A partition-free approach to transient and steady-state charge currents

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Abstract

We construct a non-equilibrium steady state and calculate the corresponding current for a mesoscopic Fermi system in the *partition-free* setting. To this end we study a small sample coupled to a finite number of semi-infinite leads. Initially, the whole system of quasi-free fermions is in a grand canonical equilibrium state. At $t = 0$ we turn on a potential bias on the leads and let the system evolve. We study how the charge current behaves in time and how it stabilizes itself around a steady state value, which is given by a Landauer-type formula.

1 Introduction

At the present time one can essentially distinguish two different ways of constructing non equilibrium steady states (NESS) for composed systems.

The first method consists of preparing a *partitioned* initial state for the total system containing several sub-systems, each of which being in a different state of thermal equilibrium, and then put them into contact with each other at $t = 0$, and let the coupled total system evolve in time until it reaches a steady state. In the mathematical physics community this method goes back to D. Ruelle [30], [31]. It was seriously promoted during the recent years through numerous papers, see e.g. [29, 1, 16, 31, 28, 5] and references therein. One can allow the carriers to interact in the sample [15], and the theory still works. Note that even if one chooses to turn on the coupling between the reservoirs in a time dependent way (for example *adiabatically*), the results remain the same [13].

The second method deals with those situations in which the initial state is an equilibrium state for the already coupled (i.e. *partition-free*) total system. The partition-free approach goes back at least to M.Cini [9]. This means that the initial state is not "partitioned" into a direct sum of equilibrium sub-states associated to e.g. different leads. The system is taken out of equilibrium by switching on an electrical bias between subsystems (leads) like for example turning on a d.c. battery, which in a certain way can be seen as changing the electro-chemical potentials of the leads coupled via a small sample. In contrast to the first method, there are almost no rigorous mathematical results on the second method beyond the linear response theory, or at least we are not aware of the existence of such results.

Although these two methods seem very similar, especially if one suddenly switches on the parameter bias in the partition-free system at $t = 0$, their implementations are different. One of the aims of this paper is to illustrate this observation.

The main result of the present paper is that now we are able to construct a NESS and to study charge currents in the partition-free setting and for the full response. Let us describe in words what we do.

For simplicity, in this paper we only consider two semi-infinite leads which are both coupled with the same small sample when $t < 0$. The full system is in a Gibbs equilibrium state at a

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given temperature and chemical potential. At $t = 0$ we turn on a time-dependent potential bias $V(t)$ between the leads, modeling a transient regime of a d.c. battery. At time $t_1 > 0$ the bias is stabilized and remains constant in time afterwards. The statistical density matrix $\rho(t)$ is found as the solution of a quantum Liouville equation, with an initial condition given by our global Gibbs state at $t = 0$. The time-dependent charge current from one lead to the other is defined as the mean value of a current operator in the state $\rho(t)$, see (2.8)-(2.12) for details. A priori the current depends on time, on the way we switch on the bias, and the point where we make the measurement.

In Theorem 2.4 we show the existence and compute the ergodic limit of this charge current. The limit depends neither on the way we switch on the bias, nor on the point where we measure the current. We also obtain an explicit Landauer-type formula for this limiting charge current value, involving the transmission coefficients between the leads.

Establishing Landauer-Büttiker type formulas (see e.g. [6, 7, 2, 3]) starting from first principles but in the partition free setting was the original motivation of a number of remarkable physical papers, see for example [14], [22], [4] and references therein. Probably the state of the art of this subject seen from a physical perspective is to be found in two papers by Stefanucci and collaborators [33, 34] in which the partition free approach is combined with the Green-Keldysh theory and a number of very current interesting formulas are proposed.

A first mathematically sound derivation of the Landauer-Büttiker formula in the partition free approach under the linear response approximation was obtained in [11] and further investigated in [12]. In [10] we significantly improved the method of proof of [11], which also allowed us to extend the results to the continuous case. Another challenging open problem is to extend the formalism in order to accommodate more efficient numerical current computations in transient regimes (see [24, 25, 26, 27] and references therein), and locally interacting fermions.

The structure of the rest of the paper is the following:

- In Section 2 we introduce the model and define the transient charge current in (2.12). The main result is formulated in Theorem 2.4.
- Section 3 starts with a list of well-known facts about the spectral and scattering theory of mesoscopic systems coupled to semi-infinite leads. The second part of the section is dedicated to the proof of our main theorem. At the end we give a list of open problems.

2 Set up and main results

We work with a discrete model in a one-particle Hilbert space $\mathcal{H}$. Following the physical convention we define the scalar product to be linear with respect to the second variable.

Our carriers are quasi-free fermions (electrons). A small sample S is modeled by $\Gamma \subset \mathbb{Z}^2$, chosen to be a finite subset of $\mathbb{Z}^2$. We couple S to two "one-dimensional" semi-infinite discrete leads $\alpha = 1, 2$. The sites of a lead (building its standard basis) are indexed by the set $\mathbb{N}_\alpha := \{0, 1, 2, ...\}$. Thus, $|j_\alpha\rangle$ denotes the basis element at the site with the number j of the lead α, see Fig.1. The total one-particle Hilbert space is a direct sum of the space modeling the sample $\Gamma \subset \mathbb{Z}^2$, and two spaces corresponding to the leads $\{\mathbb{N}_\alpha\}_{\alpha=1,2}$:

$$\mathcal{H} := l^2(\Gamma) \oplus l^2(\mathbb{N}_1) \oplus l^2(\mathbb{N}_2) \ . \tag{2.1}$$

We denote by $\{|m, n\rangle\}_{(m,n)\in\mathbb{Z}^2}$ and by $\{|j_\alpha\rangle\}_{j_\alpha\in\mathbb{N}_\alpha}$ the corresponding orthonormal bases of the spaces $l^2(\mathbb{Z}^2)$ and $l^2(\mathbb{N}_\alpha)$, where $\alpha = 1, 2$.

Now we describe our one-particle Hamiltonian. For the sample S we may choose any self-adjoint bounded operator H^S. For example, we can choose H^S to be the restriction to $l^2(\Gamma)$, of a lattice Harper-type operator with Dirichlet boundary conditions on Γ, but the concrete model for H^S does not play any role in the proof of our results. Notice that Γ is chosen to be finite, but can be arbitrarily large.

