_x,$$

where $\mathcal{O}_x=\mathrm{M}_2(\mathbb{C})$ is the algebra of 2×2 complex matrices. Together with the identity $\mathbb{1}_x\in\mathcal{O}_x$, the Pauli matrices

$$\sigma_x^{(1)}=\begin{bmatrix}0&1\\1&0\end{bmatrix},\quad\sigma_x^{(2)}=\begin{bmatrix}0&-\mathrm{i}\\\mathrm{i}&0\end{bmatrix},\quad\sigma_x^{(3)}=\begin{bmatrix}1&0\\0&-1\end{bmatrix},$$

form a basis of $\mathcal{O}_x$ satisfying the well known relations

$$\sigma_x^{(j)}\sigma_x^{(k)} = \delta_{jk}\mathbb{1}_x + \mathrm{i}\varepsilon^{jkl}\sigma_x^{(l)}.$$

For $D \subset \Lambda$ we set $\mathbb{1}_D = \otimes_{x\in D}\mathbb{1}_x$. We shall identify $T_x \in \mathcal{O}_x$ with the element $T_x \otimes \mathbb{1}_{\Lambda\setminus\{x\}}$ of $\mathcal{O}_\Lambda$. With this convention, one has the relations

$$\sigma_x^{(j)}\sigma_x^{(k)} = \delta_{jk}\mathbb{1}_\Lambda + \mathrm{i}\varepsilon^{jkl}\sigma_x^{(l)}, \qquad [\sigma_x^{(j)}, \sigma_y^{(k)}] = 2\mathrm{i}\delta_{xy}\varepsilon^{jkl}\sigma_x^{(l)}. \tag{6.22}$$

Moreover, any element of $\mathcal{O}_\Lambda$ can be written as a finite sum

$$\sum_a \prod_{x\in\Lambda} T_x^{(a)},$$

with $T_x^{(a)} \in \{\mathbb{1}_\Lambda, \sigma_x^{(1)}, \sigma_x^{(2)}, \sigma_x^{(3)}\}$. Since $\mathbb{1}_\Lambda = \sigma_x^{(j)2}$, it follows that the smallest $*$-subalgebra of $\mathcal{O}_\Lambda$ containing the set $\mathfrak{S}_\Lambda = \{\sigma_x^{(j)} \,|\, x \in \Lambda, j = 1,2,3\}$ is $\mathcal{O}_\Lambda$. By von Neumann's bicommutant theorem (Theorem 6.5), we conclude that $\mathfrak{S}_\Lambda'' = \mathcal{O}_\Lambda$ and hence $\mathfrak{S}_\Lambda' = \mathbb{C}\mathbb{1}_\Lambda$.

The dynamics of a spin chain is completely determined by its Hamiltonian H_Λ, a self-adjoint element of $\mathcal{O}_\Lambda$. The equilibrium state of the system at inverse temperature β is given by the density matrix

$$\omega_{\beta\Lambda} = \frac{\mathrm{e}^{-\beta H_\Lambda}}{\mathrm{tr}\,(\mathrm{e}^{-\beta H_\Lambda})}.$$

The particular example we shall consider in the remaining part of this section is the XY-chain on the finite 1D-lattice $\Lambda = [A, B] \subset \mathbb{Z}$. It is defined by the XY-Hamiltonian

$$H_\Lambda = -\frac{1}{4}\sum_{x\in[A,B[} J\left(\sigma_x^{(1)}\sigma_{x+1}^{(1)} + \sigma_x^{(2)}\sigma_{x+1}^{(2)}\right) - \frac{1}{2}\sum_{x\in[A,B]}\lambda\sigma_x^{(3)}, \tag{6.23}$$

where $J \in \mathbb{R}$ is the nearest-neighbor coupling constant and $\lambda \in \mathbb{R}$ is the strength of an external magnetic field in direction (3)[1]. The case $J > 0$ corresponds to a ferromagnetic coupling while $J < 0$ describes an anti-ferromagnetic system.

6.7.2 The Jordan-Wigner representation

The natural "spin" interpretation of the $*$-algebra $\mathcal{O}_\Lambda$ described in the previous section is not very convenient for computational purposes. In this section, following Jordan and Wigner [JW], we shall see that $\mathcal{O}_\Lambda$ also carries an irreducible representation of a CAR algebra. Moreover, it turns out that the XY Hamiltonian (6.23) takes a particularly simple form in this representation. In fact, we shall see that the XY-spin chain can be mapped to a free Fermi gas.

Let $\sigma_x^{(\pm)} = (\sigma_x^{(1)} \pm \mathrm{i}\sigma_x^{(2)})/2$ denote the spin raising/lowering operators at $x \in \Lambda$. Note that $\sigma_x^{(-)}$ and $\sigma_x^{(+)} = \sigma_x^{(-)*}$ satisfy the anti-commutation relations

$$\{\sigma_x^{(+)}, \sigma_x^{(+)}\} = \{\sigma_x^{(-)}, \sigma_x^{(-)}\} = 0 \qquad \{\sigma_x^{(+)}, \sigma_x^{(-)}\} = \mathbb{1}_{\mathcal{H}_\Lambda}.$$

Thus, if Λ reduces to the singleton $\{x\}$, then the maps $\alpha \mapsto \alpha\sigma_x^{(+)}$ and $\alpha \mapsto \overline{\alpha}\sigma_x^{(-)}$ define a representation of the CAR over the Hilbert space $\mathbb{C} = \ell^2(\{x\})$ (and one easily checks that this representation is irreducible). This does not directly generalize to larger Λ. Indeed, if Λ contains two distinct sites $x \neq y$ one has

$$[\sigma_x^{(+)}, \sigma_y^{(+)}] = [\sigma_x^{(-)}, \sigma_y^{(-)}] = 0 \qquad [\sigma_x^{(+)}, \sigma_y^{(-)}] = 0,$$

i.e., operators at distinct sites commute whereas they should anti-commute to define a representation of the CAR over $\ell^2(\Lambda)$.

[1]The name XY comes from the coupling between components $(1) = (X)$ and $(2) = (Y)$ of the spins.

To transform commutation at distinct sites into anti-commutation, we make the following observation: for $T_x \in \mathcal{O}_x$ and $S_y \in \mathcal{O}_y$ one has

$$\{\sigma_A^{(3)} \cdots \sigma_{x-1}^{(3)} T_x, \sigma_A^{(3)} \cdots \sigma_{y-1}^{(3)} S_y\} = \begin{cases} \{\sigma_x^{(3)}, T_x\}\sigma_{x+1}^{(3)} \cdots \sigma_{y-1}^{(3)} S_y & \text{for } x < y, \\ \{T_x, S_x\} & \text{for } x = y, \\ \{\sigma_y^{(3)}, S_y\}\sigma_{y+1}^{(3)} \cdots \sigma_{x-1}^{(3)} T_x & \text{for } x > y. \end{cases}$$

Since $\{\sigma_x^{(3)}, \sigma_x^{(\pm)}\} = 0$, it follows that the Jordan-Wigner operators

$$b_x = \sigma_A^{(3)} \cdots \sigma_{x-1}^{(3)} \sigma_x^{(-)}, \qquad b_x^* = \sigma_A^{(3)} \cdots \sigma_{x-1}^{(3)} \sigma_x^{(+)}, \tag{6.24}$$

satisfy

$$\{b_x, b_y\} = \{b_x^*, b_y^*\} = 0, \qquad \{b_x, b_y^*\} = \delta_{xy} \mathbb{1}_\Lambda.$$

Hence, the maps $\ell^2(\Lambda) \ni \alpha \mapsto b^*(\alpha) = \sum_x \alpha_x b_x^*$ and $\ell^2(\Lambda) \ni \alpha \mapsto b(\alpha) = \sum_x \overline{\alpha}_x b_x$ define a representation of the CAR over $\ell^2(\Lambda)$ on the Hilbert space $\mathcal{H}_\Lambda$. We shall call it the Jordan-Wigner representation.

