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by

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A rigorous proof for the Landauer-Büttiker formula

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Recently, Avron *et al* in [1],...,[5] shed new light on the question of quantum transport in mesoscopic samples coupled to particle reservoirs by semi-infinite leads. They rigorously treat the case when the sample undergoes an adiabatic evolution thus generating a current through the leads, and prove the so called BPT formula, see [9].

Using a discrete model, we complement their work by giving a rigorous proof of the Landauer-Büttiker formula, which deals with the current generated by an adiabatic evolution on the leads. As it is well known in physics, these formulae link the conductance coefficients for such systems to the S-matrix of the associated scattering problem.

As an application, we discuss the resonant transport through a quantum dot. The single charge tunneling processes are mediated by extended edge states simultaneosly localized near several leads.

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1 Introduction

Mesoscopic systems have been extensively studied in the last two decades, both from theoretical and experimental point of view. Much effort has been devoted to the understanding of transport phenomena through quantum rings, wires or dots (see the monographs [11] and [14]). These nanodevices display several non-trivial effects like Aharonov-Bohm conductance oscillations, quantum Hall effect, single charge tunneling. Consequently, various theories have been developed in order to explain them. Among such theories, the scattering approach to the transport problem initiated by Landauer [19] and accomplished by Büttiker [8] is perhaps the most frequently utilized in the physical literature. The basic idea of the nowadays called Landauer-Büttiker (LB) formalism is that the charge transport through a finite system connected to several (usually semi-infinite) leads is a scattering process: the incident electrons are either transmitted between leads or reflected in the same lead. By a counting argument, the conductance of a two-lead system G is related to its transmittance $\mathcal{T}$ (which still remains to be computed from the S matrix of the problem) by the Landauer formula at zero temperature:

$$G = \frac{e^2}{h}\mathcal{T}. \tag{1.1}$$

As shown by Büttiker, this formula admits a generalization to a multi-lead geometry and also to the case when a magnetic field is present. In particular a four-terminal setup is the natural way to put into evidence the quantization of the Hall resistance in strong magnetic fields.

Alternatively, the conductance G can be found from the linear-response theory. Therefore it is a natural question whether the Landauer formula can be derived directly from the Kubo formalism. This problem was addressed in a series of papers in the 80's ([13],[16],[20],[18]). All those papers used the Kubo formula as given for macroscopic samples. Later on, Baranger and Stone [6] argued for a Kubo formula adapted to mesoscopic systems with leads. They also presented a formal justification of the equivalence between the linear response theory and the LB approach.

The main aim of our work is to provide a rigorous derivation of this equivalence, following their ideas. Secondly, we use the LB formalism to describe the resonant transport through a mesoscopic sample weakly coupled to leads, the so-called quantum dot (see [17] for a review). These steps are behind the formulae used in [21] for studying specific properties of such systems.

Now let us describe the strategy followed to achieve the results. First, we establish a Kubo formula for the conductance, and then we perform the thermodynamic and adiabatic limits. Second, we compute the transmission between different leads from scattering theory. A comparison of the two results lead us to the Landauer-Büttiker formula.

We stress that in the present approach we use a tight-binding representation (i.e. a discrete model) for Hamiltonians. This makes some of the delicate technical points easier to work with. For instance, due to the particular form of the current operator (which has finite rank), the trace implied by the Kubo formula is reduced to a simple product of matrix elements of an effective resolvent R_{eff} that comes from the Feshbach formula. Its associated Hamiltonian acts only in the Hilbert space of the finite system and is non-hermitian, due to a supplementary term that embodies the effect of the leads. This term is well known in the physical literature as the 'self-energy' of the leads (see [11]). Roughly speaking, it controls the imaginary part of the effective Hamiltonian coming from the Feshbach formula and is proportional to the square of the hopping integral between the leads and the sample. As a consequence, a weak coupling generates resonances located near the real axis and a peak in the conductance as given by the LB formula, each time the energy of the incident electron equals an eigenvalue of the isolated dot. These peaks are nothing else but the so-called Coulomb oscillations in quantum dots (see [17] for an introduction to the subject). In fact, our approach shows that actually the peaks are *not* of Coulomb origin but a purely resonant effect (as shown numerically in [21] they are very sensitive to the lead-dot coupling, the interaction adding quantitative differences only).

Other interesting geometric, topological and adiabatic aspects of transport problems through mesoscopic samples were given by Avron *et al* in [2],..., [5]. Note that the authors work with adiabatic pumps, i.e. the perturbation occurs on the sample and not on the leads (the analog of LB formula in that case is the so called BPT formula [9]). They also give a very nice "pedestrian" argument of why the BPT formula should hold.

In [1], roughly the same authors rigorously prove the BPT formula. They chose to work from the beginning with infinite leads. A difficulty which appears there is that the one particle fermionic density matrix is no longer trace class, and one has to be careful when defining the currents. In our paper we manage to bypass this difficulty, by starting with the grand canonical density matrix in the associated Fock space for *finite* leads. Due to the absence of self interactions, we manage to define one particle currents in a natural way. Then we let the leads' length go to infinity, and finally we perform the adiabatic limit.

The content of the paper is organised as follows: Section 2 sets notation and gives the main result, Section 3 presents some relevant spectral properties of our system, while Section 4 contains the proof of our main theorem. Section 5 is devoted to a simple application of the formalism to the resonant transport through non-interacting quantum dots. Several technical tools are left to appendices.

2 Preliminaries and results

2.1 The model

We use the tight-binding approximation and thus a discrete model throughout the paper. The system through which the current will run is modelled by Γ, chosen to be a finite subset of $\mathbb{Z}^2$ (we can also identify it with a finite subset of $\mathbb{N}$). We couple Γ to several "one-dimensional" leads. The sites of each lead are modelled by $\mathcal{N} \subseteq \mathbb{N}$; when $\mathcal{N} = \mathbb{N}$ the lead is semi-infinite. In the sequel the finite system described by Γ will be named 'sample' while the name "system" will be given to the whole structure "sample+leads".

The total one-particle Hilbert space is a direct sum between the space modelling the sample, and M spaces corresponding to our leads:

$$\mathcal{H} = l^2(\Gamma) \oplus l^2(\mathcal{N}) \oplus \dots l^2(\mathcal{N}). \tag{2.1}$$

Let us describe the one-particle Hamiltonian. In the sample we may have any selfadjoint bounded operator H^S. For example, we can choose H^S to be the restriction of a Harper-type operator to $l^2(\Gamma)$ with Dirichlet boundary conditions:

$$\begin{aligned} H^S &= \sum_{(m,n)\in\mathbb{Z}^2} \Big(E_0 |m,n\rangle\langle m,n| + t_1 (e^{-i\frac{Bm}{2}} |m,n\rangle\langle m,n+1| + h.c.) \\ &+ t_2 (e^{-i\frac{Bn}{2}} |m,n\rangle\langle m+1,n| + h.c.) \Big) . \end{aligned} \tag{2.2}$$

Here $h.c.$ means hermitian conjugate, E_0 is the reference energy, B is a magnetic field from which the magnetic phases appear (the symmetric gauge was used), while t_1 and t_2 are hopping integrals between nearest neighbor sites.

As for the leads, the dynamics in each of them is governed by the one-dimensional discrete Laplacian with Dirichlet boundary conditions on $l^2(\mathcal{N})$

(see Appendix 1). The Hamiltonian on the leads will be ($t_L > 0$ is the hopping integral on leads)

$$H^L = \sum_{\alpha=1}^{M} H^L_\alpha, \quad H^L_\alpha = \sum_{n_\alpha \in \mathbb{Z}} t_L \cdot (|n_\alpha\rangle\langle n_\alpha + 1| + h.c.)\,. \tag{2.3}$$

The "coupling" between the sample and leads is described by the tunneling Hamiltonian

$$H^T = \tau \sum_{\alpha=1}^{M} |0_\alpha\rangle\langle\alpha_S| + \tau \sum_{\alpha=1}^{M} |\alpha_S\rangle\langle 0_\alpha| =: H^{LS} + H^{SL}. \tag{2.4}$$

Here $\tau > 0$ is the hopping integral between each lead and the sample, and simulates a quantum point constriction or a tunneling barrier. Moreover, $|0_\alpha\rangle$ is the first site on the lead α, and $|\alpha_S\rangle$ is the site from the sample through which the coupling with the lead α is realized.

Then the total one-particle Hamiltonian is the sum $H^S + H^L + H^T$. In the case when the leads are *semi-infinite*, we introduce a special notation for it:

$$K := H^S + \sum_{\alpha=1}^{M} H^L_\alpha + H^T = H^S + H^L + H^{LS} + H^{SL}. \tag{2.5}$$

2.2 Adiabatic currents and conductivity

Here we deal with electronic transport through the system. We first take the leads to be finite (i.e. each lead consists of $N < \infty$ sites), although their length can be arbitrarily large. However, the thermodynamic limit $N \to \infty$ is to be taken at a certain point in our argument.

We will only work in the grand canonical ensemble. This means that our system is in contact with a reservoir of energy and particles. Having this in mind, we will study the linear response of a system of non-interacting fermions at temperature T and chemical potential μ subjected to a perturbation, which is switched on adiabatically (to insure that the system is at equilibrium at all times).

Let χ_η, $\eta > 0$, be a smooth switching function $0 \le \chi_\eta(t) \le 2$:

$$\chi_\eta(t) = \begin{cases} e^{\eta t} & \text{if} \quad t \le 0 \\ 1 & \text{if} \quad t > 1 \end{cases}\,. \tag{2.6}$$

Then the perturbation is given by (i_α denotes the i-th site from the lead α)

$$V(N,t) := \chi_\eta(t) \sum_{\alpha=1}^{M} V_\alpha \sum_{i_\alpha=0}^{N} |i_\alpha\rangle\langle i_\alpha|. \tag{2.7}$$

Notice that $V(N,t)$ models the adiabatic application of a constant voltage V_α on the lead α. This will generate a charge transfer between the leads via the sample.

The relevant one-particle Hamiltonians then are:

$$\begin{aligned} H_0(N) &:= H^S + H^L(N) + H^T \\ H(N,t) &:= H_0(N) + V(N,t). \end{aligned} \tag{2.8}$$

Here $H^L(N)$ is the Hamiltonian acting on the finite leads, while $H_0(N)$ is the same thing as in (2.5) but the different notation indicates that it describes the initial equilibrium state for finite leads.

Now we are interested in deriving the current response of the system due to the perturbation. Since we work in the grand-canonical ensemble, we have to consider all our operators in the second quantization; see Appendix 2 for further notation and properties.

At $t = -\infty$ our system is characterized by the Gibbs equilibrium state, and its corresponding statistical operator (density matrix) is the well-known one (see (6.6)). The statistical operator describing the equilibrium state at time t for the sample coupled with the finite leads is denoted by $\hat{\rho}^{(N)}(t)$ and is defined as the (trace-class) solution of the quantum Liouville equation

$$i\frac{\partial \hat{\rho}^{(N)}(t)}{\partial t} = [d\Gamma(H(N,t)), \hat{\rho}^{(N)}(t)], \tag{2.9}$$

which satisfies the initial condition $\lim_{t\to-\infty} \hat{\rho}^{(N)}(t) = \hat{\rho}_0^{(N)}$, where $\hat{\rho}_0^{(N)}$ is as in (6.6), but with $H_0(N)$ instead of H. We stress here the fact that if the leads are infinite, these operators are no longer trace-class.

