Dissipative Transport: Thermal Contacts and Tunnelling Junctions

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Abstract

The general theory of simple transport processes between quantum mechanical reservoirs is reviewed and extended. We focus on thermoelectric phenomena, involving exchange of energy and particles. The theory is illustrated on the example of two reservoirs of free fermions coupled through a local interaction. We construct a stationary state and determine energy and particle currents with the help of a convergent perturbation series.

We explicitly calculate several interesting quantities to lowest order, such as the entropy production, the resistance, and the heat conductivity. Convergence of the perturbation series allows us to prove that they are *strictly positive* under suitable smallness and regularity assumptions on the interaction between the reservoirs.

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1 Introduction

1.1 Description of the problems

Simple transport processes, such as those observed near a spatially localized thermal contact or tunnelling junction between two macroscopically extended metals at different temperatures and chemical potentials, have been studied experimentally and theoretically for a long time; see e.g. [Ma]. One is interested, for example, in measuring or predicting energy and charge transport through a contact between two metals, as well as the rate of entropy production. The natural theoretical description of such processes is provided by quantum theory, more precisely by non-equilibrium quantum statistical mechanics. The results of experiments or theoretical calculations can, however, often be expressed in the language of thermodynamics. In this paper we attempt to study such transport processes in a mathematically precise way, extending or complementing results in [DFG, EPR, JP1, JP2, Ru1, Ru2].

In recent years, interest in transport processes has been driven by various experimental and theoretical developments in mesoscopic physics and the discovery of rather unexpected phenomena. Among them we mention dissipation-free transport in incompressible Hall fluids [La, TKNN, BES, ASS, FST], or in ballistic quantum wires [vW, Bee, ACF, FP1]. In such systems, "transport in thermal equilibrium" and the quantization of conductances are observed. Further interesting transport processes are electron tunnelling into an edge of a Hall fluid [CPW, CWCPW, LS, LSH], and tunnelling processes between two different quantum Hall edges through a constriction leading to measurements of fractional electric charges of quasi-particles (see, e.g., [SGJE], and [FP2] for theoretical considerations). At present, these processes are only partially understood theoretically. Other examples are Josephson junctions and Andreev scattering [SR1, SR2], or energy transport in chains (see, e.g., [Af] and references given there).

In this paper, the main emphasis is put, however, on conceptual aspects of the theory of simple dissipative transport processes between two quantum-mechanical reservoirs and on an illustration of the general theory in a simple example, namely transport of energy and charge between two simple metals, described as non-interacting electron liquids, at different temperatures and chemical potentials. Of particular interest to us are connections between theoretical descriptions based on non-equilibrium quantum statistical mechanics, on the one hand, and on thermodynamics, on the other hand. Our quantum-mechanical description involves equilibrium and non-equilibrium states of macroscopic reservoirs with many degrees of freedom. We show that, on intermediate time scales, tunnelling processes can be described in terms of non-equilibrium stationary states (NESS), examples of which have recently been studied in [DFG, EPR, JP1, JP2, Ru1, Ru2, BLR]. Our construction of non-equilibrium stationary states is based on methods of algebraic scattering theory and is inspired by ideas in [He, Rob, BR, BM, Ha]. Links between quantum statistical mechanics and thermodynamics are constructed by providing precise definitions of energy and particle currents and of entropy production and by deriving a suitable form of the first and second law of thermodynamics. The general theory developed in Sect. 2 reviews ideas and results scattered over numerous articles and books and represents an attempt to provide a somewhat novel and, we believe, rather clear synthesis. A more complete version, including the treatment of systems with time-dependent Hamiltonians, appears in [FMSU] and in a forthcoming paper. It is illustrated on the example of two reservoirs of non-interacting electrons coupled through local many-body interactions (Sects 3 through 5). Examples of non-equilibrium stationary states supporting particle and/or energy currents are constructed with the help of a convergent perturbation (Dyson) series in the many-body interaction terms. The currents and the entropy production rate are calculated quite explicitly to leading order. This enables us to show that, under natural hypotheses, they are strictly positive. Onsager reciprocity relations are established to lowest non-trivial order in the many-body interaction terms. Positivity of the entropy production rate has also been established recently in [AP, MO] for XY chains, and in [CNP] for wave turbulence.

1.2 Contents of paper

In Section 2.1, quantum-mechanical reservoirs are introduced, whose time evolution is given in terms of a one-parameter group of $*$automorphisms of a kinematical C^*-algebra of operators. Conservation laws of reservoirs are described by commuting conserved charges. The equilibrium states of such reservoirs are introduced and parametrized by temperature and chemical potentials. Two general assumptions, (A1) and (A2), are formulated. They state that the thermodynamic limits of the time evolution and of the gauge transformations of operators in the kinematical algebra of an infinite system and of the equilibrium states exist.

In Section 2.2 we study two interacting reservoirs at different temperatures and chemical potentials. Each reservoir is required to satisfy the assumptions formulated in Sect. 2.1. A class of many-body interactions coupling the two reservoirs is introduced. It is assumed that the thermodynamic limit of the interactions and of the corresponding time evolutions exist. Energy and charge currents for finite and infinite systems are then defined.

Connections between quantum statistical mechanics and thermodynamics are elucidated in Section 2.3. The entropy production rate is defined and expressed in terms of the currents and of thermodynamic parameters. An inequality expressing the positivity of relative entropy is shown to imply that the total entropy production is non-negative (see also [Ru2, JP1]).

In Section 2.4, non-equilibrium stationary states for coupled reservoirs are introduced. They can be construced with the help of scattering (Møller) endomorphisms of the kinematical algebra of the infinite coupled system. A precise assumption concerning the existence of scattering endomorphisms is formulated. Our approach has its roots in Hepp's work on the Kondo problem [He] and Robinson's analysis of return to equilibrium in the XY spin chain [Rob]. Robinson's ideas have been put into a general context in [BR, Ha]. The scattering approach is the starting point for numerous heuristic studies of thermal contacts and tunnelling junctions (see, e.g., [Ma]). The first mathematically rigorous implementation of this approach in a study of energy transport in the XY spin chain and of tunnelling between free-fermion reservoirs appeared in [DFG].

In Section 2.5, long-time stability properties of equilibrium and non-equilibrium stationary states against perturbations of the initial state of the coupled system are studied, and conditions for the existence of temperature or density profiles in non-equilibrium stationary states are identified.

The general theory of Section 2 is illustrated in Sections 3,4 and 5 on the example of two coupled free-electron reservoirs.

In Section 3, the quantum theory of finite and infinite reservoirs of free electrons is briefly recalled, and a class of local many-body interactions between two such reservoirs satisfying the general assumptions formulated in Section 2 is introduced.

Our main technical result, the existence of scattering (Møller) endomorphisms, defined on an appropriate kinematical C^*-algebra describing two infinite free-electron reservoirs, is established in Section 4. A similar result has previously been proven in [BM]. We show that, under appropriate smallness and regularity assumptions on the many-body interaction terms, the scattering endomorphisms are given by a (norm-) convergent Dyson series. As a consequence, non-equilibrium stationary states can be constructed with the help of a convergent perturbation expansion.

The results of Section 4 are used in Section 5 to derive explicit expressions for the energy and charged particle-currents to leading order in the many-body interaction terms. These expresssions, along with the convergence of the Dyson series prove that, for small coupling constants, the entropy production rate is strictly positive, Ohm's law holds to leading order in the voltage drop between the reservoirs, with a resistance whose temperature dependence can be determined, and the Onsager reciprocity relations hold to leading order.

We conclude this introduction with explicit formulae for the leading contributions to the particle current, $\mathcal{J}$, and to the energy current, $\mathcal{P}$, between two reservoirs, I and II, of free electrons coupled to each other by a quadratic local interaction term with a form factor $\widehat{w}((-\boldsymbol{k}, II), (\boldsymbol{l}, I))$ and a brief discussion of the qualitative implications of these formulae. These currents are given by

$$\begin{aligned}
\mathcal{J} &\simeq 2\pi\int_{\mathbb{R}^6} d\boldsymbol{k}\; d\boldsymbol{l}\; \delta(|\boldsymbol{k}|^2 - |\boldsymbol{l}|^2)\, |\widehat{w}((-\boldsymbol{k}, II), (\boldsymbol{l}, I))|^2\, (\rho_{II}(\boldsymbol{k}) - \rho_I(\boldsymbol{k}))\,, \\
\mathcal{P} &\simeq 2\pi\int_{\mathbb{R}^6} d\boldsymbol{k}\; d\boldsymbol{l}\; |\boldsymbol{k}|^2\delta(|\boldsymbol{k}|^2 - |\boldsymbol{l}|^2)\, |\widehat{w}((-\boldsymbol{k}, II), (\boldsymbol{l}, I))|^2\, (\rho_{II}(\boldsymbol{k}) - \rho_I(\boldsymbol{k}))\,, (*)
\end{aligned}$$

where $\rho_r(\boldsymbol{k})$ is the Fermi distribution of the free electron gas ($r = I, II$ labels the reservoirs), and $\widehat{w}((-\boldsymbol{k}, II), (\boldsymbol{l}, I))$ is the interaction kernel describing scattering of a particle in an initial state with energy $|\boldsymbol{l}|^2$ localized in reservoir I to a final state with energy $|\boldsymbol{k}|^2$ localized in reservoir II.

If both reservoirs have the same chemical potential and the temperatures satisfy $T^I < T^{II}$ then $\mathcal{J}$ and $\mathcal{P}$ are positive; particles and energy flow from the hotter to the colder reservoir. Similarly, if the reservoirs have the same temperature, then particles and energy flow from the reservoir with the higher chemical potential to the other one.

Formulae $(*)$ prove that the leading contribution to the entropy production rate is strictly positive, unless both reservoirs are at the same temperature and at the same chemical potential.

Another consequence of $(*)$ is that, to leading order in the interaction, and for a small voltage drop, $\Delta\mu = \mu^{II} - \mu^{I}$ (at a fixed temperature, T, for both reservoirs), *Ohm's law* is valid, i.e., the voltage drop is proportional to the current,

$$\Delta\mu \simeq R(\mu^I, T)\mathcal{J}.$$

Our calculations show that the resistance $R(\mu^I, T)$ grows linearly in T, for large T, it has a positive value at $T = 0$ and may increase or decrease in T, at small temperatures, depending on properties of the interaction kernel $\widehat{w}$ modelling the junction between the two reservoirs.

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2 Elements of a general theory of junctions and of non-equilibrium stationary states

2.1 Quantum theory of reservoirs

We start our general analysis by describing *"quantum-mechanical reservoirs"*. A reservoir is a quantum system with very many degrees of freedom, e.g., an electron liquid in a normal metal, a superconductor, a gas of atoms, or a large array of coupled, localized spins, but with a small number of observable physical quantities. It is confined to a macroscopically large, but compact subset, Λ, of physical space $\mathbb{R}^3$. Its pure states correspond, as usual, to unit rays in a *separable Hilbert space*, $\mathcal{H}^\Lambda$, and its dynamics is generated by a selfadjoint *Hamiltonian*, H^Λ, acting on the space $\mathcal{H}^\Lambda$. The kinematics of the reservoir is encoded into an algebra, $\mathcal{A}^\Lambda$, of operators contained in (or equal to) the algebra of all bounded operators on $\mathcal{H}^\Lambda$ [1]. The time evolution of an operator a on $\mathcal{H}^\Lambda$ is given, in the Heisenberg picture, by

$$\alpha_t^\Lambda(a) \ := \ e^{itH^\Lambda/\hbar}\, a\, e^{-itH^\Lambda/\hbar}, \tag{2.1}$$

and it is assumed that $\alpha_t^\Lambda(a) \in \mathcal{A}^\Lambda$, for every $a \in \mathcal{A}^\Lambda$.

There may exist a certain number of linearly independent, commuting *conservation laws*, which are represented by selfadjoint operators $Q_1^\Lambda, \ldots, Q_M^\Lambda$ on $\mathcal{H}^\Lambda$ commuting with the dynamics of the reservoir, i.e.,

$$\left[H^\Lambda, Q_j^\Lambda\right] \ = \ 0, \ \left[Q_i^\Lambda, Q_j^\Lambda\right] \ = \ 0, \ \left[Q_i^\Lambda, a\right] \ = \ 0, \tag{2.2}$$

for all $i, j, = 1, \ldots, M$, and for all "observables" $a \in \mathcal{A}^\Lambda$. More precisely, one assumes that all operators $\exp itH^\Lambda/\hbar$, $\left\{\exp i\, s_j\, Q_j^\Lambda\right\}_{j=1}^M$ commute with one another, for arbitrary real values of $t, s_1, \ldots, s_M$.

A typical example of a conservation law is the *particle number operator*, N^Λ, of a reservoir consisting of a gas of non-relativistic atoms.

On the algebra, $B(\mathcal{H}^\Lambda)$, of all bounded operators on the Hilbert space $\mathcal{H}^\Lambda$, we define *"gauge transformations of the first kind"* by setting

$$\varphi_{\boldsymbol{s}}^\Lambda(a) \ := \ e^{i\boldsymbol{s}\cdot\boldsymbol{Q}^\Lambda}\, a\, e^{-i\,\boldsymbol{s}\cdot\boldsymbol{Q}^\Lambda}, \tag{2.3}$$

for $a \in B(\mathcal{H}^\Lambda)$, where

$$\boldsymbol{s}\cdot\boldsymbol{Q}^\Lambda \ := \ \sum_{j=1}^M s_j\, Q_j^\Lambda \ . \tag{2.4}$$

Then $\left\{\varphi_{\boldsymbol{s}}^\Lambda \,\middle|\, \boldsymbol{s} \in \mathbb{R}^M\right\}$ is an M-parameter abelian group of *automorphisms (see (2.16), below) of the algebra $B(\mathcal{H}^\Lambda)$, and

$$\alpha_t^\Lambda\left(\varphi_{\boldsymbol{s}}^\Lambda(a)\right) \ = \ \varphi_{\boldsymbol{s}}^\Lambda\left(\alpha_t^\Lambda(a)\right), \tag{2.5}$$

for all $a \in B(\mathcal{H}^\Lambda)$, by (2.2). It is natural to define the "observable algebra" $\mathcal{A}^\Lambda$ as the algebra of all those operators $a \in B(\mathcal{H}^\Lambda)$ for which

$$\varphi_{\boldsymbol{s}}^\Lambda(a) \ = \ a\,, \text{ for all } \boldsymbol{s} \in \mathbb{R}^M. \tag{2.6}$$

To every conservation law Q_j^Λ there corresponds a conjugate thermodynamic parameter, μ_j, commonly called a *chemical potential*.

Thermal equilibrium of the reservoir at inverse temperature β and chemical potentials $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_M)$ is described by a mixed state, or *density matrix*, given by

$$\left(\Xi_{\beta,\boldsymbol{\mu}}^\Lambda\right)^{-1} \exp -\beta\left[H^\Lambda - \boldsymbol{\mu}\cdot\boldsymbol{Q}^\Lambda\right], \tag{2.7}$$

[1]The algebra $\mathcal{A}^\Lambda$ is sometimes called algebra of "observables", a commonly used, but unfortunate expression.

where

$$\Xi^{\Lambda}_{\beta,\boldsymbol{\mu}} \;:=\; \mathrm{tr}\left(\exp -\beta\left[H^{\Lambda} - \boldsymbol{\mu}\cdot\boldsymbol{Q}^{\Lambda}\right]\right) \tag{2.8}$$

is the grand-canonical partition function. Of course, it is assumed that the operators

$$\exp -\beta\left[H^{\Lambda} - \boldsymbol{\mu}\cdot\boldsymbol{Q}^{\Lambda}\right]$$

are trace-class, for all chemical potentials $\boldsymbol{\mu}$ in a region $\mathcal{M} \subseteq \mathbb{R}^M$, for all $\beta > 0$, and for arbitrary compact subsets Λ of physical space $\mathbb{R}^3$. It is also commonly assumed that reservoirs are *thermodynamically stable*, in the sense that the thermodynamic potential, G, given by

$$\beta G\left(\beta,\boldsymbol{\mu},V\right) \;:=\; -\ln\left(\Xi^{\Lambda}_{\beta,\boldsymbol{\mu}}\right) \tag{2.9}$$

is *extensive*, i.e., proportional to the volume, V, of the set Λ, up to boundary corrections, for arbitrary $\beta > 0, \boldsymbol{\mu} \in \mathcal{M}$.

The expectation value of an operator $a \in B(\mathcal{H}^{\Lambda})$ in the equilibrium state corresponding to the density matrix (2.7) is given by

$$\omega^{\Lambda}_{\beta,\boldsymbol{\mu}}(a) \;:=\; \left(\Xi^{\Lambda}_{\beta,\boldsymbol{\mu}}\right)^{-1}\mathrm{tr}\left(e^{-\beta\left[H^{\Lambda}-\boldsymbol{\mu}\cdot\boldsymbol{Q}^{\Lambda}\right]}\,a\right). \tag{2.10}$$

The state $\omega^{\Lambda}_{\beta,\boldsymbol{\mu}}$ has some remarkable properties to be discussed next.

It is *time-translation invariant*, i.e.,

$$\omega^{\Lambda}_{\beta,\boldsymbol{\mu}}\left(\alpha^{\Lambda}_t(a)\right) \;=\; \omega^{\Lambda}_{\beta,\boldsymbol{\mu}}(a), \tag{2.11}$$

for arbitrary $a \in B(\mathcal{H}^{\Lambda})$. It obeys the celebrated KMS *condition*

$$\omega^{\Lambda}_{\beta,\boldsymbol{\mu}}\left(\alpha^{\Lambda}_t(a)\,b\right) \;=\; \omega^{\Lambda}_{\beta,\boldsymbol{\mu}}\left(b\,\alpha^{\Lambda}_{t+i\beta\hbar}\left(\varphi^{\Lambda}_{-i\beta\boldsymbol{\mu}}(a)\right)\right), \tag{2.12}$$

for arbitrary a and b in $B(\mathcal{H}^{\Lambda})$. In particular, if $a \in \mathcal{A}^{\Lambda}$ then

$$\omega^{\Lambda}_{\beta,\boldsymbol{\mu}}\left(\alpha^{\Lambda}_t(a)\,b\right) \;=\; \omega^{\Lambda}_{\beta,\boldsymbol{\mu}}\left(b\,\alpha^{\Lambda}_{t+i\beta\hbar}\left(a\right)\right), \tag{2.13}$$

for arbitrary $b \in B(\mathcal{H}^{\Lambda})$; see (2.6). Eq. (2.12) is an easy consequence of eqs. (2.10) and (2.3) and of the cyclicity of the trace, i.e.,

$$\mathrm{tr}\left(a\,b\right) \;=\; \mathrm{tr}\left(b\,a\right).$$

For further details concerning these standard facts of quantum statistical mechanics we refer the reader to [Ru 3, BR].

Next, we recall some conventional wisdom concerning the *thermodynamic limit* of a reservoir. We are interested in understanding asymptotics of physical quantities, as the region Λ to which the reservoir is confined increases to all of $\mathbb{R}^3$, or to an infinite half-space

$$\mathbb{R}^3_{\pm} \;:=\; \left\{(x,y,z) \in \mathbb{R}^3 \;\middle|\; x \gtrless 0\right\}. \tag{2.14}$$

We use the notation "$\Lambda \nearrow \infty$" to mean that $\Lambda \nearrow \mathbb{R}^3$ (or $\Lambda \nearrow \mathbb{R}^3_{\pm}$), in the sense of Fisher (meaning, in essence, that the ratio between the surface and the volume goes to zero); see [Ru 3].