One easily inverts Relations (6.24) to express the spin operators in terms of the Jordan-Wigner operators:

$$\sigma_x^{(1)} = V_x(b_x + b_x^*), \qquad \sigma_x^{(2)} = \mathrm{i} V_x(b_x - b_x^*), \qquad \sigma_x^{(3)} = 2b_x^* b_x - \mathbb{1}_\Lambda, \tag{6.25}$$

where

$$V_x = \begin{cases} \mathbb{1}_\Lambda & \text{if } x = A, \\ \prod_{y \in [A,x[} (2b_y^* b_y - 1) & \text{otherwise.} \end{cases}$$

If follows in particular that $\mathfrak{B}_\Lambda = \{b_x^\# \,|\, x \in \Lambda\}$ satisfies $\mathfrak{B}_\Lambda' = \mathfrak{S}_\Lambda' = \mathbb{C}\mathbb{1}_\Lambda$. Hence, the Jordan-Wigner representation is irreducible. By Proposition 6.3, there exists a unitary operator $U : \Gamma(\ell^2(\Lambda)) \to \mathcal{H}_\Lambda$ such that $b^\#(\alpha) = U a^\#(\alpha) U^*$, where the $a^\#$ are the usual creation/annihilation operators on the fermionic Fock space $\Gamma(\ell^2(\Lambda))$.

A simple calculation shows that

$$\sigma_x^{(1)} \sigma_{x+1}^{(1)} + \sigma_x^{(2)} \sigma_{x+1}^{(2)} = -2(b_{x+1}^* b_x + b_x^* b_{x+1}),$$

so that we can rewrite the XY-Hamiltonian as

$$H_\Lambda = \frac{J}{2} \sum_{x \in [A,B[} (b_{x+1}^* b_x + b_x^* b_{x+1}) - \frac{\lambda}{2} \sum_{x \in [A,B]} (2b_x^* b_x - \mathbb{1}).$$

By Part (8) of Proposition 6.2 we thus have $H_\Lambda = U \mathrm{d}\Gamma(h_\Lambda) U^*$, up to an irrelevant additive constant, where the one-particle Hamiltonian h_Λ is the self-adjoint operator on $\ell^2(\Lambda)$ given by

$$h_\Lambda = \frac{J}{2} \sum_{x \in [A,B[} (|\delta_{x+1}\rangle\langle\delta_x| + |\delta_x\rangle\langle\delta_{x+1}|) - \lambda \sum_{x \in [A,B]} |\delta_x\rangle\langle\delta_x| = \frac{J}{2} \Delta_\Lambda + (J - \lambda)\mathbb{1},$$

Δ_Λ being the discrete Laplacian on Λ with Dirichlet boundary conditions (1.1). Thus, the unitary map U provides an equivalence between the XY-chain on Λ and the free Fermi gas with one particle Hamiltonian h_Λ. In particular, it maps the equilibrium state $\omega_{\beta\Lambda}$ to the quasi-free state on the CAR algebra over $\ell^2(\Lambda)$ with density

$$T_{\beta\Lambda} = (\mathbb{1} + \mathrm{e}^{\beta h_\Lambda})^{-1}.$$

Exercise 6.19.

1. Use the Jordan-Wigner representation of the XY-chain to show that, for all $x \in \Lambda$,

$$\omega_{\beta\Lambda}(\sigma_x^{(1)}) = \omega_{\beta\Lambda}(\sigma_x^{(2)}) = 0, \qquad \frac{1}{2}\omega_{\beta\Lambda}(\mathbb{1}_\Lambda + \sigma_x^{(3)}) = \frac{2}{|\Lambda|} \sum_{\xi \in \Lambda^*} \frac{\sin^2(\xi(x - A + 1))}{1 + \mathrm{e}^{\beta(J\cos\xi - \lambda)}},$$

where $\Lambda^* = \{n\pi/(|\Lambda|+1) \,|\, n = 1, \dots, |\Lambda|\}$, $|\Lambda| = B - A + 1$.

2. Show that the mean magnetization per spin is given by

$$m_\Lambda(\beta, J, \lambda) = \frac{1}{|\Lambda|} \sum_{x \in \Lambda} \omega_{\beta\Lambda}(\sigma_x^{(3)}) = \frac{1}{|\Lambda|} \sum_{\xi \in \Lambda^*} \tanh(\beta(\lambda - J\cos\xi)/2).$$

3. Show that, in the thermodynamic limit,

$$\lim_{\Lambda \to \mathbb{Z}} m_\Lambda(\beta, J, \lambda) = \frac{2\sinh(\beta\lambda/2)}{\pi} \int_0^\pi \frac{\mathrm{d}\xi}{\cosh(\beta\lambda/2) + \cosh(\beta(J\cos\xi - \lambda/2))}.$$

Hint: use the discrete Fourier transform to diagonalize the Laplacian Δ_Λ.

6.7.3 The open XY-chain

To construct a model of open XY-chain we shall consider the same geometry as in the classical harmonic chain of Chapter 1: a finite system $\mathcal{C}$, consisting of the XY-chain on $\Lambda = [-N, N]$, is coupled at its left and right ends to two reservoirs $\mathcal{R}_L$ and $\mathcal{R}_R$ which are themselves XY-chains on $\Lambda_L = [-M, -N-1]$ and $\Lambda_R = [N+1, M]$ (see Figure 6.2). The size N will be kept fixed and we shall discuss the thermodynamic limit $M \to \infty$.

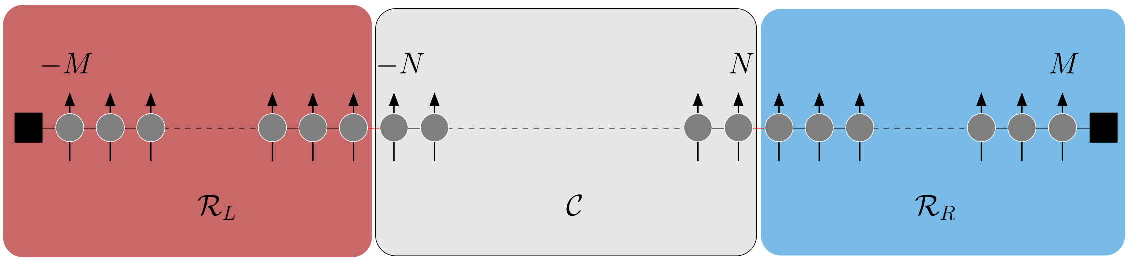

Figure 6.2: The XY-chain $\mathcal{C}$ coupled at its left and right ends to the reservoirs $\mathcal{R}_L$ and $\mathcal{R}_R$.

The Hamiltonian of the decoupled joint system $\mathcal{R}_L + \mathcal{C} + \mathcal{R}_R$ is given by

$$H_0 = H_{\Lambda_L} + H_\Lambda + H_{\Lambda_R}.$$

The coupled Hamiltonian is

$$H = H_{\Lambda_L \cup \Lambda \cup \Lambda_R} = H_0 + V_L + V_R,$$

with the coupling terms

$$V_L = -\frac{J}{4}\left(\sigma_{-N-1}^{(1)}\sigma_{-N}^{(1)} + \sigma_{-N-1}^{(2)}\sigma_{-N}^{(2)}\right), \qquad V_R = -\frac{J}{4}\left(\sigma_N^{(1)}\sigma_{N+1}^{(1)} + \sigma_N^{(2)}\sigma_{N+1}^{(2)}\right).$$