Let us now write the perturbation in the "interaction picture":

$$\tilde{V}(N,s) := e^{isH_0(N)} V(N,s) e^{-isH_0(N)}. \tag{2.10}$$

To describe the solution of the Liouville equation we consider the following equation:

$$\frac{dW}{ds}(s) = iW(s)d\Gamma(\tilde{V}(N,s)), \quad W(-\infty) = \mathrm{Id},$$

where the unitary $W(s)$ is given by the usual Dyson series with respect to $d\Gamma(\tilde{V}(N,s))$. By direct computation and using (6.9) for $\tilde{V}(N,s)$ one can verify that

$$\hat{\rho}^{(N)}(t) = e^{-itd\Gamma(H_0(N))}W^*(t)\hat{\rho}_0^{(N)}W(t)e^{itd\Gamma(H_0(N))} \tag{2.11}$$

is the unique solution to the Liouville equation, providing us with a positive and trace-class operator. Expanding the Dyson series up to the first order, and using (6.8) and (6.9), a straightforward computation gives

$$\hat{\rho}^{(N)}(t) = \hat{\rho}_0^{(N)} - i\int_{-\infty}^{t}[d\Gamma(e^{i(s-t)H_0(N)}V(N,s)e^{-i(s-t)H_0(N)}), \hat{\rho}_0^{(N)}]ds + \mathcal{O}(V^2). \tag{2.12}$$

Let us introduce the one-particle charge operator in a given lead α (which is nothing but minus the projector corresponding to the lead, the sign taking into account the fact that we deal with electrons):

$$Q_\alpha^{(N)} = -\sum_{i=0}^{N}|i_\alpha\rangle\langle i_\alpha|. \tag{2.13}$$

Denote by ${\mathbf{Q}_\alpha}^{(N)} = d\Gamma(Q_\alpha^{(N)})$ its second quantization. Since we work in the grand-canonical ensemble, the average charge in the lead α is given by

$$\mathcal{Q}_\alpha(t) := \mathrm{Tr}_{\mathcal{F}_a}\left(\hat{\rho}^{(N)}(t)\mathbf{Q}_\alpha\right). \tag{2.14}$$

Then the average charge is smooth in t, and we can define the current in the lead α as the charge transfer in the unit of time, namely

$$\mathcal{I}_\alpha(t) := \frac{d}{dt}\mathcal{Q}_\alpha(t). \tag{2.15}$$

We will see that at $t = 0$, this current can be written as

$$\mathcal{I}_\alpha(0) = \sum_\beta g_{\alpha\beta}(T,\mu,\eta,N)V_\beta + \mathcal{O}(V^2) \tag{2.16}$$

where $g_{\alpha\beta}(T,\mu,\eta,N)$ are the so-called conductance coefficients [11], and at this stage they depend on the temperature, chemical potential, the adiabatic coefficient, and the length of the leads. What we do in the rest of the paper is to study the connection of $g_{\alpha\beta}$ with the transmittance of the problem, defined just below.

2.3 The transmittance

Now we briefly switch to an apparently unrelated scattering problem, associated to the pair of Hamiltonians (H_0, K) where $H_0 = H^L$ and $K = H_0 + W = H_0 + H^S + H^T$. Thus the "free" system consists here of the *semi-infinite* leads, while the complete evolution is that of the coupled system (leads and sample). The wave operators are defined as

$$\Omega_{\pm} = s - \lim_{t\to\mp\infty} e^{itK} e^{-itH_0} P_{ac}(H_0), \tag{2.17}$$

where $P_{ac}(H_0)$ projects onto the leads' subspace $\bigoplus_{\alpha=1}^{M} l^2(\mathbb{N})$. Since $K - H_0 = H^T + H^S$ is trace class, the wave operators $\Omega_{\pm}$ exist and are complete by the Kato-Rosenblum theorem (see ([25])).

The generalized eigenfunctions of H^L on the semi-infinite leads are (here $k \in (0, \pi)$, $\lambda = 2t_L \cos(k)$ and $1 \le \alpha \le M$):

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

The generalized Fourier transform associated to these eigenvectors is defined as

$$\begin{aligned} &F : \oplus_{\alpha=1}^{M} l^2(\mathbb{N}) \mapsto \oplus_{\alpha=1}^{M} L^2([-2t_L, 2t_L]), \\ &[F(\Phi)]_\alpha(\lambda) = \langle \Psi_\alpha(\lambda), \Phi_\alpha\rangle_{l^2(\mathbb{N})} = \sum_{m\ge 0} \overline{\Psi(\lambda; m)} \Phi_\alpha(m). \end{aligned} \tag{2.18}$$

Its adjoint is given by

$$\begin{aligned} &F^* : \oplus_{\alpha=1}^{M} L^2([-2t_L, 2t_L]) \mapsto \oplus_{\alpha=1}^{M} l^2(\mathbb{N}), \\ &[F^*(\Xi)]_\alpha(m) = \int_{-2t_L}^{2t_L} \Xi_\alpha(\lambda)\Psi(\lambda; m) d\lambda. \end{aligned} \tag{2.19}$$

We see that F is a unitary operator, and that FH^LF^* is just the multiplication with λ:

$$FH^LF^* = 2t_L \cos(k)\,\mathrm{Id}. \tag{2.20}$$

Then the S-matrix is unitary and given by $S = \Omega_-^*\Omega_+$, and the T-matrix is defined by $T := S - \mathrm{Id}$. In the spectral representation of H_0, the T-operator is just a λ-dependent $M \times M$ matrix. Spelled out (see (4.4)) this means

$$\sum_\beta t_{\alpha\beta}(\lambda)\Xi_\beta(\lambda) = [F(S - \mathrm{Id})F^*\Xi]_\alpha(\lambda). \tag{2.21}$$

The transmittance between the leads α and β at energy λ is finally defined as

$$\mathcal{T}_{\alpha\beta}(\lambda) := |t_{\alpha\beta}(\lambda)|^2. \tag{2.22}$$

2.4 The Landauer-Büttiker formula and the main theorem

We can finally give the main result of our paper.

Theorem 2.1. *Consider the conductance $g_{\alpha\beta}(T, \mu, \eta, N)$ between the leads α and β ($\alpha \neq \beta$), at temperature $T > 0$, chemical potential $\mu \in (-2t_L, 2t_L)$, adiabatic switch-on coefficient $\eta > 0$ and length of the leads $N < \infty$. Assume that the point spectrum of K (the one from (2.5), with $N = \infty$) is disjoint from the thresholds $-2t_L$ and $2t_L$. Then if we first take the limit $N \to \infty$, and after that $\eta \searrow 0$, we have:*

$$g_{\alpha\beta}(T, \mu) := \lim_{\eta\searrow 0}[\lim_{N\to\infty} g_{\alpha\beta}(T, \mu, \eta, N)] = -\frac{1}{2\pi}\int_{-2t_L}^{2t_L} dE \frac{\partial f_{F-D}(E)}{\partial E}\mathcal{T}_{\alpha\beta}(E), \tag{2.23}$$

where $\mathcal{T}_{\alpha\beta}(\cdot)$ is real analytic on $(-2t_L, 2t_L)$ and equal to zero outside this interval. The function f_{F-D} is the usual Fermi-Dirac function (see (6.7)). If the temperature also tends to zero, (2.23) yields the Landauer formula

$$g_{\alpha\beta}(0_+, \mu) = \frac{1}{2\pi}\mathcal{T}_{\alpha\beta}(\mu). \tag{2.24}$$

3 The Feshbach formula and spectral analysis for the system with semi-infinite leads

We assume throughout this section that the leads are semi-infinite, thus by $R^L(z)$ we denote the resolvent of the leads as a block diagonal matrix in $\bigoplus_{\alpha=1}^{M} l^2(\mathbb{N})$. Some of its properties are given in Appendix 1.

We use the Feshbach formula [15, 22] in order to express the full resolvent in terms of an effective Hamiltonian which describes the mesoscopic system in the presence of the leads. More explicitely, the resolvent reads (see also (2.5)):

$$R(z) = (K - z)^{-1} = R^L(z) + (1 - R^L(z)H^{LS})(H_{\text{eff}}(z) - z)^{-1}(1 - H^{SL}R^L(z)) \tag{3.1}$$

where the effective Hamiltonian is defined as

$$H_{\text{eff}}(z) := H^S - H^{SL}R_L(z)H^{LS}, \quad z \in \mathbb{C} \setminus \mathbb{R}. \tag{3.2}$$

The spectral problem for K is thus reduced to the spectral problem for H_L and H_{eff}. Remark that $H_{\text{eff}}(z)$ is not hermitian. If Π^S denotes the projection onto the subspace corresponding to the "system" $l^2(\Gamma)$, then we have

$$(H_{\text{eff}}(z) - z)^{-1} = \Pi^S(K - z)^{-1}\Pi^S, \quad \Im(z) \neq 0. \tag{3.3}$$

Using (2.4), the explicit expression for the matrix elements of $R^L(z)$ that we gave in (6.1), and Proposition 6.1 iii, we can write

$$\begin{aligned} H_{\text{eff}}(z) &= H^S - \tau^2 \sum_{\alpha=1}^{M} |\alpha_S\rangle\langle 0_\alpha|R^L(z)|0_\alpha\rangle\langle\alpha_S| \\ &= H^S - \frac{\tau^2}{t_L}\zeta_1(z)\sum_{\alpha=1}^{M} |\alpha_S\rangle\langle\alpha_S| \, . \end{aligned} \tag{3.4}$$

We need some more notation. For $\epsilon > 0$, define the strip

$$\Omega_\epsilon := \{x + iy \in \mathbb{C} : \ -2t_L + \epsilon < x < 2t_L - \epsilon, \ |y| < 1/\epsilon\}. \tag{3.5}$$

Finally, introduce the orthogonal projection

$$\Pi^T := \sum_{\alpha=1}^{M} |\alpha_S\rangle\langle\alpha_S|. \tag{3.6}$$

We can write:

$$H_{\text{eff}}(z) = H^S - \frac{\tau^2}{t_L}\zeta_1(z)\Pi^T.$$

Then the main result of this section is the following:

Proposition 3.1. *Let $|\beta_S\rangle$ and $|\gamma_S\rangle$ be the coupling points between the sample and leads β and γ. Define*

$$u_{\beta\gamma}(z) = \langle\beta_S, \left[H^S - z - (\tau^2/t_L)\zeta_1(z)\Pi^T\right]^{-1}\gamma_S\rangle, \quad \Im(z) > 0. \tag{3.7}$$

Then for all positive τ and ϵ, the function $u_{\beta\gamma}$ admits a meromorphic extension $u^+_{\beta\gamma}$ to $\mathbb{C}_+ \cup \Omega_\epsilon$, and all its poles have negative imaginary part. In particular, the restriction of $u^+_{\alpha\beta}$ to the interval $(-2t_L, 2t_L)$ is real analytic.

Proof. Before anything else, notice that $u^+_{\beta\gamma}$ is the key term appearing in the transmittance formula (see (4.6)). Now introduce the notation (see (6.4)):

$$H_+(z) := H^S - \frac{\tau^2}{t_L}\zeta_+(z)\Pi^T. \tag{3.8}$$

Then $u^+_{\beta\gamma}(z) = \langle \beta_S, [H_+(z) - z]^{-1}\gamma_S\rangle$ is the meromorphic extension we are looking for. Since $l^2(\Gamma)$ is finite dimensional, the set of poles is included in the set of solutions of $\det(H_+(z)-z) = 0$. Clearly, because of (3.3), the poles cannot be in the upper complex half-plane.