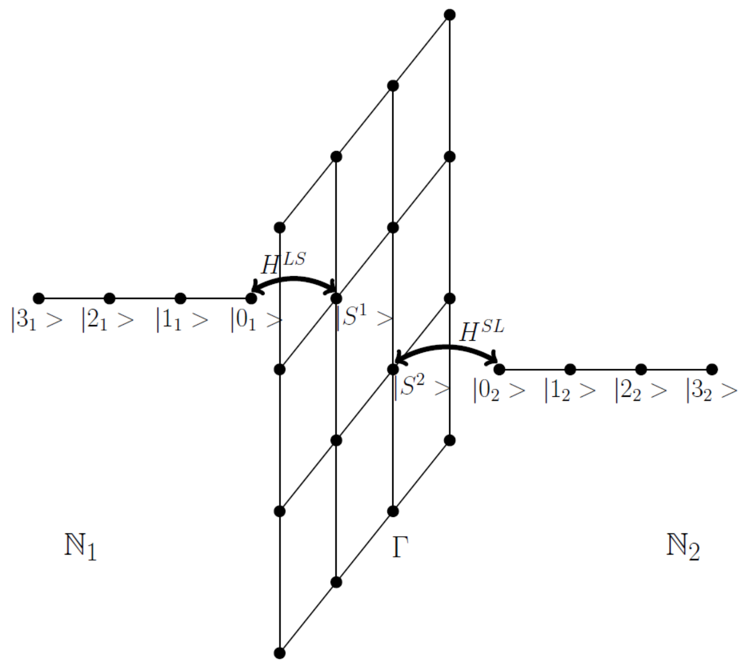

Figure 1: A sample Γ connected to two semi-infinite leads $\mathbb{N}_1$ and $\mathbb{N}_2$. Here $|j_\alpha\rangle$ denotes a basis element at the site with the number j of the lead α

On each lead $\alpha = 1, 2$ we define the identical one-dimensional discrete Laplacians acting on the functions from $l^2(\mathbb{N}_\alpha)$ with Dirichlet boundary conditions on $\mathbb{N}_\alpha$:

$$
\begin{aligned}
&(H^L_\alpha \Psi)(n) := t_L \left\{\Psi(n+1) + \Psi(n-1)\right\}, \quad n \geq 1; \quad (H^L_\alpha \Psi)(0) := t_L \Psi(1), \\
&H^L := \sum_{\alpha=1}^{2} H^L_\alpha,
\end{aligned}
\tag{2.2}
$$

where $t_L > 0$ is a hopping constant. In the following, we denote the Hamiltonian corresponding to these three *disconnected* subsystems by:

$$
H_0 := H^L + H^S.
$$

The coupling between the sample and leads is described by the *tunneling* Hamiltonian (see Fig.1):

$$
H^T := \tau \sum_{\alpha=1}^{2} \{|0_\alpha\rangle\langle \mathcal{S}^\alpha| + |\mathcal{S}^\alpha\rangle\langle 0_\alpha|\} =: H^{LS} + H^{SL}. \tag{2.3}
$$

Here $\tau > 0$ is the hopping parameter between leads and the sample. The interaction (2.3) simulates a quantum point constriction, or a tunneling barrier. Here $|0_\alpha\rangle$ is the *first* site on the lead α, and $|\mathcal{S}^\alpha\rangle$ is the corresponding *contact* site $|m_\alpha, n_\alpha\rangle$ on the sample coupled to the lead α.

Then the total one-particle Hamiltonian takes the form:

$$
H := H^S + \sum_{\alpha=1}^{2} H^L_\alpha + H^T = H^S + H^L + H^{LS} + H^{SL} =: H_0 + H^T. \tag{2.4}
$$

Remark 2.1. As we mentioned before, our results can be extended through verbatim to more general choices of Hamiltonians H^L and H^T. The key properties that we need are: the *absolutely continuous* spectrum in the leads, and a *finite rank* operator coupling between a finite sample and the leads.

2.1 The state and charge current

At $t < 0$ the total coupled system (2.4) is at equilibrium for a given temperature $1/\beta \geq 0$ and a chemical potential μ. Since we work with non-interacting fermions, the corresponding one-particle *Fermi-Dirac* equilibrium density matrix is the operator

$$f(H) = \frac{1}{e^{\beta(H-\mu)} + 1}\ ,\ \mu \in \mathbb{R}\ , \tag{2.5}$$

defined on the Hilbert space (2.1).

At the moment $t = 0$ we turn on a bias on lead number *one* in the following way. We fix $t_1 > 0$ and choose a real and continuous function ϕ which has the property that $\phi(t) = 0$ if $t < 0$ and $\phi(t) = 1$ if $t > t_1$. Let $v > 0$. Denote by $P_1 : \mathcal{H} \mapsto l^2(\mathbb{N}_1)$ the projection on the lead number *one*. Then define the time dependent potential bias as:

$$V_1(t) := v\phi(t)P_1\ . \tag{2.6}$$

Denote by $U(t)$ the unitary evolution associated to $H+V_1(t)$ through the time dependent Schrödinger equation:

$$i\partial_t U(t) = (H + V_1(t))U(t), \quad U(0) = \mathbb{I}\ . \tag{2.7}$$

The density matrix at time $t > 0$ is a solution of the Liouville equation and be expressed by:

$$\rho(t) := U(t)f(H)U(t)^*\ . \tag{2.8}$$

Denote by $P_2^{(n)} : \mathcal{H} \mapsto l^2(\{n, n+1, \ldots\})$, the projection on the second lead from which we exclude the first n sites. If $n = 0$, then it is just the projection P_2 on the lead 2. We define the current operator modeling the measurement of the charge flow at site n by:

$$j_n := i[H + V_1(t), P_2^{(n)}] = i[H, P_2^{(n)}]\ , \quad j_0 = i[H^T, P_2]\ . \tag{2.9}$$

Remark 2.2. Clearly, the current operator has finite rank, thus it is trace class. This is one important feature which is only true in the *discrete* setting. It significantly simplifies the technical estimates compared to the *continuous* case.