We consider the family of initial states

$$\omega_X = \frac{\mathrm{e}^{-\beta H + X_L H_{\Lambda_L} + X_R H_{\Lambda_R}}}{\mathrm{tr}(\mathrm{e}^{-\beta H + X_L H_{\Lambda_L} + X_R H_{\Lambda_R}})}, \tag{6.26}$$

with control parameter $X = (X_L, X_R) \in \mathbb{R}^2$. The entropy production observable is

$$\sigma_X = X_L \Phi_L + X_R \Phi_R,$$

where the heat fluxes from $\mathcal{R}_{L/R}$ to $\mathcal{C}$ are easily computed using the commutation relations (6.22),

$$\Phi_L = -\mathrm{i}[H, H_{\Lambda_L}] = \frac{J^2}{8}\left(\sigma_{-N-2}^{(2)}\sigma_{-N}^{(1)} - \sigma_{-N-2}^{(1)}\sigma_{-N}^{(2)}\right)\sigma_{-N-1}^{(3)} + \frac{\lambda J}{4}\left(\sigma_{-N-1}^{(1)}\sigma_{-N}^{(2)} - \sigma_{-N-1}^{(2)}\sigma_{-N}^{(1)}\right),$$
$$\Phi_R = -\mathrm{i}[H, H_{\Lambda_R}] = \frac{J^2}{8}\left(\sigma_{N}^{(1)}\sigma_{N+2}^{(2)} - \sigma_{N}^{(2)}\sigma_{N+2}^{(1)}\right)\sigma_{N+1}^{(3)} + \frac{\lambda J}{4}\left(\sigma_{N+1}^{(1)}\sigma_{N}^{(2)} - \sigma_{N+1}^{(2)}\sigma_{N}^{(1)}\right).$$

In the Jordan-Wigner representation, the decoupled system is a free Fermi gas with one particle Hilbert space $\ell^2(\Lambda_L \cup \Lambda \cup \Lambda_R) = \ell^2(\Lambda_L) \oplus \ell^2(\Lambda) \oplus \ell^2(\Lambda_R)$ and one particle Hamiltonian

$$h_0 = h_{\Lambda_L} \oplus h_\Lambda \oplus h_{\Lambda_R}.$$

The one particle Hamiltonian of the coupled system is

$$h = h_{\Lambda_L \cup \Lambda \cup \Lambda_R} = h_0 + v_L + v_R,$$

where the coupling terms

$$v_L = \frac{J}{2}\left(|\delta_{-N-1}\rangle\langle\delta_{-N}| + |\delta_{-N}\rangle\langle\delta_{-N-1}|\right), \qquad v_R = \frac{J}{2}\left(|\delta_N\rangle\langle\delta_{N+1}| + |\delta_{N+1}\rangle\langle\delta_N|\right),$$

are finite rank operators. The initial state ω_X is quasi-free with density

$$T_X = \left(\mathbb{1} + \mathrm{e}^{-k_X}\right)^{-1},$$

where

$$k_X = -\beta h + X_L h_{\Lambda_L} + X_R h_{\Lambda_R} = -\beta(h_\Lambda + v_L + v_R) - (\beta - X_L)h_{\Lambda_L} - (\beta - X_R)h_{\Lambda_R}.$$

It is now apparent that the results of Section 6.6 apply to the open XY-chain. By Part (2) of Exercise 6.8, the generalized entropic pressure is given by

$$e_t(X,Y) = \log\det\left(\mathbb{1} + T_X\left(\mathrm{e}^{-k_X}\mathrm{e}^{k_{X-Y}+k_{Y,t}-k_0} - \mathbb{1}\right)\right),$$

where $k_{X,t} = \mathrm{e}^{-\mathrm{i}th}k_X\mathrm{e}^{\mathrm{i}th}$. The same formula holds in the thermodynamic limit, provided k_X is replaced by its strong limit. The large time limit follows from Part (5) of Exercise 6.11,

$$\begin{aligned} e_+(X,Y) &= \lim_{t\to\infty}\frac{1}{t}\,e_t(X,Y) \\ &= \int_0^\pi \log\det\left(\mathbb{1} + T_X(\xi)(\mathrm{e}^{-k_X(\xi)}\mathrm{e}^{k_{X-Y}(\xi)+s(\xi)k_Y(\xi)s^*(\xi)-k_0(\xi)} - \mathbb{1})\right)\frac{\mathrm{d}\varepsilon(\xi)}{2\pi}, \end{aligned}$$

where $\varepsilon(\xi) = 1 - \cos\xi$, $k_X(\xi)$ is the diagonal 2×2 matrix with entries $(\beta - X_j)(\lambda - J\cos(\xi))$ and $T_X(\xi) = (\mathbb{1} + \mathrm{e}^{-k_X(\xi)})^{-1}$. Using the explicit form

$$s(\xi) = \mathrm{e}^{\pm 2\mathrm{i}N\xi}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$

of the scattering matrix (see Section 1.9, the sign $\pm$ is opposite to the sign of the coupling constant J), we obtain

$$e_+(X,Y) = \frac{1}{J\pi}\int_{u_-}^{u_+}\log\left(1 - \frac{\sinh(u\Delta Y)\sinh(u(\Delta X - \Delta Y))}{\cosh(u(\beta - X_L))\cosh(u(\beta - X_R))}\right)\mathrm{d}u,$$

where we have set $\Delta X = X_R - X_L$, $\Delta Y = Y_R - Y_L$ and $u_\pm = (\lambda \pm J)/2$. The steady heat current through the chain is given by

$$\langle\Phi_L\rangle_+ = \lim_{t\to\infty}\omega_{X,t}(\Phi_L) = -\partial_{Y_L}e_+(X,Y)|_{Y=0} = \frac{1}{J\pi}\int_{u_-}^{u_+}u\left(\tanh(\beta_L u) - \tanh(\beta_R u)\right)\mathrm{d}u,$$

where $\beta_{L/R} = \beta - X_{L/R}$. It follows that the entropy production

$$\langle\sigma\rangle_+ = \frac{1}{J\pi}\int_{u_-}^{u_+} (\beta_L u - \beta_R u)\,(\tanh(\beta_L u) - \tanh(\beta_R u))\,\mathrm{d}u,$$

is strictly positive iff $\beta_L \neq \beta_R$ and $J \neq 0$.

Exercise 6.20. Develop the linear response theory of the open XY-chain.

Exercise 6.21. Instead of (6.26) consider the reference state

$$\omega = \frac{\mathrm{e}^{-\beta_L H_{\Lambda_L} - \beta H_\Lambda - \beta_R H_{\Lambda_R}}}{\mathrm{tr}(\mathrm{e}^{-\beta_L H_{\Lambda_L} - \beta H_\Lambda - \beta_R H_{\Lambda_R}})}.$$

In this case, up to irrelevant scaling, the Jordan-Wigner transformation maps the XY-chain to the EBB model considered in Exercise 6.17. Show that for $p \in [1, \infty]$,

$$e_{\mathrm{naive},+}(\alpha) = e_{p,+}(\alpha) = \frac{1}{J\pi}\int_{u_-}^{u_+} \log\left(1 - \frac{\sinh(\alpha u\Delta\beta)\sinh((1-\alpha)u\Delta\beta)}{\cosh(u\beta_L)\cosh(u\beta_R)}\right)\mathrm{d}u, \tag{6.27}$$

where $\Delta\beta = \beta_R - \beta_L$ (see Figure 6.3). Note that $e_{p,+}(\alpha) = e_+(X, \alpha X)$.

The formula (6.27) can be rewritten in terms of Euler's dilogarithm

$$\mathrm{Li}_2(z) = -\int_0^z \frac{\log(1-w)}{w}\,\mathrm{d}w,$$

an analytic function on the cut plane $\mathbb{C} \setminus [1, \infty[$ with a branching point at $z = 1$ (see [Le]). More precisely, one has

$$e_{p,+}(\alpha) = G(\overline{\beta} + (\alpha - 1/2)\Delta\beta) + G(\overline{\beta} - (\alpha - 1/2)\Delta\beta) - G(\beta_L) - G(\beta_R),$$

where $\overline{\beta} = (\beta_L + \beta_R)/2$ and

$$G(x) = \frac{\mathrm{Li}_2\left(-\mathrm{e}^{2xu_+}\right) - \mathrm{Li}_2\left(-\mathrm{e}^{2xu_-}\right)}{\pi x(u_+ - u_-)}.$$

It follows that $e_{p,+}(\alpha)$ is analytic on the strip $|\mathrm{Im}\,\alpha| < \frac{\pi}{(|\lambda|+|J|)|\Delta\beta|}$.