We introduce an operator algebra $\mathcal{F}^r$, called the *"field algebra"*, convenient for the description of the thermodynamic limit of a reservoir:

$$\mathcal{F}^r \;:=\; \overline{\bigvee_{\Lambda\nearrow\infty} B(\mathcal{H}^\Lambda)}, \tag{2.15}$$

where $\bigvee_{\Lambda\nearrow\infty} B(\mathcal{H}^\Lambda)$ is the algebra generated by all the operators in the increasing sequence of algebras

$$\ldots \subseteq\; B\big(\mathcal{H}^\Lambda\big) \;\subseteq\; B\big(\mathcal{H}^{\Lambda'}\big) \;\subseteq\; \ldots,$$

$\Lambda \subseteq \Lambda'$, and $\overline{(\cdot)}$ denotes the closure in the operator norm. Technically speaking, $\mathcal{F}^r$ is a C*-algebra, [BR]. The superscript ^{r} stands for "reservoir". Below, we consider two interacting reservoirs, labelled by $r = I, II$.

A group $\{\tau_{\boldsymbol{t}} \mid \boldsymbol{t} \in \mathbb{R}^n\}$ of *homomorphisms*, of a C*-algebra $\mathcal{F}$ is an *n-parameter* **automorphism group* of $\mathcal{F}$ iff

$$\tau_{\boldsymbol{t}=0}(a) \;=\; a, \;\; \tau_{\boldsymbol{t}}\left(\tau_{\boldsymbol{t}'}(a)\right) \;=\; \tau_{\boldsymbol{t}+\boldsymbol{t}'}(a),$$

and

$$\tau_{\boldsymbol{t}}(a)^* \;=\; \tau_{\boldsymbol{t}}(a^*), \tag{2.16}$$

for all $a \in \mathcal{F}$ and arbitrary $\boldsymbol{t}, \boldsymbol{t}' \in \mathbb{R}^n$.

For the purposes of this paper we shall require the following two assumptions concerning the existence of the thermodynamic limit.

(A1) Existence of the thermodynamic limit of the dynamics and the gauge transformations.

For every operator $a \in \mathcal{F}^r$, the limits in operator norm

$$n - \lim_{\Lambda\nearrow\infty} \alpha_t^\Lambda(a) \;=:\; \alpha_t(a) \tag{2.17}$$

and

$$n - \lim_{\Lambda\nearrow\infty} \varphi_{\boldsymbol{s}}^\Lambda(a) \;=:\; \varphi_{\boldsymbol{s}}(a) \tag{2.18}$$

exist, for all $t \in \mathbb{R}$, $\boldsymbol{s} \in \mathbb{R}^M$, and define *automorphism groups of the field algebra $\mathcal{F}^r$. The convergence in (2.17) and (2.18) is assumed to be uniform for t in any compact interval of $\mathbb{R}$ and for $\boldsymbol{s}$ in any compact subset of $\mathbb{R}^M$, respectively. The *automorphism groups α_t and $\varphi_{\boldsymbol{s}}$ may be assumed to be norm-continuous in t and $\boldsymbol{s}$, respectively; (but "weak* continuity" will usually be sufficient).

We define the *"kinematical algebra"*, $\mathcal{A}^r$, to be the largest subalgebra of $\mathcal{F}^r$ *pointwise invariant* under $\{\varphi_{\boldsymbol{s}}\}_{\boldsymbol{s}\in\mathbb{R}^M}$, i.e.,

$$\mathcal{A}^r \ := \ \left\{ a \in \mathcal{F}^r \ \middle| \ \varphi_{\boldsymbol{s}}(a) \ = \ a, \text{ for all } \ \boldsymbol{s} \in \mathbb{R}^M \right\}. \tag{2.19}$$

Since, by (2.5), (2.17) and (2.18), α_t and $\varphi_{\boldsymbol{s}}$ commute, $\alpha_t(a) \in \mathcal{A}^r$, for every $a \in \mathcal{A}^r$.

(A2) Existence of the thermodynamic limit of the equilibrium state.
For every $a \in \mathcal{F}^r$,

$$\lim_{\Lambda \nearrow \infty} \omega^{\Lambda}_{\beta,\boldsymbol{\mu}}(a) \ =: \ \omega_{\beta,\boldsymbol{\mu}}(a) \tag{2.20}$$

exists and is time-translation invariant, i.e.,

$$\omega_{\beta,\boldsymbol{\mu}} \ (\alpha_t(a)) \ = \ \omega_{\beta,\boldsymbol{\mu}}(a), \tag{2.21}$$

for all $a \in \mathcal{F}^r$, $t \in \mathbb{R}$.

We assume that $\mathcal{F}^r$ contains a norm-dense subalgebra $\overset{\circ}{\mathcal{F}^r}$ with the property that the operator $\alpha_t(\varphi_{\boldsymbol{s}}(a))$ extends to an entire function of $t \in \mathbb{C}$, $\boldsymbol{s} \in \mathbb{C}^M$, for every $a \in \overset{\circ}{\mathcal{F}^r}$. If α_t and $\tau_{\boldsymbol{s}}$ are norm-continuous in t and $\boldsymbol{s}$, respectively, the existence of an algebra $\overset{\circ}{\mathcal{F}^r} \subset \mathcal{F}^r$ with these properties is an easy theorem.

From the KMS condition (2.12), and from (2.17), (2.18), (2.20), it follows that the infinite-volume state $\omega_{\beta,\boldsymbol{\mu}}$ on $\mathcal{F}^r$ obeys the KMS *condition*

$$\omega_{\beta,\boldsymbol{\mu}}(\alpha_t(a)\, b) \ = \ \omega_{\beta,\boldsymbol{\mu}}(b \ \alpha_{t+i\beta\hbar} \ (\varphi_{-i\beta\boldsymbol{\mu}}(a))), \tag{2.22}$$

for all $a \in \overset{\circ}{\mathcal{F}^r}$, $b \in \mathcal{F}^r$. If $a \in \mathcal{A}^r \cap \overset{\circ}{\mathcal{F}^r}$ then eq. (2.22) simplifies to

$$\omega_{\beta,\boldsymbol{\mu}}(\alpha_t(a)\, b) \ = \ \omega_{\beta,\boldsymbol{\mu}}(b \ \alpha_{t+i\beta\hbar}(a)). \tag{2.23}$$

2.2 Thermal contacts and tunnelling junctions between macroscopic reservoirs

We consider two reservoirs, I and II, with all the properties described in Sect. 2.1. These reservoirs may or may not have the same physical properties. For example, they may be ordinary metals located in two complementary half-spaces of $\mathbb{R}^3$; or I may be a metal and II a superconductor, etc. Later, we shall consider the example where I and II are ordinary metals, i.e., non-interacting electron liquids. In the following, "I" will be a shorthand notation for (I, Λ^I), and "II" for (II, Λ^{II}), where Λ^I and Λ^{II} are arbitrary compact subsets of $\mathbb{R}^3$. Realistically Λ^I and Λ^{II} should not intersect; but we shall ignore this constraint.

The Hilbert space of the system obtained by composing the two reservoirs is given by

$$\mathcal{H} \;=\; \mathcal{H}^I \otimes \mathcal{H}^{II} \tag{2.24}$$

and the dynamics, *before* the reservoirs are brought into contact, is generated by the Hamiltonian

$$H^0 \;:=\; H^I \otimes \mathbb{1} \;+\; \mathbb{1} \otimes H^{II}. \tag{2.25}$$

The natural algebra of operators of the coupled system is given by $B(\mathcal{H}^I) \otimes B(\mathcal{H}^{II})$ and, in the thermodynamic limit ($\Lambda^I \nearrow \mathbb{R}^3_-$ and $\Lambda^{II} \nearrow \mathbb{R}^3_+$, or $\Lambda^I \nearrow \mathbb{R}^3$ and $\Lambda^{II} \nearrow \mathbb{R}^3$), by

$$\mathcal{F} \;:=\; \overline{\mathcal{F}^I \otimes \mathcal{F}^{II}}, \tag{2.26}$$

where $\mathcal{F}^I$ and $\mathcal{F}^{II}$ are the field algebras of the two reservoirs (see (2.15)), and the closure is taken in the operator norm.

A *contact* or *tunnelling junction* between the two reservoirs is described in terms of a *perturbed Hamiltonian*, H, of the coupled system. The operator H has the form

$$H \;=\; H^0 + W(\Lambda^I, \Lambda^{II}) \tag{2.27}$$

where $W(\Lambda^I, \Lambda^{II})$ is a bounded, selfadjoint operator on $\mathcal{H}$ for each choice of Λ^I and Λ^{II}. We shall *always* require the following assumption.

(A3) Existence of the thermodynamic limit of the contact interaction.

$$n - \lim_{\substack{\Lambda^I \nearrow \infty \\ \Lambda^{II} \nearrow \infty}} W\left(\Lambda^I, \Lambda^{II}\right) \;=:\; W \tag{2.28}$$

exists (as a selfadjoint operator in $\mathcal{F}$).

Let $\alpha_t^{\Lambda^I}$ and $\alpha_t^{\Lambda^{II}}$ be the time evolutions of the reservoirs before they are brought into contact; see eq. (2.1). The time evolution of operators in $B(\mathcal{H}^I) \otimes B(\mathcal{H}^{II})$ is then given by $\alpha_t^{\Lambda^I} \otimes \alpha_t^{\Lambda^{II}}$ and is generated by the Hamiltonian H^0 introduced in (2.25). After the interaction $W(\Lambda^I, \Lambda^{II})$ has been turned on the time evolution of operators in the Heisenberg picture is given by

$$\alpha_t^{I \cup II}(a) \;=\; e^{i(tH/\hbar)}\, a\, e^{-i(tH/\hbar)}, \tag{2.29}$$

with H as in (2.27), for $a \in B(\mathcal{H}^{I}) \otimes B(\mathcal{H}^{II})$.

It follows from assumptions (A1) and (A3), Eqs. (2.17) and (2.28), that the thermodynamic limit of the time evolution of the coupled reservoirs exists: For arbitrary $a \in \mathcal{F}$ the limits

$$\alpha_t^0(a) \;=\; n - \lim_{\substack{\Lambda^I \nearrow \infty \\ \Lambda^{II} \nearrow \infty}} \alpha_t^{\Lambda^I} \otimes \alpha_t^{\Lambda^{II}}(a) \tag{2.30}$$

and

$$\alpha_t(a) \;=\; n - \lim_{\substack{\Lambda^I \nearrow \infty \\ \Lambda^{II} \nearrow \infty}} \alpha_t^{I \cup II}(a) \tag{2.31}$$

exist, and the convergence is *uniform* on arbitrary compact intervals of the time axis.

Given (2.30), (2.31) follows by using the *Lie-Schwinger series* for $\alpha_t(\alpha_{-t}^0(a))$. We distinguish between *different types of contacts or junctions* between the two reservoirs, according to symmetry properties of the contact interactions $W(\Lambda^I, \Lambda^{II})$.

(J1) Thermal contacts. The interaction $W(\Lambda^I, \Lambda^{II})$ commutes with *all* the conservation laws $\{Q_j^{\Lambda^I} \otimes \mathbb{1}\}_{j=1}^{M^I}$ and $\{\mathbb{1} \otimes Q_j^{\Lambda^{II}}\}_{j=1}^{M^{II}}$ of the reservoirs, i.e.,

$$\varphi_{\boldsymbol{s}}^{\Lambda^I}\big(W\big(\Lambda^I, \Lambda^{II}\big)\big) \;=\; \varphi_{\boldsymbol{s}}^{\Lambda^{II}}\big(W\big(\Lambda^I, \Lambda^{II}\big)\big) \;=\; W\big(\Lambda^I, \Lambda^{II}\big), \tag{2.32}$$

for *arbitrary* Λ^I and Λ^{II}, where $\varphi_{\boldsymbol{s}}^{\Lambda^I}$ is a shorthand notation for $\varphi_{\boldsymbol{s}}^{\Lambda^I} \otimes \mathrm{id}$, and $\varphi_{\boldsymbol{s}}^{\Lambda^{II}}$ stands for $\mathrm{id} \otimes \varphi_{\boldsymbol{s}}^{\Lambda^{II}}$; (see eq. (2.3)). It follows from (2.27) and (2.2) that the operators $\{Q_j^{\Lambda^I} \otimes \mathbb{1}\}$ and $\{\mathbb{1} \otimes Q_i^{\Lambda^{II}}\}$ are conservation laws of the perturbed dynamics.

By assumption (A1), the limits

$$n - \lim_{\Lambda^r \nearrow \infty} \varphi_{\boldsymbol{s}}^{\Lambda^r}(a) \;=:\; \varphi_{\boldsymbol{s}}^{r}(a) \tag{2.33}$$

exist for $r = I$ or II and for all $a \in \mathcal{F}$. By assumption (A3) and (2.32) it follows that

$$\varphi_{\boldsymbol{s}}^{I}(W) \;=\; \varphi_{\boldsymbol{s}}^{II}(W) \;=\; W, \tag{2.34}$$

in the thermodynamic limit.

Energy appears to be the only thermodynamic quantity that can be exchanged through a thermal contact.

(J2) Tunnelling junctions. There are $m \leq \min(M^I, M^{II})$ linear combinations, $\widetilde{Q}_1^{\Lambda^I}, \ldots, \widetilde{Q}_m^{\Lambda^I}$ and $\widetilde{Q}_1^{\Lambda^{II}}, \ldots, \widetilde{Q}_m^{\Lambda^{II}}$, of conservation laws of the two reservoirs with the property that the operators

$$Q_j^{I \cup II} \;:=\; \widetilde{Q}_j^{\Lambda^I} \otimes \mathbb{1} + \mathbb{1} \otimes \widetilde{Q}_j^{\Lambda^{II}}, \tag{2.35}$$

$j = 1, \ldots, m$, are *conservation laws* of the *perturbed dynamics* generated by the Hamiltonian H of eq. (2.27). Without loss of generality, we may assume that $\widetilde{Q}_j^{\Lambda^I} = Q_j^{\Lambda^I}$ and $\widetilde{Q}_j^{\Lambda^{II}} = Q_j^{\Lambda^{II}}$, for $j = 1, \ldots, m$. Of course, there may be further conservation laws of the reservoirs, $Q_i^{\Lambda^I} \otimes \mathbb{1}$, $\mathbb{1} \otimes Q_j^{\Lambda^{II}}$, for some $i > m$ and/or some $j > m$, which are conservation laws of the perturbed dynamics. "Leaky junctions" are contacts where the interaction $W(\Lambda^I, \Lambda^{II})$ *violates some* of the conservation laws $Q_i^{\Lambda^I} \otimes \mathbb{1}$ and/or $\mathbb{1} \otimes Q_j^{\Lambda^{II}}$, $i, j > m$. For convenience, we shall sometimes assume that the operators $Q_j^{I \cup II}$, $j = 1, \ldots, m$, are the *only* conservation laws of the perturbed dynamics, and $M^I = M^{II} = m$. Let $\boldsymbol{s} = (s_1, \ldots, s_m, 0, \ldots, 0)$. We define

$$\varphi_{\boldsymbol{s}}^{I \cup II}(a) \; := \; \varphi_{\boldsymbol{s}}^{\Lambda^I} \otimes \varphi_{\boldsymbol{s}}^{\Lambda^{II}}(a), \tag{2.36}$$

for $a \in B(\mathcal{H}^I) \otimes B(\mathcal{H}^{II})$, and

$$\varphi_{\boldsymbol{s}}(a) \; := \; n - \lim_{\substack{\Lambda^I \nearrow \infty \\ \Lambda^{II} \nearrow \infty}} \varphi_{\boldsymbol{s}}^{I \cup II}(a), \tag{2.37}$$

for $a \in \mathcal{F}$; see assumptions (A1), eq. (2.18).

Tunnelling junctions can then be characterized by the requirement that

$$\varphi_{\boldsymbol{s}}^{I \cup II}\big(W\big(\Lambda^I, \Lambda^{II}\big)\big) \; = \; W\big(\Lambda^I, \Lambda^{II}\big), \tag{2.38}$$

for arbitrary Λ^I, Λ^{II}, and hence, using (2.18) and (2.28), we find that, in the thermodynamic limit,

$$\varphi_{\boldsymbol{s}}(W) \; = \; W. \tag{2.39}$$

As an *initial state* of a tunnelling junction we shall usually choose a state ω close to a tensor product state, $\omega_{\beta^I, \boldsymbol{\mu}^I}^{\Lambda^I} \otimes \omega_{\beta^{II}, \boldsymbol{\mu}^{II}}^{\Lambda^{II}}$, of two equilibrium states of the uncoupled reservoirs, where β^I, $\boldsymbol{\mu}^I$ and β^{II}, $\boldsymbol{\mu}^{II}$ are arbitrary, (with $\boldsymbol{\mu}^I \in \mathcal{M}^I$, $\boldsymbol{\mu}^{II} \in \mathcal{M}^{II}$).

Two reservoirs joined by a tunnelling junction can exchange energy and "charge" (as measured by the conservation laws $Q_j^{\Lambda^I} \otimes \mathbb{1}$, $\mathbb{1} \otimes Q_j^{\Lambda^{II}}$, $j = 1, \ldots, m$), or leak some "charge" corresponding to $Q_j^{\Lambda^I} \otimes \mathbb{1}$, or to $\mathbb{1} \otimes Q_j^{\Lambda^{II}}$, for some $j > m$.

Energy current. The operator corresponding to a measurement of the *gain of internal energy per second* of reservoir r, with $r = I$ or II, at time t is conveniently defined in the Heisenberg picture by

$$\begin{aligned} P^r(t) \; &:= \; \frac{d}{dt}\, \alpha_t^{I \cup II}(H^r) \\ &= \; \frac{i}{\hbar}\, \alpha_t^{I \cup II}([H, H^r]), \end{aligned} \tag{2.40}$$

where $\alpha_t^{I \cup II}$ is as in (2.29), and $H^r = H^I \otimes \mathbb{1}$ or $= \mathbb{1} \otimes H^{II}$, for $r = I$ or II, respectively. By (2.25) and (2.27),

$$P^r(t) \; = \; \frac{i}{\hbar}\, \alpha_t^{I \cup II}\big(\big[W(\Lambda^I, \Lambda^{II}), H^r\big]\big). \tag{2.41}$$

By (2.17), (2.28) and (2.31), the operator corresponding to the energy gain per second of reservoir r has a thermodynamic limit given by

$$P^r(t) \;=\; -\frac{d}{ds}\,\alpha_t\left(\alpha_s^r(W)\right)\Big|_{s=0}, \tag{2.42}$$

where α_s^r is the time evolution of reservoir r in the thermodynamic limit, in the absence of any contacts. It follows from (2.41) and (2.42) that

$$\begin{aligned} P^I(t)+P^{II}(t) &= \frac{i}{\hbar}\,\alpha_t^{I\cup II}\left(\left[W(\Lambda^I,\Lambda^{II}),H^0\right]\right) \\ &= \frac{i}{\hbar}\,\alpha_t^{I\cup II}\big(\left[W(\Lambda^I,\Lambda^{II}),H\right]\big) \\ &= -\frac{d}{dt}\,\alpha_t^{I\cup II}\big(W(\Lambda^I,\Lambda^{II})\big), \end{aligned} \tag{2.43}$$

where H^0 and H are as in eqs. (2.25), (2.27), and, in the thermodynamic limit,

$$P^I(t)+P^{II}(t) \;=\; -\frac{d}{dt}\,\alpha_t(W), \tag{2.44}$$

with $W\in\mathcal{F}$.

We observe that if ω is an *arbitrary time-translation invariant state* of the coupled system, we have that

$$\omega\left(P^I(t)+P^{II}(t)\right) \;=\; 0, \tag{2.45}$$

for all times.