Remark 2.3. To obtain (2.9) we used some evident support properties of the projections $P_2^{(n)}$, which imply:

$$[P_1, P_2^{(n)}] = 0, \quad P_2^{(n)}P_2^{(n+1)} = P_2^{(n+1)}, \quad [H^S, P_2^{(n)}] = 0, \quad \forall n \geq 0, \tag{2.10}$$

and also:

$$[H^L, P_2] = 0\ ,\ [H^L, P_2^{(n)}] \neq 0, \quad [H^T, P_2^{(n)}] = 0 \quad \forall n \geq 1. \tag{2.11}$$

These properties make the commutators in (2.9) nontrivial, and are important for the study of the current propagation (see the proof of the point *(ii)* of our main theorem).

The charge current flowing through the second lead at time $t > 0$ and measured at site n is the expectation of the operator j_n from (2.9) in the quasi-free state defined by the time dependent one-particle density matrix $\rho(t)$:

$$I(t, n) := \mathrm{Tr}\{\rho(t)j_n\}. \tag{2.12}$$

2.2 The main theorem

Now we are ready to formulate our main results, collected in one theorem.

Theorem 2.4. (i) *The following ergodic limit exists and is independent of n, t_1 and ϕ:*

$$I_\infty := \lim_{T\to\infty} \frac{1}{T} \int_0^T I(t,n)dt. \tag{2.13}$$

(ii) *Fix $t \geq 0$. Then the current vanishes if we measure it infinitely far inside the lead 2:*

$$\lim_{n\to\infty} I(t,n) = 0. \tag{2.14}$$

(iii) *Assume that the operator $H + vP_1$ has only finitely many eigenvalues. If we measure the current very far inside the second lead (but not infinitely far), the transient/oscillatory effects will be weaker and weaker and the current defined in (2.12) will slightly fluctuate around the value (2.13). More precisely:*

$$\lim_{n\to\infty} \limsup_{t\to\infty} |I(t,n) - I_\infty| = 0. \tag{2.15}$$

(iv) *Denote by $\mathcal{T}_{12}^{(v)}(\lambda)$ the transmittance coefficient between the two leads at bias v for the spectral parameter λ (see* (3.19) *for a rigorous definition). Then we establish the following Landauer-type formula:*

$$I_\infty = 2\pi \int_{[-2t_L+v, 2t_L+v]\cap[-2t_L, 2t_L]} \{f(\lambda) - f(\lambda - v)\} \, \mathcal{T}_{12}^{(v)}(\lambda) d\lambda \ . \tag{2.16}$$

Remark 2.5. From *(ii)* one concludes that if we fix the time of measurement t and push the measuring point n to infinity, the current tends to zero. Although this does not imply that the propagation speed of the current is *finite*, a property which we cannot expect to hold true because of the non-relativistic dynamics on the leads. On the other hand, in *(iii)* we prove that if the current measuring device is placed further and further away from the sample, after waiting a very long time the current becomes non-zero and has weaker and weaker fluctuations around its steady-state mean value. In other words, the limits $t \to \infty$ and $n \to \infty$ do not commute.

Conjecture 2.6. *As a complement to Remark 2.5, we conjecture that the group-velocity of the spatial correlations in our model is finite, i.e. if A is any observable supported in a neighborhood of the sample, then there exist some positive constants C, M and ν such that the Lieb-Robinson type bound* [23]:

$$\|[A, U(t)^* P_2^{(n)} U(t)]\| \leq C e^{-M(n-\nu t)} \tag{2.17}$$

holds true for every $t > 0$ and $n \geq 0$. The exponential bound sounds as a strong one, i.e. one can not exclude a priori *a power-like decay.*

Remark 2.7. Our proofs are exclusively based on one-body scattering methods. We do not use the many-body language, which is unavoidable only if the carriers interact.

Remark 2.8. By the same reasons, one can completely characterize the many-body states $\omega(\cdot)$ on the Fermi algebra CAR($\mathcal{H}$), (algebra of the Canonical Anticommutation Relations) by a one-particle density-matrix operator ρ defined on $\mathcal{H}$. If at $t = 0$ the state $\omega(\cdot)$ is the grand-canonical equilibrium state on CAR($\mathcal{H}$) of a non-interacting Fermi system (2.4) (equilibrium quasi-free state), then the density-matrix operator is equal to $\rho(t = 0) = f(H)$ (2.5). The evolution (2.7) preserves this property, i.e. it transforms this state into a non-equilibrium quasi-free state (2.8).

3 Proof of the main theorem

We start this section with a list of well known facts about the spectral and scattering theory of mesoscopic, systems coupled to semi-infinite leads. This will help us to fix notation and streamline the proof of the theorem.

3.1 Some spectral and scattering background

First we recall some elements of the stationary scattering problem associated with the pair of Hamiltonians $(H + vP_1, H_0 + vP_1)$, where $H := H_0 + H^T$. In this case the free system consists of the leads with a bias v localized on the first lead together with the *decoupled* inner sample, and it is described by the Hamiltonian $H_0 + vP_1$. The perturbed system also contains the coupling H^T.

The operator $H_0 = H^L + H^S$ has as a subspace of absolute continuity $\mathcal{H}^{ac}(H_0) = \bigoplus_{\alpha=1}^2 l^2(\mathbb{N}_\alpha)$. Since the operator $H - H_0$ is of finite rank, the trace class scattering theory implies that the Møller wave operators

$$\Omega_\pm^{(v)} = \underset{t\to\mp\infty}{s\text{-lim}}\, e^{it(H+vP_1)}e^{-it(H_0+vP_1)}E_{\rm ac}(H_0 + vP_1)\ , \tag{3.1}$$

exist and are complete, see e.g. [32], [36]. Here $E_{\rm ac}(H_0 + vP_1) = E_{\rm ac}(H_0)$ denotes the projection on the absolutely continuous subspace $\mathcal{H}^{ac}(H_0 + vP_1) \subset \mathcal{H}$, or $\mathcal{H}^{ac}(H_0) \subset \mathcal{H}$ of the corresponding operators. The location and nature of the spectrum of operators like H was extensively studied in [11]; one can prove under generic conditions that there are only finitely many eigenvalues, while the singular continuous spectrum is always absent.

