

Dissipative Transport: Thermal Contacts and Tunnelling Junctions

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Abstract

The subject of this talk is the theory of transport processes between quantum mechanical reservoirs. We focus on thermoelectric phenomena that includes exchange of particles and energy between two fermionic reservoirs at different temperatures and chemical potentials in a steady-state [1]. We show that in some cases the entropy production rate is not only non-negative but strictly positive. The talk will focus on physical measurable quantities and the proofs will only be sketched or be presented during the talk.

1 Introduction

We are interested in simple transport processes, such as those observed near a spatially localized thermal contact or tunnelling junction between two macroscopically extended metals at different temperatures or chemical potential. The aim is to find expressions for e.g. the energy current, charge transport or the rate of entropy production. Part of the purpose is also proving the convergence to a non-equilibrium steady-state using scattering endomorphisms. We will describe the reservoirs according to quantum mechanics. We first define what we mean when we talk about a reservoir and make some first assumptions. In a next step, two reservoirs are connected and a local perturbation in the generator of the dynamics is introduced. Then we will try to connect our knowledge with thermodynamics and find that the entropy production rate of our system is non-negative. Our next assumption is the existence of a scattering endomorphism which tells us that stationary states in the thermodynamic limit (TDL) exist. This assumption is proven in a later chapter for two reservoirs of fermions which are coupled through a local interaction. As a first example we will look at reservoirs of non-interacting fermions and find that, under certain assumptions, an equilibrium state exists for non-negative temperature. Our next task will be to sketch the proof of the existence of a scattering endomorphism and its consequences. In the last section we will explicitly calculate resistance, the Onsager reciprocity relations and currents.

2 General theory of junctions and of non-equilibrium stationary states

2.1 Quantum theory of reservoirs

In this section we are interested in general properties of quantum mechanical reservoirs. Later we will consider a specific example where all the assumptions we will make are verified. A reservoir is a quantum system with many degrees of freedom (superconductor, gas of atoms) but with a small number of observable physical quantities. Our system is confined to a finite region $\Lambda \subset \mathbb{R}^3$ of real space. Pure states are unit rays in a separable Hilbert space \mathcal{H}^Λ , mixed states correspond to density matrices. Its dynamics is generated by a selfadjoint Hamiltonian H^Λ . The \mathbb{C}^* -algebra \mathcal{A}^Λ defines the kinematics of the system and is a subset of $\mathcal{B}(\mathcal{H}^\Lambda)$, the algebra of all bound operators on \mathcal{H}^Λ . The time evolution (in the Heisenberg representation) of any operator $a \in \mathcal{A}^\Lambda$ is given by

$$\alpha_t^\Lambda(a) = e^{itH^\Lambda} a e^{-itH^\Lambda}$$

with the assumption that this time evolution is in \mathcal{A}^Λ again. We set $\hbar = 1$ in this paper.

We represent conservation laws by selfadjoint operators Q_j on \mathcal{H}^Λ where $1 \leq j \leq M$. These conserved charges commute with each other, H^Λ and elements of \mathcal{A}^Λ . More precisely, one assumes that all operators e^{itH^Λ} and $e^{is_j Q_j^\Lambda}$ commute with one another for arbitrary values $s_j \in \mathbb{R}$, $j = 1, \dots, M$. A gauge transformation of the first kind is defined by

$$\varphi_{\mathbf{s}}^\Lambda(a) = e^{i\mathbf{s} \cdot \mathbf{Q}^\Lambda} a e^{-i\mathbf{s} \cdot \mathbf{Q}^\Lambda}$$

for $a \in \mathcal{B}(\mathcal{H}^\Lambda)$ and $\mathbf{s} \cdot \mathbf{Q}^\Lambda = \sum_{j=1}^M s_j Q_j^\Lambda$. By a simple calculation one finds that

$$\alpha_t^\Lambda[\varphi_{\mathbf{s}}^\Lambda(a)] = \varphi_{\mathbf{s}}^\Lambda[\alpha_t^\Lambda(a)],$$

which means that the time evolution and the gauge transformation commute. We define the observable algebra \mathcal{A}^Λ as the algebra of all the operators $a \in \mathcal{B}(\mathcal{H}^\Lambda)$ which are gauge invariant, which means $\varphi_{\mathbf{s}}^\Lambda(a) = a$.

We know that thermal equilibrium is described by a density matrix

$$Z^{-1} e^{-\beta[H^\Lambda - \mu \mathbf{Q}^\Lambda]}$$

where $\beta = \frac{1}{T}$ is the inverse temperature, μ the chemical potential (conjugate to the conservation laws) and $Z = Z_{\beta, \mu}^\Lambda$ the grand canonical partition function given by

$$Z = \text{tr}(e^{-\beta[H^\Lambda - \mu \mathbf{Q}^\Lambda]})$$

where $tr(\cdot)$ means the trace. The expectation value of $a \in \mathcal{B}(\mathcal{H}^\Lambda)$ in equilibrium in terms of the density matrix is

$$\omega_{\beta, \mu}^\Lambda(a) = Z^{-1} tr(e^{-\beta[H^\Lambda - \mu Q^\Lambda]} a).$$

The expectation value has some interesting properties. The expectation value is time-translation invariant, $\omega_{\beta, \mu}^\Lambda(\alpha_t^\Lambda(a)) = \omega_{\beta, \mu}^\Lambda(a)$, it obeys the KMS condition and in particular, if $a \in \mathcal{A}^\Lambda$ then $\omega_{\beta, \mu}^\Lambda(\alpha_t^\Lambda(a)b) = \omega_{\beta, \mu}^\Lambda(b\alpha_{t+i\beta}^\Lambda(a))$. Let's now turn to the task of defining of what we need in the thermodynamic limit. We want to understand the asymptotics of physical quantities. We let Λ , the physical space, increase to \mathbb{R}^3 or to an infinite half-space such that the ratio between surface and volume goes to zero. We introduce an operator algebra \mathcal{F}^r , called the field algebra, convenient for the description of the thermodynamic limit of a reservoir:

$$\mathcal{F}^r = \overline{\bigvee_{\Lambda \rightarrow \infty} \mathcal{B}(\mathcal{H}^\Lambda)}$$

i.e. the algebra is generated by all the operators in the increasing sequence of the bound algebra $\mathcal{B}(\mathcal{H}^\Lambda)$. The superscript r stands for reservoir (labeled with 1 and 2 later).