Charge current. The operator corresponding to a measurement of the gain of charge Q_j^r per second at time t, in reservoir r, is conveniently defined by

$$\begin{aligned} I_j^r(t) &= \frac{d}{dt}\,\alpha_t^{I\cup II}\left(Q_j^r\right) \\ &= \frac{i}{\hbar}\,\alpha_t^{I\cup II}\left([H,Q_j^r]\right), \end{aligned} \tag{2.46}$$

for $j=1,\dots,m$, $r=I,II$, with $Q_j^I := Q_j^{\Lambda^I}\otimes\mathbb{1}$, and $Q_j^{II} := \mathbb{1}\otimes Q_j^{\Lambda^{II}}$. Since H is given by

$$H \;=\; H^I\otimes\mathbb{1} \;+\; \mathbb{1}\otimes H^{II} \;+\; W\big(\Lambda^I,\Lambda^{II}\big),$$

and since $H^I\otimes\mathbb{1}$ and $\mathbb{1}\otimes H^{II}$ commute with Q_i^r, it follows that

$$I_j^r(t) \;=\; \frac{i}{\hbar}\,\alpha_t^{I\cup II}\left(\left[W\left(\Lambda^I,\Lambda^{II}\right),Q_j^r\right]\right). \tag{2.47}$$

In the thermodynamic limit,

$$I_j^r(t) \;=\; -\frac{1}{\hbar}\,\frac{\partial}{\partial\, s_j}\,\alpha_t\big(\varphi^r_{\boldsymbol{s}}(W)\big)\big|_{\boldsymbol{s}=0} \tag{2.48}$$

with $\varphi^r_{\boldsymbol{s}}$ as in (2.33); $r = I, II$, $j = 1, \ldots, M^r$. Recall that, for $j = 1, \ldots, m$, the operators $Q_j^{I\cup II} = Q_j^{\Lambda^I} \otimes \mathbb{1} + \mathbb{1} \otimes Q_j^{\Lambda^{II}}$ are conservation laws of the perturbed dynamics, see (2.38), and therefore

$$I_j^I(t) \,+\, I_j^{II}(t) \;=\; \frac{i}{\hbar}\,\alpha_t^{I\cup II}\big(\big[W\left(\Lambda^I, \Lambda^{II}\right), Q_j^{I\cup II}\big]\big) = 0, \tag{2.49}$$

for $j = 1, \ldots, m$; this can be transferred to the thermodynamic limit. Apparently, charge lost by one reservoir is gained by the other one.

For $j > m$, (2.49) does *not* hold in general and the operators $I_j^r(t), r = I, II$, describe the leakage of charge Q_j^r at the junction.

2.3 Connections with thermodynamics

We start by recalling the **1st and 2nd law of thermodynamics**.

For the reservoir r, the first and second law of thermodynamics can be summarized in the equation

$$dU^{\Lambda^r} \;=\; T^r\, dS^{\Lambda^r} \;+\; \boldsymbol{\mu}^r \,\cdot\, d\boldsymbol{q}^{\Lambda^r} - p^r\, dV^r, \tag{2.50}$$

where U^{Λ^r} is the expectation value of the Hamiltonian H^r in a state of reservoir r *close to*, or *in* thermal equilibrium, i.e., U^{Λ^r} is the *internal energy* of the reservoir r; T^r the *temperature*; S^{Λ^r} the *entropy*; $q_j^{\Lambda^r}$ is the expectation value of the charge Q_j^r, $j = 1, \ldots, M^r$, in the state describing the reservoir; p^r is the *pressure*, and $V^r = \mathrm{vol}(\Lambda^r)$ the volume. The differential "*d*" indicates that we consider the variation of U^{Λ^r}, S^{Λ^r}, etc. under small, reversible changes of the state of reservoir r (which may include small changes of the region Λ^r).

We shall be interested in studying small, slow changes in time of the state of reservoirs I and II, at approximately fixed values of the thermodynamic parameters T^r, $\boldsymbol{\mu}^r$ and p^r, brought about by opening a *contact* or *junction* between the two reservoirs. Then $U^{\Lambda^r}, S^{\Lambda^r}, \ldots$ are *time-dependent*, and (2.50) becomes

$$\dot U^{\Lambda^r} \;=\; T^r \dot S^{\Lambda^r} \;+\; \boldsymbol{\mu}^r \cdot \dot{\boldsymbol{q}}^{\Lambda^r} - p^r\, \dot V^r, \tag{2.51}$$

where the "dots" indicate time derivatives. By (2.40), the energy gain per second, $\dot U^{\Lambda^r}$, of the reservoir r is given by

$$\dot U^{\Lambda^r}(t) \;=\; \omega^{I\cup II}\left(P^r(t)\right), \tag{2.52}$$

and the gain in the j^{th} charge per second by

$$\dot{q}_j^{\Lambda^r}(t) \;=\; \omega^{I\cup II}\left(I_j^r(t)\right), \tag{2.53}$$

see (2.46), where $\omega^{I\cup II}$ is the state of the system consisting of the two reservoirs. By (2.51), the change in entropy per second of reservoir r is given by $(\beta^r := 1/T^r)$

$$\dot{S}^{\Lambda^r} \;=\; \beta^r\left(\dot{U}^{\Lambda^r} - \boldsymbol{\mu}^r\cdot\dot{\boldsymbol{q}}^{\Lambda^r} + p^r\dot{V}^r\right). \tag{2.54}$$

We define the *entropy production rate*, $\mathcal{E}^{I\cup II}$, by

$$\mathcal{E}^{I\cup II} \;:=\; \dot{S}^{\Lambda^I} + \dot{S}^{\Lambda^{II}}. \tag{2.55}$$

The main property of $\mathcal{E}^{I\cup II}$ is *its sign*: thermodynamic systems should exhibit positive entropy production,

$$\mathcal{E}^{I\cup II} \;\geq\; 0, \tag{2.56}$$

in the limit where $\Lambda^I \nearrow \infty$ and $\Lambda^{II} \nearrow \infty$. In [Ru2], Ruelle has proven (2.56) for the special case of thermal contacts between infinitely large reservoirs. Below, we shall derive (2.56), under more general conditions, from the positivity of "relative entropy"; see also [JP1].

We consider a situation in which the state of the system consisting of reservoirs I and II, *before* a contact or junction is opened, is given by the tensor product of two equilibrium states

$$\omega^{I\cup II}(a) \;=\; \omega^{\Lambda^I}_{\beta^I,\boldsymbol{\mu}^I}\otimes\omega^{\Lambda^{II}}_{\beta^{II},\boldsymbol{\mu}^{II}}(a), \tag{2.57}$$

for any operator $a \in B(\mathcal{H}^{\Lambda^I})\otimes B(\mathcal{H}^{\Lambda^{II}})$, where the equilibrium states $\omega^{\Lambda^r}_{\beta^r,\boldsymbol{\mu}^r}$ have been defined in (2.10). The state $\omega^{I\cup II}$ is invariant under the unperturbed time evolutions $\alpha_t^{\Lambda^r}$, $r = I, II$, of the reservoirs.

At some time t_0, the contact between the reservoirs is opened, and we are interested in the evolution of the state $\omega^{I\cup II}$ under the *perturbed* time evolution, $\alpha_t^{I\cup II}$, introduced in (2.27), (2.29). In particular, we are interested in calculating the rate of energy gain, or loss, $\dot{U}^{\Lambda^r}(t)$, the gain or loss of charge j, $\dot{q}_j^{\Lambda^r}(t)$, $j = 1,\ldots,M^r$, per second and the entropy production rate $\mathcal{E}^{I\cup II}(t)$, under the perturbed time evolution, in the state $\omega^{I\cup II}$. By eqs. (2.40) and (2.41),

$$\begin{aligned}\dot{U}^{\Lambda^r}(t) \;&=\; \omega^{I\cup II}(P^r(t))\\ &=\; \frac{i}{\hbar}\,\omega^{I\cup II}\big(\alpha_t^{I\cup II}\big(\big[W(\Lambda^I,\Lambda^{II}),H^r\big]\big)\big)\end{aligned} \tag{2.58}$$

and, by (2.46),

$$\begin{aligned}\dot{q}_j^{\Lambda^r}(t) \;&=\; \omega^{I\cup II}\big(I_j^r(t)\big)\\ &=\; \frac{i}{\hbar}\,\omega^{I\cup II}\big(\alpha_t^{I\cup II}\big(\big[W(\Lambda^I,\Lambda^{II}),Q_j^r\big]\big)\big).\end{aligned} \tag{2.59}$$

By assumption (A2), see (2.20), the states $\omega^{I\cup II}$ have a thermodynamic limit

$$\omega^0(a) \;=\; \lim_{\substack{\Lambda^I\nearrow\infty\\ \Lambda^{II}\nearrow\infty}} \;\omega^{I\cup II}(a), \tag{2.60}$$

for $a \in \mathcal{F} = \mathcal{F}^I \otimes \mathcal{F}^{II}$. It follows from this property, from assumption (A3), and from equations (2.31), (2.42), and (2.48), that the quantities $\dot{U}^{\Lambda^r}(t)$ and $\dot{q}_j^{\Lambda^r}(t)$ have thermodynamic limits

$$\begin{aligned} \mathcal{P}^r(t) \;&:=\; \lim_{\substack{\Lambda^I\nearrow\infty\\ \Lambda^{II}\nearrow\infty}} \;\dot{U}^{\Lambda^r}(t) \\ &=\; -\frac{d}{ds}\,\omega^0\big(\alpha_t\big(\alpha_s^r(W)\big)\big)\big|_{s=0} \end{aligned} \tag{2.61}$$

and

$$\begin{aligned} \mathcal{J}_j^r(t) \;&:=\; \lim_{\substack{\Lambda^I\nearrow\infty\\ \Lambda^{II}\nearrow\infty}} \;\dot{q}_j^{\Lambda^r}(t) \\ &=\; -\frac{1}{\hbar}\,\frac{\partial}{\partial s_j}\,\omega^0\big(\alpha_t\big(\varphi_{\boldsymbol{s}}^r(W)\big)\big)\big|_{\boldsymbol{s}=0}\,. \end{aligned} \tag{2.62}$$

These limits are *uniform* on compact intervals of the time axis. By (2.43) and (2.49),

$$\mathcal{P}^I(t) + \mathcal{P}^{II}(t) \;=\; -\frac{d}{dt}\,\omega^0\big(\alpha_t(W)\big) \tag{2.63}$$

and

$$\mathcal{J}_j^I(t) + \mathcal{J}_j^{II}(t) \;=\; 0, \tag{2.64}$$

for $j = 1, \ldots, m$.

Next, we study the entropy production rate for finite reservoirs. Let

$$\rho^r \;:=\; \big(\Xi_{\beta^r,\boldsymbol{\mu}^r}^{\Lambda^r}\big)^{-1}\;\exp - \beta^r\left[H^r - \boldsymbol{\mu}^r\cdot\boldsymbol{Q}^{\Lambda^r}\right] \tag{2.65}$$

be the density matrix corresponding to the equilibrium state, $\omega_{\beta^r,\boldsymbol{\mu}^r}^{\Lambda^r}$, for the reservoir r; see (2.10). Then

$$-\ln\,\rho^r \;=\; \beta^r\left[H^r - \boldsymbol{\mu}^r\cdot\boldsymbol{Q}^{\Lambda^r}\right] - \beta^r G\left(\beta^r,\boldsymbol{\mu}^r,V^r\right)\;\cdot\;\mathbb{1}\,, \tag{2.66}$$

where the thermodynamic potential G is as in (2.9). If the confinement region Λ^r is kept constant in time, so that $\dot{V}^r = 0$, then it follows from (2.51), (2.52), (2.53) and (2.66) that

$$\begin{aligned} \dot{S}^{\Lambda^r} \;&=\; \beta^r\left(\dot{U}^{\Lambda^r} - \boldsymbol{\mu}^r\cdot\dot{\boldsymbol{q}}^{\Lambda^r}\right) \\ &=\; -\frac{d}{dt}\,\omega^{I\cup II}\left(\alpha_t^{I\cup II}\left(\ln\rho^r\right)\right) \\ &=\; -\frac{d}{dt}\,\mathrm{tr}\,\left(\rho^I\otimes\rho^{II}\,\alpha_t^{I\cup II}\left(\ln\rho^r\right)\right)\,. \end{aligned} \tag{2.67}$$

Thus, by (2.55),

$$\begin{aligned} \dot{S}^{I\cup II}(t) &:= \mathcal{E}^{I\cup II}(t) \\ &= -\frac{d}{dt}\,\mathrm{tr}\,\left(\rho^{I}\otimes\rho^{II}\,\alpha_t^{I\cup II}\left(\ln\rho^{I}\otimes\rho^{II}\right)\right)\,. \end{aligned} \tag{2.68}$$

By (2.61) and (2.62) this quantity has a thermodynamic limit

$$\mathcal{E}(t) = \sum_{r=I,II}\beta^r\left[\mathcal{P}^r(t)-\boldsymbol{\mu}^r\cdot\boldsymbol{\mathcal{J}}^r(t)\right]\,. \tag{2.69}$$

Integrating (2.68) in time, we find that

$$S^{I\cup II}(t)-S^{I\cup II}(0) = -\mathrm{tr}\,\left(\rho^{I}\otimes\rho^{II}\left[\alpha_t^{I\cup II}\left(\ln\rho^{I}\otimes\rho^{II}\right)-\ln\rho^{I}\otimes\rho^{II}\right]\right)\,. \tag{2.70}$$

This equation shows that $S^{I\cup II}(t)-S^{I\cup II}(0)$ is nothing but the *relative entropy* of the density matrix $\alpha_t^{I\cup II}(\rho^{I}\otimes\rho^{II})$ with respect to the density matrix $\rho^{I}\otimes\rho^{II}$; see e.g. [BR, vol II] for a definition of relative entropy, which differs from ours by the sign, and [JP1] for similar, independent considerations. If A is a non-negative matrix and B is a strictly positive matrix then

$$-\mathrm{tr}\,\left(A\ln B-A\ln A\right) \geq \mathrm{tr}\,(A-B), \tag{2.71}$$

see Lemma 6.2.21 of [BR, vol II]. Setting $A=\rho^{I}\otimes\rho^{II}$ and $B=\alpha_t^{I\cup II}(\rho^{I}\otimes\rho^{II})$, we find that

$$S^{I\cup II}(t)-S^{I\cup II}(0) \geq \mathrm{tr}\left(\rho^{I}\otimes\rho^{II}-\alpha_t^{I\cup II}(\rho^{I}\otimes\rho^{II})\right) = 0, \tag{2.72}$$

by the unitarity of time evolution and the cyclicity of the trace. It follows that

$$\frac{1}{T}\int_0^T\mathcal{E}^{I\cup II}(t)\,\mathrm{dt} = \frac{1}{T}\left(S^{I\cup II}(T)-S^{I\cup II}(0)\right) \geq 0, \tag{2.73}$$

and this inequality remains obviously valid in the thermodynamic limit:

$$\frac{1}{T}\int_0^T\mathcal{E}(t)\,\mathrm{dt} \geq 0\,. \tag{2.74}$$

Thus, if the limit

$$\lim_{t\to\infty}\mathcal{E}(t) =: \mathcal{E} \tag{2.75}$$

exists then

$$\mathcal{E} = \lim_{T\to\infty}\frac{1}{T}\int_0^T\mathcal{E}(t)\,\mathrm{dt} \geq 0\,, \tag{2.76}$$

i.e., the *entropy production rate* $\mathcal{E}$, in the thermodynamic limit, is non-negative, as time t tends to ∞; see [Ru1]. In Sect. 5, we shall study examples where $\mathcal{E}$ is *strictly positive*.

Let us assume that the entropy production rate $\mathcal{E}(t)$ converges as $t \to \infty$. It follows from (2.74) and (2.76) that it is *nonnegative*.

Let us set

$$\mathcal{P} \;:=\; \mathcal{P}^{I} \;=\; -\mathcal{P}^{II} \tag{2.77}$$

and, for $j = 1, \ldots, m$,

$$\mathcal{J}_j \;:=\; \mathcal{J}_j^{I} \;=\; -\mathcal{J}_j^{II}. \tag{2.78}$$

In the case where each reservoir has precisely m conservation laws $\{Q_j^r\}_{j=1}^m$, $r = I, II$ (that is, $M^I = M^{II} = m$ and $\{Q_j^I \otimes \mathbb{1} + \mathbb{1} \otimes Q_j^{II}\}_{j=1}^m$ are conservation laws of the coupled system), nonnegativity of the entropy production rate implies that

$$\mathcal{E} \;=\; \left(\beta^{I} - \beta^{II}\right) \mathcal{P} - \left(\beta^{I} \boldsymbol{\mu}^{I} - \beta^{II} \boldsymbol{\mu}^{II}\right) \cdot \boldsymbol{\mathcal{J}} \;\geq\; 0\,. \tag{2.79}$$

The currents $\mathcal{J}_j^r$ vanish for thermal contacts, and (2.79) shows that energy is transferred from the hotter to the colder reservoir — as expected.

The thermoelectric situation corresponds to $M^I = M^{II} = m = 1$, and $Q_1^r = N^r$ is the particle number operator. For identical temperatures but different chemical potentials, (2.79) shows that particles are transferred from the reservoir with the higher chemical potential to the reservoir with the lower chemical potential. Notice that energy may flow from the colder reservoir to the hotter one when the chemical potentials are different (consider e.g. $\beta^I \mu^I \gg \beta^{II} \mu^{II}$ but $\beta^I > \beta^{II}$).

Also interesting is the case of *adiabatic* thermal contacts between two reservoirs, i.e., without heat exchange. A general discussion of systems with time-dependent interactions confined to time-dependent regions is given in [FMSU], and will be elaborated upon in a forthcoming paper.

2.4 Existence of stationary states in the thermodynamic limit

The above considerations, and in particular (2.61), (2.62), and (2.75), suggest to study the question whether the infinite-volume states

$$\omega_t(a) \;:=\; \omega^0\left(\alpha_t(a)\right), \;\; a \in \mathcal{F}\,, \tag{2.80}$$

have a limit, as $t \to \infty$.

The state ω^0, defined in (2.60), is obviously invariant under the unperturbed time evolution α_t^0 defined in (2.30). Thus

$$\omega_t(a) \;=\; \omega^0\left(\alpha_{-t}^0\left(\alpha_t(a)\right)\right), \; a \in \mathcal{F}. \tag{2.81}$$

A sufficient condition for the existence of a *stationary* (i.e., time-translation invariant) *limiting state*,

$$\omega_{\mathrm{stat}}(a) \;=\; \lim_{t\to\infty} \omega_t(a), \;\; a \in \mathcal{F} \,, \tag{2.82}$$

is given in

(A4) Existence of a scattering endomorphism.
The limits

$$\sigma_\pm(a) \;=\; n - \lim_{t\to\pm\infty} \alpha^0_{-t}\,(\alpha_t(a)) \tag{2.83}$$

exist, for all $a \in \mathcal{F}$*, and define* **endomorphisms of* $\mathcal{F}$*, i.e.,* $\sigma_\pm$ *are homomorphisms of the* C^**-algebra* $\mathcal{F}$ *with the property that* $\sigma_\pm(a)^* = \sigma_\pm(a^*)$*, for all* $a \in \mathcal{F}$*.*

The usefulness of these so-called *scattering (or Møller) endomorphisms* has first been recognized in [He, Rob]; interesting examples have been constructed in [BM]. In the context of thermal contacts and tunnelling junctions, they have first been used in [DFG]; see also [Ma].