Remark. We were able to compute the TD and large time limits of the entropic functionals of the XY-chain thanks to its Fermi-gas representation. We note however that the operator

$$V_x = (2b_{-M}^* b_{-M} - \mathbb{1}) \cdots (2b_{x-1}^* b_{x-1} - \mathbb{1}),$$

has no limit in the CAR algebra over $\ell^2(\mathbb{Z})$ as $M \to \infty$, and the Jordan-Wigner transformation (6.25) does not survive the TD limit. In fact, to recover the full spin algebra in the TD limit, one needs to enlarge the CAR algebra over $\ell^2(\mathbb{Z})$ with an element V formally equal to

$$\lim_{M\to\infty} (2b_{-M}^* b_{-M} - \mathbb{1}) \cdots (2b_{-1}^* b_{-1} - \mathbb{1}).$$

We refer to Araki [A] for a complete exposition of this construction. An alternative resolution of the TD limit/Jordan-Wigner transformation conflict goes as follows.

We set $\Lambda_M = [-M, M] \subset \mathbb{Z}$. The operator $W = \sigma_{-M}^{(3)} \cdots \sigma_M^{(3)} \in \mathcal{O}_{\Lambda_M}$ satisfies $W = W^* = W^{-1}$. It implements the rotation by an angle π around the (3)-axis of all the spins of the chain,

$$W\sigma_x^{(j)}W^* = \begin{cases} -\sigma_x^{(j)} & \text{for } j = 1 \text{ or } j = 2, \\ \sigma_x^{(j)} & \text{for } j = 3. \end{cases}$$

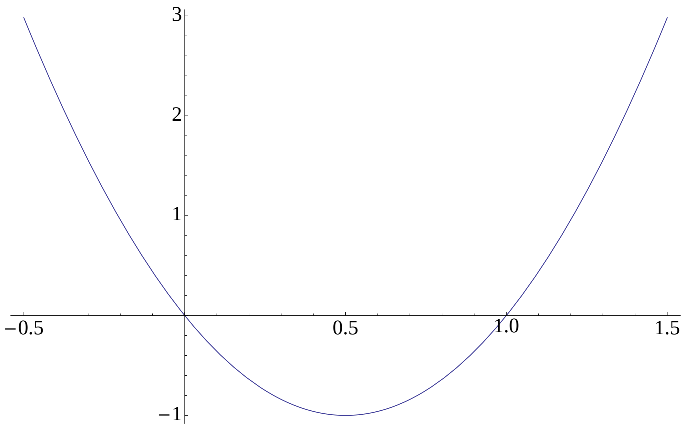

Figure 6.3: The entropic functional $e_{p,+}(\alpha)$ of the open XY-chain.

Thus, $\theta(A) = WAW^*$ defines an involutive $*$-automorphism of $\mathcal{O}_{\Lambda_M}$. In the fermionic picture, θ is completely characterized by $\theta(b_x) = -b_x$.

Since θ is a linear involution on the vector space $\mathcal{O}_{\Lambda_M}$, it follows that $\mathcal{O}_{\Lambda_M} = \mathcal{O}_{\Lambda_M+} \oplus \mathcal{O}_{\Lambda_M-}$, where

$$\mathcal{O}_{\Lambda_M\pm} = \{A \in \mathcal{O}_{\Lambda_M} \,|\, \theta(A) = \pm A\},$$

are vector subspaces. Note that $\mathcal{O}_{\Lambda_M+}$ is a $*$-subalgebra of $\mathcal{O}_{\Lambda_M}$. Since $H_\Lambda \in \mathcal{O}_{\Lambda_M+}$, the dynamics $\tau_\Lambda^t(A) = \mathrm{e}^{\mathrm{i}tH_\Lambda} A \mathrm{e}^{-\mathrm{i}tH_\Lambda}$ satisfies $\tau_\Lambda^t \circ \theta = \theta \circ \tau_\Lambda^t$ and, in particular, it preserves both subspaces $\mathcal{O}_{\Lambda_M\pm}$. Moreover, our initial state satisfies $\omega_X \circ \theta = \omega_X$ which implies that $\omega_X|_{\mathcal{O}_{\Lambda_M-}} = 0$. Thus, observables with non-trivial expectation belong to the subalgebra $\mathcal{O}_{\Lambda_M+}$ and we may restrict ourselves to such observables.

In the fermionic picture, $\mathcal{O}_{\Lambda_M+}$ is the $*$-algebra of all polynomials in the $b_x^\#$ which contain only monomials of even degree. In the spin picture, it is generated by the operators $\sigma_x^{(3)}$ and $\sigma_x^{(s)}\sigma_{x'}^{(s')}$ with $s, s' \in \{-, +\}$ and $x < x'$, which have a Jordan-Wigner representation surviving the TD limit, *e.g.*,

$$\sigma_x^{(-)}\sigma_y^{(+)} = b_x(2b_{x+1}^* b_{x+1} - \mathbb{1}) \cdots (2b_{y-1}^* b_{y-1} - \mathbb{1}) b_y^*.$$

Thus, at the price of restricting the dynamical system to the even subalgebra $\mathcal{O}_{\Lambda_M+}$, the XY-chain remains equivalent to a free Fermi gas in the TD limit. This fact is a starting point in the construction of the NESS of the XY-chain. We refer the reader to [AH, AP] for the details of this construction and to [AB1, AB2] for additional information about the NESS of the XY-chain.

Appendix A: Large deviations

In this first appendix, we formulate some well known large deviation results that were used in these lecture notes. We provide a proof in the simplest case of scalar random variables.

A.1 Fenchel-Legendre transform

In this section, we shall use freely some well known properties of convex real functions of a real variable, see, *e.g.*, [RV].

Let $I = [a, b] \subset \mathbb{R}$ be a closed finite interval, denote by $\mathrm{int}(I) =]a, b[$ its interior, and let $e : I \to \mathbb{R}$ be a continuous convex function. Then e admits finite left and right derivatives

$$D^{\pm}e(s) = \lim_{h\downarrow 0} \frac{e(s \pm h) - e(s)}{\pm h},$$

at every $s \in \mathrm{int}(I)$. $D^+e(a)$ and $D^-e(b)$ exist, although they may be respectively $-\infty$ and $+\infty$. By convention, we set $D^-e(a) = -\infty$ and $D^+e(b) = +\infty$. The functions $D^{\pm}e(s)$ are increasing on I and satisfy $D^-e(s) \le D^+e(s)$. Moreover, $D^-e(s) = D^+e(s) = e'(s)$ outside a countable set in $\mathrm{int}(I)$. If $e'(s)$ exists for all $s \in \mathrm{int}(I)$, then it is continuous on $\mathrm{int}(I)$ and

$$\lim_{s\downarrow a} e'(s) = D^+e(a), \qquad \lim_{s\uparrow b} e'(s) = D^-e(b).$$

The subdifferential of e at $s_0 \in I$, denoted $\partial e(s_0)$, is the set of $\theta \in \mathbb{R}$ such that the affine function $\underline{e}(s) = e(s_0) + \theta(s - s_0)$ satisfies $e(s) \ge \underline{e}(s)$ for all $s \in I$, *i.e.*, the graph of $\underline{e}$ is tangent to the graph of e at the point $(s_0, e(s_0))$. For any $s_0 \in I$, one has $\partial e(s_0) = [D^-e(s_0), D^+e(s_0)] \cap \mathbb{R}$.

It is convenient to extend the function e to $\mathbb{R}$ by setting $e(s) = +\infty$ for $s \notin I$. Then the function $e(s)$ is convex and lower semi-continuous on $\mathbb{R}$, *i.e.*,

$$e(s_0) = \liminf_{s\to s_0} e(s),$$

holds for all $s_0 \in \mathbb{R}$. The subdifferential of e is naturally extended by setting $\partial e(s) = \emptyset$ for $s \notin I$.

The function

$$\varphi(\theta) = \sup_{s\in I}(\theta s - e(s)) = \sup_{s\in\mathbb{R}}(\theta s - e(s)) \tag{A.1}$$

is called the Fenchel-Legendre transform of $e(s)$. $\varphi(\theta)$ is finite and convex (hence continuous) on $\mathbb{R}$. Obviously, if $a \ge 0$ then $\varphi(\theta)$ is increasing and if $b \le 0$ then $\varphi(\theta)$ is decreasing. The subdifferential of φ at $\theta \in \mathbb{R}$ is $\partial\varphi(\theta) = [D^-\varphi(\theta), D^+\varphi(\theta)]$. The basic properties of the pair (e, φ) are summarized in:

Theorem A.1 (1) $\theta s \le e(s) + \varphi(\theta)$ *for all* $s, \theta \in \mathbb{R}$.

