Linear response theory in quantum statistical mechanics

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Dedicated to Barry Simon on the occasion of his 60th birthday

Abstract

This note is a continuation of our recent paper [JOP1] where we have proven the Green-Kubo formula and the Onsager reciprocity relations for heat fluxes. In this note we extend the derivation of the Green-Kubo formula to heat and charge fluxes and discuss some other generalizations of the model and results of [JOP1].

1 Introduction

The mathematical justification of transport theory is an outstanding problem of mathematical physics. Section 4 of Barry Simon's article "Fifteen Problems in Mathematical Physics" [S] is devoted to this problem and there one finds the following specific formulations:

> *Problem 4 A (Fourier's heat law) Find a mechanical model in which a system of size* L *has a temperature* ΔT *between its ends and in which the rate of heat transfer in the infinite* L *limit goes as* L^{-2}
>
> *Problem 4 B (Kubo formula) Either justify Kubo's formula in a quantum model, or else find an alternate theory of conductivity*

This paper is the second in a series that deals with Problem 4 B and linear response theory in quantum statistical mechanics (for information about Problem 4 A we refer the reader to [BLRB]).

The development of linear response theory is a part of a much wider research program initiated in [Ru1, Ru2, Ru3, JP1, JP2, JP3]. This program deals with mathematical foundations of non-equilibrium quantum statistical mechanics in the framework of algebraic quantum statistical mechanics. Within this program transport problems can be formulated explicitly and precisely. The specific transport phenomena one studies concern heat and charge fluxes induced by thermodynamical (i.e. "non-mechanical") perturbations of equilibrium such as deviations of temperature and chemical potential from their equilibrium values.

The essential difficulty of any attempt at rigorous justification of the transport theory was clearly pointed by Barry in the opening paragraph of Section 4 in [S]:

> *At some level, the fundamental difficulty of the transport theory is that it is a steady state rather then equilibrium problem, so that the powerful formalism of equilibrium statistical mechanics is unavailable, and one does not have any way of precisely identifying the steady state and thereby computing things in it.*

Motivated by the developments in classical non-equilibrium statistical mechanics (see the review [Ru4]), we address the central issue of non-equilibrium steady states (NESS) in two independent steps.

(A) The existence and analytic properties of NESS are assumed as an *axiom*. On the basis of this axiom one develops the mathematical theory of non-equilibrium quantum statistical mechanics in an abstract setting. This step is primarily concerned with the mathematical structure of the theory and its relation to the fundamental physical aspects of non-equilibrium (see [DGM, KTH]).

(B) The second step concerns study of specific physically relevant models. Relaxation to a NESS and analytical properties of this NESS are detailed dynamical problems which can be answered only in the context of concrete models. Once these fundamental problems are solved, the thermodynamics and the transport theory of the model are derived from the general structural results established in (A).

So far, the main focus of the program has been the second law of thermodynamics (positivity of the entropy production). In this case the part (A) has been settled in [Ru2, JP1, JP4], where the entropy production has been defined in the abstract framework of algebraic quantum statistical mechanics. In these works various structural properties of the entropy production have been established and in particular it was shown that the entropy production of any NESS is non-negative. The strict positivity of the entropy production is a problem which belongs to the category (B). At the moment there are two classes of non-trivial models whose NESS are well-understood and which have strictly positive entropy production. The first class of models describes an N-level quantum system coupled to finitely many independent free Fermi gas reservoirs [Da, LeSp, JP2]. The second class describes finitely many free Fermi gas reservoirs coupled by local interactions [BM, AM, FMU]. Some exactly solvable spin or fermion models with strictly positive entropy production have been studied in [AH, AP, AJPP1, AJPP2].

The natural next step in this program is the development of linear response theory and in particular the derivation of the Green-Kubo formulas (abbreviated GKF). In [JOP1] we have derived the GKF for heat fluxes in the axiomatic framework of algebraic quantum statistical mechanics. In this note we discuss a derivation which applies to both heat *and* charge fluxes and complete the step (A). Concerning (B), the examples to which our derivation directly applies include all models for which the strict positivity of the entropy production has been established. These applications are discussed in the forthcoming papers [JOP2, JOP3, JOPP].

A fundamental open question concerns (B) and the class of examples to which our derivation applies. The existing examples are limited to quasi-free systems coupled by local interactions. Although these examples include some important models of physical interest, it is of fundamental importance to understand NESS of interacting systems coupled by local interactions (this point has been repeatedly emphasized by David Ruelle). Only after that is achieved one may claim that a significant progress toward the resolution of Problem 4 B has been made.

This note is organized as follows. For notational purposes, in Section 2 we quickly review a few basic notions of algebraic quantum statistical mechanics. In Section 3 we introduce the model and review basic concepts of non-equilibrium statistical mechanics (the reader may complement this section with reviews [JP3, AJPP1]). Linear response theory is discussed in Section 4. Our main result is stated in Subsection 4.2. Its proof follows closely the arguments in [JOP1] and is outlined in Subsection 4.3. Various generalizations of our model and results are discussed in Section 5.

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2 Basic notions

Let $\mathcal{O}$ be a C^*-algebra with identity $\mathbb{1}$ and τ^t, $t \in \mathbb{R}$, a strongly continuous group of $*$-automorphisms of $\mathcal{O}$. The group τ and the pair $(\mathcal{O}, \tau)$ are often called C^*-dynamics and C^*-dynamical system. A state ω on $\mathcal{O}$ is called τ-invariant if $\omega \circ \tau^t = \omega$ for all $t \in \mathbb{R}$. An anti-linear involutive $*$-automorphism $\Theta : \mathcal{O} \to \mathcal{O}$ is called *time-reversal* of $(\mathcal{O}, \tau)$ if $\Theta \circ \tau^t = \tau^{-t} \circ \Theta$ for all $t \in \mathbb{R}$. A state ω on $\mathcal{O}$ is called time-reversal invariant if $\omega(\Theta(A)) = \omega(A^*)$ for all $A \in \mathcal{O}$.

We call quantum dynamical system a triple $(\mathcal{O}, \tau, \omega)$ where ω is a given state on $\mathcal{O}$. The state ω describes the initial (or reference) thermodynamical state of the system and is not necessarily τ-invariant (for a discussion of this point we refer the reader to Section 2 of [AJPP1]). Under normal conditions, i.e., under natural ergodicity assumptions, all ω-normal states are thermodynamically equivalent reference states in the sense that they lead to the same NESS.

We denote by $\mathrm{Ent}(\eta_1|\eta_2)$ the Araki relative entropy of two states η_1 and η_2. We use the sign and ordering convention of [BR2, Don, DJP] (hence, $\mathrm{Ent}(\eta_1|\eta_2) \in [-\infty, 0]$). The Araki relative entropy has played an important role in recent developments in non-equilibrium quantum statistical mechanics.

Let $\beta > 0$. A state ω is called a (τ, β)-KMS state if for all $A, B \in \mathcal{O}$ there exists a function $F_{A,B}(z)$, analytic in the strip $S_\beta = \{z \in \mathbb{C} \,|\, 0 < \mathrm{Im}\, z < \beta\}$, bounded and continuous on its closure, and satisfying the KMS-boundary condition

$$F_{A,B}(t) = \omega(A\tau^t(B)), \qquad F_{A,B}(t + \mathrm{i}\beta) = \omega(\tau^t(B)A).$$

As usual, we write $\omega(A\tau^z(B)) = F_{A,B}(z)$ for $z \in \overline{S}_\beta$ even when $\tau^z(B)$ is not well-defined. A (τ, β)-KMS states describes a physical system in thermal equilibrium at inverse temperature β.