Now let us prove that the poles are neither on the real axis. If there are no solutions for $\det(H_+(z)-z) = 0$ in $(-2t_L, 2t_L)$ then we are done. Now assume that there exists $\lambda \in (-2t_L, 2t_L)$, such that $H_+(\lambda) - \lambda$ is not invertible. Then $H_+(\lambda) - \lambda$ is not injective; denote by p_λ the orthogonal projection corresponding to the null-space of $H_+(\lambda) - \lambda$. For every $\phi_\lambda \in \mathrm{Ran}(p_\lambda)$ we have

$$(H^S - \lambda)\phi_\lambda - \frac{\tau^2}{t_L}\zeta_+(\lambda)\Pi^T\phi_\lambda = 0.$$

Taking the scalar product with ϕ_λ and estimating the imaginary part we have (use (6.4))

$$\langle \phi_\lambda, \Pi^T\phi_\lambda\rangle = ||\Pi^T\phi_\lambda||^2 = 0.$$

This implies that $\Pi^T\phi_\lambda = 0$ and thus ϕ_λ must also be an eigenfunction for H^S, corresponding to the eigenvalue λ. Notice that this does not say that all eigenvectors of H^S corresponding to λ are in the range of p_λ.

Because $p_\lambda\Pi^T = 0$, and because $\mathrm{Ran}(p_\lambda)$ is spanned by eigenvectors of H^S, it means that p_λ commutes with $H_+(z)$ and we can write (here $q_\lambda = \mathrm{Id} - p_\lambda$)

$$H_+(z)-z = p_\lambda(H_+(z)-z)p_\lambda+q_\lambda(H_+(z)-z)q_\lambda = (\lambda-z)p_\lambda+q_\lambda(H_+(z)-z)q_\lambda. \tag{3.9}$$

The range of q_λ is generated by eigenvectors of H^S, which either correspond to other eigenvalues than λ, or correspond to λ but are orthogonal to $\mathrm{Ran}(p_\lambda)$. Now $q_\lambda(H_+(\lambda) - \lambda)q_\lambda$ is one to one on $\mathrm{Ran}(q_\lambda)$ thus invertible, and so is $q_\lambda(H_+(z) - z)q_\lambda$ for z close to λ (by simple perturbation theory and the Neumann series). Moreover, its inverse is holomorphic near λ. Therefore,

$$(H_+(z) - z)^{-1} - (\lambda - z)^{-1}p_\lambda \tag{3.10}$$

is holomorphic around λ. In conclusion, since $p_\lambda\gamma_S = 0$,

$$u^+_{\beta\gamma}(z) = \langle \beta_S, [H_+(z) - z]^{-1}\gamma_S - (\lambda - z)^{-1}p_\lambda\gamma_S\rangle \tag{3.11}$$

is also holomorphic near λ and we are done. A similar reasoning gives a meromorphic extension to $\mathbb{C}_- \cup \Omega_\epsilon$ which we denote by $u^-_{\beta\gamma}$. It is also easy to see (use (3.3) and (3.7) that

$$\overline{u^+_{\beta\gamma}(\overline{z})} = u^-_{\gamma\beta}(z). \tag{3.12}$$

□

Remark. The above proposition does not rule out real poles for the effective Hamiltonian. It only says that its eventual real poles are not singularities for functions like $u_{\beta\gamma}$. Notice that we allowed τ to be arbitrarily large.

4 Proof of the main theorem

As we have already announced in the introduction, the strategy of the proof consists in computing the conductance and transmittance separately, and then showing that they are related as in (2.23). Since the transmittance involves less work, we start with it.

4.1 A formula for the transmittance

We will use the notation introduced in paragraph 2.3. The S-matrix $S : \mathcal{H}^L \to \mathcal{H}^L$ can be written as (see [23], Chapter 4, p.176):

$$\begin{aligned} S &= \Omega_-^* \Omega_+ &(4.1)\\ &= \mathrm{Id} + \frac{2i}{\pi}\int_{-2t_L}^{2t_L} \Im[(H^L - x + i0)^{-1}]T(x+i0)\Im[(H^L - x + i0)^{-1}]dx, \end{aligned}$$

where we used the fact that H^L has purely absolutely continuous spectrum, and $T(z) = W - W(K-z)^{-1}W$. In fact, since H^S lives in a subspace orthogonal to $\mathcal{H}^L$, we can take $T(z) = H^T - H^T(K-z)^{-1}H^T$. Moreover, using the Feshbach formula we get

$$\begin{aligned} S &= \mathrm{Id} - \frac{2i\tau^2}{\pi}\sum_{\alpha,\beta=1}^{M}\int_{-2t_L}^{2t_L} \left(\Im[(H^L - x + i0)^{-1}]|0_\alpha\rangle\right)\\ &\times\ \langle \alpha_S, R_{\rm eff}(x+i0)\beta_S\rangle\\ &\times\ \left(\langle 0_\beta|\Im[(H^L - x + i0)^{-1}]\right)dx. &(4.2) \end{aligned}$$

Take $\Xi \in \bigoplus_{\alpha=1}^{M} C_0^\infty((-2t_L, 2t_L))$. Using the formulae (2.20), (2.18), (2.19), and (3.7), we have

$$\begin{aligned}
[F(S-\mathrm{Id})F^*\Xi]_\alpha(\lambda) &= -\frac{2i\tau^2}{\pi}\sum_{\beta=1}^{M}\int_{-2t_L}^{2t_L} dx\,\big(\Im[(\lambda-x+i0)^{-1}]\Psi(\lambda;0)\big) \\
&\times\ u_{\alpha\beta}^{+}(x) \qquad (4.3)\\
&\times\ \left(\int_{-2t_L}^{2t_L}\Im[(\lambda'-x+i0)^{-1}]\Psi(\lambda';0)\Xi_\beta(\lambda')d\lambda'\right).
\end{aligned}$$

Using twice Sohotsky's formula $1/(t+i0) = \mathrm{P.V.}(1/t) - i\pi\delta$ we get

$$[F(S-\mathrm{Id})F^*\Xi]_\alpha(\lambda) = 2\pi\tau^2 i\sum_{\beta=1}^{M}|\Psi(\lambda;0)|^2 u_{\alpha\beta}^{+}(\lambda)\Xi_\beta(\lambda). \qquad (4.4)$$

Therefore, the T-operator is a matrix in the spectral representation of H^L with elements

$$t_{\alpha\beta}(\lambda) = \frac{2\tau^2}{t_L} i\sin(k)u_{\alpha\beta}^{+}(\lambda). \qquad (4.5)$$

Then the transmittance between the leads α and β at energy $\mu =: 2t_L\cos(k_\mu)$ is (see (2.22)):

$$\mathcal{T}_{\alpha\beta}(\mu) = \frac{4\tau^4}{t_L^2}\sin^2(k_\mu)|u_{\alpha\beta}^{+}(\mu)|^2. \qquad (4.6)$$

4.2 Conductivities via the linear response theory

We now concentrate on the left hand side of (2.23). Our main goal here is obtaining a more detailed version of formula (2.16), and to put into evidence the conductivities $g_{\alpha\beta}$ between different leads. Then we perform the thermodynamic and adiabatic limits.

4.2.1 Deriving the linear response: a Kubo formula

Differentiating in (2.15), using the Liouville equation (2.9), trace properties (i.e. $\mathrm{Tr}\,([A,B]C) = -\mathrm{Tr}\,(B[A,C])$), and (6.8) we have

$$\begin{aligned}\mathcal{I}_\alpha(t) &= \mathrm{Tr}_{\mathcal{F}_a}\left(\frac{d\hat{\rho}^{(N)}(t)}{dt}\mathbf{Q}_\alpha^{(N)}\right)\\ &= i\mathrm{Tr}_{\mathcal{F}_a}\left(\hat{\rho}^{(N)}(t)[\mathbf{H}(N,t),\mathbf{Q}_\alpha^{(N)}]\right)\\ &= i\mathrm{Tr}_{\mathcal{F}_a}\left(\hat{\rho}^{(N)}(t)d\Gamma([H(N,t),Q_\alpha^{(N)}])\right)\\ &= \mathrm{Tr}_{\mathcal{F}_a}\left(\hat{\rho}^{(N)}(t)d\Gamma(j_\alpha(t))\right)\end{aligned} \tag{4.7}$$

where the one-particle current operator is

$$j_\alpha(t) := i[H(N,t),Q_\alpha^{(N)}] \tag{4.8}$$

and has a simple explicit form, independent of time (because $Q_\alpha^{(N)}$ and $V(N,t)$ commute):

$$j_\alpha = i\tau(|0_\alpha\rangle\langle\alpha_S| - |\alpha_S\rangle\langle 0_\alpha|). \tag{4.9}$$

We remark that j_α is a finite rank operator. Notice also that even if the leads are semiinfinite, j_α is the *same*, this fact justifying the absence of N in its notation.

Now we continue to compute the current, using the decomposition (2.12). Introduce the notation (see also (2.8) and (6.7), and put $t=0$)

$$\begin{aligned}\mathcal{I}^{(0)}(0) &:= \mathrm{Tr}_{\mathcal{H}}\left(f_{F-D}(H_0(N))j_\alpha\right), \qquad (4.10)\\ \mathcal{I}^{(1)}(0) &:= i\int_{-\infty}^0 \mathrm{Tr}_{\mathcal{F}_a}\left(\hat{\rho}_0^{(N)}[d\Gamma(\tilde{V}(N,s)),d\Gamma(j_\alpha)]\right)ds.\end{aligned}$$

Inserting (2.12) in (4.7), and using (6.10) for the first term and trace commutation properties for the second one, we obtain:

$$\mathcal{I}_\alpha(0) = \mathcal{I}^{(0)}(0) + \mathcal{I}^{(1)}(0) + \mathcal{O}(V^2). \tag{4.11}$$

Introduce the notation:

$$Q_\beta^{(N)}(-s) := e^{-isH_0(N)}Q_\beta^{(N)}e^{+isH_0(N)}. \tag{4.12}$$

We continue rewriting $\mathcal{I}^{(1)}(0)$ employing (6.8), (6.9), (6.10), which leads to

$$\begin{aligned}\mathcal{I}^{(1)}(0) &= i\int_{-\infty}^0 \mathrm{Tr}_{\mathcal{F}_a}\left(\hat{\rho}_0^{(N)}[d\Gamma(e^{isH_0(N)}V(N,s)e^{-isH_0(N)}),d\Gamma(j_\alpha)]\right)ds\\ &= -i\sum_\beta\int_0^\infty \chi_\eta(-s)\mathrm{Tr}_{\mathcal{F}_a}\left(\hat{\rho}_0^{(N)}[d\Gamma(Q_\beta(-s),d\Gamma(j_\alpha)]\right)V_\beta ds\\ &= -i\sum_\beta\int_0^\infty ds\chi_\eta(-s)\mathrm{Tr}_{\mathcal{F}_a}\left(\hat{\rho}_0^{(N)}d\Gamma[Q_\beta(-s),j_\alpha]\right)V_\beta\\ &= -i\sum_\beta\int_0^\infty ds\chi_\eta(-s)\mathrm{Tr}_{\mathcal{H}}\left(f_{F-D}(H_0(N))[Q_\beta(-s),j_\alpha]\right)V_\beta.\end{aligned}$$

Notice that the minus appears because the charge is negative, and we replaced the projector on each lead with the corresponding charge operator. The average current at time $t = 0$ then becomes

$$\begin{aligned} \mathcal{I}_\alpha(0) &= \mathcal{I}^{(0)}(0) + \mathcal{I}^{(1)}(0) + \mathcal{O}(V^2) = \mathrm{Tr}_{\mathcal{H}}\left(f_{F-D}(H_0(N))j_\alpha\right) \\ &- i\sum_\beta \int_0^\infty ds e^{-\eta s}\mathrm{Tr}_{\mathcal{H}}\left(f_{F-D}(H_0(N))[Q_\beta^{(N)}(-s), j_\alpha]\right) V_\beta \\ &+ \mathcal{O}(V^2). \end{aligned} \tag{4.13}$$

If we compare this expression with the one announced in (2.16) we see that we are almost in place with the exception of the term $\mathcal{I}^{(0)}(0)$. This term represents the current in the equilibrium state when all V_α's are zero. Let us now prove that this term is always zero. Indeed, up to the use of Stone's formula (or other type of functional calculus with the resolvent), it is enough to prove the following lemma:

Lemma 4.1. *Let $z \in \mathbb{C} \setminus \mathbb{R}$. Then*

$$\mathrm{Tr}_{\mathcal{H}}\left((H_0(N) - z)^{-1} j_\alpha\right) = 0. \tag{4.14}$$

In particular, $\mathcal{I}^{(0)}(0) = 0$.