(2) $\theta s = e(s) + \varphi(\theta) \Leftrightarrow \theta \in \partial e(s)$.

(3) $e(s) = \sup_{\theta\in\mathbb{R}}(\theta s - \varphi(\theta))$.

(4) $\theta \in \partial e(s) \Leftrightarrow s \in \partial\varphi(\theta)$.

(5) *If* $0 \in]a, b[$, *then* $\varphi(\theta)$ *is decreasing on* $]-\infty, D^-e(0)]$, *increasing on* $[D^+e(0), \infty[$, $\varphi(\theta) = -e(0)$ *for* $\theta \in \partial e(0)$, *and* $\varphi(\theta) > -e(0)$ *for* $\theta \notin \partial e(0)$.

Proof. (1) Follows directly from the definition of φ.

(2) Combining the inequality (1) with the equality $\theta s_0 = e(s_0)+\varphi(\theta)$ we obtain that $e(s) \geq e(s_0)+\theta(s-s_0)$ for all $s \in \mathbb{R}$ which implies $\theta \in \partial e(s_0)$. Reciprocally, if $\theta \in \partial e(s_0)$ then $e(s) \geq e(s_0) + \theta(s - s_0)$ holds for all $s \in \mathbb{R}$ and hence $\theta s_0 \geq e(s_0) + \sup_s(\theta s - e(s)) = e(s_0) + \varphi(\theta)$. Combined with inequality (1), this yields $\theta s_0 = e(s_0) + \varphi(\theta)$.

(3) It follows from Exercise 2.11 that the function $\tilde{e}(s) = \sup_{\theta\in\mathbb{R}}(\theta s - \varphi(\theta))$ is lower semi-continuous on $\mathbb{R}$. (1) implies that $\tilde{e}(s) \leq e(s)$ for any $s \in \mathbb{R}$. $\partial e(s) \neq \emptyset$ for $s \in]a, b[$ we conclude from (2) that $\tilde{e}(s) = e(s)$.

Note that $-e(s) \leq -\min_{u\in I}(-e(u)) = \varphi(0)$. Thus, for $\theta > 0$, we have $\varphi(\theta) = \sup_{s\in[a,b]}(\theta s - e(s)) \leq \theta b + \varphi(0)$ and hence $\theta s - \varphi(\theta) \geq \theta(s - b) - \varphi(0)$. It follows that $\tilde{e}(s) = +\infty = e(s)$ for $s > b$. A similar argument applies to the case $s < a$.

Consider now the case $s = a$. From our previous conclusions, we can write $\tilde{e}(a) = \liminf_{s\to a} \tilde{e}(s) = \lim_{s\downarrow a} \tilde{e}(s) = \lim_{s\downarrow a} e(s) = e(a)$. A similar argument applies to $s = b$.

(4) By (2), $\theta_0 \in \partial e(s)$ is equivalent to the equality $s\theta_0 = e(s)+\varphi(\theta_0)$ which, combined with the inequality (1) yields $\varphi(\theta) \geq \varphi(\theta_0) + s(\theta - \theta_0)$ for all $\theta \in \mathbb{R}$ and hence $s \in \partial\varphi(\theta_0)$. Reciprocally, if $s \in \partial\varphi(\theta_0)$ then $\varphi(\theta) \geq \varphi(\theta_0)+s(\theta-\theta_0)$ for all $\theta \in \mathbb{R}$ and we conclude from (3) that $e(s) \leq \sup_\theta(\theta s-\varphi(\theta_0)-s(\theta-\theta_0)) = -\varphi(\theta_0) + s\theta_0$. Using (1) and (2), we conclude that $\theta_0 \in \partial e(s)$.

(5) It follows from (4) that if $\theta_0 \in \partial e(0) = [D^-e(0), D^+e(0)]$ then $0 \in \partial\varphi(\theta_0)$, *i.e.*, $\varphi(\theta) \geq \varphi(\theta_0)$ for all $\theta \in \mathbb{R}$. Thus, $\varphi(\theta_0) = \min_\theta \varphi(\theta) = -e(0)$ and since $D^\pm\varphi(\theta)$ are increasing, φ is decreasing for $\theta \leq D^-e(0)$ and increasing for $\theta \geq D^+e(0)$. □

A.2 Gärtner-Ellis theorem in dimension $d = 1$

Let $\mathcal{I} \subset \mathbb{R}_+$ be an unbounded index set, $(M_t, \mathcal{F}_t, P_t)$, $t \in \mathcal{I}$, a family of measure spaces, and $X_t : M_t \to \mathbb{R}$ a family of measurable functions. We assume that the measures P_t are finite for all t. For $s \in \mathbb{R}$ let

$$e_t(s) = \log \int_{M_t} \mathrm{e}^{sX_t}\mathrm{d}P_t.$$

$e_t(s)$ is a convex function taking values in $]-\infty, \infty]$. We make the following assumption:

(LD) For $s \in I = [a, b]$ the limit

$$e(s) = \lim_{t\to\infty} \frac{1}{t} e_t(s),$$

exists and is finite. Moreover, the function $e(s)$ is continuous on I.

Until the end of this section we shall assume that (LD) holds and set $e(s) = \infty$ for $s \notin I$. The function $\varphi(\theta)$ is defined by (A.1).

Proposition A.2 (1) *Suppose that* $0 \in [a, b[$. *Then*

$$\limsup_{t\to\infty} \frac{1}{t} \log P_t(\{x \in M_t \,|\, X_t(x) > t\theta\}) \leq \begin{cases} -\varphi(\theta) & \text{if } \theta \geq D^+e(0) \\ e(0) & \text{if } \theta < D^+e(0). \end{cases}$$

(2) *Suppose that* $0 \in]a, b]$. *Then*

$$\limsup_{t\to\infty} \frac{1}{t} \log P_t(\{x \in M_t \,|\, X_t(x) < t\theta\}) \leq \begin{cases} -\varphi(\theta) & \text{if } \theta \leq D^-e(0) \\ e(0) & \text{if } \theta > D^-e(0). \end{cases}$$

Proof. We shall prove (1), the proof of (2) follows from (1) applied to $-X_t$ and $-\theta$. For $s \in]0, b]$,

$$P_t(\{x \in M_t \,|\, X_t(x) > t\theta\}) = P_t(\{x \in M_t \,|\, \mathrm{e}^{sX_t(x)} > \mathrm{e}^{st\theta}\}) \leq \mathrm{e}^{-st\theta} \int_{M_t} \mathrm{e}^{sX_t} \mathrm{d}P_t,$$

and so

$$\limsup_{t\to\infty} \frac{1}{t} \log P_t(\{x \in M_t \,|\, X_t(x) > t\theta\}) \leq -\sup_{0\leq s\leq b} (\theta s - e(s)).$$

For $\theta < D^+e(0)$ and $s \geq 0$, one has $e(s) \geq e(0) + sD^+e(0) \geq e(0) + \theta s$, so that

$$-e(0) \leq \sup_{0\leq s\leq b} (\theta s - e(s)) \leq \sup_{0\leq s\leq b} (\theta s - e(0) - \theta s) = -e(0),$$

and hence $\sup_{0\leq s\leq b}(\theta s - e(s)) = -e(0)$. One shows in a similar way that $\sup_{a\leq s\leq 0}(\theta s - e(s)) = -e(0)$ for $\theta \geq D^+e(0)$. It follows that

$$\varphi(\theta) = \sup_{a\leq s\leq b} (\theta s - e(s)) = \max\left(-e(0), \sup_{0\leq s\leq b} (\theta s - e(s))\right) = \sup_{0\leq s\leq b} (\theta s - e(s)).$$