The general theory of chemical potential in quantum statistical mechanics is discussed in Section 5.4.3 of [BR2]. In our study of linear response theory we will only consider the chemical potential associated to the usual $U(1)$ gauge invariance of quantum mechanics. We will call charge flux the current associated to the corresponding conserved charge. The extension of our results to more general gauge groups is straightforward. Since we only need a fraction of the mathematical structures commonly associated to the chemical potential we shall be brief. Let ϑ^φ be a C^*-dynamics on $\mathcal{O}$ such that $\tau^t \circ \vartheta^\varphi = \vartheta^\varphi \circ \tau^t$ for all $t, \varphi \in \mathbb{R}$. ϑ is the gauge-group and its elements ϑ^φ are gauge transformations. Physical observables are invariant under gauge transformations and are therefore elements of

$$\mathcal{O}_\vartheta = \{A \in \mathcal{O} \,|\, \vartheta^\varphi(A) = A \text{ for all } \varphi \in \mathbb{R}\}. \tag{2.1}$$

Note that $\mathcal{O}_\vartheta$ is a τ-invariant C^*-subalgebra of $\mathcal{O}$ and so $(\mathcal{O}_\vartheta, \tau)$ is a C^*-dynamical system. Let $\mu \in \mathbb{R}$ and

$$\alpha^t = \tau^t \circ \vartheta^{-\mu t}.$$

We say that a state ω on $\mathcal{O}$ is a $(\tau, \vartheta, \beta, \mu)$-KMS state if it is an (α, β)-KMS state. Although this last terminology is not common, it is convenient for our purposes. A $(\tau, \vartheta, \beta, \mu)$-KMS state describes a physical system in equilibrium at inverse temperature β and chemical potential μ. Note that if ω is a $(\tau, \vartheta, \beta, \mu)$-KMS state on $\mathcal{O}$ then its restriction to the gauge-invariant subalgebra $\mathcal{O}_\vartheta$ is a (τ, β)-KMS state on $\mathcal{O}_\vartheta$.

3 The model and the framework

3.1 The model

Our starting point are two C^*-dynamical systems $(\mathcal{O}_{\rm L}, \tau_{\rm L})$ and $(\mathcal{O}_{\rm R}, \tau_{\rm R})$ with gauge-groups $\vartheta_{\rm L}$ and $\vartheta_{\rm R}$. For convenience we shall call them the left, L, and the right, R, system. We denote the generators of $\tau_{\rm L}$, $\tau_{\rm R}$, $\vartheta_{\rm L}$ and $\vartheta_{\rm R}$ by $\delta_{\rm L}$, $\delta_{\rm R}$, $\xi_{\rm L}$ and $\xi_{\rm R}$.

The C^*-algebra of the joint system L + R is $\mathcal{O} = \mathcal{O}_{\rm L} \otimes \mathcal{O}_{\rm R}$ and its decoupled (non-interacting) dynamics is $\tau_0 = \tau_{\rm L} \otimes \tau_{\rm R}$. The generator of τ_0 is $\delta_0 = \delta_{\rm L} \otimes I + I \otimes \delta_{\rm R}$. In the sequel, whenever the meaning is clear within the context, we shall write $\delta_{\rm L}$ for $\delta_{\rm L} \otimes I$, $\delta_{\rm R}$ for $I \otimes \delta_{\rm R}$, etc.

The gauge-group of the joint system is $\vartheta = \vartheta_{\rm L} \otimes \vartheta_{\rm R}$ and its generator is $\xi = \xi_{\rm L} + \xi_{\rm R}$. We denote by $\mathcal{O}_\vartheta$ the corresponding gauge-invariant subalgebra of $\mathcal{O}$.

Let $V \in \mathcal{O}_\vartheta$ be a self-adjoint element describing the interaction of L and R. The interacting C^*-dynamics τ is generated by $\delta = \delta_0 + {\rm i}[V, \cdot\,]$ and commutes with the gauge-group ϑ. The coupled (interacting) joint system L + R is described by the C^*-dynamical system $(\mathcal{O}, \tau)$.

3.2 The reference states

We set $I_\epsilon(x) = (x - \epsilon, x + \epsilon)$ and write $I_\epsilon(0) = I_\epsilon$.

Let $\beta_{\rm eq} > 0$ and $\mu_{\rm eq} \in \mathbb{R}$ be given reference (equilibrium) values of the inverse temperature and the chemical potential. We make the following assumptions concerning the initial states of L and R.

> **(A1)** $\omega_{\rm L}$ is the unique $(\tau_{\rm L}, \vartheta_{\rm L}, \beta_{\rm eq}, \mu_{\rm eq})$-KMS state on $\mathcal{O}_{\rm L}$. The reference states of R are parametrized by $\beta \in I_{\epsilon_1}(\beta_{\rm eq})$ and $\mu \in I_{\epsilon_2}(\mu_{\rm eq})$ and $\omega_{{\rm R},\beta,\mu}$ is the unique $(\tau_{\rm R}, \vartheta_{\rm R}, \beta, \mu)$-KMS state on $\mathcal{O}_{\rm R}$. We shall denote $\omega_{{\rm R},\beta_{\rm eq},\mu_{\rm eq}}$ by $\omega_{\rm R}$.

Throughout the paper we shall assume that (A1) holds. The reference states of our model are $\omega_{\rm L} \otimes \omega_{{\rm R},\beta,\mu}$, $\beta \in I_{\epsilon_1}(\beta_{\rm eq})$, $\mu \in I_{\epsilon_2}(\mu_{\rm eq})$. For our purposes it is convenient to introduce the parameters (thermodynamical forces)

$$X = \beta_{\rm eq} - \beta, \qquad Y = \beta\mu - \beta_{\rm eq}\mu_{\rm eq},$$

and to parametrize the reference states by X and Y, i.e., we write

$$\omega_{X,Y,0} = \omega_{\rm L} \otimes \omega_{{\rm R},\beta,\mu}.$$

Since we are interested in linear response theory, without loss of generality we may restrict the values of X, Y to I_ϵ, where $\epsilon > 0$ is a small positive number. Note that $\omega_{0,0,0}$ is the unique $(\tau_0, \vartheta, \beta_{\rm eq}, \mu_{\rm eq})$-KMS state on $\mathcal{O}$.

As we have already mentioned, under normal conditions all $\omega_{X,Y,0}$-normal states are thermodynamically equivalent reference states of L + R. We now describe a particular $\omega_{X,Y,0}$-normal reference state which will play an important role in our discussion of linear response theory.

Set

$$\alpha_{\rm L}^t = \tau_{\rm L}^t \circ \vartheta_{\rm L}^{-\mu_{\rm eq} t}, \qquad \alpha_{{\rm R},\mu}^t = \tau_{\rm R}^t \circ \vartheta_{\rm R}^{-\mu t}.$$

Assumption (A1) implies that $\omega_{\rm L}$ is the unique $(\alpha_{\rm L}, \beta_{\rm eq})$-KMS state on $\mathcal{O}_{\rm L}$ and that $\omega_{{\rm R},\beta,\mu}$ is the unique $(\alpha_{{\rm R},\mu}, \beta)$-KMS state on $\mathcal{O}_{\rm R}$. Set

$$\alpha_{X,Y,0}^t = \alpha_{\rm L}^t \otimes \alpha_{{\rm R},\mu}^{\beta t/\beta_{\rm eq}}.$$

Then $\omega_{X,Y,0}$ is the unique $(\alpha_{X,Y,0}, \beta_{\rm eq})$-KMS state on $\mathcal{O}$. Let $\delta_{X,Y,0}$ be the generator of $\alpha_{X,Y,0}$ and

$$\delta_{X,Y} = \delta_{X,Y,0} + {\rm i}[V, \cdot\,].$$

The subalgebra ${\rm Dom}\,(\delta_{\rm L}) \cap {\rm Dom}\,(\xi_{\rm L}) \cap {\rm Dom}\,(\delta_{\rm R}) \cap {\rm Dom}\,(\xi_{\rm R})$ is a core for $\delta_{X,Y,0}$ and $\delta_{X,Y}$. On this subalgebra $\delta_{X,Y,0}$ acts as

$$\delta_{X,Y,0} = \delta_0 - \mu_{\rm eq}\xi - \frac{X}{\beta_{\rm eq}}\delta_{\rm R} - \frac{Y}{\beta_{\rm eq}}\xi_{\rm R}. \tag{3.2}$$

Let $\alpha_{X,Y}$ be the C^*-dynamics generated by $\delta_{X,Y}$. Araki's perturbation theory yields that there exists a unique $(\alpha_{X,Y}, \beta_{\rm eq})$-KMS state $\omega_{X,Y}$ on $\mathcal{O}$.