It is known that the set of (normalized) generalized eigenfunctions of H^L on the semi-infinite leads $\alpha = 1, 2$ have the form:

$$\Psi_\alpha(\lambda) = \sum_{m\geq 0} \Psi(\lambda; m)|m_\alpha\rangle, \quad \Psi(\lambda; m) = \frac{\sin(k(m + 1))}{\sqrt{\pi t_L \sin(k)}}. \tag{3.2}$$

Here the spectral parameter $\lambda = \lambda_k(:= 2t_L \cos(k))$ for $k \in (-\pi, \pi)$. The generalized Fourier transformation associated to these eigenvectors is defined by

$$F\colon \bigoplus_{\alpha=1}^{2} l^2(\mathbb{N}_\alpha) \to \bigoplus_{\alpha=1}^{2} L^2([-2t_L, 2t_L]), \tag{3.3}$$

$$[F(\Phi)]_\alpha(\lambda) = \langle \Psi_\alpha(\lambda), \Phi_\alpha\rangle_{l^2(\mathbb{N}_\alpha)} = \sum_{m\geq 0} \overline{\Psi(\lambda; m)}\Phi_\alpha(m). \tag{3.4}$$

Its adjoint is given by

$$F^*\colon \bigoplus_{\alpha=1}^{2} L^2([-2t_L, 2t_L]) \to \bigoplus_{\alpha=1}^{2} l^2(\mathbb{N}_\alpha), \tag{3.5}$$

$$[F^*(\Xi)]_\alpha(m) = \int_{-2t_L}^{2t_L} \Xi_\alpha(\lambda)\Psi(\lambda; m)d\lambda. \tag{3.6}$$

We see that F is a unitary operator, and that FH^LF^* is just the multiplication by $\lambda\mathbb{I}$ on the space which is a direct integral $\int_{[-2t_L,2t_L]}^{\oplus} \mathbb{C}^2 d\lambda \cong \bigoplus_{\alpha=1}^2 L^2([-2t_L, 2t_L])$, i.e.

$$FH^LF^* \cong \int_{[-2t_L,2t_L]}^{\oplus} \lambda\mathbb{I}\ d\lambda. \tag{3.7}$$

If the bias is present on the first lead, the situation is changed. Since $\mathcal{H}^{ac}(H_0) = \mathcal{H}^{ac}(H^L)$, the generalized eigenfunctions of $H_0 + vP_1$ are chosen to be

$$\Psi_1^{(v)}(\lambda; m) := \Psi(\lambda - v; m), \quad \lambda \in [-2t_L + v, 2t_L + v], \quad m \geq 0, \tag{3.8}$$

$$\Psi_2^{(v)}(\lambda; m) := \Psi(\lambda; m), \quad \lambda \in [-2t_L, 2t_L], \quad m \geq 0. \tag{3.9}$$

The corresponding generalized Fourier transformations are:

$$F_v\colon \bigoplus_{\alpha=1}^{2} l^2(\mathbb{N}_\alpha) \to L^2([-2t_L + v, 2t_L + v]) \oplus L^2([-2t_L, 2t_L]) \tag{3.10}$$

$$[F_v(\Phi)]_1(\lambda) = \sum_{m\geq 0} \overline{\Psi(\lambda - v; m)}\Phi_1(m), \quad [F_v(\Phi)]_2(\lambda) = \sum_{m\geq 0} \overline{\Psi(\lambda; m)}\Phi_2(m)\ . \tag{3.11}$$

Therefore, we can construct generalized eigenfunctions of $H + vP_1$, as solutions of the Lippmann-Schwinger equation:

$$\Phi_\alpha^{(v)}(\lambda;\cdot) = \Psi_\alpha^{(v)}(\lambda;\cdot) - (H_0 + vP_1 - \lambda - i0_+)^{-1} H^T \Phi_\alpha^{(v)}(\lambda;\cdot) \ . \tag{3.12}$$

These generalized eigenfunctions have the following very useful *intertwining properties* between the subspaces of absolute continuity of the operators H_0+vP_1 and $H+vP_1$, which can be formally written as:

$$\Phi_\alpha^{(v)}(\lambda;\cdot) = \Omega_+^{(v)} \Psi_\alpha^{(v)}(\lambda;\cdot) \ , \tag{3.13}$$

$$\Psi_\alpha^{(v)}(\lambda;\cdot) = \{\Omega_+^{(v)}\}^* \Phi_\alpha^{(v)}(\lambda;\cdot) \ . \tag{3.14}$$

The scattering operator $S^{(v)} : \mathcal{H}^{ac}(H_0 + vP_1) \mapsto \mathcal{H}^{ac}(H_0 + vP_1)$ is a unitary map acting on $\mathcal{H}^{\rm ac}(H_0 + vP_1) = \mathcal{H}^{\rm ac}(H_0) = \bigoplus_{\alpha=1}^2 l^2(\mathbb{N}_\alpha)$, and it is given by $S^{(v)} = \{\Omega_-^{(v)}\}^* \Omega_+^{(v)}$. Then the corresponding transition T-operator is defined by $2\pi i T^{(v)} := \mathbb{I} - S^{(v)}$. In the spectral representation of $H^L + vP_1$ in the space $\int_{[-2t_L,2t_L]}^{\oplus} \mathbb{C}^2 d\lambda$, the T-operator is a λ-dependent 2×2 matrix with elements denoted by $t_{\alpha\beta}^{(v)}(\lambda)$. Using (3.6) one gets the representation:

$$\sum_{\beta=1,2} t_{\alpha\beta}^{(v)}(\lambda)\Xi_\beta(\lambda) = \frac{1}{2\pi i}[F(\mathbb{I} - S^{(v)})F^*\Xi]_\alpha(\lambda) \ . \tag{3.15}$$

Then with the help of the generalized eigenfunctions we can express the T-matrix elements as:

$$t_{\alpha\beta}^{(v)}(\lambda) := \langle \Psi_\alpha^{(v)}(\lambda;\cdot), H^T \Phi_\beta^{(v)}(\lambda;\cdot)\rangle. \tag{3.16}$$

Since S is unitary, one gets the relation $i(T - T^*) = 2\pi T^* T = 2\pi T T^*$ (Optical Theorem), which implies:

$$\mathrm{Im}\{t_{22}^{(v)}(\lambda)\} = \pi \left(|t_{22}^{(v)}(\lambda)|^2 + |t_{12}^{(v)}(\lambda)|^2 \right) , \tag{3.17}$$

$$|t_{21}^{(v)}(\lambda)|^2 = |t_{12}^{(v)}(\lambda)|^2. \tag{3.18}$$

The *transmittance* $\mathcal{T}_{\alpha\beta}^{(v)}(\lambda)$ between the leads α and β for a given energy λ is defined by:

$$\mathcal{T}_{\alpha\beta}^{(v)}(\lambda) := |t_{\alpha\beta}^{(v)}(\lambda)|^2 \ . \tag{3.19}$$

Note that by definitions (3.8), (3.9) and (3.16) the transmittance $\mathcal{T}_{12}^{(v)}(\lambda) = 0$ if $\lambda \notin [-2t_L + v, 2t_L + v] \cap [-2t_L, 2t_L]$.