Definition. A group $\{\tau_{\mathbf{t}} | \mathbf{t} \in \mathbb{R}^n\}$ of homomorphism of \mathcal{F} is a **automorphism group of \mathcal{F} iff for all $a \in \mathcal{F}$*

$$\tau_{\mathbf{t}=0}(a) = a, \tau_{\mathbf{t}}(\tau_{\mathbf{t}'}(a)) = \tau_{\mathbf{t}+\mathbf{t}'}(a) \text{ and } \tau_{\mathbf{t}}(a)^* = \tau_{\mathbf{t}}(a^*).$$

For the purposes of this paper we need to make some assumptions on the existence of the thermodynamic limit. The first two are

Assumption 1 (Existence of the TDL of the dynamics and the gauge transformations). *For every operator $a \in \mathcal{F}^r$, we assume that the following two limits exist*

$$n - \lim_{\Lambda \rightarrow \infty} \alpha_t^\Lambda(a) =: \alpha_t(a)$$

$$n - \lim_{\Lambda \rightarrow \infty} \varphi_s^\Lambda(a) =: \varphi_s(a)$$

and define **automorphism groups of the field algebra.*

We can now look at the kinematical algebra \mathcal{A}^Λ , the algebra of observables, as the largest subalgebra of \mathcal{F} pointwise invariant under gauge transformations.

Assumption 2 (Existence of the TDL of the equilibrium state). *For every operator $a \in \mathcal{A}^r$,*

$$\lim_{\Lambda \rightarrow \infty} \omega_{\beta, \mu}^{\Lambda}(a) =: \omega_{\beta, \mu}(a)$$

exists and is time-translation invariant.

2.2 Thermal contacts and tunnelling junctions

After we have defined all properties of a reservoir we now can consider two reservoirs with all the properties of the previous section. An example of such a system is two ordinary metals located in two complementary half-spaces of our physical space. We will write "1" resp. "2" when the system $(1, \Lambda^1)$ resp. $(2, \Lambda^2)$ is meant. The Hilbert space of the system is given by $\mathcal{H} = \mathcal{H}^1 \otimes \mathcal{H}^2$ and the dynamics before the reservoirs are brought into contact is generated by $H^0 := H^1 \otimes 1 + 1 \otimes H^2$. The algebra of bounded operators of finite coupled systems is given by $\mathcal{B}(\mathcal{H}^1) \otimes \mathcal{B}(\mathcal{H}^2)$ and in the TDL is $\overline{\mathcal{F}^1 \otimes \mathcal{F}^2}$. We describe a contact or tunnelling junction between the two reservoirs in terms of a perturbed generator of the coupled dynamics H . The operator H has the following form:

$$H = H^0 + W(\Lambda^1, \Lambda^2)$$

where the operator W is bound and selfadjoint. We will always require the following assumption (we write $1, 2 \rightarrow \infty$ for $\Lambda^1 \rightarrow \infty, \Lambda^2 \rightarrow \infty$):

Assumption 3 (Existence of the TDL of the contact interaction).

The norm limit

$$n - \lim_{1, 2 \rightarrow \infty} W(\Lambda^1, \Lambda^2) =: W$$

exists as a selfadjoint operator in the field algebra.

Let $\alpha_t^{\Lambda^1}$ and $\alpha_t^{\Lambda^2}$ be the time evolution of the reservoirs before they are brought into contact. Then the time evolution of the whole system is given by $\alpha_t^{\Lambda^1} \otimes \alpha_t^{\Lambda^2}$ and is generated by the Hamiltonian H^0 . After the interaction W has been turned on, the time evolution is given by $\alpha_t^{1 \cup 2}(a) = e^{itH} a e^{-itH}$ with H the perturbed Hamiltonian H^0 . From our assumptions it follows that the TDL for the time evolution in both cases exist [1]; i.e. for the connected system we get

$$\alpha_t(a) := n - \lim_{1, 2 \rightarrow \infty} \alpha_t^{1 \cup 2}(a)$$

and for the uncoupled system

$$\alpha_t^0(a) := n - \lim_{1, 2 \rightarrow \infty} \alpha_t^{\Lambda^1} \otimes \alpha_t^{\Lambda^2}(a).$$

We now have a look at two different cases of contacts.

Thermal contacts

First we will consider the contact to be thermal, i.e. the perturbation W commutes with all conservation laws and is therefore gauge invariant. So the conservation laws $Q_j^{\Lambda^1}$ of the first reservoir becomes a conserved charge $Q_j^{\Lambda^1} \otimes 1$ of the connected system (similarly $1 \otimes Q_j^{\Lambda^1}$ a conserved charge for the second reservoir). Due to our first assumption, the TDL for the gauge transformation exists. Taking our third assumption we obtain that $\varphi_s^1(W) = \varphi_s^2(W) = W$.

