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by

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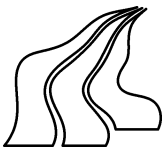

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Adiabatically switched-on electrical bias in continuous systems, and the Landauer-Büttiker formula

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Abstract

Consider a three dimensional system which looks like a cross-connected pipe system, i.e. a small sample coupled to a finite number of leads. We investigate the current running through this system, in the linear response regime, when we adiabatically turn on an electrical bias between leads. The main technical tool is the use of a finite volume regularization, which allows us to define the current coming out of a lead as the time derivative of its charge. We finally prove that in virtually all physically interesting situations, the conductivity tensor is given by a Landauer-Büttiker type formula.

1 Introduction

In any experiment which involves running a current through a microscopic sample, having a good quantum description of various conductivity coefficients is a priority. Such a description has been first derived by Landauer [21] and then generalized by Büttiker [8]; this is what one now calls the Landauer-Büttiker formalism. The main idea is that the conductivity of mesoscopic samples connected to ideal leads where the carriers are quasi free fermions, is completely characterized by a one particle scattering matrix.

Many people have since contributed to the justification of this formalism, starting from the first principles of non-equilibrium quantum statistical mechanics. In this respect, there are two different ways to model such a conduction problem, and let us briefly discuss both of them.

The first approach is the one in which one starts with several decoupled semi-infinite leads, each of them being at equilibrium [19]. Let us assume for simplicity that they are in grand canonical Gibbs states having the same temperature but different chemical potentials. Then at $t = 0$ they are suddenly joint together with a sample, and the new composed system is allowed to evolve freely until it reaches a steady state at $t = \infty$. Then one can define a current as the (Cesaro limit of the) time derivative of a regularized charge operator, and after lifting this regularization one obtains the L-B formula. This procedure is by now very well understood and completely solved in a series of very recent works (see [1], [25] and references therein). Let us mention that in this approach a crucial ingredient is the fact that the perturbation introduced by the sample and coupling is localized in space. One can even allow the carriers to interact in the sample [18], and the theory still works (even though the L-B formula must be replaced by something more complicated). Note that even if we choose to adiabatically turn on the coupling between the semi-infinite leads, the result will be the same. A rigorous proof of this fact is in preparation [14].

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The second approach is the one in which the leads (*long, but finite*) are already coupled with the sample, and at $t = -\infty$ the full system is in a Gibbs equilibrium state at a given temperature and chemical potential. Then we adiabatically turn on a potential bias between the leads, modeling in this way a gradual appearance of a difference in the chemical potentials. The statistical density matrix is found as the solution of a quantum Liouville equation. The current coming out of a given lead is defined to be the time derivative at $t = 0$ of its mean charge. Then one performs the linear response approximation with respect to the bias thus obtaining a Kubo-like formula [6], and finally the thermodynamic and adiabatic limits. The current is given by the same L-B formula, specialized to the linear response case. Note that in contrast to the previously discussed approach, the perturbation introduced by the electrical bias is not spatially localized, and this makes the adiabatic limit for the full state (i.e. without the linear response approximation) rather difficult.

Some significant papers from the physics literature which initiated the second approach are [10], [27], [28], [17], [22] and [5]. They contain many nice and interesting physical ideas, even for systems which allow local self-interactions, but with no real mathematical substance, also due to the fact that many techniques were not yet available at this time.

A first mathematically sound derivation of the L-B formula on a discrete model was obtained in [12] and further investigated in [13]. In the current paper we greatly improve the method of proof of [12], which also allows us to extend the results to the continuous case.

There are many interesting and hard questions which remain to be answered. Namely, can one compute the adiabatic limit in the second approach without the linear response approximation? If yes, then what is the connection with the first approach? Are the two steady states identical? If not, on which class of observables do they have equal expectations? Can one say anything rigorous about transient currents (see [23] and references therein)?

A distinct issue is the time dependent coupling and/or bias introduction, eventually periodic in time, closely related to the pumping problem. We here mainly refer to the so called BPT formula [9], rigorously investigated and justified in a series of papers by Avron *et al* [2], [3]. We also note that Landauer type formulas are universal in a way, and can be met in various other contexts like for example in the viscosity experienced by a topological swimmer [4].

The paper is organized as follows.

Section 2 introduces the mathematical model, and derives a current formula (2.44) via linear response theory, finite volume regularization and adiabatic switching of the electrical bias between leads.

Section 3 contains the proof of the thermodynamic limit (i.e. the length of the leads is taken to infinity). The new current formula is given in (3.25).

Section 4 contains the adiabatic limit of the current, and makes the connection with the stationary scattering objects in (4.14).

In Section 5 we derive the usual Landauer-Büttiker formula from (4.14); we state our main results in Theorem 5.2. We also derive a continuity equation in subsection 5.1, which shows that the steady current is the same, no matter where we measure it on a given lead.

2 The finite volume regularization

Since our results can be easily extended to one and two dimensions, we will only consider the three dimensional case. The small device through which the current flows is modelled by a bounded domain of $\mathbb{R}^3$, not necessarily simply connected, but with a regular enough boundary. This is the "sample", which is linked to a finite number of "leads" (which can be cylinders of length L and radius 1). Let us for simplicity only consider two leads, both cylinders being parallel to the first coordinate axis and located in $-L - a < x_1 < -a$ (the left lead) and $a < x_1 < L + a$ (the right lead). Here a is a nonnegative number. The sample is a subset of the slab $-a < x_1 < a$. Note that one possible system is just the union of the two leads, when $a = 0$ and the sample is absent. If $a > 0$ we demand the sample to be smoothly pasted to the leads, so that the boundary of their union is at least C^2.

2.1 The equilibrium state

The union between the leads and sample will be denoted by $\mathcal{X}_L$. The one particle Hamilton operator is given by $\mathbf{H}_L := -\Delta_L + w$, where $-\Delta_L$ is the Laplace operator with Dirichlet boundary conditions in $\mathcal{X}_L$. The potential w is smooth and compactly supported in the region where the sample is located, i.e. $\mathcal{X}_L \cap \{\mathbf{x} \in \mathbb{R}^3 : \ -a < x_1 < a\}$. Without loss of generality, we put $w \geq 0$. The one particle Hilbert space is $\mathcal{H}^L := L^2(\mathcal{X}_L)$.

Denote by $\mathbb{H}_D(\mathcal{X}_L) := H_0^1(\mathcal{X}_L) \cap H^2(\mathcal{X}_L)$, where $H_0^1(\mathcal{X}_L)$ and $H^2(\mathcal{X}_L)$ are the usual Sobolev spaces on the open domain $\mathcal{X}_L \subset \mathbb{R}^3$. Since we assumed enough regularity on the boundary of $\mathcal{X}_L$, the operators:

$$-\Delta_L : \mathbb{H}_D(\mathcal{X}_L) \to \mathcal{H}^L \tag{2.1}$$

$$\mathbf{H}_L := -\Delta_L \, + \, w(Q) : \mathbb{H}_D(\mathcal{X}_L) \to \mathcal{H}^L \tag{2.2}$$

are self-adjoint on $\mathbb{H}_D(\mathcal{X}_L)$. It is also very well known that their spectrum is purely discrete and accumulates to $+\infty$. Due to our assumptions on w, the Hamiltonian $\mathbf{H}_L$ in (2.2) is a positive operator and its resolvent is denoted by

$$\mathbf{R}_L(z) \, := \, (\mathbf{H}_L \, - \, z)^{-1} \tag{2.3}$$

for all $z \in \mathbb{C} \setminus \mathbb{R}_+$; we shall simply denote $\mathbf{R}_L := \mathbf{R}_L(-1)$.

We only consider the grand-canonical ensemble. In the remote past, $t \to -\infty$, the electron gas is in thermodynamic equilibrium at a temperature $T = \frac{1}{\beta} > 0$ and a chemical potential μ. The appropriate framework is the second quantization. Here the Hilbert space is $\mathfrak{F}_L := \bigoplus\limits_{n \in \mathbb{N}} (\mathcal{H}^L)^{\wedge n}$, where $(\mathcal{H}^L)^{\wedge n}$ is the n times antisymmetric tensor product of $\mathcal{H}^L$ with itself. Let $\mathfrak{n}_L = d\Gamma(\mathbf{1}_L)$ be the number operator (where $\mathbf{1}_L$ is the identity operator on $\mathcal{H}^L$).

The second quantization of $\boldsymbol{H}_L$ is denoted by $\mathfrak{h}_L := d\Gamma(\mathbf{H}_L)$. Let

$$\mathfrak{u}_L(t) \, := \, \Gamma(e^{-it\mathbf{H}_L}) \, = \, e^{-it\mathfrak{h}_L}$$

be the associated time-evolution of the system. Under our conditions, the operator $e^{-\beta \mathbf{H}_L} \in \mathbb{B}_1[\mathcal{H}^L]$, the ideal of trace-class operators on $\mathcal{H}^L$, and this property extends itself to the second quantized operators.

The associated Gibbs equilibrium state is:

$$\mathfrak{p}_L := \frac{e^{-\beta(\mathfrak{h}_L - \mu \mathfrak{n}_L)}}{\mathrm{Tr}\left\{e^{-\beta(\mathfrak{h}_L - \mu \mathfrak{n}_L)}\right\}}. \tag{2.4}$$

It is a standard fact (see Proposition 5.2.23 in [7]) that if we denote by $\rho(\lambda) := \left(e^{\beta(\lambda - \mu)} + 1\right)^{-1}$, then for any bounded operator $\mathbf{T} \in \mathbb{B}[\mathcal{H}^L]$ we have:

$$\mathrm{Tr}_{\mathfrak{F}_L}\left\{\mathfrak{p}_L \, d\Gamma(\mathbf{T})\right\} \, = \, \mathrm{Tr}_{\mathcal{H}^L}\left\{\rho(\mathbf{H}_L)\, \mathbf{T}\right\}. \tag{2.5}$$

2.2 Turning on the bias

Let us introduce three projections defined by natural restrictions on the left lead, sample, and right lead respectively:

$$\begin{aligned}
&\Pi_- : \mathcal{H}^L \to L^2(\mathcal{X}_L \cap \{\mathbf{x} \in \mathbb{R}^3 : \ -L - a < x_1 < -a\}), \\
&\Pi_+ : \mathcal{H}^L \to L^2(\mathcal{X}_L \cap \{\mathbf{x} \in \mathbb{R}^3 : \ a < x_1 < L + a\}), \\
&\Pi_0 : \mathcal{H}^L \to L^2(\mathcal{X}_L \cap \{\mathbf{x} \in \mathbb{R}^3 : \ -a < x_1 < a\}).
\end{aligned} \tag{2.6}$$

If $v_\pm \in \mathbb{R}$, define the bias between leads as

$$V := v_- \Pi_- + v_+ \Pi_+. \tag{2.7}$$

We will now consider the Hamiltonian describing the evolution under an adiabatic introduction of the electric bias. Consider a smooth switch-on function χ which fulfills $\chi, \chi' \in L^1((-\infty, 0))$, $\chi(0) = 1$ (note that the first two conditions imply $\lim_{t\to-\infty} \chi(t) = 0$). Let $\eta > 0$ be the adiabatic parameter, and define $\chi_\eta(t) := \chi(\eta t)$, $V_\eta(t, x) := \chi_\eta(t)V(x)$. At the one-body level we have

$$\mathbf{K}_{L,\eta}(t) \;:=\; \mathbf{H}_L + V_\eta(t, Q) \;=\; \mathbf{H}_L + \chi(\eta t)V(Q) \tag{2.8}$$

where $V(Q)$ denotes the bounded self-adjoint operator of multiplication with the step function $V(x)$. We shall use the notation $\mathbf{K}_{L,\eta} := \mathbf{K}_{L,\eta}(0) = \mathbf{H}_L + V(Q)$. The evolution defined by this time-dependent Hamiltonian is described by a unitary propagator $W(t, s)$, strong solution on the domain of $\mathbf{H}_L$ of the following Cauchy problem:

$$\begin{cases} -i\partial_t W_{L,\eta}(t, s) = -\mathbf{K}_{L,\eta}(t)W_{L,\eta}(t, s) \\ W_{L,\eta}(s, s) = 1 \end{cases} \tag{2.9}$$

for $(s, t) \in \mathbb{R}^2$.