The states $\omega_{X,Y,0}$ and $\omega_{X,Y}$ are mutually normal. The reference states $\omega_{X,Y}$ will play a central role in our study of linear response theory. Note that $\omega_{0,0}$ is the unique $(\tau, \vartheta, \beta_{\rm eq}, \mu_{\rm eq})$-KMS state on $\mathcal{O}$. We denote this state by $\omega_{\rm eq}$. The next assumption concerns the $(\tau, \beta_{\rm eq})$-KMS state induced by $\omega_{\rm eq}$ on the gauge invariant subalgebra $\mathcal{O}_\vartheta$.

(A2) For all $A, B \in \mathcal{O}_\vartheta$,

$$\lim_{|t|\to\infty} \omega_{\rm eq}(\tau^t(A)B) = \omega_{\rm eq}(A)\omega_{\rm eq}(B).$$

A well-known consequence of the KMS condition and Assumption (A2) is the relation

$$\lim_{t\to+\infty} \int_{-t}^{t} \omega_{\rm eq}([\tau^s(A), B]){\rm d}s = 0, \tag{3.3}$$

which holds for all $A, B \in \mathcal{O}_\vartheta$ (see Theorem 5.4.12 in [BR2]). This relation plays a key role in the derivation of the Onsager reciprocity relations.

3.3 Non-equilibrium steady states and regular observables

We postulate relaxation to a NESS as follows:

(A3) For all $X, Y \in I_\epsilon$ there exists a state $\omega_{X,Y,+}$ on $\mathcal{O}_\vartheta$ such that for all $A \in \mathcal{O}_\vartheta$,

$$\lim_{t\to+\infty} \omega_{X,Y}(\tau^t(A)) = \omega_{X,Y,+}(A).$$

Assumptions (A2) and (A3) are strong ergodic hypotheses which are difficult to verify in concrete models. In typical physical situations one expects more, namely that

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

for all $\omega_{X,Y,0}$-normal states η and $A \in \mathcal{O}_\vartheta$. Indeed, such strong form of approach to NESS has been established in all examples we consider in [JOP2, JOP3, JOPP]. However, we will not need such an assumption in our axiomatic study of linear response theory.

The observables for which we establish the Green-Kubo formulas are characterized by the following regularity properties.

Definition 3.1 *Assume that (A3) holds. Let* $A \in \mathcal{O}_\vartheta$ *be an observable such that the function*

$$(X, Y) \mapsto \omega_{X,Y}(\tau^t(A)),$$

is differentiable at $(0,0)$ *for all* t*. We call such an observable regular if the function*

$$(X, Y) \mapsto \omega_{X,Y,+}(A),$$

is also differentiable at $(0,0)$ *and*

$$\begin{aligned}\lim_{t\to+\infty} \partial_X \omega_{X,Y}(\tau^t(A))\big|_{X=Y=0} &= \partial_X \omega_{X,Y,+}(A)\big|_{X=Y=0},\\ \lim_{t\to+\infty} \partial_Y \omega_{X,Y}(\tau^t(A))\big|_{X=Y=0} &= \partial_Y \omega_{X,Y,+}(A)\big|_{X=Y=0}.\end{aligned} \tag{3.4}$$

3.4 Time-reversal invariance

Our next assumption concerns time-reversal.

> **(A4)** There exists a time-reversal Θ of $(\mathcal{O}, \tau_0)$ such that $\Theta(V) = V$ and
>
> $$\Theta \circ \tau_{\mathrm{L}}^t = \tau_{\mathrm{L}}^{-t} \circ \Theta, \qquad \Theta \circ \tau_{\mathrm{R}}^t = \tau_{\mathrm{R}}^{-t} \circ \Theta, \qquad \Theta \circ \vartheta_{\mathrm{L}}^\varphi = \vartheta_{\mathrm{L}}^{-\varphi} \circ \Theta, \qquad \Theta \circ \vartheta_{\mathrm{R}}^\varphi = \vartheta_{\mathrm{R}}^{-\varphi} \circ \Theta,$$
>
> for all $t, \varphi \in \mathbb{R}$.

Clearly, Θ is a time-reversal of $(\mathcal{O}, \vartheta)$ and $(\mathcal{O}, \alpha_{X,Y,0})$. In particular it leaves $\mathcal{O}_\vartheta$ invariant. It is not difficult to show that Θ is also a time-reversal of $(\mathcal{O}, \tau)$ and $(\mathcal{O}, \alpha_{X,Y})$, and that the states $\omega_{X,Y,0}$ and $\omega_{X,Y}$ are time-reversal invariant. The proofs of these facts are the same as the proof of Lemma 3.1 in [JOP1].

3.5 Fluxes

To define the flux observables we need:

> **(A5)** $V \in \mathrm{Dom}\,(\delta_{\mathrm{R}}) \cap \mathrm{Dom}\,(\xi_{\mathrm{R}})$.

If (A5) holds, we set

$$\Phi = \delta_{\mathrm{R}}(V), \qquad \mathcal{J} = \xi_{\mathrm{R}}(V).$$

The observable Φ describes the heat flux out of the system R. The observable $\mathcal{J}$ describes the charge flux out of R. Since $V \in \mathcal{O}_\vartheta$ and τ_{R}, ϑ_{R} commute with ϑ we have $\Phi, \mathcal{J} \in \mathcal{O}_\vartheta$. If the time-reversal assumption (A4) holds, then

$$\Theta(\Phi) = -\Phi, \qquad \Theta(\mathcal{J}) = -\mathcal{J}.$$

3.6 Entropy balance equation

In the recent literature the entropy balance equation has been always discussed with respect to the product reference state $\omega_{X,Y,0}$ [Ru2, Ru3, JP1, JP3, JP4]. The finite time entropy balance equation w.r.t. the reference state $\omega_{X,Y}$ has the following form.

Theorem 3.2 *Assume that* $V \in \mathrm{Dom}\,(\delta_{\mathrm{L}}) \cap \mathrm{Dom}\,(\xi_{\mathrm{L}}) \cap \mathrm{Dom}\,(\delta_{\mathrm{R}}) \cap \mathrm{Dom}\,(\xi_{\mathrm{R}})$. *Then*

$$\mathrm{Ent}(\omega_{X,Y} \circ \tau^t | \omega_{X,Y}) = -X \int_0^t \omega_{X,Y}(\tau^s(\Phi))\mathrm{d}s - Y \int_0^t \omega_{X,Y}(\tau^s(\mathcal{J}))\mathrm{d}s. \tag{3.5}$$

Proof. The assumptions of the theorem imply that $V \in \mathrm{Dom}\,(\delta_{X,Y})$. Since $V \in \mathcal{O}_\vartheta$ implies $\xi(V) = 0$, we have

$$\beta_{\rm eq}\delta_{X,Y}(V) = \beta_{\rm eq}\delta(V) - X\Phi - Y\mathcal{J}. \tag{3.6}$$

The entropy balance equation of [JP1, JP4] yields

$$\begin{aligned}
\mathrm{Ent}(\omega_{X,Y} \circ \tau^t|\omega_{X,Y,0}) &= \mathrm{Ent}(\omega_{X,Y}|\omega_{X,Y,0}) + \beta_{\rm eq}\int_0^t \omega_{X,Y}(\tau^s(\delta_{X,Y}(V)))\mathrm{d}s \\
&= \mathrm{Ent}(\omega_{X,Y}|\omega_{X,Y,0}) + \beta_{\rm eq}\omega_{X,Y}(\tau^t(V)) - \beta_{\rm eq}\omega_{X,Y}(V) \\
&\quad - X\int_0^t \omega_{X,Y}(\tau^s(\Phi))\mathrm{d}s - Y\int_0^t \omega_{X,Y}(\tau^s(\mathcal{J}))\mathrm{d}s.
\end{aligned} \tag{3.7}$$