Tunnelling junctions

Next we look at tunnelling junctions. Let there be $m < \min(M^1, M^2)$ linear combinations $R_1^{\Lambda^1}, \dots, R_m^{\Lambda^1}$ and $R_1^{\Lambda^2}, \dots, R_m^{\Lambda^2}$ of conservation laws of the two reservoirs with the property that the operators $Q_j^{1\cup 2} = R_j^{\Lambda^1} \otimes 1 + 1 \otimes R_j^{\Lambda^2}$ are conservation laws for the perturbed dynamics for every j . Without loss of generality we can chose the m conservation laws of each reservoir to be the first m conservation laws $Q_1^{\Lambda^i}, \dots, Q_m^{\Lambda^i}$ for $i = 1, 2$. Setting $\mathbf{s} = \{s_1, \dots, s_m, 0, \dots, 0\}$ we define the gauge transformation for the coupled system

$$\varphi_{\mathbf{s}}^{1\cup 2}(a) := \varphi_{\mathbf{s}}^{\Lambda^1} \otimes \varphi_{\mathbf{s}}^{\Lambda^2}(a)$$

and by assumption one

$$\varphi_{\mathbf{s}}(a) := n - \lim_{1,2 \rightarrow \infty} \varphi_{\mathbf{s}}^{1\cup 2}(a).$$

Tunnelling junctions can then be characterized by the requirement that $\varphi_{\mathbf{s}}^{1\cup 2}(W(\Lambda^1, \Lambda^2)) = W(\Lambda^1, \Lambda^2)$ and we obtain in the TDL that $\varphi_{\mathbf{s}}(W) = W$. Thermal contacts can only exchange energy, tunnelling junctions 'charge' as well.

Our next task is to find expressions for the energy and charge current, from the point of view of quantum mechanics. We will make the discussion for finite systems, and then take the thermodynamic limit of well defined quantities.

Energy current

We are interested in the gain of internal energy per second and introduce an operator $P^r(t)$ which is conveniently defined in the Heisenberg picture by

$$P^r(t) := \frac{d}{dt} \alpha_t^{1\cup 2}(H^r).$$

We obtain after some straightforward calculations that

$$P^r(t) = i\alpha_t^{1\cup 2}([W(\Lambda^1, \Lambda^2), H^r]),$$

and further

$$P^r(t) = -\frac{d}{ds}\alpha_t(\alpha_s^r(W))|_{s=0}.$$

The operator corresponding to the energy gain per second of reservoir r has a thermodynamic limit, where α_s^r is the time evolution of reservoir r in the TDL, in the absence of any contacts. It follows directly (by applying the formulas before) that the total gain of energy is given by

$$P^1(t) + P^2(t) = -\frac{d}{dt}\alpha_t^{1\cup 2}(W(\Lambda^1, \Lambda^2)) \quad (1)$$

and in the TDL we obtain

$$P^1(t) + P^2(t) = -\frac{d}{dt}\alpha_t(W).$$

The first notation is for finite systems, the second for infinite systems.

Charge current for tunnelling junctions

We expect that the total gain of charge will be zero in a connected system; charge lost by one reservoir has to be gained by the other. Similar to the previous section we introduce an operator $I^r(t)$ corresponding to a measurement of the gain of charge Q^r per second at time t , in reservoir r . It is defined as

$$I^r(t) := \frac{d}{dt}\alpha_t^{1\cup 2}(Q^r) = i\alpha_t^{1\cup 2}([H, Q^r])$$

with $Q^1 = Q^{\Lambda^1} \otimes 1$ and $Q^2 = 1 \otimes Q^{\Lambda^2}$. Since

$$H = H^1 \otimes 1 + 1 \otimes H^2 + W(\Lambda^1, \Lambda^2)$$

and since $H^1 \otimes 1$ and $1 \otimes H^2$ commute with Q^r , it follows that

$$I^r(t) = i\alpha_t^{1\cup 2}([W(\Lambda^1, \Lambda^2), Q^r])$$

and in TDL

$$I^r(t) = -i\frac{d}{ds}\alpha_t([\varphi_s^r(W)])|_{s=0}.$$

We are interested in the total gain of charge of the connected system. Similar to the arguments of the energy gain we obtain

$$I^1(t) + I^2(t) = i\alpha_t^{1\cup 2}([W(\Lambda^1, \Lambda^2), Q^{1\cup 2}]) = 0. \quad (2)$$

This can be transformed to the TDL and tells us that the charge lost by one reservoir is gained by the other one, as expected.

2.3 Connections with thermodynamics

We want to find the connection between what we already observed and the knowledge of thermodynamics. What we will find in this section is that the entropy production rate is non-negative. Let's start with the first and second laws of thermodynamics summarized in the following equation

$$dU^{\Lambda^r} = T^r dS^{\Lambda^r} + \boldsymbol{\mu}^r d\mathbf{q}^{\Lambda^r} - p^r dV^r$$

where U is the expectation value of the Hamiltonian H in a state of a reservoir. The differential 'd' indicates that we only look at small and reversible changes of U , S , etc. If we open a contact between two reservoirs the equation has a time dependency and the previous equation becomes

$$\dot{U}^{\Lambda^r} = T^r \dot{S}^{\Lambda^r} + \boldsymbol{\mu}^r \dot{\mathbf{q}}^{\Lambda^r} - p^r \dot{V}^r, \quad (3)$$

where dots indicate time derivatives. According to what we've found in the previous section we can write the energy and charge gain per second when the two systems are coupled as

$$\dot{U}^{\Lambda^r} = \omega^{1\cup 2}(P^r(t))$$

$$\dot{q}^{\Lambda^r} = \omega^{1\cup 2}(I^r(t)).$$

As we are interested in the change of entropy per second of reservoir r , we rewrite Eq. (3) and obtain

$$\dot{S}^{\Lambda^r} = \beta^r (\dot{U}^{\Lambda^r} - \boldsymbol{\mu}^r \dot{\mathbf{q}}^{\Lambda^r} - p^r \dot{V}^r),$$

where we set β to the inverse temperature. Our main task is to investigate the entropy production rate, which is defined as

$$e^{1\cup 2} := \dot{S}^{\Lambda^1} + \dot{S}^{\Lambda^2}$$

Since $e^{1\cup 2}$ describes in the TDL the entropy production rate of a thermodynamic system, it should be non-negative. We will proof this now.