It is important to note that scattering endomorphisms do not exist in *finite* volume, because the free and the perturbed time evolutions of the two reservoirs are generated by Hamiltonians

$$\begin{aligned} H^0 &= H^{I} \otimes \mathbb{1} + \mathbb{1} \otimes H^{II}, \\ H &= H^0 + W(\Lambda^{I}, \Lambda^{II}), \end{aligned}$$

see (2.25) and (2.27), with *pure-point* spectra when Λ^{I} and Λ^{II} are compact. It is thus natural to wonder about the meaning of scattering endomorphisms for large but finite reservoirs. Let us sketch the answer to this question. We fix an arbitrarily small, but positive number ε. For every operator $a \in \mathcal{F}$, there exist compact regions $\Lambda^r(\varepsilon, a)$, $r = I, II$, and an operator $a_\varepsilon \in B(\mathcal{H}^{\Lambda^{I}}) \otimes B(\mathcal{H}^{\Lambda^{II}})$, with $\Lambda^r = \Lambda^r(\varepsilon, a)$, $r = I, II$, such that

$$\|a - a_\varepsilon\| \;<\; \frac{\varepsilon}{4}\,.$$

Then, by (2.82) and (2.83), there is some $T(\varepsilon, a) < \infty$ such that

$$\left|\omega_{\mathrm{stat}}(a) - \omega_t(a_\varepsilon)\right| \;<\; \frac{\varepsilon}{2}\,,$$

for all $t > T(\varepsilon, a)$. Assumption (A3), eq. (2.31), tells us that, for an arbitrary $T < \infty$, there are compact sets $\Lambda^r(\varepsilon, a, T) \supseteq \Lambda^r(\varepsilon, a)$ such that if $\Lambda^r \supset \Lambda^r(\varepsilon, a, T)$, $r = I, II$, then

$$\|\alpha_t(a_\varepsilon) - \alpha_t^{I\cup II}(a_\varepsilon)\| \;<\; \frac{\varepsilon}{4}\,,$$

for all $t \in [0, T]$. Finally, by assumption (A2), one can choose $\Lambda^r(\varepsilon, a, T)$ so large that

$$\left|\omega^{I\cup II}\left(\alpha_t^{I\cup II}(a_\varepsilon)\right) - \omega^0\left(\alpha_t^{I\cup II}(a_\varepsilon)\right)\right| \;<\; \frac{\varepsilon}{4}\,,$$

provided $\Lambda^r \supset \Lambda^r(\varepsilon, a, T)$, $r = I, II$, for *all* times $t \in [0, T]$. It follows that, for any T, with $0 \;<\; T(\varepsilon, a) \;<\; T \;<\; \infty$, and for $\Lambda^r \;\supset\; \Lambda^r(\varepsilon, a, T),\;\; r \;=\; I, II,$

$$\left|\omega_{\mathrm{stat}}(a) - \omega^{I\cup II}\left(\alpha_t^{I\cup II}(a_\varepsilon)\right)\right| \;<\; \varepsilon\;, \tag{2.84}$$

for all times t, with $T(\varepsilon, a) < t < T$.

These simple considerations, combined with (2.44) and (2.48), show that the energy-gain rates $\dot{U}^{\Lambda^r}(t)$ and the currents $\dot{q}_j^{\Lambda^r}(t)$ of two very large, but finite reservoirs, $r = I, II$, are well approximated by the energy-gain rates

$$\mathcal{P}^r \;:=\; \lim_{t\to\infty}\; \mathcal{P}^r(t) \;=\; -\frac{d}{ds}\,\omega_{\mathrm{stat}}\left(\alpha_s^r(W)\right)\big|_{s=0} \tag{2.85}$$

and the currents

$$\mathcal{J}_j^r \;:=\; \lim_{t\to\infty}\; \mathcal{J}_j^r(t) \;=\; -\frac{1}{\hbar}\,\frac{\partial}{\partial s_j}\,\omega_{\mathrm{stat}}\left(\varphi_{\boldsymbol{s}}^r(W)\right)\big|_{\boldsymbol{s}=0}\,, \tag{2.86}$$

respectively, for a large range of *sufficiently large*, but *not exceedingly large* times t; (see (2.61), (2.62)).

Remark. It is usually much easier to prove that the limits

$$\sigma'_\pm(a) \;:=\; n - \lim_{t\to\pm\infty}\; \alpha_{-t}\left(\alpha_t^0(a)\right) \tag{2.87}$$

exist and are operators in $\mathcal{F}$, for arbitrary $a \in \mathcal{F}$, rather than to establish the existence of the scattering endomorphisms $\sigma_\pm$ in (2.83). If the unperturbed dynamics of the reservoirs is dispersive, (as for non-interacting, non-relativistic electrons), one may hope to prove (2.87) by using a simple Cook argument; see e.g. [He, Rob, CFKS]. If both limits (2.83) and (2.87) exist then

$$\sigma_\pm\left(\sigma'_\pm(a)\right) \;=\; \sigma'_\pm\left(\sigma_\pm(a)\right) \;=\; a\,, \tag{2.88}$$

i.e., $\sigma'_\pm$ is a left and right inverse of $\sigma_\pm$, and hence $\sigma_\pm$ is a **automorphism* of $\mathcal{F}$. This will turn out to hold in the examples discussed in subsequent sections.

2.5 Uniqueness and stability properties of stationary states

We first describe the property of return to equilibrium for a single reservoir. Let ω be a state on the field algebra of a single reservoir, $\mathcal{F}^r$, i.e., ω is a positive, linear functional on $\mathcal{F}^r$ normalized such that $\omega(\mathbb{1}) = 1$. From $\mathcal{F}^r$ and ω one can construct a Hilbert space $\mathcal{H}_\omega$, a representation π_ω of $\mathcal{F}^r$ on $\mathcal{H}_\omega$, and a unit vector $\Omega \in \mathcal{H}_\omega$ (unique up to a phase) such that

$$\mathcal{H}_\omega \;=\; \overline{\left\{\pi_\omega(a)\Omega \;\middle|\; a \in \mathcal{F}^r\right\}}, \tag{2.89}$$

where the closure is taken in the norm on $\mathcal{H}_\omega$, i.e., Ω is "cyclic" for $\pi_\omega(\mathcal{F}^r)$, and

$$\omega(a) \;=\; \big\langle \Omega, \pi_\omega(a)\,\Omega \big\rangle, \tag{2.90}$$

where $\langle \cdot, \cdot \rangle$ is the scalar product on $\mathcal{H}_\omega$. This is the content of the *Gel'fand-Naimark-Segal* (GNS) *construction*. If the state ω is time-translation invariant then there exists a one-parameter unitary group $\left\{U_\omega(t) \;\middle|\; t \in \mathbb{R}\right\}$ on $\mathcal{H}_\omega$ such that

$$\pi_\omega(\alpha_t(a)) \;=\; U_\omega(t)\,\pi_\omega(a)\,U_\omega(t)^*,$$

and

$$U_\omega(t)\,\Omega \;=\; \Omega\,. \tag{2.91}$$

Under standard continuity assumptions on $U_\omega(t)$, we can summon Stone's theorem to conclude that

$$U_\omega(t) \;=\; e^{it\,L_\omega/\hbar}, \tag{2.92}$$

where the generator L_ω is a selfadjoint operator on $\mathcal{H}_\omega$ with $L_\omega\,\Omega = 0$.

A state ρ on $\mathcal{F}^r$ is called *normal* relative to ω iff there exists a density matrix, P, on $\mathcal{H}_\omega$ such that

$$\rho\,(a) \;=\; \mathrm{tr}_{\mathcal{H}_\omega}\left(P\,\pi_\omega(a)\right), \tag{2.93}$$

for all $a \in \mathcal{F}^r$.

Let $\omega \;:=\; \omega_{\beta,\boldsymbol{\mu}}$ be an infinite-volume equilibrium state on $\mathcal{F}^r$ obeying the KMS condition (2.22). We assume that the Hilbert space $\mathcal{H}_\omega$ obtained from the GNS construction is *separable* and that the cyclic vector $\Omega \in \mathcal{H}_\omega$ is the *only eigenvector* (up to phases) of the operator L_ω of (2.92), which, in this context, is called the *Liouvillian* or *thermal Hamiltonian*. In other words, the spectrum of L_ω is purely continuous, except for a simple eigenvalue at 0.

This assumption implies the property of *"return to equilibrium"*: If ρ is an arbitrary state *normal* relative to $\omega = \omega_{\beta,\boldsymbol{\mu}}$ then

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \mathrm{d}t\,\rho\,(\alpha_t(a)) \;=\; \omega(a), \tag{2.94}$$

for all $a \in \mathcal{F}^r$. If the spectrum of L_ω is *absolutely continuous*, except for a simple eigenvalue at 0, then

$$\lim_{t\to\infty} \rho\;(\alpha_t(a)) \;=\; \omega(a), \tag{2.95}$$

for all $a \in \mathcal{F}^r$. Eqs. (2.94) and (2.95) follow from our assumptions on the spectrum of L_ω and the KMS condition (2.22); see e.g. [BFS].

Assuming the existence of the endomorphism σ_+, see (A4), we now address the question of uniqueness and dynamical stability of the stationary state ω_{stat} in (2.82).

We suppose that the property of return to equilibrium, (2.95), holds for each reservoir separately; (this can be shown for reservoirs consisting of free fermions as considered in Sections 3 and 4). Recalling that the reference state ω^0 is a product of two KMS states (see (2.60), (2.57)), it is not difficult to extend the arguments in Sect. III, D of [BFS] to show that if ρ is an arbitrary state on $\mathcal{F}$ normal relative to the state ω^0 in (2.60) then

$$\lim_{t\to\infty} \rho\left(\alpha_t^0(a)\right) \;=\; \omega^0(a), \;\; a \in \mathcal{F}\,, \tag{2.96}$$

where α_t^0 is the time evolution of the reservoirs before they are coupled; see (2.30).

Eq. (2.96) and the existence of a scattering endomorphism σ_+, see eq. (2.83), now imply that

$$\begin{aligned}\lim_{t\to\infty} \rho_t(a) \;&=\; \lim_{t\to\infty} \rho(\alpha_t(a)) \\ &=\; \lim_{t\to\infty} \rho\big(\alpha_t^0\big(\sigma_+(a)\big)\big) \\ &=\; \omega^0\big(\sigma_+(a)\big) \\ &=\; \omega_{\text{stat}}(a)\,,\end{aligned} \tag{2.97}$$

for $a \in \mathcal{F}$. Thus, if the initial state ρ is an *arbitrary* state *normal* relative to ω^0 then the states ρ_t tend to the stationary state ω_{stat}, as $t \to \infty$, (*uniqueness*).

Next, let ρ be an *arbitrary* state *normal* relative to ω_{stat}. We claim that if eq. (2.95) holds for each reservoir then

$$\lim_{t\to\infty} \rho_t(a) \;=\; \omega_{\text{stat}}(a), \; a \in \mathcal{F}. \tag{2.98}$$

Eq. (2.98) is the property of *"return to the stationary state" (stability)*, for states ρ *normal* relative to ω_{stat}. To prove eq. (2.98), we follow the arguments in Sect. III, D of [BFS]: Since ρ is normal relative to ω_{stat}, there exist non-negative numbers, $p_n,\ n = 1,2,3,\ldots$, with $\sum_{n=1}^{\infty} p_n = 1$, and nets of operators $\{u_n^\alpha\}_{\alpha\in I_n}$, $n = 1,2,3,\ldots$, with $u_n^\alpha \in \mathcal{F}$, for all α and all n, such that

$$\rho(a) \;= \sum_{n=1}^{\infty} p_n \lim_{\alpha,\alpha'} \left\langle \pi\big(u_n^\alpha\big)\Omega, \pi(a)\,\pi\big(u_n^{\alpha'}\big)\Omega \right\rangle$$

where π is the GNS representation and Ω the cyclic vector corresponding to $(\omega_{\text{stat}}, \mathcal{F})$; see (2.89), (2.90), and (2.93). Then

$$\rho_t(a) \;= \sum_{n=1}^{\infty} p_n \lim_{\alpha,\alpha'} \left\langle \pi\big(u_n^\alpha\big)\Omega,\; \pi\big(\alpha_t(a)\big)\pi\big(u_n^{\alpha'}\big)\Omega \right\rangle .$$

Let

$$b_1 := u_n^\alpha , \;\; b_2 := u_n^{\alpha'} ,$$

for some fixed n, α, α'. Then

$$\big\langle \pi(b_1)\Omega,\, \pi\big(\alpha_t(a)\big)\, \pi(b_2)\Omega \big\rangle \;=\; \omega_{\rm stat}\big(b_1^* \alpha_t(a) b_2\big) \,. \tag{2.99}$$

Since $\omega_{\rm stat}(a) \;=\; \omega^0\big(\sigma_+(a)\big)$, and since, by eq. (2.83),

$$\sigma_+\big(\alpha_t(a)\big) \;=\; \alpha_t^0\big(\sigma_+(a)\big) \,, \tag{2.100}$$

for arbitrary $a \in \mathcal{F}$, the R.S. of (2.99) is given by

$$\omega_{\rm stat}\big(b_1^* \alpha_t(a) b_2\big) \;=\; \omega^0\big(\sigma_+(b_1^*)\, \alpha_t^0\big(\sigma_+(a)\big)\, \sigma_+(b_2)\big) \,.$$

It follows from (2.96) by polarization that

$$\begin{aligned} \lim_{t\to\infty} \omega^0\big(\sigma_+(b_1^*)\, \alpha_t^0\big(\sigma_+(a)\big)\, \sigma_+(b_2)\big) &= \omega^0\big(\sigma_+(b_1^*)\, \sigma_+(b_2)\big)\, \omega^0\big(\sigma_+(a)\big) \\ &= \omega_{\rm stat}\big(b_1^*\, b_2\big)\, \omega_{\rm stat}(a) \\ &= \big\langle \pi(b_1)\Omega, \pi(b_2)\Omega \big\rangle\, \omega_{\rm stat}(a) \,. \end{aligned} \tag{2.101}$$

Our contention, eq. (2.98), follows from this.

2.6 Cluster properties and profiles in d>2 dimensional systems

The last question we wish to address, in this summary of the general theory, concerns *cluster properties* of the stationary state $\omega_{\rm stat}$, which will show that $\omega_{\rm stat}$ *cannot* be an equilibrium (KMS) state for the dynamics, α_t, of the coupled reservoirs and is, in general, *not* normal relative to the product state, ω^0, of the uncoupled reservoirs.

We consider two increasing families of reservoirs confined to regions $\Lambda^r \subset \mathbb{R}^3$, with

$$\Lambda^r \nearrow \mathbb{R}^3 \,, \;\; r \;=\; I, II \,, \tag{2.102}$$

joined together by a thermal contact or a tunnelling junction localized near the origin, $\boldsymbol{x} = 0$, of physical space. The more realistic situation where the reservoirs are confined to two complementary half spaces, $\mathbb{R}^3_+$ and $\mathbb{R}^3_-$, respectively, with a junction localized near the origin, has been considered in [DFG]; see also [Ru1, Ru2]. It will be studied in more detail elsewhere. In order to describe spatial properties of the system, we make the following assumption.

(A5) Existence of space translations.

For each reservoir $r = I, II$, there exists a *automorphism (semi-) group

$$\left\{ \tau^r_{\boldsymbol{x}} \;\middle|\; \boldsymbol{x} \in \mathbb{R}^3_{(\pm)} \right\} \tag{2.103}$$

of the field algebra $\mathcal{F}^r$, representing space translations of $\mathbb{R}^3$ ($\mathbb{R}^3_\pm$, respectively) on $\mathcal{F}^r$.

For the system of two coupled reservoirs,

$$\tau_{\boldsymbol{x}} \; := \; \tau^{I}_{\boldsymbol{x}} \otimes \tau^{II}_{\boldsymbol{x}} \; , \quad \boldsymbol{x} \in \mathbb{R}^3 \; , \tag{2.104}$$

defines a representation of space translations as a 3-parameter group of *automorphisms on the field algebra $\mathcal{F} = \overline{\mathcal{F}^I \otimes \mathcal{F}^{II}}$. It is plausible that space translations satisfy the following assumption.

(A6) Asymptotic abelianness of space translations, and homogeneity of reservoirs.

The action of $\tau_{\boldsymbol{x}}$ on $\mathcal{F}$ is norm-continuous in $\boldsymbol{x} \in \mathbb{R}^3$ and for all operators a and b in $\mathcal{F}$,

$$\lim_{|\boldsymbol{x}|\to\infty} \; \| \, [\tau_{\boldsymbol{x}}(a), b] \, \| \; = \; 0 \; . \tag{2.105}$$

Furthermore, the dynamics and the equilibrium states of the uncoupled reservoirs are homogeneous, in the sense that

$$\alpha^0_t\big(\tau_{\boldsymbol{x}}(a)\big) \;=\; \tau_{\boldsymbol{x}}\big(\alpha^0_t(a)\big) \tag{2.106}$$

and

$$\omega^0\big(\tau_{\boldsymbol{x}}(a)\big) \;=\; \omega^0(a) \; , \tag{2.107}$$

for all $a \in \mathcal{F}$.

The local nature of the perturbation, W, of the dynamics of the system due to the contact or junction, see Assumption (A3), eqs. (2.27) and (2.28), and assumption (A6), then imply that, for all $a \in \mathcal{F}$,

$$\lim_{|\boldsymbol{x}|\to\infty} \; \|\alpha_t\big(\tau_{\boldsymbol{x}}(a)\big) - \alpha^0_t\big(\tau_{\boldsymbol{x}}(a)\big)\| \;=\; 0 \; , \tag{2.108}$$

for all times t. A proof of (2.108) follows from the Lie-Schwinger series for $\alpha_{-t}(\alpha^0_t(a))$ and use of (2.28) and (2.105). Relation (2.108) shows that observables localized far from the junction evolve according to the non-interacting dynamics.

It is tempting, and can be justified in examples, to strengthen assumption (A4) (existence of scattering endomorphism) as follows.

(A7) Cluster properties of the scattering endomorphism.
The limits

$$n - \lim_{t\to\pm\infty} \alpha^0_{-t}\big(\alpha_t\big(\tau_{\boldsymbol{x}}(a)\big)\big) \;=\; \sigma_\pm\big(\tau_{\boldsymbol{x}}(a)\big) \tag{2.109}$$

are uniform in $\boldsymbol{x} \in \mathbb{R}^3$*, for every* $a \in \mathcal{F}$*.*

Equations (2.108) and (2.109) imply that

$$\lim_{|\boldsymbol{x}|\to\infty} \|\sigma_\pm\big(\tau_{\boldsymbol{x}}(a)\big) - \tau_{\boldsymbol{x}}(a)\| \;=\; 0\;, \tag{2.110}$$

for every $a \in \mathcal{F}$. From this property we conclude that

$$\begin{aligned}\lim_{|\boldsymbol{x}|\to\infty} \omega_{\mathrm{stat}}\big(\tau_{\boldsymbol{x}}(a)\big) \;&=\; \lim_{|\boldsymbol{x}|\to\infty} \omega^0\big(\sigma_+\big(\tau_{\boldsymbol{x}}(a)\big)\big)\\ &=\; \lim_{|\boldsymbol{x}|\to\infty} \omega^0\big(\tau_{\boldsymbol{x}}(a)\big)\\ &=\; \omega^0(a),\;\; a \in \mathcal{F}\;,\end{aligned} \tag{2.111}$$

i.e., very far from the junction, the stationary state ω_{stat} resembles the product state ω^0 of the uncoupled reservoirs.

Remark. It is not hard to understand that if the two reservoirs occupy complementary half spaces, $\mathbb{R}^3_+$ and $\mathbb{R}^3_-$, then (2.111) is replaced by

$$\lim_{x\to-\infty} \omega_{\mathrm{stat}}\big(\tau_{(x,0,0)}\big(a\otimes \mathbb{1}\big)\big) \;=\; \omega_{\beta^I,\boldsymbol{\mu}^I}(a)\;,$$

for $a \in \mathcal{F}^I$, and

$$\lim_{x\to+\infty} \omega_{\mathrm{stat}}\big(\tau_{(x,0,0)}\big(\mathbb{1}\otimes b\big)\big) \;=\; \omega_{\beta^{II},\boldsymbol{\mu}^{II}}(b)\;,$$

for $b \in \mathcal{F}^{II}$. This may prove the presence of a *profile* of temperature, density, or ... in the stationary state, ω_{stat}, of the system.

In the examples studied in subsequent sections, which concern junctions between ordinary *three-dimensional* metals, assumptions (A6) and (A7) can be verified. Instead of three-dimensional reservoirs, we could consider *one-dimensional* (wires), or *two-dimensional* (layers) reservoirs joined by a thermal contact or a tunnelling junction. Our analysis in Sect. 4 will show that, in dimensions $d = 1, 2$, assumption (A7) will *fail*, in general. In fact, the example of the one-dimensional XY spin chain treated in [DFG, AP] and the example of quantum wires studied in [ACF] show that, in *one* dimension, ω_{stat} may well be space-translation invariant, i.e., it does not exhibit any profile. In the example of quantum wires, ω_{stat} is actually a *homogeneous thermal equilibrium state*.