The fundamental formula of Araki [Ar1, Ar2] (see also [BR2, Don, DJP]) yields that

$$\begin{aligned}
\mathrm{Ent}(\omega_{X,Y} \circ \tau^t|\omega_{X,Y}) &= \mathrm{Ent}(\omega_{X,Y} \circ \tau^t|\omega_{X,Y,0}) - \beta_{\rm eq}\omega_{X,Y}(\tau^t(V)) + C, \\
\mathrm{Ent}(\omega_{X,Y}|\omega_{X,Y,0}) &= \beta_{\rm eq}\omega_{X,Y}(V) - C,
\end{aligned} \tag{3.8}$$

where C is a constant expressible in terms of the modular structure (we do not need its explicit form here). The relations (3.7) and (3.8) yield the statement. □

The entropy production of the NESS $\omega_{X,Y,+}$ is defined by

$$\mathrm{Ep}(\omega_{X,Y,+}) = -\lim_{t\to+\infty}\frac{\mathrm{Ent}(\omega_{X,Y} \circ \tau^t|\omega_{X,Y})}{t}.$$

Theorem 3.2 yields

$$\mathrm{Ep}(\omega_{X,Y,+}) = X\omega_{X,Y,+}(\Phi) + Y\omega_{X,Y,+}(\mathcal{J}) \geq 0, \tag{3.9}$$

and this relation is the second law of thermodynamics for our model. Of course, if $(X, Y) \neq (0, 0)$, then under normal conditions one expects that $\mathrm{Ep}(\omega_{X,Y,+}) > 0$, i.e., that the fluxes are non-vanishing. The strict positivity of entropy production is a detailed dynamical question which can be answered only in the context of specific models.

3.7 Centered observables

An observable $A \in \mathcal{O}$ is called *centered* if $\omega_{X,Y}(A) = 0$ for all $X, Y \in I_\epsilon$. We denote by $\mathcal{C}$ the set of all centered observables. Obviously, $\mathcal{C}$ is a norm-closed vector subspace of $\mathcal{O}$. Our derivation of the Green-Kubo formula applies only to centered observables.

If Assumption (A4) holds, then any self-adjoint observable A satisfying $\Theta(A) = -A$ is centered. Indeed, since $\omega_{X,Y}$ is time-reversal invariant, $\omega_{X,Y}(A) = \omega_{X,Y}(\Theta(A)) = -\omega_{X,Y}(A)$, and so $\omega_{X,Y}(A) = 0$. In particular, if (A4) holds, then the flux observables Φ and $\mathcal{J}$ are centered.

It is an important fact that the flux observables are centered irrespectively of the time-reversal assumption. This fact will play a central role in our discussion of the Green-Kubo formula for systems which are not time-reversal invariant.

Proposition 3.3 *Assume that* $V \in \mathrm{Dom}\,(\delta_{\rm R}) \cap \mathrm{Dom}\,(\xi_{\rm R})$. *Then for all* $X, Y \in I_\epsilon$,

$$\omega_{X,Y}(\Phi) = \omega_{X,Y}(\mathcal{J}) = 0.$$

Proof. Assume first that

$$V \in \mathrm{Dom}\,(\delta_{\mathrm{L}}) \cap \mathrm{Dom}\,(\xi_{\mathrm{L}}) \cap \mathrm{Dom}\,(\delta_{\mathrm{R}}) \cap \mathrm{Dom}\,(\xi_{\mathrm{R}}). \tag{3.10}$$

Note that C^*-dynamics $\alpha_{X,Y}$ is well-defined for all $X, Y \in \mathbb{R}$. The following generalization of the entropy balance equation (3.5) holds: for all $X, Y \in I_\epsilon$ and $Z, U \in \mathbb{R}$,

$$\mathrm{Ent}(\omega_{X,Y} \circ \alpha^t_{Z,U} | \omega_{X,Y}) = -(X - Z) \int_0^t \omega_{X,Y}(\alpha^s_{Z,U}(\Phi))\mathrm{d}s - (Y - U) \int_0^t \omega_{X,Y}(\alpha^s_{Z,U}(\mathcal{J}))\mathrm{d}s. \tag{3.11}$$

The proof of this relation is essentially the same as the proof of (3.5). The only difference is that the relation (3.6) is now replaced with

$$\beta_{\mathrm{eq}}\delta_{X,Y}(V) = \beta_{\mathrm{eq}}\delta_{Z,U}(V) - (X - Z)\Phi - (Y - U)\mathcal{J}. \tag{3.12}$$

The entropy balance equation of [JP1, JP4] yields

$$\mathrm{Ent}(\omega_{X,Y} \circ \alpha^t_{Z,U} | \omega_{X,Y,0}) = \mathrm{Ent}(\omega_{X,Y} | \omega_{X,Y,0}) + \beta_{\mathrm{eq}} \int_0^t \omega_{X,Y}(\alpha^s_{Z,U}(\delta_{X,Y}(V)))\mathrm{d}s,$$

and the rest of the argument follows line by line the proof of Theorem 3.2.

The equation (3.11) yields

$$\lim_{t \downarrow 0} \frac{\mathrm{Ent}(\omega_{X,Y} \circ \alpha^t_{Z,U} | \omega_{X,Y})}{t} = -(X - Z)\omega_{X,Y}(\Phi) - (Y - U)\omega_{X,Y}(\mathcal{J}),$$

and so for all $X, Y \in I_\epsilon$ and $Z, U \in \mathbb{R}$,

$$(X - Z)\omega_{X,Y}(\Phi) + (Y - U)\omega_{X,Y}(\mathcal{J}) \geq 0.$$

This relation yields the statement.

To prove the general case, let $V \in \mathrm{Dom}\,(\delta_{\mathrm{R}}) \cap \mathrm{Dom}\,(\xi_{\mathrm{R}})$ and

$$V_j = \frac{j}{\pi} \int_{\mathbb{R}^2} \mathrm{e}^{-j(t^2+s^2)} \tau^t_{\mathrm{L}} \circ \vartheta^s_{\mathrm{L}}(V)\mathrm{d}t\mathrm{d}s, \qquad j = 1, 2, \ldots .$$

The observables V_j satisfy (3.10). Let $\omega_{X,Y,j}$ and $\Phi_j, \mathcal{J}_j$ be the reference state and the flux observables associated to V_j. We have established that for all $X, Y \in I_\epsilon$,

$$\omega_{X,Y,j}(\Phi_j) = \omega_{X,Y,j}(\mathcal{J}_j) = 0. \tag{3.13}$$

By the properties of analytic approximations (see [BR2]), $\|\omega_{X,Y,j} - \omega_{X,Y}\| \to 0$, $\|\Phi_j - \Phi\| \to 0$, $\|\mathcal{J}_j - \mathcal{J}\| \to 0$ as $j \to \infty$, and the statement follows from (3.13). □

Note that we did not use the gauge invariance of V in the above proof.

4 Linear response theory

4.1 Overview

Suppose that Assumptions (A3) and (A5) hold and that the functions

$$(X, Y) \mapsto \omega_{X,Y,+}(\Phi), \qquad (X, Y) \mapsto \omega_{X,Y,+}(\mathcal{J}),$$

are differentiable at $(0,0)$. The kinetic transport coefficients are defined by

$$\begin{aligned}
L_{\rm hh} &= \partial_X \omega_{X,Y,+}(\Phi)\big|_{X=Y=0}, \\
L_{\rm hc} &= \partial_Y \omega_{X,Y,+}(\Phi)\big|_{X=Y=0}, \\
L_{\rm ch} &= \partial_X \omega_{X,Y,+}(\mathcal{J})\big|_{X=Y=0}, \\
L_{\rm cc} &= \partial_Y \omega_{X,Y,+}(\mathcal{J})\big|_{X=Y=0},
\end{aligned} \tag{4.14}$$

where indices h/c stand for heat/charge. Linear response theory is concerned with these coefficients. An elementary consequence of the second law (Relation (3.9)) is that the matrix

$$L = \begin{bmatrix} L_{\rm hh} & L_{\rm hc} \\ L_{\rm ch} & L_{\rm cc} \end{bmatrix},$$

is positive definite on the real vector space $\mathbb{R}^2$ (this of course does not imply that $L_{\rm hc} = L_{\rm ch}$!).