The statement follows. □

Proposition A.3 *Suppose that $0 \in]a, b[$, $e(0) \leq 0$, and that $e(s)$ is differentiable at $s = 0$. Then for any $\delta > 0$ there is $\gamma > 0$ such that for t large enough,*

$$P_t(\{x \in M_t \,|\, |t^{-1}X_t(x) - e'(0)| \geq \delta\}) \leq \mathrm{e}^{-\gamma t}.$$

Proof. Part (2) of Theorem A.1 implies that $\varphi(e'(0)) = -e(0)$. By Part (5) of the same theorem, one has $\varphi(\theta) > \varphi(e'(0)) \geq 0$ for $\theta \neq e'(0)$. Since

$$\begin{aligned} P_t(\{x \in M_t \,|\, |t^{-1}X_t(x) - e'(0)| \geq \delta\}) \leq &P_t(\{x \in M_t \,|\, |X_t(x) \leq t(e'(0) - \delta)\}) \\ &+P_t(\{x \in M_t \,|\, |X_t(x) \geq t(e'(0) + \delta)\}), \end{aligned}$$

Proposition A.2 implies

$$\limsup_{t\to\infty} \frac{1}{t} \log P_t(\{x \in M_t \,|\, |t^{-1}X_t(x) - e'(0)| \geq \delta\}) \leq -\min\{\varphi(e'(0) + \delta), \varphi(e'(0) - \delta)\},$$

and the statement follows. □

Proposition A.4 *Suppose that $0 \in]a, b[$ and $e(s)$ is differentiable on $]a, b[$. Then*

$$\liminf_{t\to\infty} \frac{1}{t} \log P_t(\{x \in M_t \,|\, X_t(x) > t\theta)\} \geq -\varphi(\theta),$$

for any $\theta \in]D^+e(a), D^-e(b)[$.

Proof. Let $\theta \in]D^+e(a), D^-e(b)[$ be given and let α and ϵ be such that

$$\theta < \alpha - \epsilon < \alpha < \alpha + \epsilon < D^-e(b).$$

Let $s_\alpha \in]a, b[$ be such that $e'(s_\alpha) = \alpha$ (so $\varphi(\alpha) = \alpha s_\alpha - e(s_\alpha)$). Let

$$\mathrm{d}\hat{P}_t = \mathrm{e}^{-e_t(s_\alpha)} \mathrm{e}^{s_\alpha X_t} \mathrm{d}P_t.$$

Then $\hat{P}_t$ is a probability measure on $(M_t, \mathcal{F}_t)$ and

$$\begin{aligned} P_t(\{x \in M_t \,|\, X_t(x) > t\theta\}) &\geq P_t(\{x \in M_t \,|\, t^{-1}X_t(x) \in [\alpha - \epsilon, \alpha + \epsilon]\}) \\ &= \mathrm{e}^{e_t(s_\alpha)} \int_{\{t^{-1}X_t \in [\alpha-\epsilon,\alpha+\epsilon]\}} \mathrm{e}^{-s_\alpha X_t} \mathrm{d}\hat{P}_t \qquad \text{(A.2)} \\ &\geq \mathrm{e}^{e_t(s_\alpha) - s_\alpha t\alpha - |s_\alpha| t\epsilon} \hat{P}_t(\{x \in M_t \,|\, t^{-1}X_t \in [\alpha - \epsilon, \alpha + \epsilon]\}). \end{aligned}$$

Now, if $\hat{e}_t(s) = \log \int_{M_t} \mathrm{e}^{sX_t} \mathrm{d}\hat{P}_t$, then $\hat{e}_t(s) = e_t(s + s_\alpha) - e_t(s_\alpha)$ and so

$$\lim_{t\to\infty} \frac{1}{t}\hat{e}_t(s) = e(s + s_\alpha) - e(s_\alpha),$$

for $s \in [a - s_\alpha, b - s_\alpha]$. Since $\hat{e}(0) = 0$ and $\hat{e}'(0) = e'(s_\alpha) = \alpha$, it follows from Proposition A.3 that

$$\lim_{t\to\infty} \frac{1}{t} \log \hat{P}_t(\{x \in M_t \,|\, t^{-1}X_t(x) \in [\alpha - \epsilon, \alpha + \epsilon]\}) = 0,$$

and (A.2) yields

$$\liminf_{t\to\infty} \frac{1}{t} \log P_t(\{x \in M_t \,|\, X_t(x) > t\theta\}) \geq -s_\alpha\alpha + e(s_\alpha) - |s_\alpha|\epsilon = -\varphi(\alpha) - |s_\alpha|\epsilon.$$

The statement follows by taking first $\epsilon \downarrow 0$ and then $\alpha \downarrow \theta$. □

The following local version of the Gärtner-Ellis theorem is a consequence of Propositions A.2 and A.4.

Theorem A.5 *If $e(s)$ is differentiable on $]a, b[$ and $0 \in]a, b[$ then, for any open set $\mathbb{J} \subset]D^+e(a), D^-e(b)[$,*

$$\lim_{t\to\infty} \frac{1}{t} \log P_t(\{x \in M_t \,|\, t^{-1}X_t(x) \in \mathbb{J}\}) = -\inf_{\theta\in\mathbb{J}} \varphi(\theta).$$

Proof. *Lower bound.* For any $\theta \in \mathbb{J}$ and $\delta > 0$ such that $]\theta - \delta, \theta + \delta[\subset \mathbb{J}$ one has

$$P_t(\{x \in M_t \,|\, t^{-1}X_t(x) \in \mathbb{J}\}) \geq P_t(\{x \in M_t \,|\, t^{-1}X_t(x) \in]\theta - \delta, \theta + \delta[\}),$$

and it follows from Proposition A.4 that

$$\liminf_{t\to\infty} \frac{1}{t} \log P_t(\{x \in M_t \,|\, t^{-1}X_t(x) \in \mathbb{J}\}) \geq -\varphi(\theta - \delta).$$

Letting $\delta \downarrow 0$ and optimizing over $\theta \in \mathbb{J}$, we obtain

$$\liminf_{t\to\infty} \frac{1}{t} \log P_t(\{x \in M_t \,|\, t^{-1}X_t(x) \in \mathbb{J}\}) \geq -\inf_{\theta\in\mathbb{J}} \varphi(\theta). \tag{A.3}$$

Upper bound. Note that $e(0) = 0 \in]a, b[$. By Part (5) of Proposition A.1, we have $\varphi(\theta) = 0$ for $\theta = e'(0)$ and $\varphi(\theta) > 0$ otherwise. Hence, if $e'(0) \in \mathrm{cl}(\mathbb{J})$, then

$$\limsup_{t\to\infty} \frac{1}{t} \log P_t(\{x \in M_t \,|\, t^{-1}X_t(x) \in \mathbb{J}\}) \leq 0 = -\inf_{\theta\in\mathbb{J}} \varphi(\theta).$$

In the case $e'(0) \notin \mathrm{cl}(\mathbb{J})$, there exist $\alpha, \beta \in \mathrm{cl}(\mathbb{J})$ such that $e'(0) \in]\alpha, \beta[\subset \mathbb{R} \setminus \mathrm{cl}(\mathbb{J})$. It follows that

$$\begin{aligned}
&P_t(\{x \in M_t \,|\, t^{-1}X_t(x) \in \mathbb{J}\}) \\
&\quad\leq P_t(\{x \in M_t \,|\, t^{-1}X_t(x) < \alpha\}) + P_t(\{x \in M_t \,|\, t^{-1}X_t(x) > \beta\}) \\
&\quad\leq 2\max\left(P_t(\{x \in M_t \,|\, t^{-1}X_t(x) < \alpha\}), P_t(\{x \in M_t \,|\, t^{-1}X_t(x) > \beta\})\right),
\end{aligned}$$

and Proposition A.2 yields

$$\limsup_{t\to\infty} \frac{1}{t} \log P_t(\{x \in M_t \,|\, t^{-1}X_t(x) \in \mathbb{J}\}) \leq -\min(\varphi(\alpha), \varphi(\beta)).$$

Finally, by Part (5) of Proposition A.1, one has

$$\inf_{\theta\in\mathbb{J}} \varphi(\theta) = \min(\varphi(\alpha), \varphi(\beta)),$$

and therefore

$$\limsup_{t\to\infty} \frac{1}{t} \log P_t(\{x \in M_t \,|\, t^{-1}X_t(x) \in \mathbb{J}\}) \leq \inf_{\theta\in\mathbb{J}} \varphi(\theta), \tag{A.4}$$

holds for any $\mathbb{J} \subset]D^+e(a), D^-e(b)[$. The result follows from the bounds (A.3) and (A.4). □

A.3 Gärtner-Ellis theorem in dimension $d > 1$

Let $\mathbf{X}_t : M_t \to \mathbb{R}^d$ be a family of measurable functions w.r.t. the probability spaces $(M_t, \mathcal{F}_t, P_t)$. If $G \subset \mathbb{R}^d$ is a Borel set, we denote by $\mathrm{int}(G)$ its interior, by $\mathrm{cl}(G)$ its closure, and by ∂G its boundary. The following result is a multi-dimensional version of the Gärtner-Ellis theorem.