3.2 Proof of (i)

By (2.6) and (2.7) the evolution operator $U(t)$ obeys for $t > t_1$ the equation:

$$U(t) = e^{-i(t-t_1)(H+vP_1)} U(t_1) \ . \tag{3.20}$$

Then by $\mathcal{H} = \mathcal{H}^{pp}(H+vP_1) \oplus \mathcal{H}^{ac}(H+vP_1)$ and by (2.8) we obtain for the current (2.12) measured at site n the representation:

$$\begin{aligned} I(t,n) &= \mathrm{Tr}\{e^{-i(t-t_1)(H+vP_1)} U(t_1) f(H) U^*(t_1) e^{i(t-t_1)(H+vP_1)} j_n\} \\ &= \mathrm{Tr}\{e^{-i(t-t_1)(H+vP_1)} U(t_1) f(H) U^*(t_1) e^{i(t-t_1)(H+vP_1)} E_{\rm pp}(H + vP_1) j_n\} \\ &+ \mathrm{Tr}\{e^{-i(t-t_1)(H+vP_1)} U(t_1) f(H) U^*(t_1) e^{i(t-t_1)(H+vP_1)} E_{\rm ac}(H + vP_1) j_n\} \\ &=: I_{\rm pp}(t,n) + I_{\rm ac}(t,n) \ , \end{aligned} \tag{3.21}$$

where $E_{\rm pp}(H+vP_1)$ denotes the projection on the pure point subspace $\mathcal{H}^{pp}(H+vP_1)$. By virtue of (2.9) one gets the identity:

$$
\begin{aligned}
& e^{i(t-t_1)(H+vP_1)}E_{\rm pp}(H+vP_1)j_n e^{-i(t-t_1)(H+vP_1)} \\
&= \frac{d}{dt}\left\{E_{\rm pp}(H+vP_1)e^{i(t-t_1)(H+vP_1)}P_2^{(n)}e^{-i(t-t_1)(H+vP_1)}\right\}. \qquad (3.22)
\end{aligned}
$$

Let us for now assume that $H+vP_1$ has a finite number of eigenvalues. This means that $E_{\rm pp}(H+vP_1)$ is trace class. Now if $T>t_1$, the pure point part of (3.21) yields:

$$
\begin{aligned}
\int_0^T I_{\rm pp}(t,n)dt &= \int_0^{t_1} I_{\rm pp}(t,n)dt + \int_{t_1}^T I_{\rm pp}(t,n)dt = \int_0^{t_1} I_{\rm pp}(t,n)dt \\
&+ {\rm Tr}\left\{U(t_1)f(H)U^*(t_1)\, D(T)\, E_{\rm pp}(H+vP_1)\right\}\ , \qquad (3.23)
\end{aligned}
$$

where the operator $D(T):=e^{i(T-t_1)(H+vP_1)}P_2^{(n)}e^{-i(T-t_1)(H+vP_1)}-P_2^{(n)}$ is uniformly bounded in T. Since the first integral in the right-hand side of (3.23) is finite, the pure point spectrum does not contribute to the ergodic limit (2.13). In the case when $E_{\rm pp}(H+vP_1)$ does not have finite rank, we have to employ an $\epsilon/2$ argument based on the fact that $E_{\rm pp}(H+vP_1)j_n$ can be arbitrarily well approximated in the trace norm with an operator containing the projection on a sufficiently large (but finite) number of eigenvalues of $H+vP_1$. This approximation will be independent of T, so the previous argument can be repeated.

So, it remains to investigate $I_{\rm ac}(t,n)$ and to show that it actually converges when $t\to\infty$. To this end we start with three technical lemmas:

Lemma 3.1. *The operators* $U(t_1)-e^{-iH_0t_1-ivP_1\int_0^{t_1}\phi(\tau)d\tau}$ *and* $U^*(t_1)-e^{iH_0t_1+ivP_1\int_0^{t_1}\phi(\tau)d\tau}$ *are compact.*

Proof. Since the following Dyson-type equation:

$$
\frac{d}{dt}\left\{e^{iH_0t+ivP_1\int_0^t\phi(t)dt}U(t)\right\} = -ie^{iH_0t+ivP_1\int_0^t\phi(\tau)d\tau}H^TU(t),
$$

is equivalent to

$$
U(t_1)=e^{-iH_0t_1-ivP_1\int_0^{t_1}\phi(\tau)d\tau}-i\int_0^{t_1}e^{-iH_0(t_1-t)-ivP_1\int_t^{t_1}\phi(\tau)d\tau}H^TU(t)dt\ ,
$$

we use that H^T is a compact (finite-rank) operator in order to finish the proof. □

Lemma 3.2. *The operator* $U(t_1)f(H)U^*(t_1)-f(H_0)$ *is compact.*

Proof. It is an easy consequence of Lemma 3.1, of the fact that H_0 commutes with P_1, and of the observation that the difference $f(H)-f(H_0)$ is a compact (even trace-class) operator. □

Lemma 3.3. *Let K be a compact operator. Then the following trace-norm tends to zero:*

$$
\lim_{t\to\infty}||Ke^{i(t-t_1)(H+vP_1)}E_{\rm ac}(H+vP_1)j_n||_1=0. \qquad (3.24)
$$

Proof. Since j_n is from the trace-class (finite rank in our case), by standard $\epsilon/2$ arguments we can assume that operator K has a finite rank. Then the proof is a consequence of the Riemann-Lebesgue lemma. □