Proof. Using (4.9), the left hand side of (4.14) reads as

$$i\tau\left\{\langle \alpha_S, (H_0(N) - z)^{-1} 0_\alpha\rangle - \langle 0_\alpha, (H_0(N) - z)^{-1}\alpha_S\rangle\right\}. \tag{4.15}$$

We now make use of formula (3.1) where we replace H^L with $H^L(N)$ (see below (2.8) for the definition of $H^L(N)$). We introduce the obvious notation $R^L(N, z)$ and $H_{\mathrm{eff}}(N, z)$ which indicate that the leads have finite length. Since (see (2.4)) the only contribution from H^{LS} which survives is $|0_\alpha\rangle\langle\alpha_S|$ (and a similar term for H^{SL}), formula (3.1) leads to:

$$\begin{aligned} \langle \alpha_S, (H_0(N) - z)^{-1} 0_\alpha\rangle &= -\langle \alpha_S, (H_{\mathrm{eff}}(N, z) - z)^{-1}\alpha_S\rangle\langle 0_\alpha, R^L(N, z) 0_\alpha\rangle \\ &= \langle 0_\alpha, (H_0(N) - z)^{-1}\alpha_S\rangle, \end{aligned} \tag{4.16}$$

and the proof is finished. □

Therefore, we have finally obtained an expression for the total current as it was announced in (2.16), where the conductivities are given by

$$g_{\alpha\beta}(T, \mu, \eta, N) := -i\int_0^\infty ds e^{-\eta s}\mathrm{Tr}_{\mathcal{H}}\left(f_{F-D}(H_0(N))[Q_\beta^{(N)}(-s), j_\alpha]\right). \tag{4.17}$$

What we do in the next paragraphs is to perform the various limits required by Theorem 2.23.

4.2.2 Making the leads semi-infinite: $N \to \infty$

Define the quantity which is the natural candidate for the limit $N \to \infty$:

$$g_{\alpha\beta}(T,\mu,\eta,\infty) := -i\int_0^\infty dse^{-\eta s}\mathrm{Tr}_{\mathcal{H}}\left(f_{F-D}(K)[Q_\beta^{(\infty)}(-s),j_\alpha]\right). \quad (4.18)$$

Notice that when $N = \infty$, we have $H_0(\infty) = K$ (see (2.8) and (2.5)). Neither $f_{F-D}(K)$ nor $Q_\beta^{(\infty)}(-s)$ are trace class anymore, but since j_α is the same as in (4.9) (thus of rank two), the total operator is trace class whose trace is uniformly bounded with respect to s.

The main result of this paragraph is contained in the following lemma, which states that the speed of convergence when N grows to infinity is faster than any polynomial:

Lemma 4.2. *For every $J > 0$, there exists $C > 0$ which may depend on all other parameters but N, so that*

$$|g_{\alpha\beta}(T,\mu,\eta,N) - g_{\alpha\beta}(T,\mu,\eta,\infty)| \leq C/N^J. \quad (4.19)$$

Proof. We first reduce (4.17) to a form which is easier to work with. Replacing the expression for $Q_\beta^{(N)}(-s)$ (see (4.12) and (2.13)) we have (using trace commutation properties):

$$\begin{aligned} &g_{\alpha\beta}(T,\mu,\eta,N) = \quad (4.20)\\ &-i\int_0^\infty dse^{-\eta s}\left\{\mathrm{Tr}\left(f_{F-D}(H_0(N))e^{-isH_0(N)}Q_\beta^{(N)}e^{isH_0(N)}j_\alpha\right)\right.\\ -\;&\left.\mathrm{Tr}\left(f_{F-D}(H_0(N))e^{isH_0(N)}j_\alpha e^{-isH_0(N)}Q_\beta^{(N)}\right)\right\}. \end{aligned}$$

It is clear that it is enough to prove an estimate as in (4.19) for just one of the terms in (4.20). Define

$$A_{\alpha\beta}(N) := \int_0^\infty e^{-\eta s}\mathrm{Tr}\left(f_{F-D}(H_0(N))e^{-isH_0(N)}Q_\beta^{(N)}e^{isH_0(N)}j_\alpha\right)ds. \quad (4.21)$$

Since $||H_0(N)|| \leq const$ uniformly in N, it means that we can find an interval $[a,b]$ independent of N so that the spectrum of $H_0(N)$ is included in it. Define the function $\phi_0 \in C_0^\infty(\mathbb{R})$, $0 \leq \phi_0 \leq 1$, $\mathrm{supp}(\phi_0) \subset (-1+a, b+1)$ and

$$\phi_0(x) = \frac{1}{e^{\beta(x-\mu)}+1}, \quad x \in (a,b). \quad (4.22)$$

Also define for every $s > 0$ the function

$$\phi_s(x) := \phi_0(x)e^{-isx}. \tag{4.23}$$

Clearly, $f_{F-D}(H_0(N))e^{-isH_0(N)} = \phi_s(H_0(N))$. Assume that $\tilde{\phi}_0$ is an almost analytic extension of ϕ_0, supported in the strip

$$\text{supp}(\tilde{\phi}_0) \subset (-1+a, b+1) \times (-\eta/2, \eta/2) \subset \mathbb{C}, \tag{4.24}$$

and such that

$$\sup_{-1+a \leq x \leq b+1} |\overline{\partial}\tilde{\phi}_0(x+iy)| \leq const \cdot |y|^P, \quad |y| \leq \eta/2, \tag{4.25}$$

where P is any previously given positive integer. Because e^{-isz} is entire as function of z, an almost analytic extension for ϕ_s is simply $\tilde{\phi}_s(z) := \tilde{\phi}_0(z)e^{-isz}$. The Helffer-Sjöstrand formula reads as (see for example [12])

$$\phi_s(H_0(N)) = \frac{1}{\pi}\int_{\text{supp}(\tilde{\phi}_0)} (\overline{\partial}\tilde{\phi}_0(x+iy))e^{-isx+sy}(H_0(N)-x-iy)^{-1}dx\, dy.$$

We will use the following technical result:

Proposition 4.3. *Let $F : \mathbb{C} \to \mathbb{C} \setminus \mathbb{R}$ be smooth. Assume that for $x+iy$ in the support of $\tilde{\phi}_0$, we can find two positive integers k_1 and $k_2 \leq P$, such that we have the estimate*

$$|F(x+iy)| \leq const \cdot \frac{1}{N^{k_1}|y|^{k_2}}, \quad x+iy \in \text{supp}(\tilde{\phi}_0),\ y \neq 0. \tag{4.26}$$

Then

$$\int_{\text{supp}(\tilde{\phi}_0)} |\overline{\partial}\tilde{\phi}_0(z)| \cdot |F(z)| dxdy \leq const \cdot \frac{1}{N^{k_1}}. \tag{4.27}$$

Clearly, the proposition is immediately implied by (4.25) and (4.26) and it does not require further details.

We can introduce the expression of $\phi_s(H_0(N))$ in (4.21)and perform the integral with respect to s; the interchange of integrals is permitted because on the support of $\tilde{\phi}_0$ we have $|y| < \eta$. In order to simplify the writing, we denote $x+iy = z$ and $dx\, dy$ by d^2z. Then forgetting about irrelevant constants, we have that $A_{\alpha\beta}(N)$ is proportional to:

$$\int_{\text{supp}(\tilde{\phi}_0)} \overline{\partial}\tilde{\phi}_0(z)\ \text{Tr}\left((H_0(N)-z)^{-1}Q_\beta^{(N)}(H_0(N)-z+i\eta)^{-1}j_\alpha\right) d^2z. \tag{4.28}$$

Next we want to simplify the above trace, by expressing Q_β with the help of the current operator j_β. Denote by $z' = z - i\eta$. We have (see (4.8) and (4.9))

$$\begin{aligned} j_\beta &= -i[Q_\beta^{(N)}, H_0(N)] \\ &= -i\left(Q_\beta^{(N)}(H_0(N) - z') - (H_0(N) - z)Q_\beta^{(N)}\right) - i(z' - z)Q_\beta^{(N)}, \end{aligned}$$

then using obvious notation for the resolvents:

$$\begin{aligned} R_0(N,z)Q_\beta^{(N)}R_0(N,z') &= \frac{1}{z'-z}\{iR_0(N,z)j_\beta R_0(N,z') \\ &+ Q_\beta^{(N)}R_0(N,z') - R_0(N,z)Q_\beta^{(N)}\}. \end{aligned} \tag{4.29}$$

Inserting this back into (4.28) we have a number of terms which have to be treated separately. We only deal with one of them, namely the term proportional up to irrelevant constants with

$$\int_{\mathrm{supp}(\tilde\phi_0)} \overline{\partial}\tilde\phi_0(z)\ \mathrm{Tr}\left(R_0(N,z)Q_\beta^{(N)}j_\alpha\right) d^2z. \tag{4.30}$$

Since $Q_\beta^{(N)}j_\alpha = -i\tau\delta_{\alpha\beta}|0_\alpha\rangle\langle\alpha_S|$, introducing it back again and performing the trace, we obtain up to some constants (see (4.16))

$$\delta_{\alpha\beta}\int_{\mathrm{supp}(\tilde\phi_0)} \overline{\partial}\tilde\phi_0(z)\ \langle\alpha_S, (H_{\mathrm{eff}}(N,z) - z)^{-1}\alpha_S\rangle\langle 0_\alpha, R^L(N,z)0_\alpha\rangle d^2z. \tag{4.31}$$

The next step is to replace the quantities involving finite leads with the ones corresponding to semi-infinite leads. Let J be an arbitrarily large integer. We see that one term we have to look at in connection with (4.31) is

$$F_1(z) := \langle\alpha_S, (H_{\mathrm{eff}}(N,z) - z)^{-1}\alpha_S\rangle \cdot (\langle 0_\alpha, R^L(N,z)0_\alpha\rangle - \langle 0_\alpha, R^L(z)0_\alpha\rangle).$$

An application of (6.15) and (6.18) yields the estimate

$$\left|\langle 0_\alpha, R^L(N,z)0_\alpha\rangle - \langle 0_\alpha, R^L(z)0_\alpha\rangle\right| \leq const \cdot \frac{1}{|\Im(z)|^2} e^{-2cN|\Im(z)|}, \tag{4.32}$$

uniformly in z on the support of $\tilde\phi_0$, with $\Im(z) \neq 0$. Notice that (3.3) is also true at finite N, and this gives an upper bound of order $1/|\Im(z)|$ on the first factor in $F_1(z)$. We finally obtain:

$$|F_1(z)| \leq const \cdot \frac{1}{|\Im(z)|^3} e^{-2cN|\Im(z)|}, \tag{4.33}$$

uniformly in z on the support of $\tilde{\phi}_0$, with $\Im(z) \neq 0$. But this implies

$$|F_1(z)| \leq const \cdot \frac{1}{|\Im(z)|^{3+J}} N^{-J}. \tag{4.34}$$

Now choose $\tilde{\phi}_0$ to have a decay in y near the real axis with an exponent P larger than $J+3$ (see (4.25)). Then (4.27) implies that the integral of F_1 times $\overline{\partial}\tilde{\phi}_0$ will decay at least like N^{-J}.