Remark 2.1. For any $L < \infty$ and $\eta > 0$, the operators $\{\mathbf{K}_{L,\eta}(t)\}_{t\in\mathbb{R}}$ are self-adjoint in $\mathcal{H}^L$, having a common domain equal to $\mathbb{H}_D(\mathcal{X}_L)$. They are strongly differentiable with respect to $t \in \mathbb{R}$ with a bounded self-adjoint derivative

$$\partial_t \mathbf{K}_{L,\eta}(t) \;=\; \eta\, \chi(\eta t)V(Q).$$

The following result is standard and we state it without proof:

Proposition 2.2. *The problem* (2.9) *has a unique solution which is unitary and leaves the domain* $\mathbb{H}_D(\mathcal{X}_L)$ *invariant for any pair* $(s, t) \in \mathbb{R}^2$. *For any triple* $(s, r, t) \in \mathbb{R}^3$ *it satisfies the relation* $W_{L,\eta}(t, r)W_{L,\eta}(r, s) = W_{L,\eta}(t, s)$. *Moreover it also satisfies the equation*

$$-i\partial_s W_{L,\eta}(t, s) = W_{L,\eta}(t, s)\mathbf{K}_{L,\eta}(s). \tag{2.10}$$

Later on we will need the following simple but important result:

Proposition 2.3. *Let us define the commutator*

$$[\mathbf{H}_L, W_{L,\eta}(t, s)] = \mathbf{H}_L W_{L,\eta}(t, s) - W_{L,\eta}(t, s)\mathbf{H}_L$$

on the dense domain $\mathbb{H}_D(\mathcal{X}_L)$ *(left invariant by the evolution). Then the commutator can be extended by continuity to a bounded operator on* $\mathcal{H}^L$ *such that:*

$$\sup_{(s,t)\in\mathbb{R}^2_-} \|[\mathbf{H}_L, W_{L,\eta}(t, s)]\| < \infty, \tag{2.11}$$

$$\sup_{(s,t)\in\mathbb{R}^2_-} \left\|(\mathbf{H}_L + 1)W_{L,\eta}(t, s)(\mathbf{H}_L + 1)^{-1}\right\| < \infty. \tag{2.12}$$

Proof. Let us fix some ϕ in $\mathbb{H}_D(\mathcal{X}_L)$, and for $t \le 0$ let us consider the application

$$\begin{aligned} &(-\infty, t) \ni s \mapsto \phi(s) := [\mathbf{K}_{L,\eta}(s), W_{L,\eta}(s, t)]\phi \in L^2(\mathcal{X}_L), \\ &\mathbf{K}_{L,\eta}(s)\phi(s) \subset \mathbb{H}_D(\mathcal{X}_L)^*, \end{aligned} \tag{2.13}$$

with $\phi(t) = 0$. Due to these properties, the function $\phi(s)$ is differentiable in the weak topology on $\mathbb{H}_D(\mathcal{X}_L)^*$ and we can compute its derivative:

$$\begin{aligned} \partial_s\phi(s) &= [\partial_s\mathbf{K}_{L,\eta}(s), W_{L,\eta}(s, t)]\phi + [\mathbf{K}_{L,\eta}(s), \partial_s W_{L,\eta}(s, t)]\phi \\ &= \eta\chi'(\eta s)[V(Q), W_{L,\eta}(s, t)]\phi - i\mathbf{K}_{L,\eta}(s)[\mathbf{K}_{L,\eta}(s), W_{L,\eta}(s, t)]\phi \\ &= -i\mathbf{K}_{L,\eta}(s)\phi(s) + \psi(s), \end{aligned} \tag{2.14}$$

where $\psi(s) := \eta\chi\prime(\eta s)[V(Q), W_{L,\eta}(s,t)]\phi$. Thus, taking into account the above solution of the Cauchy problem (2.9), we can write the solution for $\phi(s)$ as

$$\phi(s) = \int_t^s W_{L,\eta}(s,r)\psi(r)\,dr.$$

Let us recall that $W_{L,\eta}(t,r)$ is unitary, the function χ' belongs to $L^1(\mathbb{R}_-)$ and $\|V(Q)\| \leq \max\{v_-, v_+\}$ so that

$$\|\phi(s)\|_{\mathcal{H}^L} \leq \|\chi'\|_{L^1(\mathbb{R}_-)} \max\{v_-, v_+\}\|\phi\|, \qquad \forall s \in (-\infty, t), \forall t \in \mathbb{R}_-.$$

Thus for any pair of functions ψ and ϕ in $\mathbb{H}_D(\mathcal{X}_L)$, dense in $\mathcal{H}^L$, we have

$$|\langle\psi, [\mathbf{K}_{L,\eta}(s), W_{L,\eta}(s,t)]\phi\rangle| \;\leq\; \|\chi'\|_{L^1(\mathbb{R}_-)} \max\{v_-, v_+\}\|\psi\|\|\phi\|.$$

After a straightforward density argument, the use of Riesz' representations theorem, and the fact that $V(Q)$ is bounded, we obtain a uniform estimate as in (2.11) if $-\infty < s \leq t \leq 0$. To obtain the same for $-\infty < t \leq s \leq 0$ we remind that $W_{L,\eta}(s,t) = W_{L,\eta}(t,s)^*$ and for ψ and ϕ in $\mathbb{H}_D(\mathcal{X}_L)$ we can write (using the invariance of the domain $\mathbb{H}_D(\mathcal{X}_L)$ under $W_{L,\eta}(t,s)$)

$$-\langle[\mathbf{H}_L, W_{L,\eta}(s,t)]\phi, \psi\rangle = \langle\phi, [\mathbf{H}_L, W_{L,\eta}(t,s)]\psi\rangle,$$

and we easily get the desired conclusion. Finally, (2.12) is an easy consequence of (2.11). □

Now let us consider the second quantization of the above time-dependent evolution.

$$d\Gamma(\mathbf{K}_{L,\eta}(t)) = \mathfrak{h}_L + \chi_\eta(t)d\Gamma(V(Q)).$$

Let us first observe that the perturbation $d\Gamma(V(Q))$ is no longer bounded on $\mathfrak{F}_L$. It is rather easy to verify that the family $\{\mathfrak{w}_{L,\eta}(t,s)\}_{(s,t)\in\mathbb{R}^2}$, that is well defined by $\mathfrak{w}_{L,\eta}(t,s) := \Gamma(W_{L,\eta}(t,s))$ gives the unique (and unitary) solution of the Cauchy problem:

$$\begin{cases} -i\partial_t\mathfrak{w}_{L,\eta}(t,s) = -d\Gamma\left(\mathbf{K}_{L,\eta}(t)\right)\mathfrak{w}_{L,\eta}(t,s) \\ \mathfrak{w}_{L,\eta}(s,s) = 1. \end{cases} \tag{2.15}$$

2.3 The nonequilibrium state

In our adiabatic approach, the nonequilibrium state is completely characterized by a density matrix which solves the Liouville equation. Its initial condition at $t = -\infty$ is the Gibbs equilibrium state $\mathfrak{p}_L$, associated to the Hamiltonian $\mathfrak{h}_L$ at temperature β^{-1} and chemical potential μ. We let the state evolve with the adiabatic time-dependent Hamiltonian $\mathbf{K}_{L,\eta}(t)$ up to $t = 0$. Then we perform the thermodynamic limit $L \to \infty$, and finally we should take the adiabatic limit $\eta \to 0$. This last step raises for the moment some important technical difficulties. We will avoid them by only considering the *linear response* behavior, i.e. the linear contribution in the bias $v_+ - v_-$. The proof of the existence of the thermodynamic and adiabatic limit for the full density matrix is a challenging open problem.

Now let us formulate and solve the Liouville equation. We first want to find a weak solution to the equation:

$$\begin{cases} i\partial_t\mathfrak{p}_{L,\eta}(t) = [d\Gamma\left(\mathbf{K}_{L,\eta}(t)\right), \mathfrak{p}_{L,\eta}(t)], \quad t < 0, \\ \lim_{t\to-\infty}\mathfrak{p}_{L,\eta}(t) = \mathfrak{p}_L. \end{cases} \tag{2.16}$$

Let us note that for a fixed s, the operator (see also (2.15))

$$\mathfrak{w}_{L,\eta}(t,s)\mathfrak{p}_L\mathfrak{w}_{L,\eta}(t,s)^*$$

solves the differential equation, but does not obey the initial condition. What we do next is to take care of this.

The state $\mathfrak{p}_L$ being defined in (2.4) commutes with any function of $\mathfrak{h}_L$. Thus we can write:

$$\begin{aligned}\mathfrak{w}_{L,\eta}(t,s)\mathfrak{p}_L\mathfrak{w}_{L,\eta}(t,s)^* &= \mathfrak{w}_{L,\eta}(t,s)e^{i(t-s)\mathfrak{h}_L}\mathfrak{p}_L e^{-i(t-s)\mathfrak{h}_L}\mathfrak{w}_{L,\eta}(t,s)^* \\ &= \Gamma\left(W_{L,\eta}(t,s)e^{i(t-s)\mathbf{H}_L}\right)\mathfrak{p}_L\Gamma\left(W_{L,\eta}(t,s)e^{-i(t-s)\mathbf{H}_L}\right)^*, \end{aligned} \tag{2.17}$$

and we can consider the two-parameter family of unitaries:

$$\Omega_{L,\eta}(t,s) \;:=\; W_{L,\eta}(t,s)e^{i(t-s)\mathbf{H}_L}, \quad (s,t)\in\mathbb{R}^2. \tag{2.18}$$

We will now show that the solution at time t is given by the following strong limit (norm limit on each sector of fixed number of particles):

$$\mathfrak{p}_{L,\eta}(t) \;=\; \lim_{s\to-\infty}\Gamma(\Omega_{L,\eta}(t,s))\mathfrak{p}_L\Gamma(\Omega_{L,\eta}(t,s))^*. \tag{2.19}$$

Let us first show that the limit exists. Due to the continuity of the application Γ, it is enough to prove the existence of the norm limit $\lim_{s\to-\infty}\Omega_{L,\eta}(t,s)$ in the one particle sector. For that we use the following differential equality, valid in strong sense on the domain of $\mathbf{H}_L$:

$$-i\partial_s\Omega_{L,\eta}(t,s) = W_{L,\eta}(t,s)(\mathbf{K}_{L,\eta}(s)-\mathbf{H}_L)e^{i(t-s)\mathbf{H}_L}. \tag{2.20}$$

If we denote $\tilde{V}(r) := e^{ir\mathbf{H}_L}V(Q)e^{-ir\mathbf{H}_L}$ we observe that

$$\begin{cases} -i\partial_s\Omega_{L,\eta}(t,s) = \chi(\eta s)\Omega_{L,\eta}(t,s)\tilde{V}(s-t) \\ \Omega(s,s)=1, \end{cases} \tag{2.21}$$

and thus

$$\Omega_{L,\eta}(t,s) = 1 \;-\; i\int_s^t \chi(\eta r)\Omega_{L,\eta}(t,r)\tilde{V}(r-t)dr. \tag{2.22}$$

Since $\Omega_{L,\eta}(t,r)$ is unitary for any pair $(s,t)\in\mathbb{R}^2_-$, $\|\tilde{V}(r-t)\|$ is uniformly bounded in r, and χ is integrable, we conclude that the limit

$$\lim_{s\to-\infty}\Omega_{L,\eta}(t,s) \;=:\; \Omega_{L,\eta}(t) \tag{2.23}$$

exists in the norm topology of $\mathbb{B}[\mathcal{H}^L]$ and thus defines a unitary operator.