Corollary 3.4. *Use the identity* $U(t_1)f(H)U^*(t_1)=(U(t_1)f(H)U^*(t_1)-f(H_0))+f(H_0)$ *in the representation of* $I_{\rm ac}(t,n)$*. Then Lemma 3.2 and Lemma 3.3 imply the limit:*

$$
\lim_{t\to\infty}|I_{\rm ac}(t,n)-{\rm Tr}\{e^{-i(t-t_1)(H+vP_1)}f(H_0)e^{i(t-t_1)(H+vP_1)}E_{\rm ac}(H+vP_1)j_n\}|=0. \qquad (3.25)
$$

Now, to prove the ergodic limit (2.13) it is enough to check that the trace appearing in (3.25) converges when $t \to \infty$. To this end we use a standard trick of inserting the free evolution and then to use the identity:

$$f(H_0) = e^{i(t-t_1)(H_0+vP_1)} f(H_0) e^{-i(t-t_1)(H_0+vP_1)}$$

in (3.25). Using (3.1) together with the fact that the wave operators are complete thus unitary, we obtain the existence of the following strong limit:

$$\{\Omega_+^{(v)}\}^* E_{\rm ac}(H+vP_1) = s - \lim_{t\to\infty} e^{-i(t-t_1)(H_0+vP_1)} e^{i(t-t_1)(H+vP_1)} E_{\rm ac}(H+vP_1),$$

where the limit operator projects onto $\mathcal{H}^{\rm ac}(H_0)$. Finally, because j_n is trace class we can conclude that the limit:

$$\lim_{t\to\infty} I_{\rm ac}(t,n) = {\rm Tr}\left\{\Omega_+^{(v)} f(H^L)\{\Omega_+^{(v)}\}^* E_{\rm ac}(H+vP_1) j_n\right\} \ , \tag{3.26}$$

exists and is finite.

Remark 3.5. We were able to replace $f(H_0) = f(H^S) \oplus f(H^L)$ by $f(H^L)$ because the inner sample is projected out by the wave operator $\{\Omega_+^{(v)}\}^*$ on the right.

Until now we proved that the ergodic limit (2.13) is independent of ϕ and t_1. The independence of n follows from the next lemma:

Lemma 3.6. *For any $n \geq 1$ one can establish the following continuity equation:*

$$\begin{aligned}{\rm Tr}\left\{\Omega_+^{(v)} f(H^L)\{\Omega_+^{(v)}\}^* E_{\rm ac}(H+vP_1) j_n\right\} &= {\rm Tr}\left\{\Omega_+^{(v)} f(H^L)\{\Omega_+^{(v)}\}^* E_{\rm ac}(H+vP_1) j_0\right\} \\ &=: I_\infty.\end{aligned} \tag{3.27}$$

Proof. Denote by $\chi_n := P_2 - P_2^{(n)}$ the projection on the first n sites of the second lead. Then (2.9) and Remark 2.3 yield $j_0 - j_n = i[H+vP_1, \chi_n]$. Hence, the identity (3.27) is equivalent to

$${\rm Tr}\left\{\Omega_+^{(v)} f(H^L)\{\Omega_+^{(v)}\}^* E_{\rm ac}(H+vP_1)[H+vP_1, \chi_n]\right\} = 0.$$

But the operator χ_n is trace-class, so we can undo the commutator. The wave operators intertwine between $H+vP_1$ and H_0+vP_1, and H_0+vP_1 commutes with H^L. It follows that $H+vP_1$ commutes with $\Omega_+^{(v)} f(H^L)\{\Omega_+^{(v)}\}^* E_{\rm ac}(H+vP_1)$. Then the trace cyclicity finishes the proof of the lemma. □

3.3 Proof of (ii)

We start by proving that the current at $t = 0$ (i.e. at equilibrium) is zero for all n. Indeed, according to (2.9) and (2.12) one has $I(0,n) = {\rm Tr}(f(H)j_n) = i{\rm Tr}(f(H)[H, P_2^{(n)}])$ for all $n \geq 0$. Now fix n and denote by H_N the Dirichlet *restriction* of the operator H to the finite leads of length $N < \infty$, where $n < N$. Denote by $P_2^{(n),N}$ the finite-rank projection corresponding to the restriction of $P_2^{(n)}$ to the bounded second lead. Then one can prove a certain "thermodynamic limit" result [11]:

$$I(0,n) = \lim_{N\to\infty} {\rm Tr}\left\{f(H_N) i[H_N, P_2^{(n),N}]\right\}. \tag{3.28}$$

To understand why (3.28) holds true, note that $j_n = i[H_N, P_2^{(n),N}] = i[H, P_2^{(n)}]$ is a finite-rank operator which is independent of N. Moreover, $f(H)$ and $f(H_N)$ differ significantly from each other only very far from the support of j_n. Details can be found in [11].

But ${\rm Tr}\left\{f(H_N) i[H_N, P_2^{(n),N}]\right\} = 0$ for all N by trace cyclicity. Thus (3.28) shows that $I(0,n) = 0$ for any $n \geq 0$.

The next step of the proof is to show that for all $t \geq 0$ one has:

$$\lim_{n\to\infty} |I(t,n) - I(0,n)| = 0 \ . \tag{3.29}$$

Then by $I(0,n)=0$ for all n, the limit in (3.29) would imply (2.14). First we present the difference in (3.29) as:

$$I(t,n)-I(0,n)=\mathrm{Tr}\{U(t)f(H)[U^*(t)-e^{itH}]j_n\}+\mathrm{Tr}\{[U(t)-e^{-itH}]f(H)e^{itH}j_n\}. \tag{3.30}$$

Then we express the propagator $U(t)$ (2.7) with the help of its time-ordered Dyson series:

$$\begin{aligned}U(t)&=e^{-itH} \\ &+e^{-itH}\sum_{k\geq 1}\frac{(-i)^k v^k}{k!}\int_0^t d\tau_1\int_0^t d\tau_2 ...\int_0^t d\tau_k \mathbb{T}\{\phi(\tau_1)e^{i\tau_1 H}P_1 e^{-i\tau_1 H}...\phi(\tau_k)e^{i\tau_k H}P_1 e^{-i\tau_k H}\}\end{aligned} \tag{3.31}$$

whereas its adjoint is given by:

$$\begin{aligned}U^*(t)&=e^{itH} \\ &+\sum_{k\geq 1}\frac{i^k v^k}{k!}\int_0^t d\tau_1\int_0^t d\tau_2 ...\int_0^t d\tau_k \widetilde{\mathbb{T}}\{\phi(\tau_1)e^{i\tau_1 H}P_1 e^{-i\tau_1 H}...\phi(\tau_k)e^{i\tau_k H}P_1 e^{-i\tau_k H}\}e^{itH}\ ,\end{aligned} \tag{3.32}$$

where $\mathbb{T}$ means time-ordering in *decreasing* order and $\widetilde{\mathbb{T}}$ means time-ordering in *increasing* order.