Thus, we observe that the validity of assumption (A7) critically depends on the *dimension* of the reservoirs. In dimension $d > 2$, this assumption can be expected to hold, while it usually fails in dimension $d = 1, 2$. For people familiar with elementary facts of scattering theory this will not come as a surprise.

In a subsequent paper, we will show that, for a large class of reservoirs, one can construct *"observables at infinity"*, see e.g. [BR, Vol. II], corresponding to the operators $P^r(t)$ and $I_j^r(t)$ defined in eqs. (2.42), (2.48), respectively. Clearly, the expectation values of these operators *vanish* in the product state ω^0 of the uncoupled reservoirs and are given by $\mathcal{P}^r$ and $\mathcal{J}_j^r$ in the stationary state, $\omega_{\rm stat}$, of the coupled reservoirs. If we can show that $\mathcal{P}^r \neq 0$, or that $\mathcal{J}_j^r \neq 0$, for $r = I$ or II and some j, then it follows that $\omega_{\rm stat}$ is *not* normal relative to ω^0. In the examples studied in Sects. 4 and 5, we shall encounter instances where $\mathcal{P}^r$ and $\mathcal{J}^r$ do *not* vanish.

3 Reservoirs of non-interacting fermions

This section serves to introduce a class of simple, but physically important examples of reservoirs to which the general theory outlined in Sect. 2 can and will be applied. Our examples describe a quantum liquid of non-interacting, non-relativistic electrons in a normal metal or a semi-conductor, possibly subject to an external magnetic field, or an ideal quantum gas of fermionic atoms or molecules. In a subsequent paper, we shall also consider examples describing chiral Luttinger liquids, which arise in connection with the quantum Hall effect.

We start by considering a system consisting of a single, non-relativistic quantum-mechanical particle confined to a region Λ of physical space $\mathbb{R}^d$, $d = 1, 2, 3$. The Hilbert space of pure state vectors of this system is given by the space

$$L^2\big(\Lambda, d^d x\big) \tag{3.1}$$

of square-integrable wave functions with support in Λ. If the particle has spin and/or if there are several species of such particles then $L^2(\Lambda, d^d x)$ must be replaced by the space

$$h^\Lambda \ := \ L^2\big(\Lambda, d^d x\big) \otimes \mathbb{C}^k \ , \tag{3.2}$$

where $k = \sum_{\alpha=1}^{l} (2S_\alpha + 1)$, S_α is the spin of species α, and l is the number of species.

The one-particle dynamics is generated by the following selfadjoint operator, t^Λ, acting on h^Λ,

$$t^\Lambda \ = \ -\frac{\hbar^2}{2M}\, \Delta \otimes \mathbb{1} \, , \tag{3.3}$$

where M is the mass of the particle and Δ is the Laplace operator on $L^2(\Lambda, d^dx)$ with selfadjoint boundary conditions (e.g. Dirichlet, Neumann, or periodic) imposed at the boundary, $\partial\Lambda$, of Λ.

In the following, we choose units in which $\hbar = 1$ and $M = \frac{1}{2}$.

Other operators are physically interesting. Electrons in semi-conductors would involve a potential operator that is diagonal in the space representation. A magnetic field could also be considered; the Laplacian should be replaced by the covariant Laplacian, and a coupling between the spin of the particle and the magnetic field should be introduced. In this paper, we restrict our attention to the situation (3.3).

Next, we consider a system consisting of n identical particles of the kind just considered, all confined to the region Λ. Its state space is given by a subspace of the n-fold tensor product of h^Λ of fixed symmetry type,

$$h_n^\Lambda \;:=\; P(h^\Lambda)^{\otimes n}, \;\; h_0^\Lambda \;:=\; \mathbb{C}\,, \tag{3.4}$$

where P is the orthogonal projection onto the subspace of wave functions of the selected symmetry type under permutations of the n particle variables. If the particles are *bosons* then $P \equiv P_+$ projects onto *completely symmetric* n-particle wave functions; while, for *fermions*, $P \equiv P_-$ projects onto *totally anti-symmetric* wave functions. In this paper, we focus our attention on fermions.

If the particles do not interact with each other the Hamiltonian, T_n^Λ of the n-particle system is given by

$$T_n^\Lambda \;:=\; \sum_{j=1}^{n} \mathbb{1} \otimes \ldots \otimes t_j^\Lambda \otimes \ldots \otimes \mathbb{1}\,, \tag{3.5}$$

where t_j^Λ acts on the j^{th} factor in the n-fold tensor product in (3.4).

If the number of particles can fluctuate (e.g., because the system is coupled to a particle reservoir such as a battery) then it is convenient to use the formalism of "second quantization", which we briefly recall.

The *Fock space* is defined by

$$\mathcal{H}^\Lambda \;:=\; \bigoplus_{n=0}^{\infty} h_n^\Lambda\,. \tag{3.6}$$

The free dynamics on $\mathcal{H}^\Lambda$ is generated by the *Hamiltonian*

$$H^\Lambda \;:=\; \bigoplus_{n=0}^{\infty} T_n^\Lambda\,, \tag{3.7}$$

with T_n^Λ as in (3.5). The *particle number operator*, N^Λ, is defined by

$$N^\Lambda := \bigoplus_{n=0}^{\infty} n \cdot \mathbb{1}\big|_{h_n^\Lambda} . \tag{3.8}$$

Let κ be a symmetric $k \times k$ matrix acting on $\mathbb{C}^k$. We set

$$K_n^\Lambda := \sum_{j=1}^{n} \mathbb{1} \otimes \ldots \otimes \left(\mathbb{1} \otimes \kappa_j\right) \otimes \ldots \otimes \mathbb{1} ,$$

where $\mathbb{1}\otimes\kappa_j$ acts on the j^{th} factor, $\simeq L^2(\Lambda, d^d x)\otimes\mathbb{C}^k$, in the n-fold tensor product defining h_n^Λ. For t^Λ as in (3.3), a typical charge operator, $Q^\Lambda \equiv Q^\Lambda(\kappa)$, is of the form

$$Q^\Lambda := \bigoplus_{n=0}^{\infty} K_n^\Lambda . \tag{3.9}$$

The operators H^Λ, N^Λ and $Q^\Lambda(\kappa)$ are unbounded, selfadjoint operators on $\mathcal{H}^\Lambda$; see e.g. [RS].

Next, we describe the structure of $\mathcal{H}^\Lambda$ in some more detail and introduce creation and annihilation operators. Let $\boldsymbol{x}, \boldsymbol{y}, \ldots$ denote points in physical space $\mathbb{R}^d$, and let $s = 1, \ldots, k$ label on orthonormal basis in $\mathbb{C}^k$. Vectors f_n in the n-particle space h_n^Λ can be represented as square-integrable wave functions,

$$f_n\left(\boldsymbol{x}_1, s_1, \ldots, \boldsymbol{x}_n, s_n\right) ,$$

with support in $\Lambda^{dn} \subset \mathbb{R}^{dn}$, which, for fermions, are totally anti-symmetric under permutations of their n arguments. Vectors $\psi, \phi, \ldots$ in Fock space correspond to sequences,

$$\psi = (f_n)_{n=0}^{\infty} , \quad \phi = (g_n)_{n=0}^{\infty} , \ldots \tag{3.10}$$

of n-particle wave functions in h_n^Λ. The scalar product on $\mathcal{H}^\Lambda$ is defined by

$$\langle \psi, \phi \rangle := \sum_{n=0}^{\infty} \sum_{s_1,\ldots,s_n} \int_\Lambda \prod_{j=1}^{n} d\boldsymbol{x}_j \overline{f_n(\boldsymbol{x}_1, s_1, \ldots, \boldsymbol{x}_n, s_n)}\, g_n(\boldsymbol{x}_1, s_1, \ldots, \boldsymbol{x}_n, s_n) . \tag{3.11}$$

The vector represented by the sequence $(f_n)_{n=0}^{\infty}$, with $f_0 = 1$, $f_n \equiv 0$, for $n \geq 1$, is denoted by Ω and is called the *vacuum (vector).*

Let $\mathcal{D} = \mathcal{D}^\Lambda$ be the linear domain of vectors $\psi = (f_n)_{n=0}^{\infty}$ in $\mathcal{H}^\Lambda$ with the property that *all* but *finitely many* f_n's *vanish*. Clearly, $\mathcal{D}$ is dense in $\mathcal{H}^\Lambda$. For $f \in h^\Lambda$, we define an *annihilation operator*, $a(f)$, by

$$\begin{aligned} &\big(a(f)\psi\big)_n\big(\boldsymbol{x}_1, s_1, \ldots, \boldsymbol{x}_n, s_n\big) := \\ &\qquad \sqrt{n+1}\sum_{s=1}^{k} \int_\Lambda d\boldsymbol{x}\, \overline{f(\boldsymbol{x}, s)}\, f_{n+1}\big(\boldsymbol{x}, s, \boldsymbol{x}_1, s_1, \ldots, \boldsymbol{x}_n, s_n\big) , \end{aligned} \tag{3.12}$$

for arbitrary $\psi = (f_n)_{n=1}^{\infty} \in \mathcal{D}$, and

$$a(f)\Omega \ := \ 0 \,. \tag{3.13}$$

The *creation operator*, $a^*(f)$, is defined to be the adjoint of $a(f)$ on $\mathcal{H}^\Lambda$ and is easily seen to be well defined on $\mathcal{D}$.

It is well known, see e.g. [RS, BR], that, for *fermions*, the following *"canonical anti-commutation relations"* (CAR) hold:

$$\left\{a^{\#}(f),\ a^{\#}(g)\right\} \ = \ 0 \,, \tag{3.14}$$

for arbitrary f, g in h^Λ where $a^{\#} = a$ or a^*, and $\{A, B\} := AB + BA$ is the anti-commutator of two operators A and B;

$$\{a(f),\ a^*(g)\} \ = \ (f, g) \cdot \mathbb{1} \,, \tag{3.15}$$

where $(f, g) := \sum_s \int_\Lambda d\boldsymbol{x}\, \overline{f(\boldsymbol{x}, s)}\, g(\boldsymbol{x}, s)$ is the scalar product on h^Λ. For bosons, (3.14) and (3.15) hold if anti-commutators are replaced by commutators (CCR). Formally,

$$a(f) \ = \sum_s \int_\Lambda d\boldsymbol{x}\ \overline{f(\boldsymbol{x}, s)}\ a(\boldsymbol{x}, s),$$

and

$$a^*(f) \ = \sum_s \int_\Lambda d\boldsymbol{x}\ a^*(\boldsymbol{x}, s)\, f(\boldsymbol{x}, s) \,,$$

with

$$\{a(\boldsymbol{x}, s),\ a^*(\boldsymbol{x}', s')\} \ = \ \delta_{ss'}\, \delta^{(d)}(\boldsymbol{x} - \boldsymbol{x}') \,. \tag{3.16}$$

A remarkable consequence of the CAR is that the operators $a(f)$ and $a^*(f)$ are *bounded* in norm by

$$\|a(f)\| \ = \ \|a^*(f)\| \ = \ \|f\| \ := \ \sqrt{(f, f)} \,. \tag{3.17}$$

To see this, we choose an arbitrary $\psi \in \mathcal{D}$ and note that

$$\begin{aligned} &\|a(f)\psi\|^2 \ + \ \|a^*(f)\psi\|^2 \\ &\qquad = \ \left\langle a(f)\psi,\, a(f)\psi\right\rangle \ + \ \left\langle a^*(f)\psi,\, a^*(f)\psi\right\rangle \\ &\qquad = \ \left\langle \psi, \{a(f),\, a^*(f)\}\, \psi\right\rangle \\ &\qquad = \ (f, f)\, \langle \psi, \psi\rangle \,, \end{aligned}$$

so that

$$\|a^{\#}(f)\psi\| \ \leq \ \|f\| \cdot \|\psi\| \,. \tag{3.18}$$

Equality in (3.18) is seen from examples.

Eq. (3.17) is false for *bosons*, $a(f)$ and $a^*(f)$ being *unbounded* operators.

For fermions, polynomials in $a(f)$, $a^*(f)$, $f \in h^\Lambda$, form a *algebra of operators on $\mathcal{H}^\Lambda$ which is weakly dense in $B(\mathcal{H}^\Lambda)$. The "observable algebra" $\mathcal{A}^\Lambda$ is the norm closure of the algebra of these polynomials in $a(f), a^*(f)$, $f \in h^\Lambda$, which commute with the number operator N^Λ and, possibly, with further charge operators $Q^\Lambda(\kappa)$, for certain choices of κ. Every monomial in a and a^* belonging to $\mathcal{A}^\Lambda$ has equally many factors of a and a^*, since it must conserve the total particle number. A general monomial in a and a^* is *Wick-ordered* if all a^*'s are to the left of all a's.

In terms of creation and annihilation operators, the operators H^Λ, N^Λ and Q^Λ can be expressed as follows.

$$H^\Lambda = \sum_s \int_\Lambda d\boldsymbol{x}\, a^*(\boldsymbol{x}, s)(t^\Lambda a)(\boldsymbol{x}, s) \;, \tag{3.19}$$

$$N^\Lambda = \sum_s \int_\Lambda d\boldsymbol{x}\, a^*(\boldsymbol{x}, s)\, a(\boldsymbol{x}, s) \;, \tag{3.20}$$

and

$$Q^\Lambda(\kappa) = \sum_{s,s'} \int_\Lambda d\boldsymbol{x}\, a^*(\boldsymbol{x}, s)\, \kappa_{ss'}\, a(\boldsymbol{x}, s') \;. \tag{3.21}$$

In the examples discussed below and in Sects. 4 and 5, we usually regard $N^\Lambda = Q^\Lambda(\kappa = \mathbb{1})$ to be the *only conservation law*, besides H^Λ, relevant for the description of the reservoirs. In a general discussion, we consider M conservation laws, $Q_j^\Lambda = Q^\Lambda(\kappa_j)$, $j = 1, \ldots, M$, and choose t^Λ as in (3.3).

The main result of this section is the following theorem.

Theorem 3.1. *For t^Λ as in (3.3), and $Q_j^\Lambda = Q_j^\Lambda(\kappa_j)$, $j = 1, \ldots, M$, with $\kappa_1, \ldots, \kappa_M$ arbitrary, commuting symmetric $k \times k$ matrices, the equilibrium states $\omega_{\beta,\boldsymbol{\mu}}^\Lambda$ introduced in eq. (2.10) exist, for arbitrary $\beta \geq 0$ and $\boldsymbol{\mu} \in \mathbb{R}^M$.*

Assumptions (A1), (A2), (A5) and (A6) of Sect. 2, concerning the existence of the thermodynamic limit, $\Lambda \nearrow \mathbb{R}^d$, hold.

The proof of Theorem 3.1 is standard. A careful exposition can be found in [BR], Sect. 5.2.

In Section 4 we shall consider a system consisting of two identical reservoirs, I and II, both composed of non-interacting, non-relativistic fermions confined to some region $\Lambda = \Lambda^I = \Lambda^{II}$ of $\mathbb{R}^d$. A convenient notation for creation and annihilation operators for the two reservoirs is the following one.

$$\begin{aligned} a^\#(\boldsymbol{x}, s, I) &:= a^\#(\boldsymbol{x}, s)\big|_{\mathcal{H}^{\Lambda^I}} \otimes \mathbb{1}\big|_{\mathcal{H}^{\Lambda^{II}}} \;, \\ a^\#(\boldsymbol{x}, s, II) &:= \mathbb{1}\big|_{\mathcal{H}^{\Lambda^I}} \otimes a^\#(\boldsymbol{x}, s)\big|_{\mathcal{H}^{\Lambda^{II}}} \;. \end{aligned} \tag{3.22}$$

We note that all the operators $a^{\#}(f,I) = a^{\#}(f)\otimes\mathbb{1}$ *commute* with all the operators $a^{\#}(f,II) = \mathbb{1}\otimes a^{\#}(f)$. If, for convenience, we prefer that they anti-commute we can accomplish this feature by a standard *Klein-Jordan-Wigner transformation*:

$$\begin{aligned} a^{\#}(f,I) &\mapsto a^{\#}(f,I)\,, \\ a^{\#}(f,II) &\mapsto a^{\#}(f,II)\; e^{i\pi(N^{\Lambda^I}\otimes\mathbb{1})}\,. \end{aligned} \tag{3.23}$$

The operators on the R.S. of (3.23) will again be denoted by $a^{\#}(f,r)$, $r = I, II$. We introduce the following notation.

$$X := (\boldsymbol{x}, s, r) \in \mathbb{R}^d \times \{1,\ldots,k\} \times \{I, II\}, \tag{3.24}$$

$$X^{(N)} := (X_1,\ldots,X_N)\;, \tag{3.25}$$

$$x^{(N)} := (\boldsymbol{x}_1,\ldots,\boldsymbol{x}_n) \in \mathbb{R}^{dN}, \tag{3.26}$$

$$s^{(N)} := (s_1,\ldots,s_N) \in \{1,\ldots,k\}^N, \tag{3.27}$$

$$r^{(N)} := (r_1,\ldots,r_N) \in \{I, II\}^N, \tag{3.28}$$

$$\int_\Lambda dX := \sum_{r=I,II}\sum_{s=1}^{k}\int_\Lambda d\boldsymbol{x}, \tag{3.29}$$

$$\int_{\Lambda^N} dX^{(N)} := \prod_{j=1}^{N}\int_\Lambda dX_j, \tag{3.30}$$

$$\mathbf{a}^{\#}(X^{(N)}) := \prod_{j=1}^{N} a^{\#}(X_j)\;, \tag{3.31}$$

with $a^{\#} = a^*$ or a.

We are now prepared to describe the interactions, $W(\Lambda^I, \Lambda^{II})$, (see eq. 2.27)), corresponding to thermal contacts or tunnelling junctions between the two reservoirs. We shall always assume that the *total* particle number of the system consisting of the two reservoirs is conserved. Thus the interaction Hamiltonian $W(\Lambda^I, \Lambda^{II})$ must commute with the operator

$$N^{I\cup II} := N^{\Lambda^I}\otimes\mathbb{1} + \mathbb{1}\otimes N^{\Lambda^{II}}\;, \tag{3.32}$$

(see eq. (2.35)). It follows that $W(\Lambda^I, \Lambda^{II})$ must have the form

$$W(\Lambda^I, \Lambda^{II}) = \sum_{N=1}^{\infty} W_N(\Lambda^I, \Lambda^{II})\;, \tag{3.33}$$

where

$$W_N(\Lambda^I, \Lambda^{II}) = \int_{\Lambda^N} dX^{(N)}\int_{\Lambda^N} dY^{(N)}\mathbf{a}^*(X^{(N)})\, w_N^{\Lambda^I,\Lambda^{II}}(X^{(N)}, Y^{(N)})\,\mathbf{a}(Y^{(N)})\;, \tag{3.34}$$

and, for each choice of $s_1, r_1, \ldots, s_N, r_N, s'_1, r'_1, \ldots, s'_N, r'_N$,

$$w_N^{\Lambda^I,\Lambda^{II}}\left(\left(x^{(N)}, s^{(N)}, r^{(N)}\right), \left(y^{(N)}, s'^{(N)}, r'^{(N)}\right)\right)$$

is a smooth function of $x^{(N)} \in \Lambda^N$ and $y^{(N)} \in \Lambda^N$ vanishing if $x^{(N)} \notin \Lambda^N$ or $y^{(N)} \notin \Lambda^N$. In Sect. 4, we introduce weighted Sobolev spaces, $\mathcal{W}_N$ equipped with norms $|||(\cdot)|||_N$ with the property that

$$\|W_N(\Lambda^I, \Lambda^{II})\| \;\leq\; |||w_N^{\Lambda^I,\Lambda^{II}}|||_N\;, \tag{3.35}$$

for all $N = 1, 2, 3, \ldots$. We shall assume that, for each N, there is a function $w_N \in \mathcal{W}_N$ such that

$$g(w) \;:=\; \sum_{N=1}^{\infty} |||w_N|||_N \;<\; \infty\;, \tag{3.36}$$

where $w = (w_N)_{N=1}^{\infty}$, and

$$\lim_{\substack{\Lambda^I \nearrow \infty \\ \Lambda^{II} \nearrow \infty}} \sum_{N=1}^{\infty} |||w_N^{\Lambda^I,\Lambda^{II}} - w_N|||_N \;=\; 0\;. \tag{3.37}$$

It then follows that

$$n - \lim_{\substack{\Lambda^I \nearrow \infty \\ \Lambda^{II} \nearrow \infty}} W(\Lambda^I, \Lambda^{II}) \;=:\; W \tag{3.38}$$

exists, and

$$\|W\| \;\leq\; g(w)\;. \tag{3.39}$$

Thus, assumption (A4), eq. (2.29), of Sect. 2 follows from (3.34), (3.35), (3.36) and (3.37).