Another type of term one needs to estimate can be put into the form

$$\begin{aligned} & F_2(z) := \langle 0_\alpha, R^L(z) 0_\alpha \rangle \\ \cdot \quad & \left[\langle \alpha_S \left(H_{\text{eff}}(N,z) - z \right)^{-1} \alpha_S \rangle - \langle \alpha_S \left(H_{\text{eff}}(z) - z \right)^{-1} \alpha_S \rangle \right]. \end{aligned} \tag{4.35}$$

Using the identity $A^{-1} - B^{-1} = A^{-1}(B-A)B^{-1}$, and the expression (3.2) which is valid for both effective Hamiltonians, we reduce the problem to the estimate from (4.32), but in addition we have some other terms which are each bounded from above by $1/|\Im(z)|$. We eventually get the estimate

$$|F_2(z)| \leq const \cdot \frac{1}{|\Im(z)|^5} e^{-2cN|\Im(z)|}, \tag{4.36}$$

and then we reason as before.

Concluding, we proved that the difference between a term as in (4.31) at finite N, and a similar term "with infinite leads", decays faster than any integer power of N. We consider that (4.19), thus the lemma, to be proven. □

4.2.3 Taking the adiabatic limit: $\eta \searrow 0$

The next limit to be performed is the adiabatic limit. Thus we define

$$g_{\alpha\beta}(T,\mu) := \lim_{\eta \searrow 0} g_{\alpha\beta}(T,\mu,\eta,\infty) \tag{4.37}$$

where $g_{\alpha\beta}(T,\mu,\eta,\infty)$ is given by (4.18). The idea is again to use the resolvent properties as we did in the previous section, one important difference now being that we have to use the Stone formula instead of Helffer-Sjöstrand's. The computations will also be more involved in this case. From (4.18) we have

$$\begin{aligned} g_{\alpha\beta}(T,\mu,\eta,\infty) &= -i \int_0^\infty ds e^{-\eta s} \text{Tr}_{\mathcal{H}} \big(f_{F-D}(K) e^{-isK} Q_\beta e^{isK} j_\alpha \\ &- j_\alpha e^{-isK} Q_\beta e^{isK} f_{F-D}(H) \big) \end{aligned}$$

We note that in the above formula appears again $f_{F-D}(K)e^{-isK}$ and its adjoint. We will express them using the Stone formula. Recall now that K can have point spectrum outside the interval $[-2t_L, 2t_L]$; we also assumed that $\pm 2t_L$ are not eigenvalues. We will see in the next section that K might have embedded eigenvalues in $(-2t_L, 2t_L)$ (see Proposition 5.4).

Consider without loss of generality that there is only one eigenvalue E_1 outside $[-2t_L, 2t_L]$, P_1 being the corresponding projector. Then from the Stone formula one has

$$\begin{aligned} f_{F-D}(K)e^{-isK} &= \lim_{\varepsilon\to 0}\int_{-2t_L}^{2t_L} dE f_{F-D}(E)e^{-isE}\frac{1}{\pi}\Im R(E+i\varepsilon) \\ &+ f_{F-D}(E_1)e^{-isE_1}P_1 \end{aligned} \tag{4.38}$$

Now we follow the same steps as in Section 4.2.2, namely we perform the integrals over s and we get

$$\begin{aligned} g_{\alpha\beta}(T,\mu,\eta,\infty) &= \frac{i}{2\pi}\lim_{\varepsilon\to 0}\int_{-2t_L}^{2t_L} dE f_{F-D}(E)\mathrm{Tr}_{\mathcal{H}}\left(M_{\alpha\beta}(E,\eta,\varepsilon)\right) \\ &+ f_{F-D}(E_1)\mathrm{Tr}_{\mathcal{H}}(P_1Q_\beta R(E_1-i\eta)j_\alpha + j_\alpha R(E_1+i\eta)Q_\beta P_1) \end{aligned} \tag{4.39}$$

where we denoted

$$\begin{aligned} M_{\alpha\beta}(E,\eta,\varepsilon) &:= (R(E+i\varepsilon)-R(E-i\varepsilon))Q_\beta R(E-i\eta)j_\alpha \\ &+ j_\alpha R(E+i\eta)Q_\beta(R(E+i\varepsilon)-R(E-i\varepsilon)) \end{aligned} \tag{4.40}$$

We start with the terms arising from the eigenvalue E_1, and show that in the limit $\eta \searrow 0$ they give no contribution. First we use again a trick to introduce current operators instead of charge operators, namely we write

$$\begin{aligned} P_1 j_\beta R(E_1-i\eta) &= iP_1[K-(E_1-i\eta), Q_\beta]R(E_1-i\eta) \\ &= -\eta P_1 Q_\beta R(E_1-i\eta) - iP_1Q_\beta \end{aligned} \tag{4.41}$$

from where we get

$$P_1Q_\beta R(E_1-i\eta) = -\frac{1}{\eta}P_1 j_\beta R(E_1-i\eta) - \frac{i}{\eta}P_1Q_\beta \tag{4.42}$$

Then replacing $P_1 Q_\beta R(E_1 - i\eta)$ and its adjoint in the second term from (4.39) we obtain

$$
\begin{aligned}
&-\mathrm{Tr}_{\mathcal{H}}(P_1 Q_\beta R(E_1 - i\eta) j_\alpha + j_\alpha R(E_1 + i\eta) Q_\beta P_1) \\
&= \frac{1}{\eta} \mathrm{Tr}_{\mathcal{H}}(j_\alpha R(E_1 + i\eta) j_\beta P_1 + j_\alpha P_1 j_\beta R(E_1 - i\eta) + i(P_1 Q_\beta j_\alpha - j_\alpha Q_\beta P_1))
\end{aligned}
$$

and we can see right away that the last two terms dissapear when $\alpha \neq \beta$. The singularities appearing in resolvents can be isolated by writing

$$
R(E_1 \pm i\eta) = \pm i \frac{P_1}{\eta} + \frac{1}{2\pi i} \int_{|z-E_1|=\epsilon} \frac{1}{z - (E_1 \pm i\eta)} (K - z)^{-1} dz \quad \text{with}\, \epsilon > \eta. \tag{4.43}
$$

We also write P_1 as a Riesz integral

$$
P_1 = \frac{i}{2\pi} \int_{|z'-E_1|=\epsilon'} R(z') dz' \quad \text{with}\, \epsilon' < \epsilon. \tag{4.44}
$$

By looking at (4.43) we see that the singular term equal to

$$
\frac{1}{\eta^2} \mathrm{Tr}_{\mathcal{H}} \{ j_\alpha P_1 j_\beta P_1 \}
$$

is in fact identically zero, due to

$$
P_1 j_\alpha P_1 = i P_1 [K, Q_\alpha] P_1 = i P_1 [K - E_1, Q_\alpha] P_1 = 0. \tag{4.45}
$$

Thus we are only left wih the regular part from (4.43). Replace it in (4.43), together with P_1 expressed as in (4.44). We have

$$
\begin{aligned}
&\frac{1}{\eta} \mathrm{Tr}_{\mathcal{H}} \{ j_\alpha R(E_1 + i\eta) j_\beta P_1 + j_\alpha P_1 j_\beta R(E_1 - i\eta) \} \\
= &\frac{1}{4\pi^2 \eta} \int_{|z-E_1|=\epsilon} dz \int_{|z'-E_1|=\epsilon'} dz' F_{\alpha\beta}(z, z', \eta),
\end{aligned} \tag{4.46}
$$

where we used the notation

$$
\begin{aligned}
F_{\alpha\beta}(z, z', \eta) \;:=\; &\frac{1}{z - (E_1 + i\eta)} \mathrm{Tr}_{\mathcal{H}} \left(j_\alpha R(z) j_\beta R(z') \right) \\
+ &\frac{1}{z - (E_1 - i\eta)} \mathrm{Tr}_{\mathcal{H}} \left(j_\alpha R(z') j_\beta R(z) \right).
\end{aligned} \tag{4.47}
$$

To go further with the computations we need a technical lemma that gives a general expression for $\mathrm{Tr}_{\mathcal{H}}\left(j_\alpha R(z) j_\beta R(z')\right)$.

Lemma 4.4. *Let $u_{\alpha\beta}(z)$ be the function introduced in Prop. 3.1. Then the following identity holds ($\alpha \neq \beta$):*

$$\mathrm{Tr}_{\mathcal{H}}(j_\alpha R(z) j_\beta R(z')) = \frac{\tau^4}{t_L^2} \left(\zeta_1(z) - \zeta_1(z')\right)^2 u_{\alpha\beta}(z) u_{\beta\alpha}(z'). \tag{4.48}$$

Proof. Taking into account the explicit form of j_α and j_β

$$\begin{aligned} & \mathrm{Tr}_{\mathcal{H}}\left((j_\alpha R(z) j_\beta R(z')\right) \\ = \; & -\tau^2 \{ \langle \alpha, R(z) 0_\beta \rangle \langle \beta, R(z') 0_\alpha \rangle - \langle \alpha, R(z)\beta \rangle \langle 0_\beta, R(z') 0_\alpha \rangle \\ - \; & \langle 0_\alpha, R(z) 0_\beta \rangle \langle \beta, R(z')\alpha \rangle + \langle 0_\alpha, R(z)\beta \rangle \langle 0_\beta, R(z')\alpha \rangle \}. \end{aligned}$$