Proposition 2.4. *The operator $\Omega_{L,\eta}(t)$ preserves the domain of $\mathbf{H}_L$, and the densely defined commutator $[\mathbf{H}_L,\Omega_{L,\eta}(t)]$ can be extended to a bounded operator on $\mathcal{H}^L$, with a norm which is uniformly bounded in $t\le 0$.*

Proof. If ψ belongs to the domain of $\mathbf{H}_L$, then for every $\phi\in\mathcal{H}^L$ we have:

$$\begin{aligned}&|\langle\mathbf{H}_L\psi,\Omega_{L,\eta}(t)(\mathbf{H}_L+1)^{-1}\phi\rangle| \\ &= \lim_{s\to-\infty}|\langle\mathbf{H}_L\psi,W_{L,\eta}(t,s)(\mathbf{H}_L+1)^{-1}e^{i(t-s)\mathbf{H}_L}\phi\rangle| \le C||\psi||\;||\phi||, \end{aligned} \tag{2.24}$$

where we used (2.18), (2.23) and (2.12). Now since $\mathbf{H}_L$ is self-adjoint, it means that $\Omega_{L,\eta}(t)(\mathbf{H}_L+1)^{-1}\phi$ belongs to the domain of $\mathbf{H}_L$, hence:

$$\sup_{t\le0}\|\mathbf{H}_L\Omega_{L,\eta}(t)(\mathbf{H}_L+1)^{-1}\| \le C. \tag{2.25}$$

Now for ψ and ϕ in the domain of $\mathbf{H}_L$ we can write

$$\begin{aligned}&|\langle\psi,[\mathbf{H}_L,\Omega_{L,\eta}(t)]\phi\rangle| \\ &= \lim_{s\to-\infty}|\langle\psi,[\mathbf{H}_L,W_{L,\eta}(t,s)]e^{i(t-s)\mathbf{H}_L}\phi\rangle| \le C||\psi||\;||\phi||, \end{aligned} \tag{2.26}$$

where we used (2.11). A density argument finishes the proof. □

Up to now we have shown that $\mathfrak{p}_{L,\eta}$ is a weak solution to the Liouville equation (2.16). This density matrix is a trace class operator. The key identity which gives the expectation of a one-body bounded observable $\mathbf{T} \in \mathbb{B}(\mathcal{H}^L)$ lifted to the Fock space is (see also (2.5)):

$$\begin{aligned}\mathrm{Tr}_{\mathfrak{F}_L}\left(\mathfrak{p}_{L,\eta}(t) d\Gamma(\mathbf{T})\right) &= \mathrm{Tr}_{\mathfrak{F}_L}\left(\mathfrak{p}_L \Gamma(\Omega_{L,\eta}(t))^* d\Gamma(\mathbf{T}) \Gamma(\Omega_{L,\eta}(t))\right) \\ &= \mathrm{Tr}_{\mathfrak{F}_L}\left(\mathfrak{p}_L d\Gamma\{\Omega^*_{L,\eta}(t)\mathbf{T}\Omega_{L,\eta}(t)\}\right) \\ &= \mathrm{Tr}_{\mathcal{H}^L}\left(\Omega_{L,\eta}(t)\rho(\mathbf{H}_L)\Omega^*_{L,\eta}(t)\mathbf{T}\right). \end{aligned} \tag{2.27}$$

We stress that all this works because $\mathcal{X}_L$ is finite. The main conclusion is that if we are only interested in expectations of one body observables, the effective one-particle density matrix is:

$$\rho_{L,\eta}(t) := \Omega_{L,\eta}(t)\rho(\mathbf{H}_L)\Omega^*_{L,\eta}(t) \in \mathbb{B}_1(\mathcal{H}^L). \tag{2.28}$$

We can now prove that the above mapping is differentiable with respect to t in the trace norm topology. We write:

$$\begin{aligned}&\rho_{L,\eta}(t) = \lim_{s\to-\infty} \Omega_{L,\eta}(t,s)\rho(\mathbf{H}_L)\Omega^*_{L,\eta}(t,s) = \lim_{s\to-\infty} W_{L,\eta}(t,s)\rho(\mathbf{H}_L)W^*_{L,\eta}(t,s) \\ &= W_{L,\eta}(t,0)\left\{\lim_{s\to-\infty} W_{L,\eta}(0,s)e^{-is\mathbf{H}_L}\rho(\mathbf{H}_L)e^{is\mathbf{H}_L}W^*_{L,\eta}(0,s)\right\}W_{L,\eta}(t,0)^* \\ &= W_{L,\eta}(t,0)\rho_{L,\eta}(0)W_{L,\eta}(t,0)^* = W_{L,\eta}(t,0)\Omega_{L,\eta}(0)\rho(\mathbf{H}_L)\Omega^*_{L,\eta}(0)W^*_{L,\eta}(t,0). \end{aligned} \tag{2.29}$$

We have $\mathbf{H}_L\rho(\mathbf{H}_L)\mathbf{H}_L \in \mathbb{B}_1[\mathcal{H}^L]$ because of the exponential decay of ρ. Using (2.25) we obtain that $\mathbf{H}_L\rho_{L,\eta}(0)\mathbf{H}_L$ is also trace class. Then using (2.9) and (2.12) we conclude that $t \mapsto \rho_{L,\eta}(t) \in \mathbb{B}_1[\mathcal{H}^L]$ is differentiable and:

$$\partial_t\, \rho_{L,\eta}(t)\,|_{t=0} \;=\; -i\,[\mathbf{K}_{L,\eta}, \rho_{L,\eta}] \;\in\; \mathbb{B}_1[\mathcal{H}^L]. \tag{2.30}$$

As we have said at the beginning of this subsection, studying the limits $L \to \infty$ and $\eta \to 0$ on the above formula for the whole state seems to be rather difficult, and we will only consider the first order correction with respect to the potential bias, obtained by considering the equation (2.22) in the limit $s \to -\infty$:

$$\begin{aligned}\Omega_{L,\eta}(t) &= 1 \,-\, i\int_{-\infty}^{t} \chi(\eta r)\Omega_{L,\eta}(t,r)\tilde{V}(r-t)\,dr \\ &\sim\; 1 \,-\, i\int_{-\infty}^{t} \chi(\eta r)\tilde{V}(r-t)\,dr \,+ \mathcal{O}(V^2). \end{aligned} \tag{2.31}$$

Let us point out here that a control of the above rest $\mathcal{O}(V^2)$ is a difficult task that we will not consider for the moment.

Having in mind the above argument, we define as the *linear response state at time 0*:

$$\tilde{\rho}_{L,\eta} := \rho(\mathbf{H}_L) - [\mathcal{V}_\eta, \rho(\mathbf{H}_L)]\,, \tag{2.32}$$

where:

$$\mathcal{V}_\eta := i\int_{-\infty}^{0} \chi(\eta r)\tilde{V}(r)\,dr. \tag{2.33}$$

2.4 The current

The main advantage of our approach is that we can define the current coming out of a lead as the time derivative of its charge. We define the *charge operators* at finite volume, to be the second quantization of projections $\Pi_\pm$ (see (2.6)):

$$\mathfrak{Q}_\pm := d\Gamma(\Pi_\pm). \tag{2.34}$$

The *average charge at time t* is given by:

$$q(t) := \mathrm{Tr}_{\mathfrak{F}_L}\left(\mathfrak{p}_{L,\eta}(t)\mathfrak{Q}_\pm\right) = \mathrm{Tr}_{\mathcal{H}^L}\left(\rho_{L,\eta}(t)\Pi_\pm\right). \tag{2.35}$$

By differentiating with respect to t and using the conclusion of the previous subsection we obtain the *average current at time* $t = 0$:

$$\begin{aligned} j_{L,\eta} &= -i\mathrm{Tr}_{\mathcal{H}^L}\left([\mathbf{K}_{L,\eta}, \rho_{L,\eta}]\ \Pi_\pm\right) \\ &= -i\mathrm{Tr}_{\mathcal{H}^L}\left([\mathbf{H}_L, \rho_{L,\eta}]\ \Pi_\pm\right) - i\mathrm{Tr}_{\mathcal{H}^L}\left([V(Q), \rho_{L,\eta}]\ \Pi_\pm\right). \end{aligned} \tag{2.36}$$

But (see (2.7)) $\mathrm{Tr}_{\mathcal{H}^L}\left([V(Q), \rho_{L,\eta}]\ \Pi_\pm\right) = -\mathrm{Tr}_{\mathcal{H}^L}\left(\rho_{L,\eta}\,[V(Q),\, \Pi_\pm]\right) = 0$ and we deduce that:

$$\begin{aligned} j_{L,\eta} &= -i\mathrm{Tr}_{\mathcal{H}^L}\left([\mathbf{H}_L, \rho_{L,\eta}]\ \Pi_\pm\right) \\ &= -i\mathrm{Tr}_{\mathcal{H}^L}\left((\mathbf{H}_L+1)\rho_{L,\eta}(\mathbf{H}_L+1)\mathbf{R}_L\Pi_\pm\ -\ \mathbf{R}_L(\mathbf{H}_L+1)\rho_{L,\eta}(\mathbf{H}_L+1)\Pi_\pm\right) \\ &= -i\mathrm{Tr}_{\mathcal{H}^L}\left((\mathbf{H}_L+1)\rho_{L,\eta}(\mathbf{H}_L+1)\ [\mathbf{R}_L, \Pi_\pm]\right). \end{aligned} \tag{2.37}$$

Because we only are interested in the *linear response*, we will use (2.32). Remember that $\rho(\mathbf{H}_L)\mathbf{H}_L^2 \in \mathbb{B}_1[\mathcal{H}^L]$. An important observation is that the following commutator defined as a sesquilinear form on $\mathbb{H}_D(\mathcal{X}_L)^2$, can be extended to a bounded operator on $L^2(\mathcal{X}_L)$ since:

$$\begin{aligned} [\mathbf{H}_L, \mathcal{V}_\eta] \ &= \ \int_{-\infty}^0 \chi(\eta s)\ \left\{\partial_s\, e^{is\mathbf{H}_L} V e^{-is\mathbf{H}_L}\right\}\, ds \\ &= \ V - \eta\int_{-\infty}^0 \chi'(\eta s) e^{is\mathbf{H}_L} V e^{-is\mathbf{H}_L}\, ds. \end{aligned} \tag{2.38}$$

Note that we do not have to commute $\mathbf{H}_L$ with V in order to get this result. In fact $[\mathbf{H}_L, V]$ is quite singular due to the sharp characteristic functions from the definition of V.

Thus the second term in (2.32) is also trace-class and we can write the *linear response average current* at time $t = 0$ as:

$$\begin{aligned} \tilde{j}_{L,\eta} \ &:= \ -i\mathrm{Tr}_{\mathcal{H}^L}\left((\mathbf{H}_L+1)\tilde{\rho}_{L,\eta}(\mathbf{H}_L+1)\ [\mathbf{R}_L, \Pi_\pm]\right) \\ &= \ -i\mathrm{Tr}_{\mathcal{H}^L}\left((\mathbf{H}_L+1)\rho(\mathbf{H}_L)(\mathbf{H}_L+1)\ [\mathbf{R}_L, \Pi_\pm]\right) \\ &+ i\,\mathrm{Tr}_{\mathcal{H}^L}\left((\mathbf{H}_L+1)\,[\mathcal{V}_\eta, \rho(\mathbf{H}_L)]\,(\mathbf{H}_L+1)\ [\mathbf{R}_L, \Pi_\pm]\right). \end{aligned} \tag{2.39}$$

The first term of the last sum is zero due to trace cyclicity. We then obtain:

$$\begin{aligned} \tilde{j}_{L,\eta} \ &= \ i\mathrm{Tr}_{\mathcal{H}^L}\left((\mathbf{H}_L+1)\,[\mathcal{V}_\eta, \rho(\mathbf{H}_L)]\,(\mathbf{H}_L+1)\ [\mathbf{R}_L, \Pi_\pm]\right) \\ &= \ i\mathrm{Tr}_{\mathcal{H}^L}\left((\mathbf{H}_L+1)\,[\mathcal{V}_\eta, \mathbf{R}_L]\,(\mathbf{H}_L+1)\ [\rho(\mathbf{H}_L), \Pi_\pm]\right), \end{aligned} \tag{2.40}$$

where the second equality is obtained by carefully developing the commutators and using the cyclicity property of the trace and the fact that $\mathbf{H}_L^2\rho(\mathbf{H}_L)$ is trace class.