Theorem A.6 *Assume that the limit*

$$h(\mathbf{Y}) = \lim_{t\to\infty} \frac{1}{t} \log \int_{M_t} \mathrm{e}^{\mathbf{Y}\cdot\mathbf{X}_t} \, \mathrm{d}P_t, \tag{A.5}$$

exists in $[-\infty, +\infty]$ *for all* $\mathbf{Y} \in \mathbb{R}^d$*, that the function* $h(\mathbf{Y})$ *is lower semi-continuous on* $\mathbb{R}^d$*, differentiable on the interior of the set* $\mathcal{D} = \{\mathbf{Y} \in \mathbb{R}^d \,|\, |h(\mathbf{Y})| < \infty\}$ *and satisfies*

$$\lim_{\mathrm{int}(\mathcal{D})\ni\mathbf{Y}\to\mathbf{Y}_0} |\boldsymbol{\nabla} h(\mathbf{Y})| = \infty,$$

for all $\mathbf{Y}_0 \in \partial\mathcal{D}$*. Suppose also that* $\mathbf{0}$ *is an interior point of* $\mathcal{D}$*. Then, for all Borel sets* $G \subset \mathbb{R}^d$ *we have*

$$\begin{aligned} -\inf_{\mathbf{Z}\in\mathrm{int}(G)} I(\mathbf{Z}) &\le \liminf_{t\to\infty} \frac{1}{t} \log P_t\left(\{x \in M_t \,|\, t^{-1}\mathbf{X}_t(x) \in G\}\right) \\ &\le \limsup_{t\to\infty} \frac{1}{t} \log P_t\left(\{x \in M \,|\, t^{-1}\mathbf{X}_t(x) \in G\}\right) \le -\inf_{\mathbf{Z}\in\mathrm{cl}(G)} I(\mathbf{Z}), \end{aligned}$$

where

$$I(\mathbf{Z}) = \sup_{\mathbf{Y}\in\mathbb{R}^d} (\mathbf{Y}\cdot\mathbf{Z} - h(\mathbf{Y})).$$

We now describe a local version of Gärtner-Ellis theorem in $d > 1$. Set

$$\overline{h}(\mathbf{Y}) = \limsup_{t\to\infty} \frac{1}{t} \log \int_{M_t} \mathrm{e}^{\mathbf{Y}\cdot\mathbf{X}_t} \, \mathrm{d}P_t,$$

$$\overline{I}(\mathbf{Z}) = \sup_{\mathbf{Y}\in\mathbb{R}^d} (\mathbf{Y}\cdot\mathbf{Z} - \overline{h}(\mathbf{Y})).$$

Let $\overline{\mathcal{D}} = \{\mathbf{Y} \in \mathbb{R}^d \,|\, \overline{h}(\mathbf{Y}) < \infty\}$ and let $\mathcal{D}$ be the set of all $\mathbf{Y} \in \mathbb{R}^d$ for which the limit (A.5) exists and is finite. Let $S \subset \mathcal{D}$ be the set of points at which $h(\mathbf{Y})$ is differentiable and let $\mathcal{F} = \{\boldsymbol{\nabla} h(\mathbf{Y}) \,|\, \mathbf{Y} \in S\}$.

Theorem A.7 *Suppose that* $\mathbf{0} \in \mathrm{int}(\overline{\mathcal{D}})$*. Then*

(1) *For any Borel set* $G \subset \mathbb{R}^d$*,*

$$\limsup_{t\to\infty} \frac{1}{t} \log P_t\left(\{x \in M \,|\, t^{-1}\mathbf{X}_t(x) \in G\}\right) \le -\inf_{\mathbf{Z}\in\mathrm{cl}(G)} \overline{I}(\mathbf{Z}).$$

(2) *For any Borel set* $G \subset \mathcal{F}$*,*

$$\liminf_{t\to\infty} \frac{1}{t} \log P_t\left(\{x \in M \,|\, t^{-1}\mathbf{X}_t(x) \in G\}\right) \ge -\inf_{\mathbf{Z}\in\mathrm{int}(G)} \overline{I}(\mathbf{Z}).$$

We refer to [DZ] for proofs and various extensions of these fundamental results.

A.4 Central limit theorem

Bryc [Br] has observed that under a a suitable analyticity assumption the central limit theorem follows from the large deviation principle. In this appendix we state and prove Bryc's result. The setup is the same as in Appendix A.3. Let

$$h_t(\mathbf{Y}) = \frac{1}{t} \log \int_{M_t} \mathrm{e}^{\mathbf{Y}\cdot\mathbf{X}_t} \, \mathrm{d}P_t,$$

and let D_ϵ be the open polydisk of $\mathbb{C}^d$ of radius ϵ centered at $\mathbf{0}$, *i.e.*,

$$D_\epsilon = \{z = (z_1, \ldots, z_d) \in \mathbb{C}^d \mid \max_j |z_j| < \epsilon\}.$$

The analyticity assumption is:

(A) For some $\epsilon > 0$ and all $t \in \mathcal{I}$ the function $\mathbf{Y} \mapsto h_t(\mathbf{Y})$ has an analytic continuation to the polydisc D_ϵ such that

$$\sup_{\substack{z \in D_\epsilon \\ t \in \mathcal{I}}} |h_t(z)| < \infty.$$

Moreover, for $\mathbf{Y} \in D_\epsilon$ real, the limit

$$h(\mathbf{Y}) = \lim_{t\to\infty} h_t(\mathbf{Y})$$

exists.

This assumption and Vitali's convergence theorem (see Appendix B below) imply that $h(\mathbf{Y})$ has analytic extension to D_ϵ and that all derivatives of $h_t(z)$ converge to corresponding derivatives of $h(z)$ as $t \to \infty$ uniformly on compact subsets of D_ϵ. We denote

$$\mathbf{m}_t = \nabla h_t(\mathbf{Y})|_{\mathbf{Y}=\mathbf{0}}, \qquad \mathbf{m} = \nabla h(\mathbf{Y})|_{\mathbf{Y}=\mathbf{0}}.$$

Clearly, Clearly, $\mathbf{m_t}$ is the expectation of $\mathbf{X}_t$ w.r.t. P_t and

$$\lim_{t\to\infty} \frac{1}{t}\mathbf{m}_t = \mathbf{m}.$$

Similarly, if $\mathbf{D}_t = [D_{jkt}]$ is the covariance of $\mathbf{X}_t$, then

$$\lim_{t\to\infty} \frac{1}{t}\mathbf{D}_t = \mathbf{D},$$

where $\mathbf{D} = [D_{jk}]$ is given by

$$D_{jk} = \partial^2_{Y_jY_k} h(\mathbf{Y})|_{\mathbf{Y}=\mathbf{0}}.$$

Theorem A.8 *Assumption* (A) *implies the central limit theorem: for any Borel set $G \subset \mathbb{R}^d$,*

$$\lim_{t\to\infty} P_t\left(\left\{x \in M_t \mid \frac{\mathbf{X}_t(x) - \mathbf{m}_t}{\sqrt{t}} \in G\right\}\right) = \mu_{\mathbf{D}}(G),$$

where $\mu_{\mathbf{D}}$ is centered Gaussian with variance $\mathbf{D}$.