If we want to describe *thermal contacts* we shall require that

$$[N^{\Lambda^I} \otimes \mathbb{1},\; W(\Lambda^I, \Lambda^{II})] \;=\; [\mathbb{1} \otimes N^{\Lambda^{II}}, W(\Lambda^I, \Lambda^{II})] \;=\; 0\;, \tag{3.40}$$

while, for *tunnelling junctions*, only

$$[N^{I \cup II}, W(\Lambda^I, \Lambda^{II})] \;=\; 0 \tag{3.41}$$

is required, for arbitrary $\Lambda^I = \Lambda^{II} = \Lambda \subset \mathbb{R}^d$.

To conclude this section, we remark that a system of two reservoirs of non-interacting fermions, with a one-particle Hamiltonian t^Λ as in eq. (3.3), and with interactions $W(\Lambda^I, \Lambda^{II})$ as in (3.34)-(3.38), satisfies Assumptions (A1)-(A3) and (A5), (A6) of Section 2. Assumptions (A4) and (A7) are established in the next section for $d \geq 3$ and small $g(w)$.

4 Existence of Møller endomorphisms

The goal of this section is to illustrate the general theory of Section 2 by providing a complete mathematical description of a concrete system, namely two coupled reservoirs of free fermions in dimension $d \geq 3$. An illustration can be found in Fig. 1. The reservoirs are infinite and without boundary, and the coupling W is localized near the origin, in the the sense that $\|W\|'$, or $\|W\|''$, is finite (see (4.3), (4.4), or (4.25)).

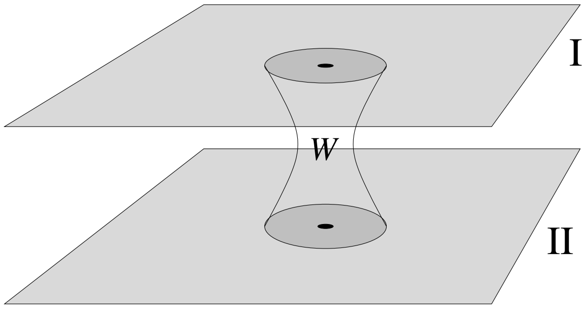

Figure 1: Two-dimensional reservoirs coupled by a local interaction W. We actually consider the three-dimensional analogue of this situation.

The Hamiltonian for each reservoir has been introduced in Section 3, see equation (3.7). The coupling between reservoirs is represented by the interaction in equations (3.33) and (3.34). As stated in Theorem 3.1, there exist time evolution automorphisms α_t^0 and α_t in the thermodynamic limit. The former corresponds to the free dynamics and the latter to the dynamics for interacting reservoirs.

In this section, we establish the existence of the Møller endomorphisms $\sigma_\pm$ defined in (2.83). We start with the Dyson series for $\alpha_{-t}^0\alpha_t$, namely

$$\alpha_{-t}^0\alpha_t(a) = \sum_{m=0}^{\infty} i^m \int_{t>t_m>\cdots>t_1>0} dt_1 \ldots dt_m \, [W(t_m), \ldots, [W(t_1), a] \ldots], \quad (4.1)$$

where we set $W(t) := \alpha_{-t}^0(W)$. Convergence of this series for finite t is clear since $\|W\| < \infty$, but we need to consider the limit $t \to \infty$. Let us define an operator $D_m(t)$ on the field algebra $\mathcal{F}$ by

$$D_m(t)a := \int_{t>t_m>\cdots>t_1>0} dt_1 \ldots dt_m \, [W(t_m), \ldots, [W(t_1), a] \ldots], \quad (4.2)$$

for arbitrary $a \in \mathcal{F}$. It is understood that $D_0 a = a$.

We define the norm of an interaction W by setting

$$\|W\|' = \sum_{N\geq 1} N 2^{(d+2)N} \sum_{s_1,\ldots,s_N=1}^{k} \sum_{s'_1,\ldots,s'_N=1}^{k} \sum_{r_1,\ldots,r_N=I,II} \sum_{r'_1,\ldots,r'_N=I,II} \|w_N\big((\cdot, s^{(N)}, r^{(N)}), (\cdot, s'^{(N)}, r'^{(N)})\big)\|'_{2dN}; \quad (4.3)$$

the function w_N is viewed above as a function on $\mathbb{R}^{2dN}$, and the norm $\|\cdot\|'_M$ is defined by

$$\|f\|'_M = \frac{1}{2^{3M/2}} \Big[\int_{\mathbb{R}^M} dx^{(M)} \overline{f(x^{(M)})} \prod_{k=1}^{M} \Big(-\frac{d^2}{dx_k^2} + x_k^2 + 1 \Big)^3 f(x^{(M)}) \Big]^{1/2}. \quad (4.4)$$

Note that the operators $-\frac{d^2}{dx_k^2} + x_k^2 + 1$ are bounded below by 2, which implies the inequality (3.35), namely $\|f\|_{L^2(\mathbb{R}^M)} \leq \|f\|'_M$; this inequality is saturated when f is a product of Gaussians centered at the origin, $f(x^{(M)}) = \prod_{k=1}^{M} e^{-x_k^2/2}$.

Theorem 4.1. *For $d \geq 3$ we have the bound*

$$\int_0^\infty \|[W(t), D_{m-1}(t)a]\| dt \leq \frac{1}{m} \Big(\frac{8\pi d}{d-2} \Big)^m \|a\|' \, (\|W\|')^m.$$

A similar statement holds for negative times. That is, one can rewrite the Dyson series in (4.1) and the operator $D_M(t)$ in (4.2) for $t < 0$ by integrating over negative times $0 > t_1 > \cdots > t_m > t$. Then Theorem 4.1 holds with an integral from $-\infty$ to 0. The proof for negative times is identical to the one of positive times.

Before proving Theorem 4.1, let us work out its main consequence, the existence of Møller endomorphisms.

Corollary 4.2. *If $\frac{8\pi d}{d-2}\|W\|' < 1$, there exist $\sigma_\pm$ such that*

$$\lim_{t\to\pm\infty} \|\alpha^0_{-t}\alpha_t(a) - \sigma_\pm(a)\| = 0$$

for all a with $\|a\|' < \infty$.

Corollary 4.2 implies the existence of a scattering automorphism, see Assumption (A4). We comment below that the norm (4.4) can be replaced by an object that is translation invariant, see (4.25). Therefore the scattering automorphism is given by a limit of infinite times, and this limit exists in norm, uniformly with respect to space translations (for both the interaction and the operator $a \in \mathcal{F}$). Hence Assumption (A7) holds.

Proof of Corollary 4.2. Observe that

$$\alpha^0_{-t}\alpha_t(a) = a + \sum_{m\geq 1} i^m \int_0^t [W(s), D_{m-1}(s)a]ds. \tag{4.5}$$

Then, for $t < t'$,

$$\|\alpha^0_{-t}\alpha_t(a) - \alpha^0_{-t'}\alpha_{t'}(a)\| \leq \sum_{m\geq 1} \int_t^{t'} \|[W(s), D_{m-1}(s)a]\|ds.$$

By Theorem 4.1 and the dominated convergence theorem, the right side vanishes as $t, t' \to \infty$. This implies the norm-convergence of $\alpha^0_{-t}\alpha_t(a)$. □

We will make use of Hermite functions in the proof of Theorem 4.1; so we collect a few useful facts on them. The Hermite functions are denoted by $\{\phi_q\}_{q\in\mathbb{N}}$, where

$$\phi_q(x) = \frac{(-1)^q}{\sqrt{2^q q!}\pi^{\frac{1}{4}}} e^{\frac{1}{2}x^2}\Big(\frac{d}{dx}\Big)^q e^{-x^2},$$

with $x \in \mathbb{R}$. These functions satisfy the equation

$$\Big(-\frac{d^2}{dx^2} + x^2\Big)\phi_q(x) = (2q+1)\phi_q(x). \tag{4.6}$$

Lemma 4.3.

(i) $\|\phi_q\|_1 \leq \sqrt{4\pi(q+1)}$.

(ii) $|(e^{it\Delta}\phi_p, \phi_q)| \leq \frac{\|\phi_p\|_1\|\phi_q\|_1}{\sqrt{4\pi|t|}}$.

Proof. By Cauchy-Schwarz and since the operator $-\frac{d^2}{dx^2}$ is positive definite, we have that

$$\begin{aligned} \|\phi_q\|_1 &= \int_{-\infty}^{\infty} \sqrt{x^2+1}\,|\phi_q(x)|\,\frac{1}{\sqrt{x^2+1}}dx \\ &\leq \Big(\phi_q, \Big(-\frac{d^2}{dx^2} + x^2 + 1\Big)\phi_q\Big)^{1/2}\Big(\int_{-\infty}^{\infty}\frac{dx}{x^2+1}\Big)^{1/2}. \end{aligned} \tag{4.7}$$

The first factor is equal to $\sqrt{2(q+1)}$ and the second one equals $\sqrt{2\pi}$, which proves (i). Claim (ii) immediately follows from

$$\Big(e^{it\Delta}\phi_p, \phi_q\Big) = \sqrt{\frac{i}{4\pi t}} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy e^{-i(x-y)^2/4t}\phi_p(y)\phi_q(x).$$

□

Hermite functions form an orthonormal basis of $L^2(\mathbb{R})$. We use them to express the interaction as a polynomial of creation and annihilation operators of fermions in states described by Hermite functions. The free time evolution of the interaction can be described as an evolution of these functions, and their decorrelation in time can be controlled using Lemma 4.3 (ii). Finally, Hermite functions will be removed at the expense of introducing differential operators in the definition of the norm of the interaction; see (4.4).

We use from now on the following notation: for $\boldsymbol{q} = (q_1, \ldots, q_d) \in \mathbb{N}^d$ and $\boldsymbol{x} = (x_1, \ldots, x_d) \in \mathbb{R}^d$,

$$\phi_{\boldsymbol{q}}(\boldsymbol{x}) = \prod_{i=1}^{d} \phi_{q_i}(x_i). \tag{4.8}$$

Proof of Theorem 4.1. We start by rewriting the interaction in the basis of Hermite functions. Let $Q^{(N)} := (Q_1, \ldots, Q_N)$, with

$$Q_j = (\boldsymbol{q}_j, s_j, r_j) \in \mathbb{N}^d \times \{1, \ldots, k\} \times \{\mathrm{I}, \mathrm{II}\}. \tag{4.9}$$

We set

$$\tilde{w}_N(Q^{(N)}, Q'^{(N)}) = \int_{\mathbb{R}^{dN}} dx^{(N)} \int_{\mathbb{R}^{dN}} dy^{(N)} w_N(X^{(N)}, Y^{(N)}) \prod_{j=1}^{N} \phi_{\boldsymbol{q}_j}(\boldsymbol{x}_j)\phi_{\boldsymbol{q}'_j}(\boldsymbol{y}_j). \tag{4.10}$$

Here, $X^{(N)}$ is determined by $Q^{(N)}$ and $x^{(N)}$, namely $X_j = (\boldsymbol{x}_j, s_j, r_j)$ if $Q_j = (\boldsymbol{q}_j, s_j, r_j)$. The interaction (3.32), (3.33) is given by a sum over

$$\boldsymbol{Q} := (N, Q^{(N)}, Q'^{(N)}),$$

$$W = \sum_{\boldsymbol{Q}} W_{\boldsymbol{Q}} = \sum_{\boldsymbol{Q}} \mathbf{a}^*(Q^{(N)})\tilde{w}_N(Q^{(N)}, Q'^{(N)})\mathbf{a}(Q'^{(N)}), \tag{4.11}$$

where $\mathbf{a}^*(Q^{(N)}) = \prod_{j=1}^{N} a^*(Q_j)$, and $a^*(Q_j)$ is the creation operator for a fermion in the state $\phi_{\boldsymbol{q}_j}$, of spin s_j, in the reservoir r_j. The annihilation operators $\mathbf{a}(Q'^{(N)})$ are defined similarly. The operator a also has a Hermite expansion

$$a = \sum_{\boldsymbol{Q}} a_{\boldsymbol{Q}} = \sum_{\boldsymbol{Q}} \mathbf{a}^*(Q^{(N)})\tilde{a}_N(Q^{(N)}, Q'^{(N)})\mathbf{a}(Q'^{(N)}). \tag{4.12}$$

With this notation, we have that

$$\int_0^\infty |||[W(t), D_{m-1}(t)a]|||dt \leq \sum_{\boldsymbol{Q}_0, \ldots, \boldsymbol{Q}_m} \int_{\infty > t_m > \cdots > t_1 > 0} dt_1 \ldots dt_m$$
$$|||[W_{\boldsymbol{Q}_m}(t_m), \ldots, [W_{\boldsymbol{Q}_1}(t_1), a_{\boldsymbol{Q}_0}] \ldots]|||. \tag{4.13}$$

The multiple commutator above involves operators W and a, which in turn involve creation and annihilation operators of particles in both reservoirs. The latter satisfy anticommutation relations for particles in the same reservoir, or commutation relations for particles in different reservoirs. This introduces a complication when estimating the multicommutator above. This complication can be avoided by using the Klein-Jordan-Wigner transformation explained in (3.23). For simplicity, we keep the same notation, but we assume from now on that all creation and annihilation operators satisfy anticommutation relations.

Because α^0_{-t} is a $*$-automorphism, its action on the interaction W simply amounts to replacing operators $a^\#(Q) = a^\#(\phi_{\boldsymbol{q}}, s, r)$ by

$$\alpha^0_{-t}(a^\#(\phi_{\boldsymbol{q}}, s, r)) = a^\#(e^{it\Delta}\phi_{\boldsymbol{q}}, s, r) := a^\#(Q, t). \tag{4.14}$$

We note that Lemma 4.3 yields the bound

$$\begin{aligned} \big\| \big\{ \alpha^0_{-t}(a^\#(Q)), \alpha^0_{-t'}(a^\#(Q')) \big\} \big\| &= |(e^{it\Delta}\phi_{\boldsymbol{q}}, e^{it'\Delta}\phi_{\boldsymbol{q}'})| \delta_{ss'}\delta_{rr'} \\ &\leq \big(1 \wedge \tfrac{4\pi}{|t-t'|}\big)^{d/2} \prod_{i=1}^d (q_i+1)^{\frac12}(q_i'+1)^{\frac12}. \end{aligned} \tag{4.15}$$

The multicommutator in (4.13) can be written as

$$\begin{aligned} &[W_{\boldsymbol{Q}_m}(t_m), \dots, [W_{\boldsymbol{Q}_1}(t_1), a_{\boldsymbol{Q}_0}] \dots] = \\ &\tilde a_{N_0}(Q_0^{(N_0)}, {Q'_0}^{(N_0)}) \prod_{j=1}^m \tilde w_{N_j}(Q_j^{(N_j)}, {Q'_j}^{(N_j)}) \big[\mathbf{a}^*(Q_m^{(N_m)}, t_m)\mathbf{a}({Q'_m}^{(N_m)}, t_m), \dots \\ &\qquad \dots, \big[\mathbf{a}^*(Q_1^{(N_1)}, t_1)\mathbf{a}({Q'_1}^{(N_1)}, t_1), \mathbf{a}^*(Q_0^{(N_0)})\mathbf{a}({Q'_0}^{(N_0)}) \big] \dots \big]. \end{aligned} \tag{4.16}$$

Here, we set

$$\mathbf{a}^\#(Q_j^{(N_j)}, t_j) = \prod_{\ell=1}^{N_j} \alpha^0_{-t_j}(\mathbf{a}^\#(Q_{j,\ell})), \tag{4.17}$$

where $Q_{j,\ell}$ is the ℓ-th element of $Q_j^{(N_j)}$.

A commutator of products of operators can be expanded according to contraction schemes. The following equation holds when $k\ell$ is even:

$$\begin{aligned} [a_1 \dots a_k, b_1 \dots b_\ell] = \sum_{\substack{1 \leq i \leq k \\ 1 \leq j \leq \ell}} (-1)^{i\ell+j+1} a_1 \dots a_{i-1} b_1 \dots b_{j-1} \\ \{a_i, b_j\} b_{j+1} \dots b_\ell a_{i+1} \dots a_k. \end{aligned} \tag{4.18}$$

The multicommutator of (4.16) can thus be expanded in contraction schemes for operators at different times. An operator at time t_1 contracts necessarily with

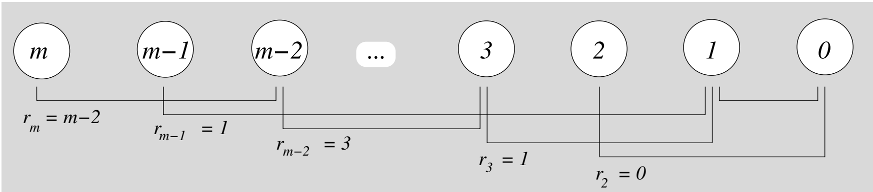

Figure 2: Illustration for the numbers $r_m, \ldots, r_2$ that occur in the choice of contractions. We see that they define a tree.

an operator at time $t_0 = 0$; an operator at time t_2 contracts with an operator at time t_{r_2} with $r_2 = 0, 1$; …; an operator at time t_m contracts with an operator at time t_{r_m} with $r_m = 0, \ldots, m-1$. See Fig. 2 for an illustration. To a set of contractions corresponds a monomial of creation and annihilation operators, multiplied by anticommutators of contracted operators.

The monomial of creation and annihilation operators is bounded in operator norm by 1. Contracted operators are estimated using (4.15). This yields a factor involving times, namely

$$\prod_{j=1}^{m} \big(1 \wedge \tfrac{4\pi}{t_j - t_{r_j}}\big)^{d/2}.$$

Second, one obtains a factor involving indices of Hermite functions for the contracted operators. An upper bound on this factor is obtained by writing a product over all indices, namely

$$\prod_{j=0}^{m} \prod_{k=1}^{N_j} \prod_{i=1}^{d} (q_{jki} + 1)^{\frac{1}{2}} (q'_{jki} + 1)^{\frac{1}{2}}.$$

Here, $\boldsymbol{q}_{jk}, \boldsymbol{q}'_{jk} \in \mathbb{N}^d$ are indices for Hermite functions determined by the k-th element of $\boldsymbol{Q}_j$.

It remains to estimate the number of contraction schemes, given $r_2, \ldots, r_m$. We define

$$e_j = \big|\{k : r_k = j\}\big| + 1 - \delta_{j0}, \quad 0 \leq j \leq m. \tag{4.19}$$

Notice that $1 \leq e_0 \leq m$ and $1 \leq e_j \leq m - j + 1$ if $j \neq 0$. e_j is the number of operators at time t_j that belong to a contraction and it is necessarily smaller than $2N_j$. Since there are $2N_j$ operators at time t_j, the number of possible contractions is

$$\prod_{j=0}^{m} \frac{(2N_j)!}{(2N_j - e_j)!}.$$

The above estimates could be improved by observing that many contraction schemes yield zero; namely, in the case where both operators are creation or annihilation operators; or if the spins are different; or if they belong to different reservoirs. It is not easy to take advantage of this, however.