The Green-Kubo formulas are at the center of linear response theory. For $A, B \in \mathcal{O}_\vartheta$ we set

$$\mathcal{L}(A,B) = \lim_{t\to+\infty} \frac{1}{2}\int_{-t}^{t} \omega_{\rm eq}(A\tau^s(B))\mathrm{d}s.$$

The GKF assert that if the system is time-reversal invariant, then

$$\begin{aligned}
L_{\rm hh} &= \mathcal{L}(\Phi,\Phi), \\
L_{\rm hc} &= \mathcal{L}(\Phi,\mathcal{J}), \\
L_{\rm ch} &= \mathcal{L}(\mathcal{J},\Phi), \\
L_{\rm cc} &= \mathcal{L}(\mathcal{J},\mathcal{J}).
\end{aligned} \tag{4.15}$$

These formulas are mathematical expressions of the fluctuation-dissipation mechanism in statistical mechanics—they link linear response to a thermodynamical force to the equilibrium correlations w.r.t. the corresponding flux observable.

The coefficients $L_{\rm hc}$ and $L_{\rm ch}$ are of particular physical importance. In words, the chemical potential difference may cause a heat flow out of R even if L and R are at the same temperature. For Y small, this flow is equal to $YL_{\rm hc} + o(Y)$. Similarly, the temperature difference may cause a charge flow out of R even if L and R have equal chemical potentials. For X small this flow is equal to $XL_{\rm ch} + o(X)$. An immediate consequence of the second and third relation in (4.15) and the formula (3.3) are the Onsager reciprocity relations

$$L_{\rm hc} = L_{\rm ch}. \tag{4.16}$$

For $A, B \in \mathcal{O}_\vartheta$ and $t \in \mathbb{R}$ we set

$$\mathfrak{L}(A,B,t) = \frac{1}{\beta_{\rm eq}}\int_0^t \mathrm{d}s \int_0^{\beta_{\rm eq}} \mathrm{d}u\, \omega_{\rm eq}(\tau^s(A)\tau^{\mathrm{i}u}(B)),$$

and

$$\mathfrak{L}(A,B) = \lim_{t\to+\infty} \mathfrak{L}(A,B,t),$$

whenever the limit exists. We remark that by the KMS condition the function

$$(s,z) \mapsto \omega_{\rm eq}(\tau^s(A)\tau^z(B)),$$

is bounded and continuous on the set $\mathbb{R} \times \overline{S}_{\beta_{\rm eq}}$. The central step in our derivation of (4.15) are the following formulas

$$\begin{aligned} L_{\rm hh} &= \mathfrak{L}(\Phi, \Phi), \\ L_{\rm hc} &= \mathfrak{L}(\Phi, \mathcal{J}), \\ L_{\rm ch} &= \mathfrak{L}(\mathcal{J}, \Phi), \\ L_{\rm cc} &= \mathfrak{L}(\mathcal{J}, \mathcal{J}). \end{aligned} \tag{4.17}$$

It is an important point that these formulas hold *without the time-reversal assumption*— they are the Green-Kubo formulas for systems which are not time-reversal invariant. The Green-Kubo formulas (4.15) are an immediate consequence of (4.17) and the following result established in [JOP1].

Proposition 4.1 *Suppose that Assumptions (A1), (A2), and (A4) hold and let* $A, B \in \mathcal{O}_\vartheta$ *be two self-adjoint observables which are both even or odd under* Θ. *Then*

$$\mathcal{L}(A, B) = \mathfrak{L}(A, B).$$

Proof. The argument follows line by line the proof of Theorem 2.3 in [JOP1]. For reader convenience we outline the main steps of the argument.

We need to prove that

$$\lim_{t\to+\infty} \frac{1}{\beta_{\rm eq}} \int_0^{\beta_{\rm eq}} \left[\int_0^t \omega_{\rm eq}(\tau^s(A)\tau^{{\rm i}u}(B)){\rm d}s \right] {\rm d}u = \lim_{t\to+\infty} \int_{-t}^t \omega_{\rm eq}(A\tau^s(B)){\rm d}s.$$

The time-reversal invariance and the KMS-condition yield that for $s \in \mathbb{R}$ and $u \in [0, \beta]$,

$$\omega_{\rm eq}(\tau^s(A)\tau^{{\rm i}u}(B)) = \omega_{\rm eq}(\tau^{-s}(A)\tau^{{\rm i}\beta_{\rm eq}-{\rm i}u}(B)),$$

and so

$$\frac{1}{\beta_{\rm eq}} \int_0^{\beta_{\rm eq}} \left[\int_0^t \omega_{\rm eq}(\tau^s(A)\tau^{{\rm i}u}(B)){\rm d}s \right] {\rm d}u = \frac{1}{2\beta_{\rm eq}} \int_0^{\beta_{\rm eq}} \left[\int_{-t}^t \omega_{\rm eq}(A\tau^{s+{\rm i}u}(B)){\rm d}s \right] {\rm d}u.$$

Since the integral of the function $z \mapsto \omega_{\rm eq}(A\tau^z(B))$ over the boundary of the rectangle with vertices $-t, t, t + {\rm i}u, -t + {\rm i}u$ is zero, we have

$$\frac{1}{\beta_{\rm eq}} \int_0^{\beta_{\rm eq}} \left[\int_0^t \omega_{\rm eq}(\tau^s(A)\tau^{{\rm i}u}(B)){\rm d}s \right] {\rm d}u = \frac{1}{2} \int_{-t}^t \omega_{\rm eq}(A\tau^s(B)){\rm d}s + \frac{1}{2\beta_{\rm eq}} \int_0^{\beta_{\rm eq}} R(t, u){\rm d}u, \tag{4.18}$$

where

$$R(t, u) = {\rm i} \int_0^u \left[\omega_{\rm eq}(A\tau^{t+{\rm i}y}(B)) - \omega_{\rm eq}(A\tau^{-t+{\rm i}y}(B)) \right] {\rm d}y.$$

Assumption (A2) implies that

$$\lim_{t\to+\infty} \omega_{\rm eq}(A\tau^{\pm t+{\rm i}y}(B)) = \omega_{\rm eq}(A)\omega_{\rm eq}(B),$$

and the dominated convergence theorem yields

$$\lim_{t\to+\infty} \sup_{0\le u\le\beta} |R(t, u)| = 0.$$

This fact and the formula (4.18) yield the statement. □

In the next subsection we state our main results concerning the Green-Kubo formulas.

4.2 The Green-Kubo formulas

We set

$$\mathcal{O}_{\vartheta,\mathrm{R}} = \mathcal{O}_{\vartheta} \cap \mathrm{Dom}\,(\delta_{\mathrm{R}}) \cap \mathrm{Dom}\,(\xi_{\mathrm{R}}),$$

$$\mathcal{O}_{\vartheta,\mathrm{R,c}} = \mathcal{O}_{\vartheta,\mathrm{R}} \cap \mathcal{C}.$$

Our key technical result is:

Theorem 4.2 *Suppose that Assumptions (A1) and (A5) hold and let* $A \in \mathcal{O}_{\vartheta,\mathrm{R,c}}$. *Then for all* $t \in \mathbb{R}$ *the function*

$$(X, Y) \mapsto \omega_{X,Y}(\tau^t(A)),$$

is differentiable at $(0, 0)$ *and*

$$\partial_X \omega_{X,Y}(\tau^t(A))\big|_{X=Y=0} = \mathfrak{L}(A, \Phi, t),$$

$$\partial_Y \omega_{X,Y}(\tau^t(A))\big|_{X=Y=0} = \mathfrak{L}(A, \mathcal{J}, t).$$

We will prove Theorem 4.2 in Subsection 4.3. The next two theorems are consequence of Theorem 4.2, definition of the regular observable, and Proposition 4.1.