Now we rewrite (2.40) in a more suitable form for taking the limits $L \to \infty$ and $\eta \to 0$.

We begin by computing the first commutator in (2.40):

$$\begin{aligned} [\mathcal{V}_\eta, \mathbf{R}_L] = \ i\int_{-\infty}^0 \chi(\eta r)\left[\tilde{V}(r), \mathbf{R}_L\right]\, dr \\ = \ i\int_{-\infty}^0 \chi(\eta r) e^{ir\mathbf{H}_L}\,[V(Q), \mathbf{R}_L]\, e^{-ir\mathbf{H}_L}\, dr. \end{aligned} \tag{2.41}$$

Now let us observe that in the strong topology on $\mathbb{B}[\mathcal{H}_L]$ we can write:

$$\partial_s\, e^{is\mathbf{H}_L}\mathbf{R}_L(z)V(Q)\mathbf{R}_L(z)e^{-is\mathbf{H}_L} \ = \ i\, e^{is\mathbf{H}_L}\,[V(Q), \mathbf{R}_L(z)]\, e^{-is\mathbf{H}_L},$$

so that we get:

$$[\mathcal{V}_\eta, \mathbf{R}_L] \;=\; \int_{-\infty}^{0} \chi(\eta s)\, \left\{\partial_s\, e^{is\mathbf{H}_L}\mathbf{R}_L V(Q)\mathbf{R}_L e^{-is\mathbf{H}_L}\right\}\, ds$$
$$= \mathbf{R}_L V(Q)\mathbf{R}_L \;-\; \eta \int_{-\infty}^{0} \chi'(\eta s)\, e^{is\mathbf{H}_L}\mathbf{R}_L V(Q)\mathbf{R}_L e^{-is\mathbf{H}_L}\, ds. \tag{2.42}$$

Inserting the first term in (2.40), we observe that it gives zero:

$$\mathrm{Tr}_{\mathcal{H}^L}\left(V(Q)\;[\rho(\mathbf{H}_L), \Pi_\pm]\right) = 0, \tag{2.43}$$

due to the trace cyclicity and the fact that $V(Q) = v_+\Pi_+ + v_-\Pi_-$ commutes with $\Pi_\pm$. Thus the final expression is:

$$\tilde{j}_{L,\eta} \;=\; -i\eta \int_{-\infty}^{0} \chi'(\eta s)\, \mathrm{Tr}_{\mathcal{H}^L}\left(e^{is\mathbf{H}_L} V(Q) e^{-is\mathbf{H}_L}\,[\rho(\mathbf{H}_L), \Pi_\pm]\right) ds. \tag{2.44}$$

3 The thermodynamic limit

3.1 The limit of the dynamics

For different values of L, the Hamiltonians $\mathbf{H}_L$ are densely defined in different Hilbert spaces $\mathcal{H}^L := L^2(\mathcal{X}_L)$. In order to study the behavior of our system at $L \to \infty$, we embed $\mathcal{H}^L$ in the unique Hilbert space $\mathcal{H} := L^2(\mathcal{X}_\infty)$ (i.e. with infinitely long leads), using the natural decomposition:

$$\mathcal{H} = \mathcal{H}^L \oplus L^2(\mathcal{X}_\infty \setminus \mathcal{X}_L). \tag{3.1}$$

We denote by Π_L the orthogonal projection corresponding to the restriction to $\mathcal{X}_L$. Its orthogonal $\Pi_L^\perp$ corresponds to the restriction to $\mathcal{X}_\infty \setminus \mathcal{X}_L$. Each operator $\mathbf{H}_L$ is self-adjoint on the domain $\mathbb{H}_D(\mathcal{X}_L)$ (see (2.2)), while the resolvent $\mathbf{R}_L(z)$ is a bounded operator. We extend $\mathbf{R}_L(z)$ to $\mathcal{H}$ by the natural formula $\Pi_L\mathbf{R}_L(z)\Pi_L$; this new z-dependent operator family is a pseudoresolvent, which vanishes on $\Pi_L^\perp\mathcal{H}$.

Let us denote by

$$\mathbf{H} := -\Delta + w(Q) \tag{3.2}$$

with $-\Delta$ minus the usual Laplacian with Dirichlet boundary conditions defined on the Sobolev space $H^2(\mathcal{X}_\infty)$. We denote by $\mathbf{R}(z)$ the resolvent $(\mathbf{H} - z)^{-1}$ (and with $\mathbf{R} := \mathbf{R}(-1)$).

Proposition 3.1. *The sequence of operators $\{\Pi_L\mathbf{R}_L\Pi_L\}_{L>1}$ converges strongly to $\mathbf{R}$.*

Proof. Fix $u \in H^2(\mathcal{X}_\infty)$. If $\psi \in C_0^\infty(\mathbb{R})$, define $\psi_3(\mathbf{x}) := \psi(x_1)$. If L is large enough such that $\mathrm{supp}(\psi_3 u) \subset \mathcal{X}_L$, then $\psi_3 u \in \mathbb{H}_D(\mathcal{X}_L)$. If we denote by D_1 the subset of $H^2(\mathcal{X}_\infty)$ with compact support in the x_1 variable, then $\mathbf{H}$ is essentially self adjoint on it. Then the subspace $\mathcal{E} := (\mathbf{H}+1)D_1$ is dense in the Hilbert space $\mathcal{H}$. For any $u \in \mathcal{E}$, there exists $L_u > 0$ such that for every $L \geq L_u$ we have $\Pi_L\mathbf{R}u = \mathbf{R}u$, $\mathbf{R}u \in \mathbb{H}_D(\mathcal{X}_L)$ and $\mathbf{H}_L\mathbf{R}u = \mathbf{H}\mathbf{R}u$, and thus we have:

$$\Pi_L\mathbf{R}_L\Pi_L u - \mathbf{R}u \;=\; \Pi_L\mathbf{R}_L\left(\Pi_L\mathbf{H} - \mathbf{H}_L\right)\mathbf{R}u = \Pi_L\mathbf{R}_L\Pi_L^\perp u.$$

As $\|\mathbf{R}\| \leq 1$ and $\|\mathbf{R}_L\| \leq 1$ for any $L > 0$, the proof follows after a density argument. □

Corollary 3.2. *The sequence of operators $\{\Pi_L e^{it\mathbf{H}_L}\Pi_L\}_{L>a}$ converges in the strong topology to $e^{it\mathbf{H}}$, uniformly for t in any compact subset of $\mathbb{R}$.*

Proof. Let us fix $u \in \mathcal{H}$ and some $t \in \mathbb{R}$. We can take u with compact support, such that $\Pi_L u = u$ for L large enough. For any continuous function which vanishes at infinity $\psi \in C_\infty(\mathbb{R})$ consider $\psi(\mathbf{H}_L)$ defined on $\mathcal{H}^L$ through functional calculus. We define the operator $\tilde{\psi}(\mathbf{H}_L) = \Pi_L\psi(\mathbf{H}_L)\Pi_L$. Let us observe that $C_\infty(\mathbb{R})$ is the norm closure of the algebra defined by the 'resolvent functions'

$\{\mathfrak{r}_z(t) := (t-z)^{-1}\}_{z\in\mathbb{C}\setminus\mathbb{R}}$ and our definition of $\tilde{\psi}(\mathbf{H}_L)$ agrees with the definition of the extension of the resolvent $\mathbf{R}_L$. Thus the strong convergence of the pseudoresolvents for $L\to\infty$ immediately implies the strong convergence of the operators $\tilde{\psi}(\mathbf{H}_L)$ to $\psi(\mathbf{H})$ defined by the usual functional calculus on $\mathcal{H}$. Now let us choose $\psi\in C_\infty(\mathbb{R})$ such that $\psi(\lambda)=1$ for $|\lambda|\leq 1$ and $\psi(\lambda)=0$ for $|\lambda|\geq 2$. For any $E>0$ let us denote by $\psi_E(\lambda):=\psi(E^{-1}\lambda)$. Using the above arguments, let us fix $\epsilon>0$ as small as we want and choose $E>0$ such that $\|(1-\psi_E(\mathbf{H}))u\|\leq\epsilon/2$. Then there exists L_ϵ large enough such that $\|(1-\widetilde{\psi_E}(\mathbf{H}_L))u\|\leq\epsilon$ for any $L\geq L_\epsilon$. Then

$$\begin{aligned}&\|(\Pi_L e^{it\mathbf{H}_L}\Pi_L - e^{it\mathbf{H}})u\|\\&\leq\|(\widetilde{e^{it\cdot}\psi_E}(\mathbf{H}_L)-\widetilde{e^{it\cdot}\psi_E}(\mathbf{H}))u\|+\|(1-\widetilde{\psi_E}(\mathbf{H}_L))u\|+\|(1-\psi_E(\mathbf{H}))u\|.\end{aligned}$$

For the first term we observe that for any fixed $t\in\mathbb{R}$ the function $\lambda\mapsto\psi(\lambda)e^{it\lambda}$ belongs to $C_0(\mathbb{R})$ and thus we can use once again the strong resolvent convergence in order to control it. Due to the continuity of the map $t\mapsto e^{it\lambda}$ (at fixed λ), we deduce that we have the strong convergence locally uniformly in $t\in\mathbb{R}$. □

3.2 The limit of the current

Let us fix some small enough $r>0$ and consider the positively oriented contour:

$$\mathcal{C}_r=\{\lambda+ir\mid\lambda\in\mathbb{R}_+\}\cup\left\{re^{i\theta}\mid\theta\in[\pi/2,3\pi/2]\right\}\cup\{\lambda-ir\mid\lambda\in\mathbb{R}_+\}\subset\mathbb{C}. \tag{3.3}$$

Then by analytic functional calculus we can write (due to the analyticity and the decay properties of the function ρ):

$$\rho(\mathbf{H}_L)\;=\;\frac{i}{2\pi}\int_{\mathcal{C}_r}\rho(z)\,\mathbf{R}_L(z)\,dz. \tag{3.4}$$

All these operators can be extended to the whole Hilbert space by the procedure $\Pi_L\rho(\mathbf{H}_L)\Pi_L$, (i.e. when considered in $\mathcal{H}$, $\rho(H_L)$ stands for $\Pi_L\rho(\mathbf{H}_L)\Pi_L$) but for notational simplicity we drop the cut-off projectors. The main result of this subsection is:

Proposition 3.3. *The operators $[\rho(\mathbf{H}_L),\Pi_+]$, $1<L\leq\infty$, are trace class. Moreover, for every $n>1$ there exists $C>0$ such that for $L>1$ we have:*

$$\|[\rho(\mathbf{H}),\Pi_+]-[\rho(\mathbf{H}_L),\Pi_+]\|_{\mathbb{B}_1(\mathcal{H})}\leq CL^{-n}.$$

Proof. Let $0\leq\chi(x_1)\leq 1$ be a C^∞ cut-off function such that $\chi=1$ on $x_1\geq a+2$ and $\chi=0$ on $x_1\leq a+1$. We have $\Pi_+\chi=\chi$, and the following identity holds:

$$[\mathbf{R}_L(z),\Pi_+]=[\mathbf{R}_L(z),\chi]+\mathbf{R}_L(z)\Pi_+(1-\chi)-\Pi_+(1-\chi)\mathbf{R}_L(z). \tag{3.5}$$