Positivity of entropy production

We look at the situation in which the state of the system, consisting of two reservoirs, before the contact is opened, is given by

$$\omega^{1\cup 2}(a) = \omega_{\beta^1, \boldsymbol{\mu}^1}^{\Lambda^1} \otimes \omega_{\beta^2, \boldsymbol{\mu}^2}^{\Lambda^2}(a)$$

where the $\omega_{\beta^r, \boldsymbol{\mu}^r}^{\Lambda^r}$ are the equilibrium states already defined and $a \in \mathcal{A}^{1\cup 2}$. At some time t_0 the contact between the two reservoirs is opened. We are interested in the evolution of the state $\omega^{1\cup 2}$ under the perturbed time evolution

and therefore the gain/loss of charge/energy and the entropy production rate.

$$\dot{U}^{\Lambda^r} = i\omega^{1\cup 2}(\alpha_t^{1\cup 2}([W(\Lambda^1, \Lambda^2), H^r]))$$

and

$$\dot{q}^{\Lambda^r} = i\omega^{1\cup 2}(\alpha_t^{1\cup 2}([W(\Lambda^1, \Lambda^2), Q_j^r])).$$

By Assumption 2 (existence of the TDL of the equilibrium state), the state $\omega^{1\cup 2}(a)$ has a thermodynamic limit $\omega^0(a)$. Then we also can define a TDL for \dot{U}^{Λ^r} and \dot{q}^{Λ^r} as

$$\mathcal{U}^r(t) := \lim_{1,2 \rightarrow \infty} \dot{U}^{\Lambda^r}(t) = -\frac{d}{ds}\omega^0(\alpha_t(\alpha_s^r(W)))|_{s=0}$$

and

$$\mathcal{Q}^r(t) := \lim_{1,2 \rightarrow \infty} \dot{q}^{\Lambda^r}(t) = -\frac{d}{ds}\omega^0(\alpha_t([\varphi_s^r(W)]))|_{s=0}.$$

By Eq. (1) and Eq. (2) we find that

$$\mathcal{U}^1(t) + \mathcal{U}^2(t) = -\frac{d}{dt}\omega^0(\alpha_t(W))$$

and

$$\mathcal{Q}^1(t) + \mathcal{Q}^2(t) = 0.$$

Now we'd like to study the entropy production rate for finite reservoirs. The density matrix is defined as

$$\rho^r = Z^{-1}e^{-\beta[H^r - \mu^r Q^r]},$$

corresponding to the equilibrium state for reservoir r . By fixing the volume V , we can write the entropy production rate as follows

$$\begin{aligned} \dot{S}^{\Lambda^r} &= \beta^r(\dot{U}^{\Lambda^r} - \mu^r \dot{q}^{\Lambda^r}) \\ &= -\frac{d}{dt}\omega^{1\cup 2}(\alpha_t^{1\cup 2}(\ln \rho^r)) \\ &= -\frac{d}{dt}\text{tr}(\rho^1 \otimes \rho^2 \alpha_t^{1\cup 2}(\ln \rho^r)). \end{aligned}$$

and by definition of the entropy production rate

$$\dot{S}^{1\cup 2} := e^{1\cup 2}(t) = -\frac{d}{dt}\text{tr}(\rho^1 \otimes \rho^2 \alpha_t^{1\cup 2}(\ln \rho^1 \otimes \rho^2)) \quad (4)$$

We know that $\mathcal{U}^r(t)$ and $\mathcal{Q}^r(t)$ have a TDL, so the TDL for the entropy production rate has to exist and

$$e(t) = \sum_{r=1,2} \beta^r [\mathcal{U}^r - \mu^r \cdot \mathcal{Q}^r(t)].$$

By integrating Eq. (4) in time we obtain

$$S^{1\cup 2}(t) - S^{1\cup 2}(0) = -\text{tr}(\rho^1 \otimes \rho^2 [\alpha_t^{1\cup 2}(\ln \rho^1 \otimes \rho^2) - \ln \rho^1 \otimes \rho^2]).$$

If A is a non-negative matrix and B is a strictly positive matrix then

$$-\text{tr}(A \ln B - A \ln A) \geq \text{tr}(A - B).$$

A proof of this can be found in [2]. Setting $A = \rho^1 \otimes \rho^2$ and $B = \alpha_t^{1\cup 2}(\rho^1 \otimes \rho^2)$ we obtain

$$S^{1\cup 2}(t) - S^{1\cup 2}(0) \geq \text{tr}(\rho^1 \otimes \rho^2 - \alpha_t^{1\cup 2}(\rho^1 \otimes \rho^2)) = 0$$

by the unitarity of time evolution and the cyclicity of the trace. Then, by integrating the entropy production rate, we find that the overall production is non-zero

$$\frac{1}{T} \int_0^T e^{1\cup 2}(t) dt = \frac{1}{T} (S^{1\cup 2}(T) - S^{1\cup 2}(0)) \geq 0.$$

If the limit $\lim_{t \rightarrow \infty} e(t) =: e$ exists then we get in the TDL

$$e = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T e(t) dt \geq 0.$$

We will show in Chapter 5 that we even have strict positive entropy production using a Dyson series expansion.

2.4 Existence of stationary states in the TDL

We will now turn to the task of studying whether the infinite-volume states $\omega_t(a) := \omega^0(\alpha_t(a))$ have a limit as t goes to infinity. The state ω^0 is invariant under the unperturbed time evolution α_t^0 and therefore $\omega_t(a) := \omega^0(\alpha_{-t}^0(\alpha_t(a)))$. We don't have to find the limit of ω_t itself. It's sufficient for the existence of a stationary limiting state $\omega_{stat}(a) = \lim_{t \rightarrow \infty} \omega_t(a)$ that there is a

Assumption 4 (Existence of scattering endomorphisms). *For all a , the limits*

$$\sigma_{\pm}(a) = n - \lim_{t \rightarrow \pm \infty} \alpha_{-t}^0(\alpha_t(a))$$

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

We only note that scattering endomorphisms do not exist in finite volume.