Theorem 4.3 *Suppose that Assumptions (A1), (A3) and (A5) hold.*
(1) *Let* $A \in \mathcal{O}_{\vartheta,\mathrm{R,c}}$ *be a regular observable. Then*

$$\partial_X \omega_{X,Y,+}(A)\big|_{X=Y=0} = \mathfrak{L}(A, \Phi),$$

$$\partial_Y \omega_{X,Y,+}(A)\big|_{X=Y=0} = \mathfrak{L}(A, \mathcal{J}).$$

(2) *If in addition (A2) and (A4) hold and* $A \in \mathcal{O}_{\vartheta,\mathrm{R}}$ *is a regular self-adjoint observable such that* $\Theta(A) = -A$, *then*

$$\partial_X \omega_{X,Y,+}(A)\big|_{X=Y=0} = \mathcal{L}(A, \Phi),$$

$$\partial_Y \omega_{X,Y,+}(A)\big|_{X=Y=0} = \mathcal{L}(A, \mathcal{J}).$$

Theorem 4.4 *Suppose that Assumptions (A1), (A3) and (A5) hold and that* $\Phi, \mathcal{J}$ *are regular observables in* $\mathrm{Dom}\,(\delta_{\mathrm{R}}) \cap \mathrm{Dom}\,(\xi_{\mathrm{R}})$. *Then the formulas (4.17) hold. If in addition (A2) and (A4) hold, then the formulas (4.15) and (4.16) hold.*

Theorem 4.2 was proven in [JOP1] in the case $\mu_{\mathrm{eq}} = 0$, $Y = 0$. The technical extensions of the proofs in [JOP1] needed to accommodate charge fluxes are relatively minor and are discussed in the next section.

4.3 Proof of Theorem 4.2

We will freely use the notation introduced in Subsection 3.1.

Lemma 4.5 (a) *The group* $\alpha_{0,0}$ *preserves* $\mathrm{Dom}\,(\delta_{\mathrm{R}}) \cap \mathrm{Dom}\,(\xi_{\mathrm{R}})$ *and for* $A \in \mathrm{Dom}\,(\delta_{\mathrm{R}}) \cap \mathrm{Dom}\,(\xi_{\mathrm{R}})$ *the functions*

$$\mathbb{R} \ni t \mapsto \delta_{\mathrm{R}}(\alpha_{0,0}^t(A)), \qquad \mathbb{R} \ni t \mapsto \xi_{\mathrm{R}}(\alpha_{0,0}^t(A)),$$

are norm continuous.
(b) *For all $t \in \mathbb{R}$ and $A \in \mathrm{Dom}\,(\delta_{\mathrm{R}}) \cap \mathrm{Dom}\,(\xi_{\mathrm{R}})$,*

$$\alpha_{X,Y}^{t}(A) - \alpha_{0,0}^{t}(A) = -\frac{X}{\beta_{\mathrm{eq}}} \int_0^t \alpha_{X,Y}^{t-s}(\delta_{\mathrm{R}}(\alpha_{0,0}^{s}(A)))\mathrm{d}s - \frac{Y}{\beta_{\mathrm{eq}}} \int_0^t \alpha_{X,Y}^{t-s}(\xi_{\mathrm{R}}(\alpha_{0,0}^{s}(A)))\mathrm{d}s.$$

(c) *For all $t \in \mathbb{R}$ and $A \in \mathcal{O}$,*

$$\lim_{(X,Y)\to(0,0)} \|\alpha_{X,Y}^{t}(A) - \alpha_{0,0}^{t}(A)\| = 0.$$

(d) *For all $A \in \mathcal{O}$,*

$$\lim_{(X,Y)\to(0,0)} \omega_{X,Y}(A) = \omega_{\mathrm{eq}}(A).$$

Proof. To simplify notation let us set $\alpha_0 = \alpha_{0,0,0}$ and $\alpha = \alpha_{0,0}$. We shall use the identity

$$\alpha^t(A) = \Gamma_t \alpha_0^t(A) \Gamma_t^*,$$

where $\Gamma_t \in \mathcal{O}$ is a family of unitary elements defined by

$$\Gamma_t = \mathbb{1} + \sum_{n\geq 1} (\mathrm{i}t)^n \int_{0\leq s_n\leq\cdots s_1\leq 1} \alpha_0^{ts_n}(V)\cdots\alpha_0^{ts_1}(V)\mathrm{d}s_1\cdots\mathrm{d}s_n,$$

see Proposition 5.4.1 in [BR2]. Since $V \in \mathrm{Dom}\,(\delta_{\mathrm{R}}) \cap \mathrm{Dom}\,(\xi_{\mathrm{R}})$, one easily shows that $\Gamma_t \in \mathrm{Dom}\,(\delta_{\mathrm{R}}) \cap \mathrm{Dom}\,(\xi_{\mathrm{R}})$ and that

$$\delta_{\mathrm{R}}(\Gamma_t) = \sum_{n\geq 1} (\mathrm{i}t)^n \int_{0\leq s_n\leq\cdots s_1\leq 1} \sum_j \alpha_0^{ts_n}(V)\cdots\alpha_0^{ts_j}(\delta_{\mathrm{R}}(V))\cdots\alpha_0^{ts_1}(V)\mathrm{d}s_1\cdots\mathrm{d}s_n,$$

$$\xi_{\mathrm{R}}(\Gamma_t) = \sum_{n\geq 1} (\mathrm{i}t)^n \int_{0\leq s_n\leq\cdots s_1\leq 1} \sum_j \alpha_0^{ts_n}(V)\cdots\alpha_0^{ts_j}(\xi_{\mathrm{R}}(V))\cdots\alpha_0^{ts_1}(V)\mathrm{d}s_1\cdots\mathrm{d}s_n.$$

These two formulas yield that the functions

$$t \mapsto \delta_{\mathrm{R}}(\Gamma_t), \qquad t \mapsto \xi_{\mathrm{R}}(\Gamma_t),$$

are norm continuous. Finally, the identities

$$\delta_{\mathrm{R}}(\alpha^t(A)) = \delta_{\mathrm{R}}(\Gamma_t)\alpha_0^t(A)\Gamma_t^* + \Gamma_t\alpha_0^t(\delta_{\mathrm{R}}(A))\Gamma_t^* + \Gamma_t\alpha_0^t(A)\delta_{\mathrm{R}}(\Gamma_t^*),$$

$$\xi_{\mathrm{R}}(\alpha^t(A)) = \xi_{\mathrm{R}}(\Gamma_t)\alpha_0^t(A)\Gamma_t^* + \Gamma_t\alpha_0^t(\xi_{\mathrm{R}}(A))\Gamma_t^* + \Gamma_t\alpha_0^t(A)\xi_{\mathrm{R}}(\Gamma_t^*),$$

yield Part (a).

If $A \in \mathrm{Dom}\,(\delta_{\mathrm{L}}) \cap \mathrm{Dom}\,(\delta_{\mathrm{R}}) \cap \mathrm{Dom}\,(\xi_{\mathrm{L}}) \cap \mathrm{Dom}\,(\xi_{\mathrm{R}})$ then,

$$\frac{\mathrm{d}}{\mathrm{d}t}\alpha_{X,Y}^{-t} \circ \alpha^t(A) = \frac{X}{\beta_{\mathrm{eq}}}\alpha_{X,Y}^{-t}(\delta_{\mathrm{R}}(\alpha^t(A))) + \frac{Y}{\beta_{\mathrm{eq}}}\alpha_{X,Y}^{-t}(\xi_{\mathrm{R}}(\alpha^t(A))),$$

and (b) follows. The case $A \in \mathrm{Dom}\,(\delta_{\mathrm{R}}) \cap \mathrm{Dom}\,(\xi_{\mathrm{R}})$ is handled by approximating A with the sequence

$$A_j = \frac{j}{\pi} \int_{\mathbb{R}^2} \mathrm{e}^{-j(t^2+s^2)} \tau_{\mathrm{L}}^t \circ \vartheta_{\mathrm{L}}^s(A)\mathrm{d}t\mathrm{d}s,$$

see the proof of Lemma 3.3 in [JOP1].