Now choose two functions $\Phi,\tilde{\Phi}\in C^\infty(\mathbb{R}^3)$ such that $0\leq\Phi,\tilde{\Phi}\leq 1$, $\Phi(\mathbf{x})=1$ if $|x_1|\leq 1/4$, $\Phi(\mathbf{x})=0$ if $|x_1|\geq 1/2$, and $\Phi^2(\mathbf{x})+\tilde{\Phi}^2(\mathbf{x})=1$ on $\mathbb{R}^3$. Denote by $\Phi_L(\mathbf{x}):=\Phi(\mathbf{x}/L)$ and $\tilde{\Phi}_L(\mathbf{x}):=\tilde{\Phi}(\mathbf{x}/L)$. We have:

$$\Phi_L^2(\mathbf{x})+\tilde{\Phi}_L^2(\mathbf{x})=1,\;\forall\mathbf{x}\in\mathbb{R}^3, \tag{3.6}$$

$$\mathrm{supp}(\Phi_L)\subset\{|\mathbf{x}|\leq L/2\},\quad\mathrm{supp}(\tilde{\Phi}_L)\subset\{|\mathbf{x}|\geq L/4\}, \tag{3.7}$$

$$\sup_{\mathbf{x}\in\mathbb{R}^3}\left\{|D^\alpha\Phi_L|(\mathbf{x})+|D^\alpha\tilde{\Phi}_L|(\mathbf{x})\right\}\leq C(\alpha)L^{-|\alpha|}. \tag{3.8}$$

If $z\in\mathbb{C}\setminus\mathbb{R}$ define:

$$S_L(z):=\Phi_L\mathbf{R}(z)\Phi_L+\tilde{\Phi}_L\mathbf{R}_L(z)\tilde{\Phi}_L. \tag{3.9}$$

The range of this operator is included in the domain of $\mathbf{H}_L$ and we can write:

$$(\mathbf{H}_L-z)S_L(z)=1+T_L(z), \tag{3.10}$$

$$T_L(z)=[-2(\nabla\Phi_L)\nabla-(\Delta\Phi_L)]\mathbf{R}(z)\Phi_L+[-2(\nabla\tilde{\Phi}_L)\nabla-(\Delta\tilde{\Phi}_L)]\mathbf{R}_L(z)\tilde{\Phi}_L. \tag{3.11}$$

This leads to a resolvent-like equation:

$$\mathbf{R}_L(z) = S_L(z) - \mathbf{R}_L(z)T_L(z). \tag{3.12}$$

Using standard Combes-Thomas estimates [11], [15], one can prove the following lemma (given without proof):

Lemma 3.4. *Denote by* $d(\mathbf{x}) := \sqrt{1+x_1^2}$. *If* $z \in \mathcal{C}_r$ *(see* (3.3)*) we denote by* $\lambda = \sqrt{1+\Re(z)^2}$. *Fix* $0 \leq \beta_2 < \beta_1 \leq 1$. *Then there exist* $\delta > 0$, $p > 0$ *and* $C > 0$ *such that uniformly in* $L > 1$ *(including* $L = \infty$*) and* $z \in \mathcal{C}_r$*:*

$$||e^{\pm\frac{\delta d}{\lambda}} D^\alpha \mathbf{R}_L(z) e^{\mp\frac{\delta d}{\lambda}}||_{B(L^2)} + ||e^{\pm\frac{\delta d}{\lambda}} \mathbf{R}_L(z) e^{\mp\frac{\delta d}{\lambda}}||_{B(L^2,L^\infty)} \leq C\lambda^p, \quad |\alpha| \leq 1, \tag{3.13}$$

$$||e^{-\beta_1\frac{\delta d}{\lambda}} \mathbf{R}_L(z) e^{\beta_2\frac{\delta d}{\lambda}}||_{HS} \leq C\lambda^p. \tag{3.14}$$

We are now ready to prove Proposition 3.3. The idea is to use (3.5) in (3.4) and prove that each term on the right hand side converge in the trace norm to the operator with $L = \infty$.

Let us first prove that $\rho(\mathbf{H})\Pi_+(1-\chi) \in \mathbb{B}_1(\mathcal{H})$. Because ρ has an exponential decay at infinity, we can integrate arbitrary many times by parts in (3.4) and replace $\mathbf{R}(z)$ by $\mathbf{R}^N(z)$, $N \geq 2$:

$$\rho(\mathbf{H}) \;=\; \frac{i}{2\pi}\int_{\mathcal{C}_r} \rho_N(z)\,\mathbf{R}^N(z)\,dz, \tag{3.15}$$

where ρ_N still decays exponentially at infinity. Take $N = 2$. Let us prove that the integrand in (3.15) becomes trace class if we multiply it by the localized multiplication operator $\phi := \Pi_+(1-\chi)$. Indeed, for $0 < \alpha_2 < \alpha_1 < 1$ we have:

$$\mathbf{R}^2(z)\phi = \left\{\mathbf{R}(z)e^{-\alpha_2\frac{\delta d}{\lambda}}\right\}\left\{e^{\alpha_2\frac{\delta d}{\lambda}}\mathbf{R}(z)e^{-\alpha_1\frac{\delta d}{\lambda}}\right\}e^{\alpha_1\frac{\delta d}{\lambda}}\phi. \tag{3.16}$$

The operator $e^{\alpha_1\frac{\delta d}{\lambda}}\phi$ is bounded, while the other two are Hilbert-Schmidt (see (3.14)). Thus:

$$||\mathbf{R}^2(z)\phi||_{\mathbb{B}_1(\mathcal{H})} \leq C\lambda^p, \quad \forall z \in \mathcal{C}_r. \tag{3.17}$$

Now since ρ_N has an exponential decay, the integral with respect to z defines a trace class operator.

Let us now prove that for any $n \geq 1$ there exists $C > 0$ such that:

$$\|\Pi_+(1-\chi)\rho(\mathbf{H}) - \Pi_+(1-\chi)\rho(\mathbf{H}_L)\|_{\mathbb{B}_1(\mathcal{H})} \leq CL^{-n}. \tag{3.18}$$

Using $\tilde{\Phi}_L\Pi_+(1-\chi) = 0$ and $\Phi_L\Pi_+(1-\chi) = \Pi_+(1-\chi)$ for $L > L_0$, and introducing equations (3.12) and (3.9) in (3.4) we obtain (denote again by $\phi = \Pi_+(1-\chi)$):

$$\phi\,\rho(\mathbf{H}) - \phi\,\rho(\mathbf{H}_L) = \phi\,\rho(\mathbf{H})(\Phi_L - 1) + \frac{i}{2\pi}\int_{\mathcal{C}_r}\rho(z)\phi\,\mathbf{R}_L(z)T_L(z)dz. \tag{3.19}$$

Both operators on the right hand side are trace class with a fast decaying trace norm. For the first one we use (3.15) with $N = 2$ and reason as in (3.16):

$$\begin{aligned}&\phi\,\mathbf{R}^2(z)(1-\Phi_L) \\ &= e^{\alpha_1\frac{\delta d}{\lambda}}\phi\left\{e^{-\alpha_1\frac{\delta d}{\lambda}}\mathbf{R}(z)e^{\alpha_2\frac{\delta d}{\lambda}}\right\}\left\{e^{-\alpha_2\frac{\delta d}{\lambda}}\mathbf{R}(z)e^{\alpha_3\frac{\delta d}{\lambda}}\right\}e^{-\alpha_3\frac{\delta d}{\lambda}}(1-\Phi_L), \\ &0 < \alpha_3 < \alpha_2 < \alpha_1 < 1.\end{aligned} \tag{3.20}$$

Again $e^{\alpha_1\frac{\delta d}{\lambda}}\phi$ is bounded, the next two operators are Hilbert-Schmidt, and the last one has a norm bounded from above by $e^{-\frac{cL}{\lambda}}$, $c > 0$, because of the support properties of $1 - \Phi_L$. Hence

$$\left\|\phi\,\mathbf{R}^2(z)(1-\Phi_L)\right\|_{\mathbb{B}_1(\mathbb{R}^3)} \leq C\lambda^p e^{-\frac{cL}{\lambda}}$$

and after integration with respect to z we obtain a decay as in (3.18) (use the exponential decay of ρ_N).

As for the other term in (3.19), we have to integrate by parts with respect to z in order to obtain products containing three resolvents. One resolvent is used to bound the momentum operator from the formula of T_L, and the other two for creating two Hilbert-Schmidt factors. Let us consider one typical term:

$$\phi\,\mathbf{R}_L(z)\Phi'_L\partial_{x_1}\mathbf{R}_L^2(z).$$

We write:

$$\begin{aligned}
&\phi\,\mathbf{R}_L(z)\Phi'_L\partial_{x_1}\mathbf{R}_L^2(z) = \left\{e^{\alpha_1\frac{\delta d}{\lambda}}\phi\right\}\left\{e^{-\alpha_1\frac{\delta d}{\lambda}}\mathbf{R}_L(z)e^{\alpha_2\frac{\delta d}{\lambda}}\right\}\\
&\cdot\left\{e^{-\alpha_2\frac{\delta d}{2\lambda}}\Phi'_L\right\}\left\{e^{-\alpha_2\frac{\delta d}{2\lambda}}\partial_{x_1}\mathbf{R}_L(z)e^{\alpha_2\frac{\delta d}{2\lambda}}\right\}e^{-\alpha_2\frac{\delta d}{2\lambda}}\mathbf{R}_L(z),\\
&0<\alpha_2<\alpha_1<1.
\end{aligned}\tag{3.21}$$

The first factor in the above product, $e^{\alpha_1\frac{\delta d}{\lambda}}\phi$, is bounded. The second and the fifth factors are Hilbert-Schmidt, while the fourth one is bounded (see again (3.13) and (3.14)). Now the operator $e^{-\alpha_2\frac{\delta d}{2\lambda}}\Phi'_L$ is again bounded by $e^{-\frac{cL}{\lambda}}$ since Φ'_L is supported in $|x_1|>L/4$. Hence the operator in (3.21) has an exponentially small trace norm, and after integration with respect to z we obtain an estimate as in the right hand side of (3.18).

Looking back at (3.4) and (3.5) we see that we also need to prove that $[\rho(\mathbf{H}),\chi]$ is trace class, and

$$\|[\rho(\mathbf{H}),\chi]-[\rho(\mathbf{H}_L),\chi]\|_{\mathbb{B}_1(\mathcal{H})}\leq CL^{-n}.\tag{3.22}$$

Since (use (3.15) with $N=2$)

$$[\rho(\mathbf{H}),\chi]\;=\;\frac{i}{2\pi}\int_{\mathcal{C}_r}\rho_2(z)\left\{\mathbf{R}^2(z)[\chi,\mathbf{H}]\mathbf{R}(z)+\mathbf{R}(z)[\chi,\mathbf{H}]\mathbf{R}^2(z)\right\}dz\tag{3.23}$$

we see that a typical contribution to the integrand is an operator of the form $\mathbf{R}(z)\chi'\partial_{x_1}\mathbf{R}^2(z)$. We can write ($0<\alpha_1<1$):

$$\begin{aligned}
&\mathbf{R}(z)\chi'\partial_{x_1}\mathbf{R}^2(z)\\
&=\left\{\mathbf{R}(z)e^{-\alpha_1\frac{\delta d}{\lambda}}\right\}\left\{\chi' e^{2\alpha_1\frac{\delta d}{\lambda}}\right\}\left\{e^{-\alpha_1\frac{\delta d}{\lambda}}\partial_{x_1}\mathbf{R}(z)e^{\alpha_1\frac{\delta d}{\lambda}}\right\}\left\{e^{-\alpha_1\frac{\delta d}{\lambda}}\mathbf{R}(z)\right\}
\end{aligned}\tag{3.24}$$

The first and last factors are Hilbert-Schmidt, the second and third ones are bounded (the support of χ' is near the origin). Hence the trace norm is polynomially bounded in λ, and the exponential decay of ρ_2 will do the rest.