One can show that the energy gain rates and currents of two very large, but finite reservoirs are well approximated by the energy gain rates

$$-\frac{d}{ds}\omega_{stat}(\alpha_s^r(W))|_{s=0}$$

and the currents

$$-\frac{d}{ds}\omega_{stat}([\varphi_s^r(W)])|_{s=0}$$

respectively, for a large range of sufficiently large, but not exceedingly large times t .

2.5 Return to equilibrium and non equilibrium stationary states

We consider a system of one reservoir first. If ρ is an arbitrary state normal relative to an infinite-volume equilibrium state $\omega = \omega_{\beta,\mu}$ on \mathcal{F}^r then

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \rho(\alpha_t(a)) = \omega(a).$$

This is the property of return to equilibrium. Now suppose that the property of return to equilibrium holds for each reservoir separately. Then one can show that for any state ρ normal relative to the state $\omega^0(a) = \lim_{1 \rightarrow \infty, 2 \rightarrow \infty} \omega^{1 \cup 2}(a)$ the following limit holds

$$\lim_{t \rightarrow \infty} \rho(\alpha_t^0(a)) = \omega^0(a),$$

where α_t^0 is the time evolution of the reservoirs before they are coupled. This equation and the existence of a scattering endomorphism σ_+ imply that

$$\begin{aligned} \lim_{t \rightarrow \infty} \rho_t(a) &= \lim_{t \rightarrow \infty} \rho(\alpha_t(a)) \\ &= \lim_{t \rightarrow \infty} \rho(\alpha_t^0(\sigma_+(a))) \\ &= \omega^0(\sigma_+(a)) \\ &= \omega_{stat}(a). \end{aligned} \tag{5}$$

So the states ρ_t tend to the stationary state ω_{stat} , as $t \rightarrow \infty$.

2.6 Three more assumptions

We consider two increasing reservoirs joined together by a thermal contact or a tunnelling junction localized near the origin $\mathbf{x} = 0$.

Assumption 5 (Existence of space translations). *For each reservoir there exists a *automorphism group $\{\tau_{\mathbf{x}} | \mathbf{x} \in \mathbb{R}^3\}$ of the field algebra \mathcal{F} , representing space translations of \mathbb{R}^3 on \mathcal{F} .*

For the system of coupled reservoirs, the direct product $\tau_{\mathbf{x}} = \tau_{\mathbf{x}}^1 \otimes \tau_{\mathbf{x}}^2$ defines a representation of space translations.

Assumption 6 (Asymptotic abelianness of space translations and homogeneity of reservoirs). *The action of $\tau_{\mathbf{x}}$ is norm-continuous in \mathbf{x} and for all operators a and b ,*

$$\lim_{|\mathbf{x}| \rightarrow \infty} \|[\tau_{\mathbf{x}}(a), b]\| = 0.$$

The dynamics and the equilibrium states of the uncoupled reservoirs are homogeneous, in the sense that $\alpha_t^0(\tau_{\mathbf{x}}(a)) = \tau_{\mathbf{x}}(\alpha_t^0(a))$ and $\omega^0(\tau_{\mathbf{x}}(a)) = \omega^0(a)$.

It is then possible to show that due to the local nature of the perturbation W

$$\lim_{|\mathbf{x}| \rightarrow \infty} \|\alpha_t(\tau_{\mathbf{x}}(a)) - \alpha_t^0(\tau_{\mathbf{x}}(a))\| = 0$$

for all times t . This relation tells us that observables localized far from the junction evolve according to the non-interacting dynamics.

Assumption 7 (Properties of the scattering endomorphism). *The limits*

$$n - \lim_{t \rightarrow \pm\infty} \alpha_{-t}^0(\alpha_t(\tau_{\mathbf{x}}(a))) = \sigma_{\pm}(\tau_{\mathbf{x}}(a))$$

are uniform in \mathbf{x} for every $a \in \mathcal{F}$.

This implies that far from a junction, the stationary state ω_{stat} resembles the product state ω^0 of the uncoupled reservoirs.

The validity of Assumption 7 critically depends on the dimension of the reservoir. In dimension $d > 2$, this assumption can be expected to hold, while it usually fails in dimension $d = 1, 2$.

3 Reservoirs of non-interacting fermions

We have developed the quantum mechanical theory of two coupled reservoirs of free non-relativistic fermions in the previous chapter so we can now apply this theory for a class of simple, but physically important examples of reservoirs. This examples describe a quantum gas of non-interacting, non-relativistic electrons or an ideal quantum gas of fermionic atoms or molecules. We will construct the Fock space, creation and annihilation operators, particle number operator and charge operators. We will see that for a family of reservoirs with certain properties, the equilibrium states exist for non-negative temperature.

We start by considering a system consisting of a single, non-relativistic quantum-mechanical particle confined to a region $\Lambda \subset \mathbb{R}$. The Hilbert space

of pure state vectors is the space of square-integrable functions $L^2(\Lambda, d^d x)$ with support in Λ . We have to consider that the particle could have spin and/or there are several species of particles. Then we have to extend our Hilbert space to $L^2(\Lambda, d^d x) \otimes \mathbb{C}^k$ with $k = \sum_{i=1}^r (2S_i + 1)$, where S_i is the spin of species i and r is the number of different species. The free and non-relativistic one-particle dynamics is generated by a selfadjoint operator

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

where we set $M = \frac{1}{2}$ for convenience.

The next step is to consider a system of n identical particles, all confined to the region Λ . The state space of these n particles is given by a direct product

$$h_n^\Lambda := P_\pm(h^\Lambda)^{\otimes n}, h_0^\Lambda = \mathbb{C},$$

where P_\pm determines the subspace of the wave functions of the selected symmetry. P_\pm is an orthogonal projection from the state space into a subspace e.g. if the particles are fermions (which we consider in this paper), P_- projects onto the completely anti-symmetric n -particles wave functions, while for bosons P_+ projects onto the completely symmetric n -particles wave functions. The Hamiltonian of non-interacting particles is given by

$$T_n^\Lambda = \sum_{j=1}^n 1 \otimes \cdots \otimes t_j^\Lambda \otimes \cdots \otimes 1$$

where t_j^Λ acts on the j^{th} factor in the state space.