Since $\mathrm{Dom}\,(\delta_{\mathrm{R}}) \cap \mathrm{Dom}\,(\xi_{\mathrm{R}})$ is dense in $\mathcal{O}$, (b) implies (c). The proof of (d) is the same as the proof of Lemma 3.4 in [JOP1]. □

Lemma 4.6 *Let $A \in \mathcal{O}_{\vartheta,\mathrm{R,c}}$. Then for all $t \in \mathbb{R}$ the function*

$$(X,Y) \mapsto \omega_{X,Y}(\tau^t(A)),$$

is differentiable at $(0,0)$, and

$$\partial_X \omega_{X,Y}(\tau^t(A))\big|_{X=Y=0} = \frac{1}{\beta_{\mathrm{eq}}}\int_0^t \omega_{\mathrm{eq}}(\delta_{\mathrm{R}}(\tau^s(A)))\mathrm{d}s,$$

$$\partial_Y \omega_{X,Y}(\tau^t(A))\big|_{X=Y=0} = \frac{1}{\beta_{\mathrm{eq}}}\int_0^t \omega_{\mathrm{eq}}(\xi_{\mathrm{R}}(\tau^s(A)))\mathrm{d}s.$$

Proof. Since A is a centered observable and $\omega_{X,Y}$ is $\alpha_{X,Y}$-invariant, we have that $\omega_{X,Y}(\alpha_{X,Y}^t(A)) = 0$ for all t. Since $\alpha_{0,0} = \tau$ on $\mathcal{O}_\vartheta$, we have that $\omega_{X,Y}(\alpha_{0,0}^t(A)) = \omega_{X,Y}(\tau^t(A))$ and $\omega_{0,0}(\tau^t(A)) = \omega_{\mathrm{eq}}(\tau^t(A)) = 0$ for all t. These observations and Part (b) of Lemma 4.5 imply

$$\omega_{X,Y}(\tau^t(A)) - \omega_{0,0}(\tau^t(A)) = \frac{X}{\beta_{\mathrm{eq}}}\int_0^t \omega_{X,Y}(\delta_{\mathrm{R}}(\tau^s(A)))\mathrm{d}s + \frac{Y}{\beta_{\mathrm{eq}}}\int_0^t \omega_{X,Y}(\xi_{\mathrm{R}}(\tau^s(A)))\mathrm{d}s.$$

This relation, Lemma 4.5, and the dominated convergence yield the statement. □

Lemma 4.7 *Assume that $A \in \mathcal{O}_{\vartheta,\mathrm{R}}$. Then*

$$\omega_{\mathrm{eq}}(\delta_{\mathrm{R}}(A)) = \int_0^{\beta_{\mathrm{eq}}} \omega_{\mathrm{eq}}(A\tau^{\mathrm{i}s}(\Phi))\mathrm{d}s,$$

$$\omega_{\mathrm{eq}}(\xi_{\mathrm{R}}(A)) = \int_0^{\beta_{\mathrm{eq}}} \omega_{\mathrm{eq}}(A\tau^{\mathrm{i}s}(\mathcal{J}))\mathrm{d}s.$$

Proof. This lemma is the central and technically most demanding step of the argument. Fortunately, its proof is identical to the proof of Lemma 3.6 in [JOP1]. This follows from the fact that $A, V, \Phi, \mathcal{J} \in \mathcal{O}_\vartheta$ and that $\omega_{\mathrm{eq}} \restriction \mathcal{O}_\vartheta$ is a $(\tau, \beta_{\mathrm{eq}})$-KMS state. □

Theorem 4.2 is an immediate consequence of Lemmas 4.6 and 4.7.

5 Some generalizations

Although we have restricted ourselves in this note to two coupled quantum dynamical systems, the model, the framework and all our results have a straightforward extension to the case of M systems. Let β_{eq} and μ_{eq} be the reference (equilibrium) values of the inverse temperature and chemical potential. For $j = 1, \ldots, M$ let $(\mathcal{O}_j, \tau_j, \omega_{j,\beta_j\mu_j})$ be quantum dynamical systems with gauge groups ϑ_j where ω_j is a $(\tau_j, \vartheta_j, \beta_j, \mu_j)$-KMS state. We denote by δ_j and ξ_j the generators of τ_j and ϑ_j. Assumption (A1) is replaced with

> **(G1)** The reference states of the j-th system are parametrized by $\beta_j \in I_\epsilon(\beta_{\mathrm{eq}})$ and $\mu_j \in I_\epsilon(\mu_{\mathrm{eq}})$ and $\omega_{j,\beta_j\mu_j}$ is the unique $(\tau_j, \vartheta_j, \beta_j, \mu_j)$-KMS state on $\mathcal{O}_j$.

Let $\mathcal{O} = \mathcal{O}_1 \otimes \cdots \otimes \mathcal{O}_M$, $\tau_0 = \tau_1 \otimes \cdots \otimes \tau_M$, $\vartheta = \vartheta_1 \otimes \cdots \otimes \vartheta_M$. The algebra $\mathcal{O}_\vartheta$ is again defined by (2.1). The pair $(\mathcal{O}, \tau_0)$ describes the uncoupled joint system. Let $V \in \mathcal{O}_\vartheta$ be a self-adjoint perturbation and τ the perturbed C^*-dynamics. The coupled joint system is described by $(\mathcal{O}, \tau)$. The thermodynamical forces are

$$X_j = \beta_{\rm eq} - \beta_j, \qquad Y_j = \beta_j \mu_j - \beta_{\rm eq}\mu_{\rm eq}.$$

We set $X = (X_1, \ldots, X_M)$, $Y = (Y_1, \ldots, Y_M)$. The reference state is $\omega_{X,Y,0} = \omega_{1,\beta_1\mu_1} \otimes \cdots \omega_{M,\beta_M\mu_M}$. $\omega_{X,Y,0}$ is the unique $\beta_{\rm eq}$-KMS state for the C^*-dynamics

$$\alpha^t_{X,Y,0} = [\tau_1^{\beta_1 t/\beta_{\rm eq}} \circ \vartheta_1^{-\mu_1\beta_1 t/\beta_{\rm eq}}] \otimes \cdots \otimes [\tau_M^{\beta_M t/\beta_{\rm eq}} \circ \vartheta_M^{-\mu_M\beta_M t/\beta_{\rm eq}}].$$

Let $\delta_{X,Y,0}$ be the generator of $\alpha_{X,Y,0}$ and $\delta_{X,Y} = \delta_{X,Y,0} + {\rm i}[V, \cdot\,]$. Let $\alpha_{X,Y}$ be the C^*-dynamics generated by $\delta_{X,Y}$ and let $\omega_{X,Y}$ be the $(\alpha_{X,Y}, \beta_{\rm eq})$-KMS state obtained from $\omega_{X,Y,0}$ by Araki's perturbation theory. The completes the setup of the model. Note that the state $\omega_{\rm eq} \equiv \omega_{0,0}$ is the unique $(\tau, \vartheta, \beta_{\rm eq}, \mu_{\rm eq})$-KMS state on $\mathcal{O}$. Assumptions (G2) has the same formulation as Assumption (A2) and Assumptions (A3), (A4) and (A5) are replaced with:

(G3) For all $X, Y \in I_\epsilon^M$ there exists a state $\omega_{X,Y,+}$ on $\mathcal{O}_\vartheta$ such that for all $A \in \mathcal{O}_\vartheta$,

$$\lim_{t\to+\infty} \omega_{X,Y}(\tau^t(A)) = \omega_{X,Y,+}(A).$$

(G4) There exists a time-reversal Θ of $(\mathcal{O}, \tau_0)$ such that $\Theta(V) = V$ and

$$\Theta \circ \tau_j^t = \tau_j^{-t} \circ \Theta, \qquad \Theta \circ \vartheta_j^t = \vartheta_j^{-t} \circ \Theta,$$

for all j.