We now gather the above estimates to obtain the bound

$$\begin{aligned}\int_0^\infty \|[W(t), D_{m-1}(t)A]\| dt \leq \\ \sum_{\boldsymbol{Q}_0,\dots,\boldsymbol{Q}_m} |\tilde{A}_{N_0}(Q_0^{(N_0)}, {Q'_0}^{(N_0)})| \prod_{j=1}^m |\tilde{w}_{N_j}(Q_j^{(N_j)}, {Q'_j}^{(N_j)})| \\ \times \prod_{j=0}^m \prod_{k=1}^{N_j} \prod_{i=1}^d (q_{jki}+1)^{\frac12} (q'_{jki}+1)^{\frac12} \int_{\infty>t_m>\dots>t_1>0} dt_1 \dots dt_m \\ \times \sum_{r_m=0}^{m-1} \sum_{r_{m-1}=0}^{m-2} \cdots \sum_{r_2=0}^{1} \prod_{j=1}^m \bigl(1 \wedge \tfrac{4\pi}{t_j - t_{r_j}}\bigr)^{d/2} \prod_{j=0}^m \frac{\chi[e_j \leq 2N_j](2N_j)!}{(2N_j - e_j)!}. \end{aligned} \tag{4.20}$$

A sequence of numbers $r_2, \dots, r_m$ can be represented by a graph with set of vertices $\{0, \dots, m\}$, and an edge between i and j whenever $r_j = i$. This graph is a tree: there are m edges, and each vertex $j \neq 0$ is directly connected to a vertex $i < j$, hence each vertex is eventually connected to 0. The numbers e_j defined in (4.19) are then the incidence numbers of the tree — e_j is the number of edges containing the vertex j. This is illustrated in Fig. 2. We can symmetrize the bound by summing over *all* trees T with $m+1$ vertices; this step will allow to deal with the time integrals. Reorganizing, we obtain

$$\begin{aligned}\int_0^\infty \|[W(t), D_{m-1}(t)a]\| dt \leq \\ \sum_{\boldsymbol{Q}_0} |\tilde{a}_{N_0}(Q_0^{(N_0)}, {Q'_0}^{(N_0)})| \prod_{k=1}^{N_0} \prod_{i=1}^d (q_{0ki}+1)^{\frac12} (q'_{0ki}+1)^{\frac12} \\ \times \int_{\infty>t_m>\dots>t_1>0} dt_1 \dots dt_m \sum_T \prod_{(i,j)\in T} \bigl(1 \wedge \tfrac{4\pi}{|t_i - t_j|}\bigr)^{d/2} \frac{\chi[e_0 \leq 2N_0](2N_0)!}{(2N_0 - e_0)!} \\ \times \prod_{j=1}^m \Bigl\{ \sum_{\boldsymbol{Q}_j} |\tilde{w}_{N_j}(Q_j^{(N_j)}, {Q'_j}^{(N_j)})| \prod_{k=1}^{N_j} \prod_{i=1}^d (q_{jki}+1)^{\frac12} (q'_{jki}+1)^{\frac12} \frac{\chi[e_j \leq 2N_j](2N_j)!}{(2N_j - e_j)!} \Bigr\}. \end{aligned} \tag{4.21}$$

Let us focus on the time integrals. The integrand is a symmetric function of $t_1, \dots, t_m$, because of the sum over arbitrary trees. We can therefore extract a factor $1/m!$, at the cost of integrating over *all* positive times $t_1, \dots, t_m$ without the ordering condition. Since there is no integral over $t_0 = 0$, we have

$$\int_0^\infty dt_1 \dots \int_0^\infty dt_m \prod_{(i,j)\in T} \left(1 \wedge \tfrac{4\pi}{|t_i - t_j|}\right)^{d/2} \le \left(\int_{-\infty}^\infty \left(1 \wedge \tfrac{4\pi}{|t|}\right)^{d/2} dt\right)^m, \qquad (4.22)$$

for any tree T. The last integral is equal to $8\pi d/(d-2)$.

The number of trees with $m+1$ vertices and incidence numbers $e_0, \dots, e_m$ is equal to

$$\binom{m-1}{e_0 - 1,\ e_1 - 1,\ \dots,\ e_m - 1} = \frac{(m-1)!}{(e_0-1)! \dots (e_m - 1)!};$$

see for instance [Ber], Théorème 2 p. 86. We sum over incidence numbers, using $\sum_{e=0}^{2N} \binom{2N}{e} = 4^N$, and we get

$$\begin{aligned}\int_0^\infty \|[W(t), D_{m-1}(t)a]\| dt \le \frac{1}{m}\Big(\frac{8\pi d}{d-2}\Big)^m \sum_{\boldsymbol{Q}_0} N_0 4^{N_0} |\tilde{a}_{N_0}(Q_0^{(N_0)}, {Q'_0}^{(N_0)})| \\ \times \prod_{k=1}^{N_0} \prod_{i=1}^{d} (q_{0ki}+1)^{\frac12} (q'_{0ki}+1)^{\frac12} \\ \times \left\{ \sum_{\boldsymbol{Q}} N 4^N |\tilde{w}_N(Q^{(N)}, Q'^{(N)})| \prod_{k=1}^{N}\prod_{i=1}^{d} (q_{ki}+1)^{\frac12}(q'_{ki}+1)^{\frac12} \right\}^m. \qquad (4.23)\end{aligned}$$

The last step consists in removing the Hermite functions. We fix N, $s^{(N)}$, $s'^{(N)}$, $r^{(N)}$, $r'^{(N)}$, and perform the summation over $q^{(N)}$ and $q'^{(N)}$. Using Cauchy-Schwarz, we obtain

$$\begin{aligned}\sum_{q^{(N)}, q'^{(N)}} \left|\tilde{w}_N(Q^{(N)}, Q'^{(N)})\right| \prod_{k=1}^{N}\prod_{i=1}^{d} (q_{ki}+1)^{\frac12}(q'_{ki}+1)^{\frac12} \\ \le \left(\sum_{q^{(N)}, q'^{(N)}} \left|\tilde{w}_N(Q^{(N)}, Q'^{(N)})\right|^2 \prod_{k=1}^{N}\prod_{i=1}^{d} (q_{ki}+1)^3 (q'_{ki}+1)^3 \right)^{1/2} \\ \times \left(\sum_{\nu \ge 0} \frac{1}{(q+1)^2}\right)^{dN}. \qquad (4.24)\end{aligned}$$

The last factor on the right side is bounded by 2^{dN}. The first factor on the right side can be viewed as an expectation value of a certain operator expressed in the basis of Hermite functions. Rewriting it in the x-space representation, we find that it is given by the square root of the following expression

$$\frac{1}{2^{6dN}} \int_{\mathbb{R}^{dN}} dx^{(N)} \int_{\mathbb{R}^{dN}} dy^{(N)} \, \overline{w_N(X^{(N)}, Y^{(N)})} \\ \times \prod_{k=1}^{N} \prod_{i=1}^{d} \Big(-\frac{d^2}{dx_{ki}^2} + x_{ki}^2 + 1 \Big)^3 \Big(-\frac{d^2}{dy_{ki}^2} + y_{ki}^2 + 1 \Big)^3 w_N(X^{(N)}, Y^{(N)}).$$

This motivates the use of the norm (4.4) and concludes the proof of Theorem 4.1. □

We end this section by remarking that an estimate can be obtained that is invariant under space translations. Such an estimate follows by repeating the steps above with translates of Hermite functions. Recall that $\tilde{w}_N$ was defined in (4.10) by integrating $2dN$ Hermite functions centered at the origin. We can choose $z \in \mathbb{R}^{2dN}$ and translate the j-th function by z_j. Lemma 4.3 still holds with translates of Hermite functions, so that the proof goes through without a change until (4.24). Since a Hermite function translated by $z \in \mathbb{R}$ satisfies the differential equation (4.6) with $(x-z)^2$ instead of x^2, one gets a bound where the differential operators in the norm (4.4) are translated by $z \in \mathbb{R}^M$. This holds for all z; let us introduce $\|\cdot\|''_M$ by

$$\|f\|''_M = \\ \frac{1}{2^{3M/2}} \inf_{y \in \mathbb{R}^M} \Big[\int_{\mathbb{R}^M} dx^{(M)} \overline{f(x^{(M)})} \prod_{k=1}^{M} \Big(-\frac{d^2}{dx_k^2} + (x_k - y_k)^2 + 1 \Big)^3 f(x^{(M)}) \Big]^{1/2}. \tag{4.25}$$

This object is translation invariant but it is not a norm. We have $\|\cdot\|''_M \leq \|\cdot\|'_M$. Theorem 4.1 holds when $\|A\|'$ and $\|W\|'$ are replaced by $\|A\|''$ and $\|W\|''$, whose definition is like (4.3) with $\|\cdot\|''_M$ instead of $\|\cdot\|'_M$.

5 Explicit perturbative calculation of particle and energy currents

In this section, we consider two reservoirs of non-relativistic non-interacting free spinless fermions. Such systems are a special case of the ones introduced in Section 3.

For explicit calculations, it is convenient to represent the system in Fourier space, see Subsection 5.1, since the one-particle energy operator $t = -\Delta$ is diagonal in this representation. Subsection 5.2 is devoted to the calculation of the particle and energy currents for tunnelling junctions, in the lowest non-vanishing order in W. This establishes the relation between the particle current and chemical potentials of the reservoirs, the *current voltage characteristics*. If the difference of chemical potentials $\Delta\mu = \mu^I - \mu^{II}$ is small, then the particle current is proportional to the voltage drop $\Delta\mu$. This linear relation is known as *Ohm's law*. We calculate the (inverse of the) proportionality factor, which is called the *resistance* of the junction. Moreover, we explicitly verify that the entropy production rate is strictly positive, provided the two reservoirs are at either different temperatures or chemical potentials.

Let us recall that the single particle Hilbert space (in the thermodynamic limit) is $h = L^2(\mathbb{R}^d, d\boldsymbol{x})$, with $\boldsymbol{x} \in \mathbb{R}^d, d \geq 3$ (see equation (3.2)). The dynamics is determined by $t = -\Delta$, see (3.3). For each reservoir, we take the particle number to be the only conservation law. Recall that for *tunnelling junctions*, the interaction W commutes with the total particle number operator, $N \otimes \mathbb{1} + \mathbb{1} \otimes N$, while for *thermal junctions*, W commutes separately with $N \otimes \mathbb{1}$ and $\mathbb{1} \otimes N$; see equations (3.41) and (3.40).

To quantify the interaction, we introduce two coupling constants, g and ξ, and set

$$W = g \sum_{N=1}^{\infty} \xi^N W_N. \tag{5.1}$$

Let $\mathcal{J}_{k,l}, \mathcal{P}_{k,l}$ denote the term of order $g^k \xi^l$ of the particle current $\mathcal{J}$ (see (2.86), (2.78) (2.81)) and the energy current $\mathcal{P}$ (see (2.85), (2.77), (2.82)). Accordingly, we define $\mathcal{E}_{k,l}$, where $\mathcal{E}$ is the entropy production rate in (2.69) and (2.75). We give now explicit expressions for some lower order terms of the currents and the entropy production rate. The calculations are presented in Subsection 5.2.

Tunnelling junctions. The lowest order terms of the particle current are given by

$$\mathcal{J}_{1,1} = \mathcal{J}_{1,2} = 0, \tag{5.2}$$

$$\mathcal{J}_{2,2} = 2\pi \int_{\mathbb{R}^{2d}} d\boldsymbol{k}\, d\boldsymbol{l}\, \delta(|\boldsymbol{k}|^2 - |\boldsymbol{l}|^2)\, |\widehat{w}_1((-\boldsymbol{k}, II), (\boldsymbol{l}, I))|^2 \left(\rho_{II}(\boldsymbol{k}) - \rho_I(\boldsymbol{k})\right), \tag{5.3}$$

where $\boldsymbol{k}, \boldsymbol{l} \in \mathbb{R}^d$, $\widehat{w}$ is the Fourier transform of w, and the function $\rho_r(\boldsymbol{k})$ is defined as

$$\rho_r(\boldsymbol{k}) = \frac{1}{e^{\beta^r(|\boldsymbol{k}|^2 - \mu^r)} + 1}.$$

We obtain for the energy current the expressions

$$\begin{aligned}\mathcal{P}_{1,1} &= \mathcal{P}_{1,2} = 0, &(5.4)\\ \mathcal{P}_{2,2} &= 2\pi \int_{\mathbb{R}^{2d}} d\boldsymbol{k}\, d\boldsymbol{l}\ |\boldsymbol{k}|^2 \delta(|\boldsymbol{k}|^2 - |\boldsymbol{l}|^2)\, |\widehat{w}_1((-\boldsymbol{k}, II), (\boldsymbol{l}, I))|^2 \left(\rho_{II}(\boldsymbol{k}) - \rho_I(\boldsymbol{k})\right). &(5.5)\end{aligned}$$

Assuming that $\widehat{w}_1$ is not identically zero, the above formulas show the following qualitative behaviour of the flows.

- If $(\beta^I, \mu^I) = (\beta^{II}, \mu^{II})$ then $\mathcal{J}_{2,2} = \mathcal{P}_{2,2} = 0$. The flows vanish if both reservoirs are at the same temperature and chemical potential.
- If $\mu^I = \mu^{II}$ and $\beta^I > \beta^{II}$ then $\rho_{II}(k) - \rho_I(k) > 0$, for all k. Consequently, $\mathcal{J}_{2,2}, \mathcal{P}_{2,2} > 0$. At constant chemical potential, there is a particle and energy flow from the hotter to the colder reservoir.
- If $\mu^I > \mu^{II}$ and $\beta^I = \beta^{II} = \beta$, then $\rho_{II}(k) - \rho_I(k) < 0$, for all k. Consequently, $\mathcal{J}_{2,2}, \mathcal{P}_{2,2} < 0$. At constant temperature, there is a particle and energy flow from the reservoir with higher chemical potential to the reservoir with lower chemical potential.

Ohm's law and the resistance of the junction. Suppose that $\beta^I = \beta^{II}$ and $\mu^I = \mu$, $\mu^{II} = \mu + \Delta\mu$, with $\Delta\mu$ small. Retaining only the leading order in $\Delta\mu$ in the expression of the particle flow yields

$$\mathcal{J}_{2,2} \approx \frac{\Delta\mu}{R(\mu, \beta)}, \tag{5.6}$$

where the *resistance* $R(\mu, \beta)$ is determined by

$$R(\mu, \beta)^{-1} = 2\pi\beta \int_{\mathbb{R}^{2d}} d\boldsymbol{k}\, d\boldsymbol{l}\ \delta(|\boldsymbol{k}|^2 - |\boldsymbol{l}|^2) \frac{|\widehat{w}_1((-\boldsymbol{k}, II), (\boldsymbol{l}, I))|^2\, e^{\beta(|\boldsymbol{k}|^2 - \mu)}}{(e^{\beta(|\boldsymbol{k}|^2-\mu)} + 1)^2}. \tag{5.7}$$

We refer to Subsection 5.2 for a qualitative discussion of the resistance, in three dimensions, $d = 3$.

Onsager reciprocity relations. Let us study the interdependence of the flows near equilibrium. The relevant parameters are the difference of the inverse temperatures, and the difference of the chemical potentials divided by the temperature. Precisely, we set $\beta^I = \beta$; $\beta^{II} = \beta - \Delta\beta$; $\nu = \beta^I\mu^I$; $\Delta\nu = \beta^I\mu^I - \beta^{II}\mu^{II}$. We consider the flows to depend on β, ν, $\Delta\beta$, and $\Delta\nu$.

One easily checks that

$$\begin{aligned}\frac{\partial}{\partial\Delta\beta}\big[\rho_{II}(\boldsymbol{k})-\rho_I(\boldsymbol{k})\big]\Big|_{\Delta\beta=\Delta\nu=0} &= \frac{e^{\beta(|\boldsymbol{k}|^2-\mu)}}{(e^{\beta(|\boldsymbol{k}|^2-\mu)}+1)^2}|\boldsymbol{k}|^2,\\ \frac{\partial}{\partial\Delta\nu}\big[\rho_{II}(\boldsymbol{k})-\rho_I(\boldsymbol{k})\big]\Big|_{\Delta\beta=\Delta\nu=0} &= -\frac{e^{\beta(|\boldsymbol{k}|^2-\mu)}}{(e^{\beta(|\boldsymbol{k}|^2-\mu)}+1)^2}.\end{aligned} \tag{5.8}$$

The first partial derivative is taken at constant β, ν, and $\Delta\nu$; the second partial derivative is at constant β, ν, and $\Delta\beta$. Then from (5.3) and (5.5) we observe that

$$\frac{\partial\mathcal{P}_{2,2}}{\partial\Delta\nu}\Big|_{\Delta\beta=\Delta\nu=0} = -\frac{\partial\mathcal{J}_{2,2}}{\partial\Delta\beta}\Big|_{\Delta\beta=\Delta\nu=0}. \tag{5.9}$$

This is an Onsager reciprocity relation and we see that it holds at lowest order.

Entropy production rate. Recall that $\mathcal{P}^{II}=-\mathcal{P}^I$ (equation (2.77)) and $\mathcal{J}^{II}=-\mathcal{J}^I$ (equation (2.78)), hence

$$\mathcal{E}=(\beta^I-\beta^{II})\mathcal{P}-(\beta^I\mu^I-\beta^{II}\mu^{II})\mathcal{J}.$$

Using the above expressions for $\mathcal{J}_{k,l}$ and $\mathcal{P}_{k,l}$, we obtain

$$\begin{aligned}\mathcal{E}_{1,1} &= \mathcal{E}_{1,2}=0,\\ \mathcal{E}_{2,2} &= (\beta^I-\beta^{II})\mathcal{P}_{2,2}-(\beta^I\mu^I-\beta^{II}\mu^{II})\mathcal{J}_{2,2}\\ &= 2\pi\int_{\mathbb{R}^{2d}} d\boldsymbol{k}\, d\boldsymbol{l}\, \delta(|\boldsymbol{k}|^2-|\boldsymbol{l}|^2)|\widehat{w}_1((-\boldsymbol{k},II),(\boldsymbol{l},I))|^2\\ &\quad\times\frac{\{(\beta^I-\beta^{II})|\boldsymbol{k}|^2-(\beta^I\mu^I-\beta^{II}\mu^{II})\}\{e^{\beta^I(|\boldsymbol{k}|^2-\mu^I)}-e^{\beta^{II}(|\boldsymbol{k}|^2-\mu^{II})}\}}{(e^{\beta^I(|\boldsymbol{k}|^2-\mu^I)}+1)(e^{\beta^{II}(|\boldsymbol{k}|^2-\mu^{II})}+1)}.\end{aligned}$$

The numerator of the fraction is of the form $(x^I-x^{II})(e^{x^I}-e^{x^{II}})$, with $x^r=\beta^r(|\boldsymbol{k}|^2-\mu^r)$, hence it is strictly positive unless $x^I=x^{II}$. We assume that

$$\int_{\mathbb{R}^d} d\boldsymbol{l}\, \delta(|\boldsymbol{k}|^2-|\boldsymbol{l}|^2)|\widehat{w}_1((-\boldsymbol{k},II),(\boldsymbol{l},I))|^2 \tag{5.10}$$

does not vanish for all $\boldsymbol{k}\in\mathbb{R}^d$. Then $\mathcal{E}_{2,2}$ is strictly positive unless $\beta^I(|\boldsymbol{k}|^2-\mu^I)=\beta^{II}(|\boldsymbol{k}|^2-\mu^{II})$ for all $\boldsymbol{k}$ in the support of (5.10). This shows that $\mathcal{E}_{2,2}$ *is strictly positive unless* $(\beta^I,\mu^I)=(\beta^{II},\mu^{II})$*, in which case* $\mathcal{E}_{2,2}$ *vanishes.*

Thermal junctions. The particle current is zero, a thermal junction allows only for an exchange of heat between the two reservoirs. Since $W_1=0$, the lowest order term which is nonvanishing is $\mathcal{P}_{2,4}$. Without loss of generality, we take the coupling function $\widehat{w}_2$ to be of the form

$$\widehat{w}_2((\boldsymbol{k}_1, r_1), (\boldsymbol{k}_2, r_2); (\boldsymbol{l}_1, s_1), (\boldsymbol{l}_2, s_2)) = \delta_{r_1,I}\ \delta_{r_2,II}\ \delta_{s_1,I}\ \delta_{s_2,II}\ \widehat{w}_2(\boldsymbol{k}_1, \boldsymbol{k}_2, \boldsymbol{l}_1, \boldsymbol{l}_2).$$

A somewhat lengthy but straightforward calculation yields

$$\begin{aligned}\mathcal{P}_{2,4} = 2\pi \int & d\boldsymbol{k}_1 d\boldsymbol{k}_2 d\boldsymbol{l}_1 d\boldsymbol{l}_2\ \delta(|\boldsymbol{k}_1|^2 + |\boldsymbol{k}_2|^2 - |\boldsymbol{l}_1|^2 - |\boldsymbol{l}_2|^2) \\ & \times |\widehat{w}_2(-\boldsymbol{k}_1, -\boldsymbol{k}_2, \boldsymbol{l}_1, \boldsymbol{l}_2)|^2 (|\boldsymbol{k}_1|^2 - |\boldsymbol{l}_1|^2) \rho_I(\boldsymbol{l}_1) \rho_{II}(\boldsymbol{l}_2)(1 - \rho_I(\boldsymbol{k}_1) - \rho_{II}(\boldsymbol{k}_2)),\end{aligned} \tag{5.11}$$

from which we obtain the following qualitative discussion.