Remark 1. In general, the large deviation principle does not imply the central limit theorem. In fact, assumption (A) cannot be significantly relaxed, see [Br] for a discussion.
Remark 2. Assumption (A) is typically difficult to check in practice. We emphasize, however, that a verification of assumptions of this type has played the central role in the works [JOP1, JOP2, JOPP].
Remark 3. The proof below should be compared with Section 1.12.
Proof. By absorbing $\mathbf{m}_t$ into $\mathbf{X}_t$ we may assume that $\mathbf{m}_t = \mathbf{0}$. Let $\mathbf{k} = (k_1, \cdots, k_d)$, $k_j \geq 0$, be a multi-index and

$$\chi_{\mathbf{k}}(t) = \frac{\partial^{k_1+\cdots+k_d}}{\partial Y_1^{k_1}\cdots\partial Y_d^{k_d}} \log \int_{M_t} \mathrm{e}^{\frac{\mathbf{Y}\cdot\mathbf{X}_t}{\sqrt{t}}} \mathrm{d}P_t\big|_{\mathbf{Y}=\mathbf{0}},$$

the $\mathbf{k}$-th cummulant of $t^{-1/2}\mathbf{X}_t$.

Set

$$\Gamma_r = \{z = (z_1, \ldots, z_d) \in \mathbb{C}^d \mid |z_j| = r \text{ for all } j\}.$$

The Cauchy integral formula for polydisc yields

$$\frac{\partial^{k_1+\cdots+k_d}}{\partial z_1^{k_1}\cdots\partial z_d^{k_d}}h(z)\big|_{z=0} = \frac{k_1!\cdots k_d!}{(2\pi\mathrm{i})^d}\oint_{\Gamma_{\frac{\epsilon}{2}}}\frac{h(z)}{z_1^{k_1+1}\cdots z_d^{k_d+1}}\,\mathrm{d}z_1\cdots\mathrm{d}z_n$$

$$= \lim_{t\to\infty}\frac{k_1!\cdots k_d!}{(2\pi\mathrm{i})^d}\oint_{\Gamma_{\frac{\epsilon}{2}}}\frac{h_t(z)}{z_1^{k_1+1}\cdots z_d^{k_d+1}}\,\mathrm{d}z_1\cdots\mathrm{d}z_n.$$

Note that

$$\oint_{\Gamma_{\frac{\epsilon}{2}}}\frac{h_t(z)}{z_1^{k_1+1}\cdots z_d^{k_d+1}}\mathrm{d}z = \oint_{\Gamma_{\frac{\epsilon}{2\sqrt{t}}}}\frac{h_t(z)}{z_1^{k_1+1}\cdots z_d^{k_d+1}}\mathrm{d}z$$

$$= t^{\frac{k_1+\cdots k_d}{2}}\oint_{\Gamma_{\frac{\epsilon}{2}}}\frac{h_t(t^{-1/2}z)}{z_1^{k_1+1}\cdots z_d^{k_d+1}}\mathrm{d}z,$$

and so

$$\frac{\partial^{k_1+\cdots+k_d}}{\partial z_1^{k_1}\cdots\partial z_d^{k_d}}h(z)\big|_{z=0} = \lim_{t\to\infty}\frac{k_1!\cdots k_d!}{(2\pi\mathrm{i})^d}t^{\frac{k_1+\cdots+k_d}{2}}\oint_{\Gamma_{\frac{\epsilon}{2}}}\frac{h_t(z)}{z_1^{k_1+1}\cdots z_d^{k_d+1}}\,\mathrm{d}z_1\cdots\mathrm{d}z_n.$$

The Cauchy formula implies

$$\chi_{\mathbf{k}}(t) = t\frac{k_1!\cdots k_d!}{(2\pi\mathrm{i})^d}\oint_{\Gamma_{\frac{\epsilon}{2}}}\frac{h_t(t^{-1/2}z)}{z_1^{k_1+1}\cdots z_d^{k_d+1}}\mathrm{d}z,$$

and we see that

$$\frac{\partial^{k_1+\cdots+k_d}}{\partial z_1^{k_1}\cdots\partial z_d^{k_d}}h(z)\big|_{z=0} = \lim_{t\to\infty}t^{\frac{k_1+\cdots+k_d}{2}-1}\chi_{\mathbf{k}}(t).$$

Hence, if $k_1+\cdots+k_d\geq 3$, then

$$\lim_{t\to\infty}\chi_{\mathbf{k}}(t) = 0.$$

and if $k_1+\cdots+k_d = 2$ with the pair k_i, k_j strictly positive, then

$$\lim_{t\to\infty}\chi_{\mathbf{k}}(t) = \frac{\partial^2}{\partial z_{k_i}\partial z_{k_j}}h(z)\big|_{z=0}.$$

Since the expectation of $\mathbf{X}_t$ is zero, we see that the cumulants of $t^{-1/2}\mathbf{X}_t$ converge to the cumulants of the centered Gaussian on $\mathbb{R}^d$ with covariance $\mathbf{D}$. This implies that the moments of $t^{-1/2}\mathbf{X}_t$ converge to the moments of the centered Gaussian with covariance $\mathbf{D}$, and theorem follows (see Section 30 in [Bi2]). □

Appendix B: Vitali convergence theorem

For $\epsilon > 0$ let D_ϵ be the open polydisk of $\mathbb{C}^n$ of radius ϵ centered at $\mathbf{0}$, *i.e.*,

$$D_\epsilon = \{z = (z_1, \dots, z_n) \in \mathbb{C}^n \mid \max_j |z_j| < \epsilon\}.$$

Theorem B.1 *Let $\mathcal{I} \subset \mathbb{R}_+$ be an unbounded set and let $F_t : D_\epsilon \to \mathbb{C}$, $t \in \mathcal{I}$, be analytic functions such that*

$$\sup_{\substack{z \in D_\epsilon \\ t > 0}} |F_t(z)| < \infty.$$

Suppose that the limit

$$\lim_{t \to \infty} F_t(z) = F(z), \tag{B.1}$$

exists for all $z \in D_\epsilon \cap \mathbb{R}^n$. Then the limit (B.1) exists for all $z \in D_\epsilon$ and is an analytic function on D_ϵ. Moreover, as $t \to \infty$, all derivatives of F_t converge uniformly on compact subsets of D_ϵ to the corresponding derivatives of F.

Proof. Set

$$\Gamma_r = \{z = (z_1, \dots, z_n) \in \mathbb{C}^n \mid |z_j| = r \text{ for all } j\}.$$

For any $0 < r < \epsilon$, the Cauchy integral formula for polydisks yields

$$\frac{\partial^{k_1 + \cdots + k_n} F_t}{\partial z_1^{k_1} \cdots \partial z_n^{k_n}}(z) = \frac{k_1! \cdots k_n!}{(2\pi \mathrm{i})^n} \oint_{\Gamma_r} \frac{F_t(w)}{(w_1 - z_1)^{k_1+1} \cdots (w_n - z_n)^{k_n+1}} \, \mathrm{d}w_1 \cdots \mathrm{d}w_n, \tag{B.2}$$

for all $z \in D_r$. It follows that the family of functions $\{F_t\}_{t \in \mathcal{I}}$ is equicontinuous on $D_{r'}$ for any $0 < r' < r$. By the Arzela-Ascoli theorem, the set $\{F_t\}$ is precompact in the Banach space $C(\mathrm{cl}(D_{r'}))$ of all bounded continuous functions on $\mathrm{cl}(D_{r'})$ equipped with the sup norm. The Cauchy integral formula (B.2), where now $z \in D_{r'}$ and the integral is over $\Gamma_{r'}$, yields that any limit point of the net $\{F_t\}_{t \in \mathcal{I}}$ (as $t \to \infty$) in $C(\mathrm{cl}(D_{r'}))$ is an analytic function on $D_{r'}$. By the assumption, any two limit functions coincide for z real, and hence they are identical. This yields the first part of the theorem. The convergence of the partial derivatives of $F_t(z)$ is an immediate consequence of the Cauchy integral formula. $\square$

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Notations

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