(G5) $V \in {\rm Dom}\,(\delta_j) \cap {\rm Dom}\,(\xi_j)$ for all j.

The observables associated to the heat and charge flux out of the j-th system are

$$\Phi_j = \delta_j(V), \qquad \mathcal{J}_j = \xi_j(V).$$

It immediately follows that

$$\sum_{j=1}^M \omega_{X,Y,+}(\Phi_j) = 0 \quad \text{and} \quad \sum_{j=1}^M \omega_{X,Y,+}(\mathcal{J}_j) = 0,$$

which are respectively the first law of thermodynamics (conservation of energy) and charge conservation. The entropy balance equation reads

$$\operatorname{Ent}(\omega_{X,Y} \circ \tau^t | \omega_{X,Y}) = -\sum_{j=1}^M X_j \int_0^t \omega_{X,Y}(\tau^s(\Phi_j)){\rm d}s - \sum_{j=1}^M Y_j \int_0^t \omega_{X,Y}(\tau^s(\mathcal{J}_j)){\rm d}s,$$

and in particular the second law holds:

$$\operatorname{Ep}(\omega_{X,Y,+}) = \sum_{j=1}^M X_j\, \omega_{X,Y,+}(\Phi_j) + \sum_{j=1}^M Y_j\, \omega_{X,Y,+}(\mathcal{J}_j) \geq 0. \tag{5.19}$$

The definition of the centered observable is the same as in Subsection 3.7. We set

$$\hat{\mathcal{O}}_\vartheta = \left(\cap_{j=1}^M {\rm Dom}\,(\delta_j)\right) \cap \left(\cap_{j=1}^M {\rm Dom}\,(\xi_j)\right) \cap \mathcal{O}_\vartheta,$$

$$\hat{\mathcal{O}}_{\vartheta,{\rm c}} = \hat{\mathcal{O}}_\vartheta \cap \mathcal{C}.$$

If $V \in \hat{\mathcal{O}}_\vartheta$, then $\Phi_j, \mathcal{J}_j \in \hat{\mathcal{O}}_{\vartheta,\mathrm{c}}$ for all j (after obvious notational changes, Proposition 3.3 applies directly to the model consider in this section).

Theorem 4.2 is replaced with:

Theorem 5.1 *Suppose that Assumptions (G1) and (G5) hold and let* $A \in \hat{\mathcal{O}}_{\vartheta,\mathrm{c}}$. *Then for all* $t \in \mathbb{R}$ *the function*

$$(X, Y) \mapsto \omega_{X,Y}(\tau^t(A)),$$

is differentiable at $(0,0)$ *and*

$$\partial_{X_j} \omega_{X,Y}(\tau^t(A))\big|_{X=Y=0} = \mathfrak{L}(A, \Phi_j, t),$$

$$\partial_{Y_j} \omega_{X,Y}(\tau^t(A))\big|_{X=Y=0} = \mathfrak{L}(A, \mathcal{J}_j, t).$$

The definition of the regular observable is the same as before, and we have:

Theorem 5.2 *Suppose that Assumptions (G1), (G3) and (G5) hold.*
(1) *Let* $A \in \hat{\mathcal{O}}_{\vartheta,\mathrm{c}}$ *be a regular observable. Then*

$$\partial_{X_j} \omega_{X,Y,+}(A)\big|_{X=Y=0} = \mathfrak{L}(A, \Phi_j),$$

$$\partial_{Y_j} \omega_{X,Y,+}(A)\big|_{X=Y=0} = \mathfrak{L}(A, \mathcal{J}_j).$$

(2) *If in addition (G2) and (G4) hold and* $A \in \hat{\mathcal{O}}_\vartheta$ *is a regular self-adjoint observable such that* $\Theta(A) = -A$, *then*

$$\partial_{X_j} \omega_{X,Y,+}(A)\big|_{X=Y=0} = \mathcal{L}(A, \Phi_j),$$

$$\partial_{Y_j} \omega_{X,Y,+}(A)\big|_{X=Y=0} = \mathcal{L}(A, \mathcal{J}_j).$$

Theorem 5.3 *Suppose that (G1), (G3) and (G5) hold and that* $\Phi_j, \mathcal{J}_j$ *are regular observables in* $\mathrm{Dom}\,(\delta_j) \cap \mathrm{Dom}\,(\xi_j)$. *Then:*
(1) *The kinetic transport coefficients*

$$L_{\mathrm{hh}}^{kj} = \partial_{X_j} \omega_{X,Y,+}(\Phi_k)\big|_{X=Y=0},$$

$$L_{\mathrm{hc}}^{kj} = \partial_{Y_j} \omega_{X,Y,+}(\Phi_k)\big|_{X=Y=0},$$

$$L_{\mathrm{ch}}^{kj} = \partial_{X_j} \omega_{X,Y,+}(\mathcal{J}_k)\big|_{X=Y=0},$$

$$L_{\mathrm{cc}}^{kj} = \partial_{Y_j} \omega_{X,Y,+}(\mathcal{J}_k)\big|_{X=Y=0},$$

satisfy

$$L_{\mathrm{hh}}^{kj} = \mathfrak{L}(\Phi_k, \Phi_j),$$

$$L_{\mathrm{hc}}^{kj} = \mathfrak{L}(\Phi_k, \mathcal{J}_j),$$

$$L_{\mathrm{ch}}^{kj} = \mathfrak{L}(\mathcal{J}_k, \Phi_j),$$

$$L_{\mathrm{cc}}^{kj} = \mathfrak{L}(\mathcal{J}_k, \mathcal{J}_j).$$

Assume in addition that (G2) and (G4) hold. Then
(2) *The Green-Kubo formulas hold:*

$$L^{kj}_{\rm hh} = \mathcal{L}(\Phi_k, \Phi_j),$$

$$L^{kj}_{\rm hc} = \mathcal{L}(\Phi_k, \mathcal{J}_j),$$

$$L^{kj}_{\rm ch} = \mathcal{L}(\mathcal{J}_k, \Phi_j),$$

$$L^{kj}_{\rm cc} = \mathcal{L}(\mathcal{J}_k, \mathcal{J}_j).$$

(3) *The Onsager reciprocity relations hold:*

$$L^{kj}_{\rm hh} = L^{jk}_{\rm hh},$$

$$L^{kj}_{\rm cc} = L^{jk}_{\rm cc},$$

$$L^{kj}_{\rm hc} = L^{jk}_{\rm ch}.$$

The remark after Theorem 4.4 applies to Theorems 5.2 and 5.3.

In the literature one often considers so called open quantum systems, where one of the quantum dynamical systems, say $(\mathcal{O}_1, \tau_1, \omega_{1,\beta_1\mu_1})$, is finite dimensional and plays a role of a "small" quantum system coupled to reservoirs described by $(\mathcal{O}_j, \tau_j, \omega_{j,\beta_j\mu_j})$, $j \geq 2$. Open quantum systems are one of the basic paradigms of non-equilibrium quantum statistical mechanics and have played an important role in the historical development of the subject. With regard to the algebraic approach described in this note, the only additional feature of open quantum systems is vanishing of heat and charge fluxes out of the small system: $\omega_{X,Y,+}(\Phi_1) = \omega_{X,Y,+}(\mathcal{J}_1) = 0$.

Many other generalizations are possible and it appears difficult to have a unified framework which covers all cases of physical interest. The Electronic Black Block Models studied in [AJPP1, AJPP2, JOPP] are examples of open quantum systems which do not fit directly into the class of models described here (the non-interacting coupled system is not a tensor product of the individual subsystems). However, the changes needed to apply our results to these models are elementary. One may also consider W^*-dynamical systems instead of C^*-dynamical systems and unbounded interactions which are only affiliated to the algebra of observables. The models where such generalization is necessary involve free bosonic reservoirs (a well-known example is the spin-boson model). One may also consider time-dependent interactions (see [Ru1, JP3, JP4, ASF]). Another possible generalization involves more general gauge groups. The important point is that although all such generalizations may require some adjustment of technique and presentation, they bring nothing conceptually new.

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