The proof of (3.22) does not contain any new ingredients. The ideas are the same: introduce (3.12) in (3.4), integrate by parts with respect to z, propagate exponential factors over resolvents, and use the fact that the distance between the support of χ' and the support of $\tilde{\Phi}_L$, $1-\Phi_L$ or Φ'_L is of order L. □

Corollary 3.5. *The linear response contribution to the current admits the thermodynamic limit and*

$$\lim_{L\to\infty}\tilde{j}_{L,\eta}=-i\eta\int_{-\infty}^{0}\chi'(\eta s)\mathrm{Tr}_{\mathcal{H}}\left(e^{is\mathbf{H}}V(Q)e^{-is\mathbf{H}}\left[\rho(\mathbf{H}),\Pi_{\pm}\right]\right)ds.\tag{3.25}$$

Proof. This is a direct consequence of Corollary 3.2, Proposition 3.3, and the Lebesgue dominated convergence theorem. □

4 The Adiabatic Limit

From now on the leads are semiinfinite; the thermodynamic limit has been taken. Hence in (2.6) one has to interpret L as infinite. The adiabatic limit $\eta\to 0$ in the formula (3.25) will in fact be

an Abel limit once we can show that the limit $\lim_{s\to\infty} e^{is\mathbf{H}}V(Q)e^{-is\mathbf{H}}$ exists, at least for the strong topology and on a certain subspace of $\mathbb{B}[\mathcal{H}]$. In view of the definition of $V(Q)$ (see (2.7)) we are reduced to studying the limits $\lim_{s\to\infty} e^{is\mathbf{H}}\Pi_{\pm}e^{-is\mathbf{H}}$.

The idea is to consider the Hamiltonian $\mathbf{H}$ as the perturbation of a *decoupled Hamiltonian* $\overset{\circ}{\mathbf{H}}_a$ that commutes with the projections $\Pi_{\pm}$. We define a *decoupled Hilbert space* $\overset{\circ}{\mathcal{H}}_a := (\Pi_-\mathcal{H}) \oplus (\Pi_0\mathcal{H}) \oplus (\Pi_+\mathcal{H})$. The decoupled Hamiltonian is simply $\mathbf{H}$ with two extra Dirichlet boundary conditions defined by the previous splitting. Let us denote it by $\overset{\circ}{\mathbf{H}}_a$. We assume that the internal boundary defined by the condition $x_1 = \pm a$ is smooth enough; it is so in the cylinder case. It is important to note that:

$$[\overset{\circ}{\mathbf{H}}_a, \Pi_{\pm}] = 0. \tag{4.1}$$

With these notations and definitions we now have:

$$e^{is\mathbf{H}}\Pi_{\pm}e^{-is\mathbf{H}} \;=\; e^{is\mathbf{H}}e^{-is\overset{\circ}{\mathbf{H}}}\Pi_{\pm}e^{is\overset{\circ}{\mathbf{H}}}e^{-is\mathbf{H}}. \tag{4.2}$$

Under our assumptions, the Hamiltonian $\mathbf{H}$ in (4.3) is nonnegative and has no singular continuous spectrum. Let us further assume that $\mathbf{H}$ has no embedded eigenvalues, and only a finite number of discrete eigenvalues of finite multiplicity located below the essential spectrum (which can arise from the geometry we chose for our system $\mathcal{X}_\infty$, [16]). Then let us denote by E_α the finite dimensional orthogonal projection corresponding to a discrete eigenvalue λ_α of $\mathbf{H}$, by E_∞ the projection corresponding to its absolutely continuous spectrum, and by $E_0 := \bigoplus_{\alpha\le N} E_\alpha = 1 - E_\infty$ the finite dimensional projection on its discrete spectrum. We can write:

$$\begin{aligned}
&\mathrm{Tr}_{\mathcal{H}}\left(e^{is\mathbf{H}}V(Q)e^{-is\mathbf{H}}\left[\rho(\mathbf{H}),\Pi_{\pm}\right]\right) = \mathrm{Tr}_{\mathcal{H}}\left(E_\infty e^{is\mathbf{H}}V(Q)e^{-is\mathbf{H}}E_\infty\left[\rho(\mathbf{H}),\Pi_{\pm}\right]\right)\\
&+\sum_{\alpha\le N}\mathrm{Tr}_{\mathcal{H}}\left(E_\alpha e^{is\mathbf{H}}V(Q)e^{-is\mathbf{H}}E_\infty\left[\rho(\mathbf{H}),\Pi_{\pm}\right]\right)\\
&+\sum_{\alpha\le N}\mathrm{Tr}_{\mathcal{H}}\left(E_\infty e^{is\mathbf{H}}V(Q)e^{-is\mathbf{H}}E_\alpha\left[\rho(\mathbf{H}),\Pi_{\pm}\right]\right)\\
&+\sum_{\alpha\le N,\beta\le N}\mathrm{Tr}_{\mathcal{H}}\left(E_\alpha e^{is\mathbf{H}}V(Q)e^{-is\mathbf{H}}E_\beta\left[\rho(\mathbf{H}),\Pi_{\pm}\right]\right).
\end{aligned} \tag{4.3}$$

Let us show that the last term does not contribute to the current after the adiabatic limit. We have the identity:

$$\begin{aligned}
&\mathrm{Tr}_{\mathcal{H}}\left(E_\alpha e^{is\mathbf{H}}V(Q)e^{-is\mathbf{H}}E_\beta\left[\rho(\mathbf{H}),\Pi_{\pm}\right]\right)\\
&= e^{is(\lambda_\alpha-\lambda_\beta)}\mathrm{Tr}_{\mathcal{H}}\left(V(Q)E_\beta[\rho(\mathbf{H}),\Pi_{\pm}]E_\alpha\right).
\end{aligned} \tag{4.4}$$

Now for $\alpha = \beta$ we have

$$E_\alpha[\rho(\mathbf{H}),\Pi_{\pm}]E_\alpha = \rho(\lambda_\alpha)(E_\alpha\Pi_{\pm}E_\alpha - E_\alpha\Pi_{\pm}E_\alpha) = 0. \tag{4.5}$$

For $\alpha \neq \beta$ we use the bound

$$\left|\mathrm{Tr}_{\mathcal{H}}\left(V(Q)E_\beta[\rho(\mathbf{H}),\Pi_{\pm}]E_\alpha\right)\right| \le \|V(Q)\|\,\|[\rho(\mathbf{H}),\Pi_{\pm}]\|_{\mathbb{B}_1}$$

and the fact that the s-integral

$$\eta\int_{-\infty}^{0}\chi'(\eta s)\,e^{is\omega}\,ds = (\mathcal{F}\chi')(\omega/\eta)\underset{\eta\to 0}{\longrightarrow} 0$$

for any $\omega \neq 0$, as the Fourier transform of a L^1-function on $\mathbb{R}$.

Now let us study the second term in (4.2) and prove that it will also disappear after the adiabatic limit. We have the identity:

$$\begin{aligned}&\mathrm{Tr}_{\mathcal{H}}\left(E_\alpha e^{is\mathbf{H}}V(Q)e^{-is\mathbf{H}}E_\infty\left[\rho(\mathbf{H}),\Pi_\pm\right]\right)\\&=\mathrm{Tr}_{\mathcal{H}}\left(V(Q)e^{-is(\mathbf{H}-\lambda_\alpha)}E_\infty\left[\rho(\mathbf{H}),\Pi_\pm\right]E_\alpha\right)\end{aligned}\tag{4.6}$$

and observe that (by interchanging the trace with the s-integral) we have

$$\begin{aligned}&\mathrm{Tr}_{\mathcal{H}}\left\{V(Q)\,\left(\eta\int_{-\infty}^{0}\chi'(\eta s)\,e^{-is(\mathbf{H}-\lambda_\alpha)}\,ds\right)\,E_\infty\left[\rho(\mathbf{H}),\Pi_\pm\right]E_\alpha\right\}\\&=\mathrm{Tr}_{\mathcal{H}}\left\{V(Q)\,\left((\mathcal{F}\chi')(\eta^{-1}\,(\mathbf{H}-\lambda_\alpha)E_\infty)\right)\left[\rho(\mathbf{H}),\Pi_\pm\right]E_\alpha\right\}.\end{aligned}\tag{4.7}$$

Due to our hypothesis on $\mathbf{H}$ and the definition of E_∞, we get:

$$(\mathbf{H}-\lambda_\alpha)E_\infty\ \geq(\inf(\sigma_{ac}(\mathbf{H}))-\lambda_\alpha)E_\infty,$$

and since $\mathcal{F}\chi'$ converges to zero at infinity we obtain:

$$\|(\mathcal{F}\chi')(\eta^{-1}(\mathbf{H}-\lambda_\alpha)E_\infty)\|_{\mathbb{B}[\mathcal{H}]}\ =\sup_{\mu\geq\inf(\sigma_{ac}(\mathbf{H}))-\lambda_\alpha}(\mathcal{F}\chi')(\mu/\eta)\ \underset{\eta\to0}{\longrightarrow}\ 0.$$

The third term in (4.3) can be treated in a similar way as the second one. Therefore only the first term can give a contribution, and let us identify it. Denote by $P_{ac}(\overset{\circ}{\mathbf{H}})=\Pi_-\oplus\Pi_+$ the projector on the absolutely continuous subspace of $\overset{\circ}{\mathbf{H}}$. We note that the incoming wave operators at $-\infty$ associated to the pair of Hamiltonians $(\overset{\circ}{\mathbf{H}},\mathbf{H})$ exist and are complete. This can be shown in a number of different of ways, but here we choose to invoke the invariance principle and the Kato-Rosenblum theorem. Indeed, the function $-\rho$ is admissible (see Thm. XI.23 [RS III]), and we have:

$$\mathbf{\Omega}_+(\overset{\circ}{\mathbf{H}},\mathbf{H})=\mathbf{\Omega}_+(-\rho(\overset{\circ}{\mathbf{H}}),-\rho(\mathbf{H}))=\mathbf{\Omega}_+(-\rho(\overset{\circ}{\mathbf{H}}),-\rho(\overset{\circ}{\mathbf{H}})-\Delta\rho),\tag{4.8}$$

where the operator $\Delta\rho:=\rho(\mathbf{H})-\rho(\overset{\circ}{\mathbf{H}})$ is trace class (more details will be given in the next section). Thus:

$$\mathbf{\Omega}_+\ :=\ s-\lim_{s\to-\infty}e^{is\mathbf{H}}e^{-is\overset{\circ}{\mathbf{H}}}P_{ac}(\overset{\circ}{\mathbf{H}}),\quad\mathrm{Ran}(\Omega_+)=E_\infty.\tag{4.9}$$

Using (4.2), (4.9) and the fact that $V(Q)=V(Q)P_{ac}(\overset{\circ}{\mathbf{H}})$, we obtain:

$$\begin{aligned}&\lim_{s\to-\infty}\mathrm{Tr}_{\mathcal{H}}\left(E_\infty e^{is\mathbf{H}}V(Q)e^{-is\mathbf{H}}E_\infty\left[\rho(\mathbf{H}),\Pi_\pm\right]\right)\\&=\lim_{s\to-\infty}\mathrm{Tr}_{\mathcal{H}}\left(E_\infty e^{is\mathbf{H}}e^{-is\overset{\circ}{\mathbf{H}}}V(Q)e^{is\overset{\circ}{\mathbf{H}}}e^{-is\mathbf{H}}E_\infty\left[\rho(\mathbf{H}),\Pi_\pm\right]\right)\\&=\mathrm{Tr}_{\mathcal{H}}\left(E_\infty\mathbf{\Omega}_+V(Q)\mathbf{\Omega}_+^*E_\infty\left[\rho(\mathbf{H}),\Pi_\pm\right]\right).\end{aligned}\tag{4.10}$$