As the number of particles can fluctuate, the description of the system is conveniently described in second quantization. Our defined state space is confined to n particles so we define the Fock space by

$$\mathcal{H}^\Lambda := \bigoplus_{n=0}^{\infty} h_n^\Lambda$$

and the dynamics on the Fock space is generated by

$$H^\Lambda := \bigoplus_{n=0}^{\infty} T_n^\Lambda.$$

We define a particle number operator by

$$N^\Lambda := \bigoplus_{n=0}^{\infty} n \cdot 1|_n$$

where $1|_n$ means that it acts only on the space h_n^Λ . We need unbounded and selfadjoint charge operators to be defined and therefore

$$Q^\Lambda(l) := Q^\Lambda = \bigoplus_{n=0}^{\infty} K_n^\Lambda$$

with

$$K_n^\Lambda = \sum_{j=1}^n 1 \otimes \cdots \otimes (1 \otimes l_j) \otimes \cdots \otimes 1$$

where l is a symmetric $k \times k$ matrix acting on \mathbb{C}^k and $1 \otimes l_j$ acts on the j^{th} factor of the tensor product defining h_n^Λ .

As we said before, we want to introduce annihilation and creation operators. We define $\mathbf{x}, \mathbf{y}, \dots$ as points in physical space and $s = 1, \dots, k$ labels an orthonormal basis in \mathbb{C}^k . Vectors in the n -particle state space can be represented as square-integrable wave functions $f_n(\mathbf{x}_1, s_1, \dots, \mathbf{x}_n, s_n)$ which for fermions is totally anti-symmetric under permutations of their n arguments. Vectors ψ in the Fock space correspond to sequences $\psi = (f_n)_{n=0}^\infty$ of the n -particle wave functions. According to Quantum Mechanics the scalar product on \mathcal{H}^Λ is defined by

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

where $\phi = (g_n)_{n=0}^\infty$. The vector represented by the sequence $(f_n)_{n=0}^\infty$, with $f_0 = 1$ and $f_n = 0$ for all $n > 0$ is denoted by Ω and is called the vacuum vector. By defining this vacuum vector we can now construct a creation operator which acts on the vacuum vector and creates a state. Similarly, we can act with an annihilation operator on a state until our state is the vacuum vector. Let D be the linear domain of vectors $\psi = (f_n)_{n=0}^\infty$ in \mathcal{H}^Λ with the property that all but finitely many f_n 's vanish. So we can define an annihilation operator $a(f)$ of f by

$$(a(f)\psi)_n(\mathbf{x}_1, s_1, \dots, \mathbf{x}_n, s_n) := \sqrt{n+1} \sum_{s=1}^k \int_{\Lambda} d\mathbf{x} \overline{f(\mathbf{x}, s)} f_{n+1}(\mathbf{x}_1, s_1, \dots, \mathbf{x}_n, s_n)$$

for any ψ and $a(f)\Omega = 0$. The creation operator $a^*(f)$ is defined to be the adjoint of $a(f)$ and is also well defined on D .

We know from Quantum Mechanics that for fermions the following anticommutation relations hold

$$\{a^\#(f), a^\#(g)\} = 0$$

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

for arbitrary f, g in h^Λ , $a^\# = a$ or a^* , $\{A, B\} = AB + BA$ and $(f, g) := \sum_s \int_{\Lambda} d\mathbf{x} \overline{f(\mathbf{x}, s)} g(\mathbf{x}, s)$ is the scalar product on h^Λ . The creation and annihilation operators are formally

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

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

with $\{a(\mathbf{x}, s), a^*(\mathbf{x}', s')\} = \delta_{ss'} \delta^{(d)}(\mathbf{x} - \mathbf{x}')$. One can easily see that the operators $a(f)$ and $a^*(f)$ are bounded in norm by

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

Note that for bosons the two operators are unbounded.

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

$$H^{\Lambda} = \sum_s \int_{\Lambda} d\mathbf{x} a^*(\mathbf{x}, s) (t^{\Lambda} a)(\mathbf{x}, s),$$

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

and

$$Q^{\Lambda} = \sum_{s, s'} \int_{\Lambda} d\mathbf{x} a^*(\mathbf{x}, s) l_{s, s'} a(\mathbf{x}, s').$$

From now on we usually regard $N^{\Lambda} = Q^{\Lambda}(l = 1)$ to be the only conservation law. The next theorem is the main result of this section and tells us something about equilibrium states and when they exist

Theorem. For $t^{\Lambda} = -\Delta \otimes 1$ and $Q_j^{\Lambda} = Q_j^{\Lambda}(l_j)$, $j = 1, \dots, M$, with l_1, \dots, l_M arbitrary, commuting $k \times k$ matrices, the equilibrium states $\omega_{\beta, \boldsymbol{\mu}}^{\Lambda}$ exist for arbitrary $\beta \geq 0$ and $\boldsymbol{\mu} \in \mathbb{R}$.

The proof of this theorem can be found, for example, in [2].