- If $(\beta^I, \mu^I) = (\beta^{II}, \mu^{II})$, then $\rho_I = \rho_{II}$, and by switching $\boldsymbol{l}_1 \leftrightarrow \boldsymbol{l}_2$, $\boldsymbol{k}_1 \leftrightarrow \boldsymbol{k}_2$ in the integral, we see that $\mathcal{P}_{2,4} = 0$.

- By splitting the integral in (5.11) into a sum of two integrals over the regions $\chi(|\boldsymbol{k}_1|^2 > |\boldsymbol{l}_1|^2)$ and $\chi(|\boldsymbol{k}_1|^2 < |\boldsymbol{l}_1|^2)$, and switching $\boldsymbol{k}_1 \leftrightarrow \boldsymbol{l}_1$, $\boldsymbol{k}_2 \leftrightarrow \boldsymbol{l}_2$, we can rewrite

$$\begin{aligned}\mathcal{P}_{2,4} = 2\pi \int & d\boldsymbol{k}_1 d\boldsymbol{k}_2 d\boldsymbol{l}_1 d\boldsymbol{l}_2\ \delta(|\boldsymbol{k}_1|^2 + |\boldsymbol{k}_2|^2 - |\boldsymbol{l}_1|^2 - |\boldsymbol{l}_2|^2) \\ & \times |\widehat{w}_2(-\boldsymbol{k}_1, -\boldsymbol{k}_2, \boldsymbol{l}_1, \boldsymbol{l}_2)|^2\ (|\boldsymbol{k}_1|^2 - |\boldsymbol{l}_1|^2)\ \chi(|\boldsymbol{k}_1|^2 > |\boldsymbol{l}_1|^2) \\ & \times \big\{\rho_I(\boldsymbol{l}_1)\rho_{II}(\boldsymbol{l}_2)[1 - \rho_I(\boldsymbol{k}_1) - \rho_{II}(\boldsymbol{k}_2)] \\ & \quad -\rho_I(\boldsymbol{l}_1)\rho_{II}(\boldsymbol{l}_2)[1 - \rho_I(\boldsymbol{k}_1) - \rho_{II}(\boldsymbol{k}_2)]\big\} \\ = \ 2\pi \int & d\boldsymbol{k}_1 d\boldsymbol{k}_2 d\boldsymbol{l}_1 d\boldsymbol{l}_2\ \delta(|\boldsymbol{k}_1|^2 + |\boldsymbol{k}_2|^2 - |\boldsymbol{l}_1|^2 - |\boldsymbol{l}_2|^2) \\ & \times |\widehat{w}_2(-\boldsymbol{k}_1, -\boldsymbol{k}_2, \boldsymbol{l}_1, \boldsymbol{l}_2)|^2\ (|\boldsymbol{k}_1|^2 - |\boldsymbol{l}_1|^2)\ \chi(|\boldsymbol{k}_1|^2 > |\boldsymbol{l}_1|^2) \\ & \times \big\{\rho_{II}(\boldsymbol{l}_2)[1 - \rho_{II}(\boldsymbol{k}_2)][\rho_I(\boldsymbol{l}_1) - \rho_I(\boldsymbol{k}_1)] \\ & \quad -\rho_I(\boldsymbol{k}_1)[1 - \rho_I(\boldsymbol{l}_1)][\rho_{II}(\boldsymbol{k}_2) - \rho_{II}(\boldsymbol{l}_2)]\big\}.\end{aligned}$$

  The first product in the round brackets $\{\ \}$ is strictly positive and tends to zero, as $\beta^{II} \to \infty$ (because in the limit $\beta^r \to \infty$, $\rho_r(k)$ tends to the characteristic function $\chi(|k|^2 < \mu^r)$). The second term in the round brackets is strictly negative and tends to zero, as $\beta^I \to \infty$. We conclude that $\mathcal{P}_{2,4} < 0$ if $\beta^I < \infty$, and β^{II} is large enough; as expected!

5.1 Fourier representation

The creation and annihilation operators in the Fourier representation are defined by

$$\begin{aligned} a^*(\boldsymbol{k},r) &= (2\pi)^{-d/2}\int_{\mathbb{R}^d} d\boldsymbol{x}\; e^{i\boldsymbol{k}\boldsymbol{x}} a^*(\boldsymbol{x},r), &(5.12)\\ a(\boldsymbol{k},r) &= (2\pi)^{-d/2}\int_{\mathbb{R}^d} d\boldsymbol{x}\; e^{-i\boldsymbol{k}\boldsymbol{x}} a(\boldsymbol{x},r), &(5.13)\end{aligned}$$

where $\boldsymbol{k}\in\mathbb{R}^d$, $r = I, II$; compare with (3.16) and (3.22). The dynamics of $a^*(\boldsymbol{k},r)$ and $a(\boldsymbol{k},r)$ is given by

$$\alpha_t^r(a^*(\boldsymbol{k},r)) = e^{i\omega t}a^*(\boldsymbol{k},r),\;\; \alpha_t^r(a(\boldsymbol{k},r)) = e^{-i\omega t}a(\boldsymbol{k},r), \tag{5.14}$$

where

$$\omega = \omega(\boldsymbol{k}) = |\boldsymbol{k}|^2.$$

The operators H^r, N^r, W_N defined in (3.19), (3.20), (3.34) are represented in Fourier space (and in the thermodynamic limit) by

$$\begin{aligned} H^r &= \int_{\mathbb{R}^d} d\boldsymbol{k}\;\omega(\boldsymbol{k})a^*(\boldsymbol{k},r)a(\boldsymbol{k},r), &(5.15)\\ N^r &= \int_{\mathbb{R}^d} d\boldsymbol{k}\; a^*(\boldsymbol{k},r)a(\boldsymbol{k},r), &\\ W_N &= \int dK^{(N)}dL^{(N)}\mathbf{a}^*(K^{(N)})\widehat{w}_N(-K^{(N)},L^{(N)})\mathbf{a}(L^{(N)}), &\end{aligned}$$

where we introduce notation analogous to (3.24)-(3.31). For $K^{(N)} = (K_1,\ldots,K_N)$, $K_j = (\boldsymbol{k}_j, r_j)\in\mathbb{R}^d\times\{I,II\}$, we set $-K^{(N)} := (-K_1,\ldots,-K_N)$, where $-K_j = (-\boldsymbol{k}_j, r_j)$. The symbol $\widehat{\ }$ denotes the Fourier transform, i.e.

$$\begin{aligned}&\widehat{w}_N(K^{(N)},L^{(N)})\\ &\quad = (2\pi)^{-dN}\int_{\mathbb{R}^{2dN}} d\boldsymbol{x}_1\cdots d\boldsymbol{y}_N e^{-i(\boldsymbol{k}_1\boldsymbol{x}_1+\cdots+\boldsymbol{l}_N\boldsymbol{y}_N)}w_N(X^{(N)},Y^{(N)}).\end{aligned}$$

We recall some properties of the state ω^0 defined in (2.60), which is given by

$$\omega^0 = \omega_{\beta^I,\mu^I}\otimes\omega_{\beta^{II},\mu^{II}}, \tag{5.16}$$

where ω_{β^r,μ^r} is the equilibrium state of reservoir $r = I, II$ in the thermodynamic limit; see also Theorem 3.1. The two-point function of ω_{β^r,μ^r} is

$$\omega_{\beta^r,\mu^r}(a^*(\boldsymbol{k},r)a(\boldsymbol{l},r)) = \delta(\boldsymbol{k}-\boldsymbol{l})\rho_r(\boldsymbol{k}),\;\;\text{where}\;\;\rho_r(\boldsymbol{k}) = \frac{1}{e^{\beta^r(|\boldsymbol{k}|^2-\mu^r)}+1}.$$

The average of a monomial in n creation and m annihilation operators is zero unless $n = m$, in which case it can be calculated recursively from the formula

$$\omega_{\beta^r,\mu^r}\left(\prod_{i=1}^{n} a^*(\boldsymbol{k}_i, r) \prod_{j=1}^{n} a(\boldsymbol{l}_j, r)\right)$$
$$= \sum_{p=1}^{n} (-1)^{n-p} \omega_{\beta^r,\mu^r}(a^*(\boldsymbol{k}_1, r)a(\boldsymbol{l}_p, r))\, \omega_{\beta^r,\mu^r}\left(\prod_{i=2}^{n} a^*(\boldsymbol{k}_i, r) \prod_{j=1, j\neq p}^{n} a(\boldsymbol{l}_j, r)\right).$$

For details, we refer to [BR]. We are now ready for explicit calculations of the currents.

5.2 Calculations for tunnelling junctions

Particle current and resistance. The particle current

$$\mathcal{J} = \omega_{\rm stat}(-i[N \otimes \mathbb{1}, W]) = \omega^0(\sigma_+(-i[N \otimes \mathbb{1}, W])) \tag{5.17}$$

has been introduced in (2.86), (2.78), see also (2.81). We set $\hbar = 1$. We see from the Dyson series expansion of σ_+, see (4.1), and the definition of $\mathcal{J}_{k,l}$ (see after (5.1)), that

$$\begin{aligned} \mathcal{J}_{1,1} &= -i\omega^0([N \otimes \mathbb{1}, W_1]), \\ \mathcal{J}_{1,2} &= -i\omega^0([N \otimes \mathbb{1}, W_2]), \\ \mathcal{J}_{2,2} &= \int_0^\infty dt\, \omega^0([W_1(t), [N \otimes \mathbb{1}, W_1]]). \end{aligned} \tag{5.18}$$

It is not difficult to verify that

$$\begin{aligned} [N \otimes \mathbb{1}, W_N] &= \int dK^{(N)} dL^{(N)} \sum_{j=1}^{N} (\delta_{r_j, I} - \delta_{r'_j, I}) \\ &\qquad \times \mathbf{a}^*(K^{(N)}) \widehat{w}_N(-K^{(N)}, L^{(N)}) \mathbf{a}(L^{(N)}), \end{aligned} \tag{5.19}$$

where δ is the Kronecker symbol and $L^{(N)} = (L_1, \ldots, L_N)$, $L_j = (\boldsymbol{l}_j, r'_j)$. Using that ω^0 is invariant under $A \mapsto e^{isN^I} A e^{-isN^I}$, we find that

$$\omega^0([N \otimes \mathbb{1}, W_l]) = 0, \quad \text{for all } l. \tag{5.20}$$

Thus $\mathcal{J}_{1,1} = \mathcal{J}_{1,2} = 0$. Next, we calculate $\mathcal{J}_{2,2}$. Recalling that $W_1(t) = \alpha^0_{-t}(W)$ and equation (5.14), we write

$$[W_1(t), [N \otimes \mathbb{1}, W_1]] = \sum_{r,r',s,s'=I,II} (\delta_{s,I} - \delta_{s',I}) \int_{\mathbb{R}^{4d}} d\boldsymbol{k}\, d\boldsymbol{l}\, d\boldsymbol{k}'\, d\boldsymbol{l}'\, e^{-i(|\boldsymbol{k}|^2 - |\boldsymbol{l}|^2)t}$$
$$\times \widehat{w}_1((-\boldsymbol{k}, r), (\boldsymbol{l}, r'))\;\; \widehat{w}_1((-\boldsymbol{k}', s), (\boldsymbol{l}', s'))\;\; [a^*(\boldsymbol{k}, r)a(\boldsymbol{l}, r'), a^*(\boldsymbol{k}', s)a(\boldsymbol{l}', s')].$$

We expand the commutator on the right side and apply the state ω^0 to obtain

$$\begin{aligned}\mathcal{J}_{2,2} = \int_0^\infty dt \int_{\mathbb{R}^{2d}} d\boldsymbol{k}\; d\boldsymbol{l}\; \widehat{w}_1((-\boldsymbol{k}, II), (\boldsymbol{l}, I))\; \widehat{w}_1((-\boldsymbol{l}, I), (\boldsymbol{k}, II)) \\ \times \left\{ e^{-i(|\boldsymbol{k}|^2 - |\boldsymbol{l}|^2)t} + e^{i(|\boldsymbol{k}|^2 - |\boldsymbol{l}|^2)t} \right\} (\rho_{II}(\boldsymbol{k}) - \rho_I(\boldsymbol{l}))\,.\end{aligned}$$

Because W_1 is selfadjoint, we have the relation

$$\overline{\widehat{w}_1((-\boldsymbol{k}, II), (\boldsymbol{l}, I))} = \widehat{w}_1((-\boldsymbol{l}, I), (\boldsymbol{k}, II));$$

using this and the formula $\int_{-\infty}^{\infty} dt\; e^{i\tau t} = 2\pi\delta(\tau)$, one sees that (5.3) holds. It is useful to keep in mind that

$$\rho_{II}(\boldsymbol{k}) - \rho_I(\boldsymbol{k}) = \frac{e^{\beta^I(|\boldsymbol{k}|^2 - \mu^I)} - e^{\beta^{II}(|\boldsymbol{k}|^2 - \mu^{II})}}{\left(e^{\beta^I(|\boldsymbol{k}|^2 - \mu^I)} + 1\right)\left(e^{\beta^{II}(|\boldsymbol{k}|^2 - \mu^{II})} + 1\right)}.$$

The resistance. Let $\beta^I = \beta^{II}$ and $\mu^I = \mu$, $\mu^{II} = \mu + \Delta\mu$, with $\Delta\mu$ small. We expand

$$\rho_{II}(\boldsymbol{k}) - \rho_I(\boldsymbol{k}) = \beta\;\Delta\mu\; e^{\beta(|\boldsymbol{k}|^2 - \mu)}(e^{\beta(|\boldsymbol{k}|^2 - \mu)} + 1)^{-2} + O((\Delta\mu)^2).$$

Retaining only the first order in $\Delta\mu$ in equation (5.3) gives (5.6) and (5.7). Let $T = 1/\beta$ denote the temperature and assume that $\mu > 0$. We see that $R(\mu, \beta) \sim T$, as $T \to \infty$. Next, we examine the dependence of the resistance on T, for small T, in three dimensions, and where $\widehat{w}_1$ is a radial function in both variables (i.e. $\widehat{w}_1$ depends only on $|\boldsymbol{k}|$ and $|\boldsymbol{l}|$). We then have

$$R(\mu, \beta)^{-1} = 8\pi^3\beta \int_0^\infty dr\; r|\widehat{w}_1((\sqrt{r}, II), (\sqrt{r}, I))|^2 \frac{e^{\beta(r-\mu)}}{\left(e^{\beta(r-\mu)} + 1\right)^2}.$$

The fraction in the integral equals $-\beta^{-1}\partial_r(e^{\beta(r-\mu)} + 1)^{-1}$ and it follows that

$$R(\mu, \beta)^{-1} = \int_0^\infty dr\; f'(r)\frac{1}{e^{\beta(r-\mu)} + 1}, \tag{5.21}$$

where f' denotes the derivative of the function

$$f(r) := 8\pi^3 r|\widehat{w}_1((\sqrt{r}, II), (\sqrt{r}, I))|^2.$$

Let us split the integral in (5.21) as

$$\begin{aligned} R(\mu, \beta)^{-1} &= \int_0^\mu f'(r)\frac{1}{e^{\beta(r-\mu)} + 1} + \int_\mu^\infty f'(r)\frac{1}{e^{\beta(r-\mu)} + 1} \\ &= f(\mu) - \int_0^\mu f'(r)\frac{1}{1 + e^{-\beta(r-\mu)}} + \int_\mu^\infty f'(r)\frac{1}{e^{\beta(r-\mu)} + 1}. \end{aligned} \tag{5.22}$$

Apply the change of variables $t = -\beta(r-\mu)$ and $t = \beta(r-\mu)$ in the first and second integral on the right side of (5.22), repectively. Then one has

$$\begin{aligned} R(\mu,\beta)^{-1} &= f(\mu) \\ &+\frac{1}{\beta}\int_0^\infty dt\ \{f'(t/\beta+\mu) - f'(-t/\beta+\mu)\chi(t\le\beta\mu)\}\,(e^t+1)^{-1} \end{aligned}$$

and using the mean value theorem,

$$R(\mu,\beta)^{-1} = f(\mu) + \frac{2}{\beta^2}\left(\int_0^\infty dt\ f''(\xi_t)\frac{t}{e^t+1} + O(e^{-\beta\mu})\right),$$

for some $\xi_t \in [-t/\beta+\mu, t/\beta+\mu]$ and where the exponentially small remainder term comes from removing the cutoff function $\chi(t \le \beta\mu)$. Retaining the main term ($\beta \to \infty$) yields

$$R(\mu,\beta)^{-1} \approx f(\mu) + \frac{\pi^2}{6\beta^2}f''(\mu)$$

and consequently,

$$R(\mu,\beta) \approx \frac{1}{f(\mu)+\pi^2T^2f''(\mu)/6}, \quad T \to 0.$$

At zero temperature, the resistance has the value $R(\mu,\infty) = f(\mu)^{-1}$ and it increases or decreases with increasing T according to whether $f''(\mu) < 0$ or $f''(\mu) > 0$.

Energy current. The energy current

$$\mathcal{P} = \omega_{\mathrm{stat}}(-i[H\otimes\mathbb{1}, W]) = \omega^0(\sigma_+(-i[H\otimes\mathbb{1}, W]))$$

has been introduced in equations (2.85), (2.77), see also (2.82). We set $\hbar = 1$. Using the CAR and expression (5.15) for H, one obtains

$$\begin{aligned} [H\otimes\mathbb{1}, W_N] &= \int dK^{(N)}dL^{(N)}\sum_{j=1}^N(|\boldsymbol{k}_j|^2\delta_{r_j,I} - |\boldsymbol{l}_j|^2\delta_{r'_j,I}) \\ &\quad\times\mathbf{a}^*(K^{(N)})\widehat{w}_N(-K^{(N)}, L^{(N)})\mathbf{a}(L^{(N)}), \end{aligned}$$

and it is readily verified that $\mathcal{P}_{1,1} = \mathcal{P}_{1,2} = 0$, and a similar calculation as for the particle current shows that

$$\mathcal{P}_{2,2} = \int_0^\infty dt\ \omega^0([W_1(t), [H\otimes\mathbb{1}, W_1]]) \tag{5.23}$$

is given by (5.5).

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