Note that in the formula (3.30) the first term on the right-hand side contains the operator $[U^*(t)-e^{itH}]j_n$; we want to show that its trace-norm goes to zero with n. By a simple support property (2.10) one has $P_2^{(n-1)}j_n=j_n$ and since j_n is a finite-rank, it is enough to prove that $[U^*(t)-e^{itH}]P_2^{(n-1)}$ converges to zero with n in the operator norm. To this end we need a technical estimate given by the following lemma:

Lemma 3.7. *For any fixed* $t\geq 0$ *one has:*

$$\lim_{n\to\infty}\sup_{|\tau|\leq t}\left\|P_1 e^{i\tau H}P_2^{(n-1)}\right\|=0. \tag{3.33}$$

Proof. Since the operator H is bounded, for any $\epsilon>0$ there exists N_ϵ such that

$$\sup_{|\tau|\leq t}\left\|e^{i\tau H}-\sum_{k=0}^{N_\epsilon}\frac{i^k\tau^k H^k}{k!}\right\|\leq\epsilon. \tag{3.34}$$

The support properties (Remark 2.3) and the one-step hopping in the Hamiltonian H^L imply that $P_1 H^k P_2^{(n-1)}=0$ if $n>N_\epsilon\geq k$. Hence, by (3.34) we obtain that for $n>N_\epsilon$

$$\sup_{|\tau|\leq t}\left\|P_1 e^{i\tau H}P_2^{(n-1)}\right\|\leq\epsilon\ , \tag{3.35}$$

which proves the lemma. □

Applying this result to the expansion (3.32), one finds that $[U^*(t)-e^{itH}]P_2^{(n-1)}$ converges to zero in norm. This convergence allows to bound from above the limit of the difference (3.30):

$$\limsup_{n\to\infty}|I(t,n)-I(0,n)|\leq\limsup_{n\to\infty}|\mathrm{Tr}\{[U(t)-e^{-itH}]f(H)e^{itH}j_n\}|. \tag{3.36}$$

To estimate the limit (3.36) we use the representation $[U(t)-e^{-itH}]f(H)e^{itH}j_n=[U(t)-e^{-itH}]\{(\mathbb{I}-P_2^{([n/2])})+P_2^{([n/2])}\}f(H)e^{itH}j_n$. Since again the function $f(H)e^{itH}$ can be approximated in operator norm by polynomials in H, we can apply to $(\mathbb{I}-P_2^{([n/2])})f(H)e^{itH}j_n$ the same line of reasoning as in Lemma 3.7 to establish:

$$\lim_{n\to\infty}\|(\mathbb{I}-P_2^{([n/2])})f(H)e^{itH}P_2^{(n-1)}\|=0, \tag{3.37}$$

since the distance between the supports of $\mathbb{I}-P_2^{([n/2])}$ and of $P_2^{(n-1)}$ tends to infinity. For the term $[U(t)-e^{-itH}]P_2^{([n/2])}f(H)e^{itH}j_n$ we use the representation (3.31) and Lemma 3.7, which imply that the norm of $[U(t)-e^{-itH}]P_2^{([n/2])}$ goes to zero with n. Together with (3.37) this proves that the limit of the right hand side of (3.36) equals zero, thus (3.29) follows.

3.4 Proof of (iii)

By virtue of (3.26) and (3.27) one has $\lim_{t\to\infty} I_{\rm ac}(t,n) = I_\infty$. Therefore, it only remains to estimate the current $I_{\rm pp}(t,n)$. This gives by (3.21):

$$\sup_{t\geq 0} |I_{\rm pp}(t,n)| \leq ||E_{\rm pp}(H+vP_1)j_n||_1 \ .$$

Note the right-hand side of this estimate can be made arbitrarily small by increasing n, since we assumed that we have finitely many eigenfunctions which are necessarily localized near the sample S, thus

$$\lim_{n\to\infty} ||E_{\rm pp}(H+vP_1)P_2^{(n-1)}|| = 0.$$

This finishes the proof of (iii). Note that in the exceptional case in which $H+vP_1$ could have infinitely many eigenvalues, this argument fails.

3.5 Proof of (iv)

To calculate the steady charge current (2.16) we use our main formula (3.27) in the form:

$$I_\infty = {\rm Tr}\left\{\Omega_+^{(v)} f(H^L)\{\Omega_+^{(v)}\}^* E_{\rm ac}(H+vP_1)j_0\right\} = {\rm Tr}\left\{f(H^L)\{\Omega_+^{(v)}\}^* E_{\rm ac}(H+vP_1)j_0\Omega_+^{(v)}\right\} \ .$$

Now using the spectral representation for $H^L + vP_1$ one can evaluate the *trace* on $l^2(\mathbb{N}_1)\oplus l^2(\mathbb{N}_2)$ with the help of its generalized eigenfunctions (see (3.8) and (3.9)). Then we obtain the representation:

$$\begin{aligned} I_\infty = &\int_{-2t_L+v}^{2t_L+v} d\lambda\ f(\lambda-v)\left\langle \Psi_1^{(v)}(\lambda;\cdot), \{\Omega_+^{(v)}\}^* E_{\rm ac}(H+vP_1)j_0\Omega_+^{(v)}\Psi_1^{(v)}(\lambda;\cdot)\right\rangle \\ &+ \int_{-2t_L}^{2t_L} d\lambda\ f(\lambda)\left\langle \Psi_2^{(v)}(\lambda;\cdot), \{\Omega_+^{(v)}\}^* E_{\rm ac}(H+vP_1)j_0\Omega_+^{(v)}\Psi_2^{(v)}(\lambda;\cdot)\right\rangle \ . \end{aligned} \tag{3.38}$$