Using (4.10) and (4.3) in (3.25) we can write a formula for the adiabatic limit of the linear response current at $t=0$ as:

$$\begin{aligned}\tilde{j}_\pm:=\lim_{\eta\to0}\tilde{j}_\eta\ &=\ i\mathrm{Tr}_{\mathcal{H}}\left(E_\infty\mathbf{\Omega}_+V(Q)\mathbf{\Omega}_+^*E_\infty\left[\rho(\mathbf{H}),\Pi_\pm\right]\right)\\&=\ v_-i\mathrm{Tr}_{E_\infty\mathcal{H}}\left(\mathbf{\Omega}_+\Pi_-\mathbf{\Omega}_+^*\left[\rho(\mathbf{H}),\Pi_\pm\right]\right)+v_+i\mathrm{Tr}_{E_\infty\mathcal{H}}\left(\mathbf{\Omega}_+\Pi_+\mathbf{\Omega}_+^*\left[\rho(\mathbf{H}),\Pi_\pm\right]\right).\end{aligned}\tag{4.11}$$

Recalling that the decoupled Hamiltonian commutes with the projections $\Pi_\pm$ (see (4.1)), we can write:

$$\left[\rho(\mathbf{H}),\Pi_\pm\right]\ =\ \left[(\rho(\mathbf{H})-\rho(\overset{\circ}{\mathbf{H}})),\Pi_\pm\right].$$

Then we have:

$$\tilde{j}_{\pm} \;=\; v_{-} i\mathrm{Tr}_{E_{\infty}\mathcal{H}}\left(\mathbf{\Omega}_{+}\Pi_{-}\mathbf{\Omega}_{+}^{*}\left[\Delta\rho,\Pi_{\pm}\right]\right)+v_{+}i\mathrm{Tr}_{E_{\infty}\mathcal{H}}\left(\mathbf{\Omega}_{+}\Pi_{+}\mathbf{\Omega}_{+}^{*}\left[\Delta\rho,\Pi_{\pm}\right]\right). \tag{4.12}$$

At this point we can show that if $v_{+}=v_{-}$, then the current is zero. Indeed, since $\Omega_{+}(\Pi_{+}+\Pi_{-})\mathbf{\Omega}_{+}^{*}=1$ on $E_{\infty}\mathcal{H}$, and because $\mathrm{Tr}_{\mathcal{H}}([\Delta\rho,\Pi_{+}])=0$ we can write:

$$\tilde{j}_{+} \;=\; (v_{-}-v_{+})i\mathrm{Tr}_{E_{\infty}\mathcal{H}}\left(\mathbf{\Omega}_{+}\Pi_{-}\mathbf{\Omega}_{+}^{*}\left[\Delta\rho,\Pi_{+}\right]\right)-i\mathrm{Tr}_{E_{\mathrm{pp}}\mathcal{H}}([\Delta\rho,\Pi_{+}]). \tag{4.13}$$

But $\mathrm{Tr}_{E_{\mathrm{pp}}\mathcal{H}}([\Delta\rho,\Pi_{+}])=\mathrm{Tr}(E_{\mathrm{pp}}(\mathbf{H})\left[\rho(\mathbf{H}),\Pi_{+}\right])=0$, therefore we obtain:

$$\tilde{j}_{+} \;=\; (v_{-}-v_{+})i\mathrm{Tr}_{E_{\infty}\mathcal{H}}\left(\mathbf{\Omega}_{+}\Pi_{-}\mathbf{\Omega}_{+}^{*}\left[\Delta\rho,\Pi_{+}\right]\right), \tag{4.14}$$

which is a close analog of the formula given by NESS type approaches (see [1] and references therein). A remark is in order here. In NESS type approaches the reservoirs (leads) are suddenly coupled at $t=0$ and the current is computed in the limit $t\to\infty$. In general, the current has an oscillatory component given by a term similar to the last term in (4.3) [19], so it does not have a definite limit at $t\to\infty$. What it is actually computed by an averaging procedure, is the steady component of the current. As we have seen above, in the adiabatic switching formalism the current itself has a limit as $\eta\to 0$. This fact confirms (in our particular setting) the basic feature of the adiabatic switching, namely that it "kills" oscillatory terms of various physical quantities.

5 The Landauer-Büttiker formula

We will now compute the trace appearing in equation (4.14) using a spectral representation of $\overset{\circ}{\mathbf{H}}$. By doing this we will obtain the L-B formula.

Let us enumerate a few technical results needed in order to justify the computations which will follow next. In the next subsection we will only give the proof of (5.1), since the other points are just well known facts which can be found in any standard book treating the stationary scattering theory.

Proposition 5.1. *Consider some $n>1/2$.*

1. *The operator $\Delta\rho=\rho(\mathbf{H})-\rho(\overset{\circ}{\mathbf{H}})$ is trace class, and if $\langle\mathbf{x}\rangle:=\sqrt{1+x_{1}^{2}}$ we have:*

$$\langle\cdot\rangle^{n}(\Delta\rho)\langle\cdot\rangle^{n}\in\mathbb{B}(\mathcal{H}). \tag{5.1}$$

2. *Denote by $E_{0}\geq 0$ the infimum of the essential spectrum of $\overset{\circ}{\mathbf{H}}$. Then $\sigma_{\mathrm{ac}}(\overset{\circ}{\mathbf{H}})=[E_{0},\infty)$. Moreover, the spectrum of $\mathbf{H}$ in $[E_{0},\infty)$ is absolutely continuous, with finitely many (possibly none) eigenvalues. The set of thresholds $\mathcal{T}$ (points where we do not have a Mourre estimate, see [24]) is discrete and contains infinitely many points. If n is large enough then the mapping*

$$\begin{aligned}&A:[E_{0},\infty)\setminus\mathcal{T}\mapsto\mathbb{B}(\mathcal{H}),\\&A(\lambda):=\lim_{\epsilon\searrow 0}\langle\cdot\rangle^{-n}(\mathbf{H}-\lambda-i\epsilon)^{-1}\langle\cdot\rangle^{-n}\end{aligned} \tag{5.2}$$

is continuously differentiable.

3. *For n large enough, the mapping*

$$\begin{aligned}&A_{\rho}:[0,\rho(E_{0})]\setminus\rho(\mathcal{T})\mapsto\mathbb{B}(\mathcal{H}),\\&A_{\rho}(t):=\lim_{\epsilon\searrow 0}\langle\cdot\rangle^{-n}(\rho(\mathbf{H})-t-i\epsilon)^{-1}\langle\cdot\rangle^{-n}\end{aligned} \tag{5.3}$$

is continuously differentiable.

4. *We can choose a family of generalized eigenfunctions for the absolutely continuous part of the operator* $\overset{\circ}{\mathbf{H}}$*, which in the case of our cylinder-like semiinfinite leads can be explicitly written down. The multiplicity of the absolutely continuous spectrum is finite when the energy is restricted to compacts, but it is not constant and increases with the energy. A given channel will be indexed by* (α, σ)*, where* $\sigma \in \{\pm 1\}$ *shows the left/right lead, and* α *indexes all other quantum numbers at a given energy. Hence for* $n > 1/2$ *we have :*

$$\langle\cdot\rangle^{-n}\overset{\circ}{\varphi}{}_E^{(\alpha,\pm)} \in \mathcal{H}, \quad \overset{\circ}{\mathbf{H}}\overset{\circ}{\varphi}{}_E^{(\alpha,\pm)} \text{"} = \text{"} E\overset{\circ}{\varphi}{}_E^{(\alpha,\pm)}, \quad E \in [E_0, \infty) \setminus \mathcal{T}. \tag{5.4}$$

5. *With this choice, we can define the corresponding generalized eigenfunctions of* $\mathbf{H}$ *either with the help of the limiting absorption principle:*

$$\begin{aligned} &\langle\cdot\rangle^{-n}\varphi_E^{(\alpha,\pm)} = \langle\cdot\rangle^{-n}\overset{\circ}{\varphi}{}_E^{(\alpha,\pm)} - A_\rho(\rho(E))\left\{\langle\cdot\rangle^n \Delta\rho \langle\cdot\rangle^n\right\}\left\{\langle\cdot\rangle^{-n}\overset{\circ}{\varphi}{}_E^{(\alpha,\pm)}\right\}, \\ &E \in [E_0, \infty) \setminus \mathcal{T}, \end{aligned} \tag{5.5}$$

or as solutions of the Lippmann-Schwinger equation (with the usual abuse of notation):

$$\begin{aligned} &\varphi_E^{(\alpha,\pm)} = \overset{\circ}{\varphi}{}_E^{(\alpha,\pm)} - (\rho(\overset{\circ}{\mathbf{H}}) - \rho(E) - i0_+)^{-1}(\Delta\rho)\varphi_E^{(\alpha,\pm)}, \\ &E \in [E_0, \infty) \setminus \mathcal{T}. \end{aligned} \tag{5.6}$$

If n *is large enough, then the map*

$$[E_0, \infty) \setminus \mathcal{T} \ni E \mapsto \langle\cdot\rangle^{-n}\varphi_E^{(\alpha,\pm)} \in \mathcal{H} \tag{5.7}$$

is continuously differentiable.

Let us now use this proposition in order to compute the current. The main idea is to compute the integral kernels of the two trace class operators in (4.12), and then to compute the trace as the integral of the diagonal values of their kernels. We use for this the generalized eigenvalues of $\mathbf{H}$. Let us choose two energies $E, E' \in \sigma_{\mathrm{ac}}(\mathbf{H}) \setminus \mathcal{T}$. Denote by $(\alpha, \pm)$ and $(\alpha', \pm)$ the quantum numbers describing the spectral multiplicity of $\mathbf{H}$ at E and E'. Then in the spectral representation of $\mathbf{H}$, an operator like $E_\infty \mathbf{\Omega}_+ \Pi_- \mathbf{\Omega}_+^*(\Delta\rho)\Pi_+$ will have the integral kernel (here $\sigma, \sigma' \in \{+, -\}$ indicate the leads):

$$\mathcal{I}(E, \alpha, \sigma; E', \alpha', \sigma') = \delta_{\sigma,+}\langle(\Delta\rho)\Pi_+\varphi_{E'}^{(\alpha',\sigma')}, \varphi_E^{(\alpha,+)}\rangle. \tag{5.8}$$

In deriving this equation we formally used the "intertwining" property

$$\mathbf{\Omega}_+^*\varphi_E^{(\alpha,\sigma)} \text{"} = \text{"} \overset{\circ}{\varphi}{}_E^{(\alpha,\sigma)} \tag{5.9}$$

since the wave operators are unitary between the absolutely continuous subspaces of $\overset{\circ}{\mathbf{H}}$ and $\mathbf{H}$. The scalar product is in fact a duality bracket between weighted spaces, and we used (5.2). This integral kernel is jointly continuous in its energy variables outside the set of thresholds, due to (5.7). Thus when we compute the trace of $E_\infty \mathbf{\Omega}_+ \Pi_- \mathbf{\Omega}_+^*(\Delta\rho)\Pi_+$, we may write:

$$\mathrm{Tr} E_\infty \mathbf{\Omega}_+ \Pi_- \mathbf{\Omega}_+^*(\Delta\rho)\Pi_+ = \lim_{S \to \sigma_{\mathrm{ac}}(\mathbf{H}) \setminus \mathcal{T}} \int_S \sum_{\alpha,\sigma} \mathcal{I}(E, \alpha, \sigma; E, \alpha, \sigma) dE, \tag{5.10}$$

where S denotes compact sets included in $\sigma_{\mathrm{ac}}(\mathbf{H}) \setminus \mathcal{T}$, and the limit means that the Lebesgue measure of $\sigma_{\mathrm{ac}}(\mathbf{H}) \setminus (\mathcal{T} \cup S)$ goes to zero.