Each term is computed then using the Feshbach formula for $R(z)$

$$\begin{aligned} \langle \alpha, R(z) 0_\beta \rangle \langle \beta, R(z') 0_\alpha \rangle &= \tau^2 \langle \alpha, R_{\text{eff}}(z)\beta \rangle \langle 0_\beta, R^L(z) 0_\beta \rangle \\ &\cdot \; \langle \beta, R_{\text{eff}}(z')\alpha \rangle \langle 0_\alpha, R^L(z') 0_\alpha \rangle \\ \langle \alpha, R(z)\beta \rangle \langle 0_\beta, R(z') 0_\alpha \rangle &= \tau^2 \langle \alpha, R_{\text{eff}}(z)\beta \rangle \langle 0_\beta, R^L(z') 0_\beta \rangle \\ &\cdot \; \langle \beta, R_{\text{eff}}(z')\alpha \rangle \langle 0_\alpha, R^L(z') 0_\alpha \rangle \\ \langle 0_\alpha, R(z) 0_\beta \rangle \langle \beta, R(z')\alpha \rangle &= \tau^2 \langle 0_\alpha, R^L(z) 0_\alpha \rangle \langle \alpha, R_{\text{eff}}(z)\beta \rangle \\ &\cdot \; \langle 0_\beta, R^L(z) 0_\beta \rangle \langle \beta, R_{\text{eff}}(z')\alpha \rangle \\ \langle 0_\alpha, R(z)\beta \rangle \langle 0_\beta, R(z')\alpha \rangle &= \tau^2 \langle 0_\alpha, R^L(z) 0_\alpha \rangle \langle \alpha, R_{\text{eff}}(z)\beta \rangle \\ &\cdot \; \langle 0_\beta, R^L(z') 0_\beta \rangle \langle \beta, R_{\text{eff}}(z')\alpha \rangle. \end{aligned}$$

Moreover, we can also use the expression for the matrix elements of the resolvent R_L, which proves the lemma. □

Now turning back to (4.47) and using the lemma we arrive at

$$\begin{aligned} \frac{t_L^2}{\tau^4} F_{\alpha\beta}(z, z', \eta) &= \frac{1}{z - (E_1 + i\eta)} \left(\zeta_1(z) - \zeta_1(z')\right)^2 u_{\alpha\beta}(z) u_{\beta\alpha}(z') \\ &+ \frac{1}{z - (E_1 - i\eta)} \left(\zeta_1(z) - \zeta_1(z')\right)^2 u_{\alpha\beta}(z') u_{\beta\alpha}(z). \end{aligned}$$

Now we have to handle the contour integrals in (4.46). Notice that $u_{\alpha\beta}(z)$ is singular around E_1. However, due to the equivalence (3.3) and relation (4.43) we have (with $\epsilon_1 > \epsilon$):

$$u_{\alpha\beta}(z) = \langle \alpha_S, P_1 \beta_S \rangle \frac{1}{E_1 - z} + \frac{1}{2\pi i} \int_{|z_1 - E_1| = \epsilon_1} dz_1 \frac{1}{z_1 - z} \langle \alpha_S, R(z_1) \beta_S \rangle . \quad (4.49)$$

Remember that we have $\epsilon_1 > \epsilon > \epsilon'$. Replacing the u's in (4.47) we obtain a lot of terms. The most singular one is of the form (we omit the contours and other constants for simplicity)

$$A_1 := \frac{1}{\eta} \int dz \int dz' \left(\frac{1}{z - (E_1 + i\eta)} + \frac{1}{z - (E_1 - i\eta)} \right) \frac{(\zeta_1(z) - \zeta_1(z'))^2}{(E_1 - z) \cdot (E_1 - z')} . \quad (4.50)$$

By the residue theorem :

$$A_1 = \frac{(2\pi)^2 i}{\eta^2} \left((\zeta_1(E_1 - i\eta) - \zeta_1(E_1))^2 - (\zeta_1(E_1 + i\eta) - \zeta_1(E_1))^2 \right) .$$

Writing the Taylor series for $\zeta_1(E_1 \pm i\eta)$, one is left inside the paranthesis with an expression of order η^3, and A_1 vanishes in the limit $\eta \to 0$.

Next, take one of the terms involving the singular part of $u_{\alpha\beta}(z)$ and the regular part of $u_{\alpha\beta}(z')$ (we omit for the moment the constants t_L,τ as well as the matrix elements of P_1)

$$A_2 = \frac{1}{\eta} \int dz \int dz' \frac{(\zeta_1(z) - \zeta_1(z'))^2}{z - (E_1 + i\eta)} \cdot \frac{1}{E_1 - z} \int \frac{dz_1}{z_1 - z'} u_{\alpha\beta}(z_1). \quad (4.51)$$

We see that the integral with respect to z' only involves analytic functions in the disk $|E_1 - z'| < \epsilon'$, therefore the integral vanishes.

Another term coming from the singular part of $u_{\alpha\beta}(z')$ and the regular part of $u_{\alpha\beta}(z)$ is the following:

$$\begin{aligned} A_3 &:= \frac{1}{\eta} \int dz \int dz' \frac{(\zeta_1(z) - \zeta_1(z'))^2}{z - (E_1 + i\eta)} \cdot \frac{1}{E_1 - z'} \int \frac{dz_1}{z_1 - z} u_{\alpha\beta}(z_1) \\ &= -\frac{2\pi i}{\eta} \int dz \frac{(\zeta_1(z) - \zeta_1(E_1))^2}{z - (E_1 + i\eta)} \int \frac{dz_1}{z_1 - z} u_{\alpha\beta}(z_1), \end{aligned} \quad (4.52)$$

where in the second line we performed the integral with respect to z'. We can also perform the integral with respect to z and get something proportional with

$$\frac{1}{\eta}\left(\zeta_1(E_1+i\eta)-\zeta_1(E_1)\right)^2\int\frac{dz_1}{z_1-E_1}u_{\alpha\beta}(z_1).$$

Using again the Taylor series we see that $A_3 \sim \eta$, thus it will dissapear as well. The same thing happens with all the other terms.

Looking back at (4.39), we continue with the contribution of $M_{\alpha\beta}$. Let us first bring $M_{\alpha\beta}(E,\eta,\varepsilon)$ to a suitable form. Using (4.29) it turns out that

$$M_{\alpha\beta}(E,\eta,\varepsilon)=M^{(1)}_{\alpha\beta}(E,\eta,\varepsilon)+M^{(2)}_{\alpha\beta}(E,\eta,\varepsilon) \tag{4.53}$$

where

$$\begin{aligned} & M^{(1)}_{\alpha\beta}(E,\eta,\varepsilon) \\ := \ & \frac{1}{\eta-\varepsilon}(j_\alpha R(E-i\varepsilon)j_\beta R(E-i\eta)-j_\alpha R(E+i\eta)j_\beta R(E+i\varepsilon)) \\ - \ & \frac{1}{\eta+\varepsilon}(j_\alpha R(E+i\varepsilon)j_\beta R(E-i\eta)-j_\alpha R(E+i\eta)j_\beta R(E-i\varepsilon)), \end{aligned} \tag{4.54}$$

while $M^{(2)}_{\alpha\beta}$ includes all terms with only one resolvent. Since $\alpha\neq\beta$, and using the trace cyclicity, the trace of $M^{(2)}_{\alpha\beta}$ is zero and we are only left with $M^{(1)}_{\alpha\beta}$:

$$g_{\alpha\beta}(T,\mu)=\lim_{\eta\searrow 0}\lim_{\epsilon\searrow 0}\frac{i}{2\pi}\int_{-2t_L}^{2t_L}dE f_{F-D}(E)\mathrm{Tr}_{\mathcal{H}}\left(M^{(1)}_{\alpha\beta}(E,\eta,\epsilon)\right). \tag{4.55}$$

Now we apply again the identity (4.48) and we use the meromorphic extensions of $u_{\alpha\beta}(z)$ (see Prop 3.1) and the properties of $\zeta_1(z)$. The result is

$$g_{\alpha\beta}(T,\mu)=\lim_{\eta\searrow 0}\lim_{\epsilon\searrow 0}\frac{\tau^4}{t_L^2}\frac{i}{2\pi}\int_{-2t_L}^{2t_L}dE f_{F-D}(E)\left(\frac{C_{\alpha\beta}(E,\eta,\epsilon)}{\eta-\epsilon}-\frac{D_{\alpha\beta}(E,\eta,\epsilon)}{\eta+\epsilon}\right). \tag{4.56}$$

with the following notations (see also (3.7) and (3.12)):

$$\begin{aligned} C_{\alpha\beta}(E,\eta,\epsilon) \ := \ & \left(\zeta_-(E-i\epsilon)-\zeta_-(E-i\eta)\right)^2 u^-_{\alpha\beta}(E-i\epsilon)u^-_{\beta\alpha}(E-i\eta) \\ - \ & \left(\zeta_+(E+i\eta)-\zeta_+(E+i\epsilon)\right)^2 u^+_{\alpha\beta}(E+i\eta)u^+_{\beta\alpha}(E+i\epsilon) \end{aligned} \tag{4.57}$$

$$\begin{aligned} D_{\alpha\beta}(E,\eta,\epsilon) \ := \ & \left(\zeta_+(E+i\epsilon)-\zeta_-(E-i\eta)\right)^2 u^+_{\alpha\beta}(E+i\epsilon)u^-_{\beta\alpha}(E-i\eta) \\ - \ & \left(\zeta_+(E+i\eta)-\zeta_-(E-i\epsilon)\right)^2 u^+_{\alpha\beta}(E+i\eta)u^-_{\beta\alpha}(E-i\epsilon) \end{aligned} \tag{4.58}$$

Since $u^{\pm}(z)$ are smooth near the real axis and $\zeta_{\pm}$ have good behavior one can take at once the limit $\epsilon \searrow 0$ in (4.57) and (4.58). In the following we show that $C_{\alpha\beta}$ vanishes in the limit $\eta \searrow 0$. To see this we write for example

$$\zeta_+(E+i\eta) - \zeta_+(E) = -i\int_0^\eta (\partial_y \zeta_+(E+iy))dy \tag{4.59}$$

and use the explicit form of ζ_+ to obtain the estimate

$$|\partial_y \zeta_+(E+iy)| \leq const \cdot \frac{1}{\sqrt{4t_L^2 - E^2}} \tag{4.60}$$

which shows that $\frac{1}{\eta} C_{\alpha\beta} \sim \eta$ from where the result follows.
The last step is to deal with

$$g_{\alpha\beta}(T,\mu) = -\lim_{\eta\searrow 0} \frac{\tau^4}{t_L^2}\frac{i}{2\pi}\int_{-2t_L}^{2t_L} f_{F-D}(E)\frac{D_{\alpha\beta}(E,\eta,0_+)}{\eta}\, dE. \tag{4.61}$$

One remarks that with the notation

$$F(E,\eta) := (\zeta_+(E+i\eta) - \zeta_-(E))^2 u_{\alpha\beta}^+(E+i\eta) u_{\beta\alpha}^-(E)$$

we have $D_{\alpha\beta}(E,\eta,0_+) = -2i\Im F(E,\eta)$ and

$$g_{\alpha\beta}(T,\mu) = -\lim_{\eta\searrow 0} \frac{\tau^4}{t_L^2}\frac{1}{\pi}\int_{-2t_L}^{2t_L} f_{F-D}(E)\frac{\Im F(E,\eta)}{\eta}\, dE. \tag{4.62}$$

Using (3.12) and (6.4) we see that $\Im F(E, i0_+) = 0$ and

$$\Re F(E,0_+) = -4[\Im\zeta_+(E)]^2 \cdot |u_{\alpha\beta}^+(E)|^2.$$

Taking the limit $\eta \searrow 0$, we obtain in the integral the term $(\partial_\eta \Im F)(E,0_+)$. Using the Cauchy-Riemann equations for u^+ and ζ_+, we get after some work that we can replace $(\partial_\eta \Im F)(E,0_+)$ by $(1/2) \times \partial_E \Re F(E,0_+)$. This also shows that F is not analytic.