By (3.13) for the scalar product in the first integral we get:

$$\begin{aligned} i\left\langle \Psi_1^{(v)}(\lambda;\cdot), \{\Omega_+^{(v)}\}^*[H^T,P_2]\Omega_+^{(v)}\Psi_1^{(v)}(\lambda;\cdot)\right\rangle &= 2\,{\rm Im}\left\langle \Phi_1^{(v)}(\lambda;\cdot), P_2H^T\Phi_1^{(v)}(\lambda;\cdot)\right\rangle \\ = 2\,{\rm Im}\left\langle P_2\{\Psi_1^{(v)}(\lambda;\cdot) - (H_0+vP_1-\lambda-i0_+)^{-1}H^T\Phi_1^{(v)}(\lambda;\cdot)\}, H^T\Phi_1^{(v)}(\lambda;\cdot)\right\rangle \ , \end{aligned} \tag{3.39}$$

where in the second line we used the Lippmann-Schwinger equation (3.12). Notice that the vector $P_2(H_0+vP_1-\lambda-i0_+)^{-1}H^T\Phi_1^{(v)}(\lambda;\cdot) \in l^2(\mathbb{N}_2)$ for almost every λ. By Remark 2.3 one has: $[H_0,P_2]=0$ and $P_2P_1=0$, which implies $P_2(H_0+vP_1-\lambda-i0_+)^{-1}H^T = P_2(H_0-\lambda-i0_+)^{-1}H^T$. Taking this and the identity: $P_2\Psi_1^{(v)}(\lambda;\cdot)=0$ into account, we can use the spectral representation of H_0 and decomposition the vector $P_2(H_0-\lambda-i0_+)^{-1}H^T\Phi_1^{(v)}(\lambda;\cdot)$ over the generalised eigenvectors $\{\Psi_2^{(v)}(\lambda';\cdot)\}_{\lambda'\in[-2t_L,2t_L]}$ to obtain

$$\begin{aligned} &2\,{\rm Im}\left\langle P_2\{\Psi_1^{(v)}(\lambda;\cdot) - (H_0+vP_1-\lambda-i0_+)^{-1}H^T\Phi_1^{(v)}(\lambda;\cdot)\}, H^T\Phi_1^{(v)}(\lambda;\cdot)\right\rangle = \\ &= -2\,{\rm Im}\int_{-2t_L}^{2t_L} d\lambda' \frac{1}{\lambda'-\lambda-i0_+}\left|\left\langle \Psi_2^{(v)}(\lambda';\cdot)H^T\Phi_1^{(v)}(\lambda;\cdot)\right\rangle\right|^2 \\ &= -2\pi\mathcal{T}_{21}^{(v)}(\lambda)\ \chi_{[-2t_L,2t_L]}(\lambda) \ . \end{aligned} \tag{3.40}$$

For the last equality we used the Sokhotskii-Plemelj formula, and definitions (3.16), (3.19).

By the same line of reasoning one gets for the second integrand in (3.38):

$$\left\langle \Psi_2^{(v)}(\lambda;\cdot), \{\Omega_+^{(v)}\}^* E_{\rm ac}(H+vP_1) j_0 \Omega_+^{(v)} \Psi_2^{(v)}(\lambda;\cdot) \right\rangle = 2\,{\rm Im} \left\langle \Phi_2^{(v)}(\lambda;\cdot), P_2 H^T \Phi_2^{(v)}(\lambda;\cdot) \right\rangle$$
$$= 2\,{\rm Im} \left\langle P_2\{\Psi_2^{(v)}(\lambda;\cdot) - (H_0+vP_1-\lambda-i0_+)^{-1} H^T \Phi_2^{(v)}(\lambda;\cdot)\}, H^T \Phi_2^{(v)}(\lambda;\cdot) \right\rangle$$
$$= 2\,{\rm Im}\{t_{22}^{(v)}(\lambda)\} - 2\,{\rm Im} \left\langle P_2(H_0-\lambda-i0_+)^{-1} H^T \Phi_2^{(v)}(\lambda;\cdot), H^T \Phi_2^{(v)}(\lambda;\cdot) \right\rangle$$
$$= 2\,{\rm Im}\{t_{22}^{(v)}(\lambda)\} - 2\pi |t_{22}^{(v)}(\lambda)|^2 = 2\pi \mathcal{T}_{12}^{(v)}(\lambda)\ , \tag{3.41}$$

where for the last identity we used (3.16) and (3.17). Note that here $\lambda \in [-2t_L, 2t_L]$. Taking into account the symmetry (3.18) and plugging (3.40), (3.41) into (3.38), we obtain (2.16).

Recall that $\mathcal{T}_{12}^{(v)}(\lambda) = 0$, if $\lambda \notin [-2t_L, 2t_L] \cap [-2t_L+v, 2t_L+v]$. □

4 Concluding remarks

In the present paper, we established a Landauer-type formula for the stationary current running through a discrete system with a (small) sample coupled to one-dimensional infinite leads. We give a rigorous proof of the existence of the ergodic limit of the charge current and then its explicit expression. Our strategy is based on the partition-free approach, it is quite general and demands a minimal information about the sample.

There are several open problems which deserve to be mentioned.

1. One of them is our Conjecture 2.6 about the Lieb-Robinson type correlation group velocity bound, which up to our knowledge it has not been studied before in this context.
2. If $V(t)$ is a time dependent bias between which after $t = t_1$ becomes a perfect monochromatic signal like $V_0 + V_1 \cos(\omega t)$, then the ergodic limit exists and is independent of t_1 and of the site where one measures the current. Furthermore, the ergodic limit is given by a Landauer-like formula [18].
3. A computation of the current $I(t, 0)$ (see (2.12)), by expressing the evolution unitaries through the functional calculus associated to the resolvents, and the resolvents with the help of the Feshbach formula as in [11, 12]. Can one obtain an "easy" formula for $I(t, n)$ at a given n? Can one study numerically the transient effects and check point (ii) in Theorem 2.4?
4. Study the resonant transport in the case of small coupling ($0 < \tau << 1$ and v a variable parameter).
5. What happens with point *(ii)* of our theorem if there are infinitely many eigenvalues?
6. Study the "wide band limit", or $t_L \to \infty$.
7. Compute the first few corrections in v of the conductivity tensor.
8. Introduce a Kohn-Sham interaction in the sample, as in Stefanucci's papers [19]. How can one properly formulate the mathematical problem in this non-linear case? Can one still prove the existence of a steady state? Is it unique?

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