We introduce the following notation

$$X := (\mathbf{x}, s, r) \in \mathbb{R}^d \times \{1 \dots k\} \times \{1, 2\},$$

$$X^{(N)} := (X_1 \dots X_N),$$

$$\mathbf{x}^{(N)} := (\mathbf{x}_1 \dots \mathbf{x}_N) \in \mathbb{R}^{dN},$$

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

$$r^{(N)} := (r_1 \dots r_N) \in \{1, 2\}^N,$$

$$\int_{\Lambda} dX = \sum_{r=1,2} \sum_{s=1}^k \int_{\Lambda} d\mathbf{x},$$

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

$$\mathbf{a}^\#(X^N) := \prod \mathbf{a}^\#(X^N).$$

We now can go into describing the interaction, $W(\Lambda^1, \Lambda^2)$ corresponding to a thermal contact or tunnelling junction between the two reservoirs. We assume that the total particle number of the system of the two reservoirs is conserved. The interaction Hamiltonian $W(\Lambda^1, \Lambda^2)$ must commute with the operator $N^{1\cup 2} := N^{\Lambda^1} \otimes 1 + 1 \otimes N^{\Lambda^2}$. It follows that the interaction Hamiltonian must have the form

$$W(\Lambda^1, \Lambda^2) = \sum_{N=1}^{\infty} W_N(\Lambda^1, \Lambda^2),$$

where

$$W_N(\Lambda^1, \Lambda^2) = \int_{\Lambda^N} dX^{(N)} \int_{\Lambda^N} dY^{(N)} \mathbf{a}^*(X^{(N)}) w_N^{\Lambda^1, \Lambda^2}(X^{(N)}, Y^{(N)}) \mathbf{a}(Y^{(N)})$$

where w_n is always a smooth function.

A system of two reservoirs of non-interacting fermions, as we considered in this section, satisfies Assumptions (A1)-(A3) and (A5), (A6).

4 Existence of a scattering endomorphism

Our next goal is to prove the existence of scattering endomorphisms for two reservoirs of free non-relativistic fermions coupled through spatially localized interactions in $d \geq 3$. The reservoirs are infinite and without boundary, and the coupling is localized near the origin. We assumed in the first chapter that the time evolutions α_t^0 for the free dynamics and α_t for the dynamic of the coupled system exist in the TDL (see [2]). We define $W(t) := \alpha_{-t}^0(W)$ and can write the Dyson series for $\alpha_{-t}^0 \alpha_t$ as

$$\alpha_{-t}^0 \alpha_t = \sum_{m=0}^{\infty} i^m \int_{t > t_m > \dots > t_1 > 0} dt_1 dt_2 \dots dt_m [W(t_m), \dots, [W(t_1), a] \dots].$$

Since we assume that $\|W\| < \infty$, the convergence of the series for finite t is clear. But we want to consider $t \rightarrow \infty$. We define the operator $D_m(t)$ on the field algebra \mathcal{F} as

$$D_m(t)a := \int_{t > t_m > \dots > t_1 > 0} dt_1 dt_2 \dots dt_m [W(t_m), \dots, [W(t_1), a] \dots]$$

where $D_0 a = a$. Before we can state the theorem we have to define two norms, one for the interaction and one for vectors in the Fock space. The norm of an interaction W is defined as

$$\begin{aligned} \|W\|' &= \sum_{N \geq 1} N 2^{(d+2)N} \sum_{s_1, \dots, s_N=1}^k \sum_{s'_1, \dots, s'_N=1}^k \\ &\quad \sum_{r_1, \dots, r_N=1,2} \sum_{r'_1, \dots, r'_N=1,2} \|w_N((\cdot, s^N, r^N), (\cdot, s'^N, r'^N))\|'_{2dN} \quad (6) \end{aligned}$$

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

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

Now we are ready for the main theorem of this chapter.

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

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

We can also write the Dyson series for negative times (in reverse time ordering) and integrate from $-\infty$ to 0 to see a similar statement for negative times. The proof of this theorem can be found in [1], we only roughly sketch it.

Proof. Rewrite the interaction in the basis of Hermite functions (they are an orthonormal basis in $L^2(\mathbb{R})$). Then it follows that we can rewrite the integral as

$$\begin{aligned} \int_0^\infty \| [W(t), D_{m-1}(t)a] \| dt &\leq \sum_{Q_0 \dots Q_M} \int_{t > t_m > \dots > t_1 > 0} dt_1 dt_2 \dots dt_m \\ &\quad [W_{Q_m}(t_m), \dots, [W_{Q_1}(t_1), a_{Q_0}] \dots]. \quad (7) \end{aligned}$$

The subscript Q_i means that we have written the quantities in Hermite functions. Rewriting the interaction in this basis makes it easier to estimate the multicommutator in the integral. \square

What we are interested in is the following

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

$$\lim_{t \rightarrow \pm\infty} \|\alpha_{-t}^0 \alpha_t - \sigma_\pm(a)\| = 0$$

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

This implies the existence of the scattering automorphism (A4).

Proof. As one can easily see

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

For $t < t'$ so we can write

$$\|\alpha_{-t}^0 \alpha_t - \alpha_{-t'}^0 \alpha_{t'}\| = \left\| \sum_{m \geq 1} i^m \int_t^{t'} [W(s), D_{m-1}(s)a] \right\|$$

and with the triangular inequality we obtain

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

As $t, t' \rightarrow \infty$ the integral has to vanish because of the theorem and the dominated convergence theorem. \square

5 Calculations

We'd like to do some explicit calculations for a system of two reservoirs of non-interacting non-relativistic free spinless fermions. The explicit calculations will be done in Fourier space as the dynamics $t = -\Delta$ is diagonal there. This means we had to transform the coupling, all operators, creation and annihilation operators into Fourier space (This is not done explicitly in this paper. Assume we have already the step from physical space to Fourier space). The Fourier transformed of a operator a is denoted by \hat{a} . For each reservoir we will take the particle number to be the only conservation law. For tunnelling junctions the interaction W commutes with the total particle number operator, $N \otimes 1 + 1 \otimes N$, while for thermal junctions, W commutes separately with $N \otimes 1$ and $1 \otimes N$. In our calculations we are only interested in leading orders so we introduce two coupling constants a and b and set

$$W = a \sum_{N=1}^{\infty} b^N W_N.$$

Let $\mathcal{Q}_{k,l}$, $\mathcal{U}_{k,l}$ denote the term of order $a^k b^l$ of the particle current \mathcal{Q} and the energy current \mathcal{U} . Accordingly we define $e_{k,l}$ where e is the entropy production rate.