Integrating by parts and noticing that $\zeta_+(\pm 2t_L) - \zeta_-(\pm 2t_L) = 0$ we proved the following lemma:

Lemma 4.5. *The conductance coefficients $g_{\alpha\beta}(T,\mu)$ defined in (4.37) are given by the relation*

$$g_{\alpha\beta}(T,\mu) = -\frac{4\tau^4}{t_L^2}\frac{1}{2\pi}\int_{-2t_L}^{2t_L} dE \frac{\partial f_{F-D}(E)}{\partial E}\left(\Im\zeta_+(E)\right)^2 |u_{\alpha\beta}^+(E)|^2. \tag{4.63}$$

4.3 Ending the proof of the main theorem

Before giving the final step for the proof of the Landauer- Büttiker formula let us briefly review what we have done in this section. We started with the scattering problem associated to the semi-infinite leads case, the transmission between two leads being found in Eq.(4.6). The rest of the work has been done to obtain explicit expressions for the conductance coefficients given by the Kubo-type formula (4.17) when the thermodynamic and adiabatic limits are taken.

To finish the proof of Theorem 2.1 there is not much to be done. First, use the explicit expressions for $\zeta_{\pm}(\cdot)$, together with the definition of the Fermi 'momentum', $E = 2t_L \cos(k_E)$ in (4.63). The result is

$$g_{\alpha\beta}(T,\mu) = -\frac{4\tau^4}{t_L^2}\frac{1}{2\pi}\int_{-2t_L}^{2t_L} dE \frac{\partial f_{F-D}(E)}{\partial E} \sin^2(k_E)|u_{\alpha\beta}^{+}(E)|^2. \tag{4.64}$$

Now comparing (4.64) and (4.6) one obtains (2.23) and we are done. Notice that when $T \to 0$ we have $-\partial_E f_{F-D} \to \delta(E-\mu)$ and (2.24) follows.

The presence of $\frac{1}{2\pi}$ in those equations is not an accident. It makes more sense if one carefully includes in computations the physical constants e and $\hbar$ (we have been working until now with the convention $e = \hbar = 1$). Without giving details, we assure the reader that in the end the equality in (2.24) becomes

$$g_{\alpha\beta}(0_+,\mu) = \frac{e^2}{2\pi\hbar}\mathcal{T}_{\alpha\beta}(\mu) = \frac{e^2}{h}\mathcal{T}_{\alpha\beta}(\mu), \tag{4.65}$$

which is nothing else but the well-known Landauer formula at zero temperature. Remark that when the total particle density is fixed, then μ represents the Fermi energy of our system. When the leads become infinite, the sample does not contribute to the thermodynamic limit thus the Fermi energy is fixed by the leads. The proof of Theorem 2.1 is complete. □

5 Resonant transport in a quantum dot

Up to now we allowed τ to be arbitrarily large, together with the assumption that the Hamilton operator for the system with semi-infinite leads K had no eigenvalues at $\pm 2t_L$. In this section we are interested in small coupling, that is when $\tau \to 0$.

Assume that the Hamiltonian describing the sample H^S has $J \geq 1$ (possibly degenerate) eigenvalues $\{E_1, \ldots, E_J\}$ so that

$$\sigma(H^S) \cap [-2t_L, 2t_L] = \{E_1, \ldots, E_J\} \subset (-2t_L, 2t_L). \tag{5.1}$$

We are not interested in possible eigenvalues outside $[-2t_L, 2t_L]$ since for small τ they will still remain discrete eigenvalues for K and we saw that they do not contribute to transport. Now we focus on the influence of $\{E_1, \dots, E_J\}$ on the transport properties when τ is small.

Let us give the main result of this section. We consider the transmittance (see (4.6)) between the leads β and γ. Assume that all eigenvalues $\{E_1, \dots, E_J\} \subset (-2t_L, 2t_L)$ of H^S are nondegenerate. The normalized eigenvector corresponding to E_j is denoted by ϕ_j.

Proposition 5.1. *(i). For every $\lambda \in (-2t_L, 2t_L) \setminus \{E_1, \dots, E_J\}$ we have*

$$\lim_{\tau \searrow 0} \mathcal{T}_{\beta\gamma}(\lambda, \tau) = 0. \tag{5.2}$$

(ii). Fix $\lambda = E_j$. If either $\langle \beta_S, \phi_j \rangle$ or $\langle \gamma_S, \phi_j \rangle$ is zero, then

$$\lim_{\tau \searrow 0} \mathcal{T}_{\beta\gamma}(E_j, \tau) = 0. \tag{5.3}$$

(iii). Fix $\lambda = E_j$. If both $\langle \beta_S, \phi_j \rangle$ and $\langle \gamma_S, \phi_j \rangle$ are different from zero, then there exists a positive constant $C_j(E_j)$ such that

$$\lim_{\tau \searrow 0} \mathcal{T}_{\beta\gamma}(E_j, \tau) = C_j \left| \frac{\langle \beta_S, \phi_j \rangle \cdot \langle \gamma_S, \phi_j \rangle}{\sum_{\alpha=1}^{M} |\langle \alpha_S, \phi_j \rangle|^2} \right|^2. \tag{5.4}$$

Remark. The physical significance of this proposition is quite transparent. It states that at small coupling, the following things happen: 1. If the energy of the incident electron is not close to the eigenvalues of H^S, it will not contribute to the current. 2. If the incident energy is close to some eigenvalue E_j, but the eigenfunction ϕ_j is not localized around both coupling points γ_S and β_S, then again there is no current. 3. In order to have a peak in the current, it is necessary for H^S to have extended edge states, which couple several leads. A numerical analysis of the Harper operator on large domains with Dirichlet boundary conditions puts into evidence such extended edge states as well as the existence of bulk states concentrated in the middle of the dot (see [21] and [27]).

Proof. We split the proof into several technical results. We will not assume that E_j's are nondegenerate unless stated otherwise.

Lemma 5.2. *Consider $u_{\beta\gamma}$ given in (3.7), and $u^+_{\beta\gamma}$ its meromorphic extension. Then*

$$\lim_{\tau \searrow 0} \left(\tau^2 \sup_{\lambda \in (-2t_L, 2t_L)} |u^+_{\beta\gamma}(\lambda, \tau)| \right) < \infty.$$

Proof. Notice that the lemma roughly says that $u^+_{\beta\gamma}(\lambda)$ cannot blow up worse than $1/\tau^2$ when τ is small. In other words, its eventual poles have an imaginary part of order τ^2 when τ is small.

Clearly, if τ is smaller than some $\tau_0 > 0$, then by usual perturbation theory we get that for all λ located outside some small discs (with radii determined by τ_0) centered at $\{E_j\}_{j=1}^J$ (the eigenvalues of H^S), we have

$$||(H_+(\lambda) - \lambda)^{-1}|| \leq C \max_{j\in\{1,\ldots,J\}} |E_j - \lambda|^{-1},$$

thus we only need to look at what happens in each interval of the form $(E_j - \epsilon, E_j + \epsilon)$.

Assume that E_j is n-fold degenerate. Denote by Π_j the n-dimensional projector corresponding to E_j. The operator $\Pi_j \Pi^T \Pi_j$ has a (possibly trivial) null space in $\mathrm{Ran}(\Pi_j)$, and denote by p_j the projector corresponding to it. Denote by $\tilde{p}_j = \Pi_j - p_j$ the projection corresponding to the orthogonal complement of $\mathrm{Ran}(p_j)$ in $\mathrm{Ran}(\Pi_j)$. It is easy to see that there exists a positive constant C_j such that

$$\tilde{p}_j \Pi^T \tilde{p}_j \geq C_j \tilde{p}_j^2. \tag{5.5}$$

Indeed, this is implied by the fact that the operator is non-negative and with trivial null space.

Denote by $q_j = \mathrm{Id} - p_j$. Since $\Pi^T p_j = 0$, and reasoning as in (3.9) we have

$$(H_+(\lambda) - \lambda)^{-1} - (E_j - \lambda)^{-1} p_j = q_j [q_j (H_+(\lambda) - \lambda) q_j]^{-1} q_j.$$

Only the right hand side will contribute to $u^+_{\beta\gamma}$ since $p_j \gamma_S = 0$. The proposition would be proven if we can show the estimate (on $\mathrm{Ran}(q_j)$)

$$||[q_j (H_+(\lambda) - \lambda) q_j]^{-1}|| \leq C/\tau^2 \tag{5.6}$$

for λ near E_j.

Notice that $q_j = \tilde{p}_j + (\mathrm{Id} - \Pi_j)$, i.e. it is the orthogonal sum of some part of Π_j and the projectors corresponding to all other eigenvalues of H^S different from E_j. Denote by $A_j := q_j (H_+(\lambda) - \lambda) q_j$.

Remark that $(\mathrm{Id} - \Pi_j) A_j (\mathrm{Id} - \Pi_j)$ is well-behaved when λ is close to E_j because it essentially equals $(\mathrm{Id} - \Pi_j)(H^S - \lambda)(\mathrm{Id} - \Pi_j)$ plus a perturbation of order τ^2. Applying the Neumann series again, we get that on $\mathrm{Ran}(\mathrm{Id} - \Pi_j)$:

$$||[(\mathrm{Id} - \Pi_j) A_j (\mathrm{Id} - \Pi_j)]^{-1}|| \leq const \tag{5.7}$$

for λ close to E_j and τ small enough. Hence if $\tilde{p}_j = 0$, this estimate implies

$$||[q_j (H_+(\lambda) - \lambda) q_j]^{-1}|| \leq const \tag{5.8}$$

which implies (5.6) and we are done.

If $\tilde{p}_j \neq 0$, we again apply the Feshbach lemma for the operator A_j, intending to reduce the problem to the subspace $\mathrm{Ran}(\tilde{p}_j)$. Then A_j is invertible in $\mathrm{Ran}(q_j)$ iff the operator

$$X_j := \tilde{p}_j A_j \tilde{p}_j - \tilde{p}_j A_j (\mathrm{Id} - \Pi_j)[(\mathrm{Id} - \Pi_j) A_j (\mathrm{Id} - \Pi_j)]^{-1} (\mathrm{Id} - \Pi_j) A_j \tilde{p}_j \quad (5.9)$$

is invertible in $\mathrm{Ran}(\tilde{p}_j)$, and their inverses will have the same estimate on their norm when τ is small. It is not difficult to see that the second term in (5.9) is of order τ^4 when λ is near E_j. We can then write

$$X_j = \tilde{p}_j A_j \tilde{p}_j + \mathcal{O}(\tau^4). \quad (5.10)$$

But the operator

$$\tilde{p}_j A_j \tilde{p}_j = E_j - \lambda - (\tau^2/t_L)\zeta_+(\lambda)\tilde{p}_j \Pi^T \tilde{p}_j \quad (5.11)$$

is one to one (thus invertible) because for every $f \in \mathrm{Ran}(\tilde{p}_j)$ with norm one we have (see also (6.4))

$$||\tilde{p}_j A_j \tilde{p}_j\, f|| \geq |\langle f, A_j f\rangle| \geq |\Im(\langle f, A_j f\rangle)| = (\tau^2/t_L)\sqrt{1 - \lambda^2/(4t_L^2)}\langle f, \Pi^T f\rangle,$$

and using (5.5) we get

$$||\tilde{p}_j A_j \tilde{p}_j\, f|| \geq (\tau^2/t_L)\sqrt{1 - \lambda^2/(4t_L^2)}C_j,$$

which leads to

$$||[\tilde{p}_j A_j \tilde{p}_j]^{-1}|| \leq \mathit{const} \cdot 1/\tau^2.$$

Using this in (5.10) by employing again the Neumann series, we get that for τ small and λ near E_j we have

$$||X_j^{-1}|| \leq \mathit{const} \cdot 1/\tau^2,$$

thus (5.6) is proven, and so is the lemma. □

Remark. We see that if $p_j \neq 0$, its range is spanned by eigenvectors of K corresponding to E_j. But they do not contribute in any way to $u^+_{\beta\gamma}$.