Now after undoing the commutator in (4.14), we compute the traces in the way we described above, keeping in mind that the energy integral has to be understood as a limit avoiding the thresholds. Thus we obtain:

$$\tilde{j}_+ = -\,i\int_{E_0}^{\infty}\sum_{\alpha}\Big\{(v_- - v_+)\langle[\Delta\rho,\Pi_+]\varphi_E^{(\alpha,-)},\varphi_E^{(\alpha,-)}\rangle\Big\}\,dE$$
$$= 2(v_- - v_+)\int_{E_0}^{\infty}\sum_{\alpha}\Big\{\Im\langle\Delta\rho\Pi_+\varphi_E^{(\alpha,-)},\varphi_E^{(\alpha,-)}\rangle\Big\}\,dE. \tag{5.11}$$

Using the Lippmann-Schwinger equation (5.6) we obtain

$$\Delta\rho\Pi_+\varphi_E^{(\alpha,-)} = -\Delta\rho\Pi_+(\rho(\overset{\circ}{\mathbf{H}}) - \rho(E) - i0_+)^{-1}(\Delta\rho)\varphi_E^{(\alpha,-)},$$

and we insert this in (5.11). Using the generalized eigenfunctions of $\overset{\circ}{\mathbf{H}}$, the limiting absorption principle, the various regularity properties listed in Proposition 5.1, and the Sokhotskii-Plemelj formula, we obtain:

$$\Im\left\langle\Pi_+(\rho(\overset{\circ}{\mathbf{H}}) - \rho(E) - i0_+)^{-1}(\Delta\rho)\varphi_E^{(\alpha,-)},(\Delta\rho)\varphi_E^{(\alpha,-)}\right\rangle \tag{5.12}$$
$$= \frac{\pi}{\rho'(E)}\sum_{\alpha'}\left|\left\langle(\Delta\rho)\varphi_E^{(\alpha,-)},\overset{\circ}{\varphi}_E^{(\alpha',+)}\right\rangle\right|^2.$$

Thus the current reads as:

$$\tilde{j}_+ = 2\pi(v_+ - v_-)\int_{E_0}^{\infty}\sum_{\alpha,\alpha'}\frac{1}{\rho'(E)}\left|\left\langle(\Delta\rho)\varphi_E^{(\alpha,-)},\overset{\circ}{\varphi}_E^{(\alpha',+)}\right\rangle\right|^2 dE. \tag{5.13}$$

We now have to relate the above integrand with the scattering matrix. We know that the S matrix commutes with $\overset{\circ}{\mathbf{H}}$, and so does the T matrix defined as $\frac{1}{2\pi i}(1-S)$. In the spectral representation of $\overset{\circ}{\mathbf{H}}$ induced by $\{\overset{\circ}{\varphi}_E^{(\alpha,\sigma)}\}_{\alpha,\sigma}$, the T operator is a direct integral with a fiber which is a finite dimensional matrix. Now using the correspondence principle (see (4.8)), and formula $(4)_{\pm}$, page 233 in [29] we can write (see also Thm. XI.42 in [26]):

$$T_{\alpha,\sigma;\alpha',\sigma'}(E) = \frac{1}{\rho'(E)}\left\langle(\Delta\rho)\varphi_E^{(\alpha',\sigma')},\overset{\circ}{\varphi}_E^{(\alpha,\sigma)}\right\rangle. \tag{5.14}$$

The Landauer-Büttiker formula becomes:

$$\tilde{j}_+ = 2\pi(v_+ - v_-)\int_{E_0}^{\infty}\sum_{\alpha,\alpha'}\rho'(E)\left|T_{\alpha',+;\alpha,-}(E)\right|^2 dE. \tag{5.15}$$

We can now state the main result of our paper:

Theorem 5.2. *Assume that the system has N leads. Then the charge variation of lead $f = 1$ defined after the thermodynamic and adiabatic limits, in the linear response regime, reads as:*

$$j_1 = \sum_{f=2}^{N}(v_f - v_1)i\mathrm{Tr}_{E_\infty\mathcal{H}}\left(\Omega_+\Pi_f\Omega_+^*[\Delta\rho,\Pi_1]\right). \tag{5.16}$$

In terms of transmittance between leads we have:

$$j_1 = 2\pi\sum_{f=2}^{N}(v_1 - v_f)\int_{E_0}^{\infty}\sum_{\alpha,\alpha'}\rho'(E)\left|T_{\alpha',1;\alpha,f}(E)\right|^2 dE. \tag{5.17}$$

5.1 A continuity equation for the current

If we go back to (2.35) and instead of $\Pi_\pm$ we use some smaller projections $\hat{\Pi}_\pm$ which have the property that $\hat{\Pi}_\pm \Pi_\pm = \hat{\Pi}_\pm$ (but still corresponding to an infinitely long portion of a lead), then we can again define a current and obtain an expression as in (2.44), where $\Pi_\pm$ are replaced by $\hat{\Pi}_\pm$. The thermodynamic and adiabatic limits can be performed in the same manner, and we would obtain a formula very similar to (5.16):

$$\hat{j}_1 = \sum_{f=2}^{N} (v_f - v_1) i \mathrm{Tr}_{E_\infty \mathcal{H}} \left(\Omega_+ \Pi_f \Omega_+^* [\rho(\mathbf{H}), \hat{\Pi}_1] \right). \tag{5.18}$$

Note that $\overset{\circ}{\mathbf{H}}$ is still defined with respect to the old decomposition imposed by Π's, and NOT by $\hat{\Pi}_1$. That is $\overset{\circ}{\mathbf{H}}$ does NOT commute with $\hat{\Pi}_1$. Another important observation is that $[\rho(\mathbf{H}), \hat{\Pi}_1]$ is already trace class even before inserting something commuting with $\hat{\Pi}_1$, as we can see from the proof of Proposition 3.3. If we subtract $\hat{j}_1$ from j_1 we obtain (denote by $\pi_1 := \Pi_1 - \hat{\Pi}_1$):

$$j_1 - \hat{j}_1 = \sum_{f=2}^{N} (v_f - v_1) i \mathrm{Tr}_{E_\infty \mathcal{H}} \left(\Omega_+ \Pi_f \Omega_+^* [\rho(\mathbf{H}), \pi_1] \right). \tag{5.19}$$

Now π_1 corresponds to the multiplication with a function with compact support. Using again the methods of Proposition 3.3, one can show that $\rho(\mathbf{H})\pi_1$ is trace-class (one can write it as a product of two Hilbert-Schmidt operators). Then

$$\mathrm{Tr}_{E_\infty \mathcal{H}} \left(\Omega_+ \Pi_f \Omega_+^* [\rho(\mathbf{H}), \pi_1] \right) = \mathrm{Tr} \left(\Omega_+ \Pi_f \Omega_+^* \rho(\mathbf{H}) \pi_1 \right) - \mathrm{Tr} \left(\Omega_+ \Pi_f \Omega_+^* \pi_1 \rho(\mathbf{H}) \right). \tag{5.20}$$

Let us show the operator $\rho(\mathbf{H})\Omega_+ \Pi_f \Omega_+^* \pi_1$ is also trace class: note first that $[\Omega_+ \Pi_f \Omega_+^*, \rho(\mathbf{H})] = 0$ (this is due to the intertwining property of wave operators and due to $[\overset{\circ}{\mathbf{H}}, \Pi_f] = 0$); second, we can put near π_1 enough resolvents in order to obtain the product of two Hilbert-Schmidt operators. Then let us prove the trace cyclicity:

$$\mathrm{Tr} \left(\Omega_+ \Pi_f \Omega_+^* \pi_1 \rho(\mathbf{H}) \right) = \mathrm{Tr} \left(\rho(\mathbf{H}) \Omega_+ \Pi_f \Omega_+^* \pi_1 \right). \tag{5.21}$$

Indeed, take π_2 with compact support such that $\pi_2 \pi_1 = \pi_1$. The usual trace cyclicity gives:

$$\mathrm{Tr} \left(\Omega_+ \Pi_f \Omega_+^* \pi_1 \rho(\mathbf{H}) \right) = \mathrm{Tr} \left(\Omega_+ \Pi_f \Omega_+^* \pi_1 \pi_2 \rho(\mathbf{H}) \right) = \mathrm{Tr} \left(\pi_2 \rho(\mathbf{H}) \Omega_+ \Pi_f \Omega_+^* \pi_1 \right). \tag{5.22}$$

Now take back π_2 to the right and (5.21) is proved. Thus we can write:

$$\mathrm{Tr} \left(\Omega_+ \Pi_f \Omega_+^* \pi_1 \rho(\mathbf{H}) \right) = \mathrm{Tr} \left(\rho(\mathbf{H}) \Omega_+ \Pi_f \Omega_+^* \pi_1 \right) = \mathrm{Tr} \left(\Omega_+ \Pi_f \Omega_+^* \rho(\mathbf{H}) \pi_1 \right) \tag{5.23}$$

where in the second equality we used that $[\Omega_+ \Pi_f \Omega_+^*, \rho(\mathbf{H})] = 0$. Use this in (5.20) and obtain

$$j_1 = \hat{j}_1,$$

which shows that the current is the same no matter where we measure it on the lead.

5.2 Sketching the proof of (5.1)

Proof. The main idea is to use the geometric perturbation theory, in the same spirit as in Proposition 3.3. With the functions introduced in (3.6) and (3.7), choose L large enough such that $\mathbf{H}\tilde{\Phi}_L = \overset{\circ}{\mathbf{H}}\tilde{\Phi}_L$. This means that the "sample" is contained in the domain where $\Phi_L = 1$. Then keep L fixed. Now for $z \in \mathbb{C} \setminus \mathbb{R}$ we define the parametrix:

$$S(z) := \Phi_L (\mathbf{H} - z)^{-1} \Phi_L + \tilde{\Phi}_L (\overset{\circ}{\mathbf{H}} - z)^{-1} \tilde{\Phi}_L. \tag{5.24}$$

We have that the range of $S(z)$ is mapped into the domain of $\mathbf{H}$ and:

$$(\mathbf{H}-z)S(z) =: 1+T(z), \tag{5.25}$$
$$T(z) = [-2(\nabla\Phi_L)\nabla - (\Delta\Phi_L)](\mathbf{H}-z)^{-1}\Phi_L$$
$$+ [-2(\nabla\tilde{\Phi}_L)\nabla - (\Delta\tilde{\Phi}_L)](\overset{\circ}{\mathbf{H}}-z)^{-1}\tilde{\Phi}_L.$$

Similarly as in (3.12) we can write:

$$(\mathbf{H}-z)^{-1} = S(z) - (\mathbf{H}-z)^{-1}T(z). \tag{5.26}$$

Thus:

$$(\mathbf{H}-z)^{-1} - (\overset{\circ}{\mathbf{H}}-z)^{-1} = \Phi_L(\mathbf{H}-z)^{-1}\Phi_L + (\tilde{\Phi}_L - 1)(\overset{\circ}{\mathbf{H}}-z)^{-1}\tilde{\Phi}_L$$
$$+ (\overset{\circ}{\mathbf{H}}-z)^{-1}(\tilde{\Phi}_L - 1) - (\mathbf{H}-z)^{-1}T(z). \tag{5.27}$$

Then using the Cauchy integral representation as in (3.15), we see that the operator $\Delta\rho$ can be expressed as an integral where the integrand consists of several terms, and we can write each of them as a product of two Hilbert-Schmidt operators, due to the support properties of our cut-off functions and the exponential decay of various integral kernels. In order to prove (5.1) we need to propagate some exponential decay near both polynomials $\langle\cdot\rangle^n$, and this can be done as in Proposition 3.3. We do not give further details. □

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