First we are interested in the consequences of the lowest order particle and energy current, where we will restrict to the case of the tunnelling junction. One can show that the first non vanishing order of the particle and energy current is of order (2, 2) and of the form

$$\mathcal{Q}_{2,2} = 2\pi \int_{\mathbb{R}^{2d}} d\mathbf{k} d\mathbf{l} \delta(|\mathbf{k}|^2 - |\mathbf{l}|^2) |\hat{w}_1((-\mathbf{k}, 2), (\mathbf{l}, 1))|^2 (\rho_2(\mathbf{k}) - \rho_1(\mathbf{k}))$$

and

$$\mathcal{U}_{2,2} = 2\pi \int_{\mathbb{R}^{2d}} d\mathbf{k} d\mathbf{l} |\mathbf{k}|^2 \delta(|\mathbf{k}|^2 - |\mathbf{l}|^2) |\hat{w}_1((-\mathbf{k}, 2), (\mathbf{l}, 1))|^2 (\rho_2(\mathbf{k}) - \rho_1(\mathbf{k}))$$

where $\mathbf{k}, \mathbf{l} \in \mathbb{R}^{2d}$, \hat{w} is the Fourier transform of w , and the function $\rho_i(\mathbf{k})$ is defined as $\rho_i(\mathbf{k}) = \frac{1}{e^{\beta^i(|\mathbf{k}|^2 - \mu^i)} + 1}$. Let's assume that \hat{w}_1 is not identically zero (which would mean that there's no interaction), then the above formulas show the following qualitative behavior of the flows.

- If the temperature and the chemical potential are equal, $(\beta^1, \mu^1) = (\beta^2, \mu^2)$, then the flows vanish $\mathcal{U}_{2,2} = \mathcal{Q}_{2,2} = 0$.
- If $\mu^1 = \mu^2$ and $\beta^1 < \beta^2$ then $\rho_2(\mathbf{k}) - \rho_1(\mathbf{k}) > 0$ for all k . So the particle and energy flow are positive what means that there is particle and energy flow from the hotter to the colder reservoir.
- If $\mu^1 > \mu^2$ and $\beta^1 = \beta^2$ then $\rho_2(\mathbf{k}) - \rho_1(\mathbf{k}) < 0$ for all k . Consequently the flows are negative what means that at constant temperature, there is a particle and energy flow from the reservoir with higher chemical potential to the reservoir with the lower chemical potential.

The resistance of the junction

Suppose both reservoirs have the same temperature, $\beta^1 = \beta^2$, and the chemical potentials have a small difference $\mu^1 = \mu$, $\mu^2 = \mu + \Delta\mu$, with $\Delta\mu$ small. As we are only interested in the leading order of $\Delta\mu$ the expression of the particle flow yields

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

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

$$R^{-1}(\mu, \beta) = 2\pi\beta \int_{\mathbb{R}^{2d}} d\mathbf{k} d\mathbf{l} \delta(|\mathbf{k}|^2 - |\mathbf{l}|^2) \frac{|\hat{w}_1((-\mathbf{k}, 2), (\mathbf{l}, 1))|^2 e^{\beta(|\mathbf{k}|^2 - \mu)}}{(e^{\beta(|\mathbf{k}|^2 - \mu)} + 1)^2}. \quad (8)$$

Onsager reciprocity relations

We want to show that the Onsager reciprocity relations hold in lowest order. Suppose we set $\beta^1 = \beta$, $\beta^2 = \beta - \Delta\beta$, $\nu = \beta^1 \mu^1$ and $\Delta\nu = \beta^1 \mu^1 - \beta^2 \mu^2$. Then it can be shown that

$$\left. \frac{\partial \mathcal{U}_{2,2}}{\partial \Delta\nu} \right|_{\Delta\beta = \Delta\nu = 0} = - \left. \frac{\partial \mathcal{Q}_{2,2}}{\partial \Delta\beta} \right|_{\Delta\beta = \Delta\nu = 0},$$

which is an Onsager reciprocity relation and it holds at lowest order.

Entropy production rate

As we have seen, the entropy production rate is given by

$$e = (\beta^1 - \beta^2)\mathcal{U} - (\beta^1\mu^1 - \beta^2\mu^2)\mathcal{Q}.$$

One can show that the first non-vanishing order of the entropy production rate is $e_{2,2}$ and that for coupled reservoirs $e_{2,2}$ is strictly positive unless not both reservoirs have the same temperature and the same chemical potential. We consider two special cases: First we want to consider a thermal contact where $\mathcal{Q} = 0$. Then $\beta^1 > \beta^2$ and therefore $\mathcal{U} > 0$. This means that heat flows from the hotter to the colder reservoir. This is Clausius' formulation of the second law of thermodynamics. The second case to consider is that of a tunnelling junction with $\beta^1 = \beta^2 = \beta$ and $\mu^1 > \mu^2$. Then it follows that $-\beta(\mu^1 - \mu^2)\mathcal{Q} > 0$. So we obtain $\mathcal{Q} < 0$, what means that particles flow from the reservoir with the higher chemical potential to the one with the lower potential.

The resistance

We'd now like to calculate the resistance for small and large temperatures. We assume that $\mu > 0$ holds. For large T we see from formula Eq. (8) the resistance goes like T . Next we examine the dependence of the resistance of T , for small T , in three dimensions, and where \hat{w}_1 is a radial function in both variables. We then have

$$R^{-1}(\mu, \beta) = 8\pi^3\beta \int_0^\infty dr r \frac{|\hat{w}_1((-r, 2), (r, 1))|^2 e^{\beta(|r|^2 - \mu)}}{(e^{\beta(|r|^2 - \mu)} + 1)^2}.$$

One can show that for $T \rightarrow 0$ the resistance is given by

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

where $f = 8\pi^3 r |\hat{w}_1((-r, 2), (r, 1))|^2$.

References

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