Corollary 5.3. *We use the notation introduced in the previous lemma. Assume that E_j is n-fold degenerate.*

(i). For every $\lambda \in (-2t_L, 2t_L)$ with $\lambda \notin \{E_1, \ldots, E_J\}$ we have

$$\lim_{\tau \searrow 0} \tau^2 |u^+_{\beta\gamma}(\lambda, \tau)| = 0. \quad (5.12)$$

(ii). Fix $\lambda = E_j$*. Assume* $\tilde{p}_j = 0$*. Then*

$$\lim_{\tau\searrow 0} \tau^2 |u^+_{\beta\gamma}(E_j, \tau)| = 0. \tag{5.13}$$

(iii). Fix $\lambda = E_j$*. Assume that* $\tilde{p}_j \neq 0$*. Then* $\tilde{p}_j \Pi^T \tilde{p}_j$ *is positive on* $\mathrm{Ran}(\tilde{p}_j)$ *and*

$$\lim_{\tau\searrow 0} \tau^2 |u^+_{\beta\gamma}(E_j, \tau)| = t_L |\langle \beta_S, \tilde{p}_j [\tilde{p}_j \Pi^T \tilde{p}_j]^{-1} \tilde{p}_j \gamma_S \rangle|. \tag{5.14}$$

Proof. (i). By regular perturbation theory, we see that $|u^+_{\beta\gamma}(\lambda, \tau)|$ remains bounded when τ tends to zero, while λ is fixed and away from the eigenvalues of H^S. Hence (5.12) is straightforward.

(ii). If $\tilde{p}_j = 0$ and $\lambda = E_j$, the estimate (5.8) implies again that $|u^+_{\beta\gamma}(E_j, \tau)|$ remains bounded when τ tends to zero, thus (5.13) follows.

(iii). If $\tilde{p}_j \neq 0$ and $\lambda = E_j$, we rely on the properties of the inverse on $\mathrm{Ran}(\tilde{p}_j)$ of the operator $\tilde{p}_j A_j \tilde{p}_j$ introduced in (5.11). A consequence of the arguments presented in the previous proposition is that for λ close to E_j we have

$$u^+_{\beta\gamma}(\lambda) - \langle \beta_S, \tilde{p}_j [\tilde{p}_j A_j \tilde{p}_j]^{-1} \tilde{p}_j \gamma_S \rangle = \mathcal{O}_\tau(1). \tag{5.15}$$

Then using (5.11) with $\lambda = E_j$, and the fact that $|\zeta_+(\lambda)| = 1$, the result follows easily. The corollary is proven. □

Ending the proof of Proposition 5.1. The proof is easily obtained by replacing (5.12), (5.13) and (5.14) in (4.6), in the nondegenerate case. We do not give more details.

We see that in the degenerate case it is not that simple to give clear criteria for which the current is zero or not in the small coupling regime. Assume that E_j is n-fold degenerate. Denote by $\{\phi_j^{(s)}\}_{s=1}^n$ the normalized eigenvectors of H^S spanning the range of Π_j. A sufficient condition for the right hand side of (5.14) to be zero for every β and γ, is Π_j to be orthogonal to Π^T. In other words, $\langle \alpha_S, \phi_j^{(r)} \rangle = 0$ for every $1 \leq \alpha \leq M$ and $1 \leq r \leq n$. Physically, this means no contact at all between the leads and the mode E_j. A necessary but not sufficient condition for the right hand side of (5.14) to be different from zero is to have $\tilde{p}_j \neq 0$. The proposition is proven. □

We continue this section with a result giving more information about the poles in the case when τ is small and we are near a nondegenerate eigenvalue of H^S.

Assume that the eigenvalue $E_1 \in (-2t_L, 2t_L)$ of H^S is nondegenerate. We denote the corresponding normalized eigenvector with ϕ_1, i.e. $H^S\phi_1 = E_1\phi_1$. It is clear that one of the following two alternatives is true:

- A_1: there exists $\alpha^1 \in \{1, \dots, M\}$ such that $\langle \phi_1, \alpha_S^1 \rangle \neq 0$,
- A_2: for every $\alpha \in \{1, \dots, M\}$ we have $\langle \phi_1, \alpha_S \rangle = 0$.

If A_1 holds, then ϕ_1 is "coupled" with at least one lead; if A_2 holds, then the coupling is absent.

Define the projection $\Pi^L = \sum_{\alpha=1}^M |0_\alpha\rangle\langle 0_\alpha|$. By direct computation we have (see (3.7) and (3.1))

$$\Pi^L(K-z)^{-1}\Pi^L = \frac{\zeta_1(z)}{t_L}\sum_{\alpha=1}^M |0_\alpha\rangle\langle 0_\alpha| + \frac{\zeta_1^2(z)}{t_L^2}\sum_{\alpha,\beta=1}^M |0_\alpha\rangle u_{\alpha\beta}(z)\langle 0_\beta|. \quad (5.16)$$

Then the weighted resolvent $\Pi^L(K-z)^{-1}\Pi^L$ admits a meromorphic extension to any domain of the form $\mathbb{C}_+ \cup \Omega_\epsilon$ (see (3.5)).

Proposition 5.4. i. *For small enough τ, the weighted resolvent $\Pi^L(K-z)^{-1}\Pi^L$ has a simple pole near E_1 (denoted by $\tilde{E}_1(\tau)$).*
ii. *If A_1 holds true, then for $\tau > 0$ small enough the pole $\tilde{E}_j(\tau)$ is a resonance for K with*

$$\lim_{\tau \searrow 0}(\Re(\tilde{E}_1(\tau)) - E_1)/\tau^2 = -\frac{E_1}{2t_L^2}\sum_{\alpha=1}^M |\langle \phi_1, \alpha_S\rangle|^2,$$

and

$$\lim_{\tau \searrow 0}\Im(\tilde{E}_1(\tau))/\tau^2 = -\frac{\sqrt{4t_L^2 - E_1^2}}{2t_L^2}\sum_{\alpha=1}^M |\langle \phi_1, \alpha_S\rangle|^2.$$

iii. *If A_2 holds for ϕ_1 then $\tilde{E}_1(\tau) = E_1$ and ϕ_1 remains an eigenvector for K, i.e. $K\phi_1 = \tilde{E}_1\phi_1$.*

Proof. Let us focus on what happens near E_1 in case when A_1 holds. Denote with P_1 the spectral projection of H^S corresponding to ϕ_1, and with $Q_1 = \mathrm{Id} - P_1$ its orthogonal. Feshbach lemma gives:

$$\begin{aligned}(H_+(z)-z)^{-1} &= (Q_1H_+Q_1 - z)^{-1} + (1 - (Q_1H_+Q_1 - z)^{-1}Q_1H_+P_1) \\ &\cdot (\tilde{H}_+(z)-z)^{-1} \cdot (1 - P_1H_+Q_1(Q_1H_+Q_1-z)^{-1}) \quad (5.17)\end{aligned}$$

where the new effective Hamiltonian $\tilde{H}_+(z)$ is defined by

$$\tilde{H}_+(z) := P_1 H_+(z) P_1 - P_1 H_+ Q_1 (Q_1 H_+ Q_1 - z)^{-1} Q_1 H_+ P_1, \tag{5.18}$$

and lives in a one dimensional space. With the notation

$$\begin{aligned} f_1(z,\tau) \ &:= \ \sum_{\alpha,\beta=1}^{M} \sum_{i,i'\neq 1} \frac{\tau^4}{t_L^2} \zeta_+^2(z) \langle \phi_1 | \alpha_S \rangle \langle \alpha_S | \phi_i \rangle \\ &\cdot \ \langle \phi_i | (Q_1 H_+ Q_1 - z)^{-1} | \phi_i' \rangle \langle \phi_i' | \beta_S \rangle \langle \beta_S | \phi_1 \rangle \end{aligned}$$

we have that for small enough τ, $H_+(z) - z$ is invertible iff the function

$$F_1(z,\tau) := E_1 - z - \frac{\tau^2}{t_L} \zeta_+(z) \sum_{\alpha=1}^{M} |\langle \phi_j, \alpha_S \rangle|^2 - f_1(z,\tau)$$

is different from zero. Notice that for τ small enough and z near E_1 we have $f_1(z,\tau) = \mathcal{O}(\tau^4)$.

For small τ and with z near E_1, the implicit function theorem provides us with a unique solution $\tilde{E}_1(\tau)$ to the equation $F_1(z,\tau) = 0$.

If we define

$$\begin{aligned} \mathcal{T}_1(z,\tau) \ &:= \ -(Q_1 H_+ Q_1 - z)^{-1} Q_1 H_+ P_1 \\ &- \ P_1 H_+ Q_1 (Q_1 H_+ Q_1 - z)^{-1} \\ &+ \ (Q_1 H_+ Q_1 - z)^{-1} Q_1 H_+ P_1 H_+ Q_1 (Q_1 H_+ Q_1 - z)^{-1}, \end{aligned}$$

then we can write

$$(H_+ - z)^{-1} = \frac{1}{F_1(z,\tau)} [P_1 + \mathcal{T}_1] + (Q_1 H_+ Q_1 - z)^{-1}. \tag{5.19}$$

It is easy to see that $\mathcal{T}_1$ is analytic in z near E_1 and of order $\mathcal{O}(\tau^2)$. Now we have to take the matrix elements $\langle \alpha_S | (H_+(z) - z)^{-1} | \beta_S \rangle$ to obtain $u_{\alpha\beta}(z)$ in Eq.(5.16). It turns out that

$$\begin{aligned} \Pi^L (K - z)^{-1} \Pi^L \ &= \ \textit{bounded \& analytic} \\ &+ \ \frac{\zeta_+^2(z)}{t_L^2} \sum_{\alpha,\beta=1}^{M} \left\{ \frac{\langle \alpha_S | \psi_1 \rangle \langle \psi_1 | \beta_S \rangle + \langle \alpha_S | \mathcal{T}_1 | \beta_S \rangle}{F_1(z,\tau)} \right\} |0_\alpha\rangle\langle 0_\beta| \end{aligned}$$

Moreover, since we can show that

$$F_1(z,\tau)/(E_1(\tau) - z) = 1 + \mathcal{O}(\tau^2)$$

for z in a small neighborhood of E_1, we conclude that

$$\begin{aligned}\Pi^L(K-z)^{-1}\Pi^L &= \textit{bounded \& analytic} \\ &+ (1+\mathcal{O}(\tau^2))\frac{\zeta_+^2(z)}{t_L^2}\sum_{\alpha,\beta=1}^{M}\frac{\langle\alpha|\psi_1\rangle\langle\psi_1|\beta\rangle+\mathcal{O}(\tau^2)}{\tilde{E}_1(\tau)-z}|0_\alpha\rangle\langle 0_\beta|.\end{aligned}$$

Therefore the second statement of the proposition is now proved up to a straightforward application of the implicit function theorem for the claimed properties of $\tilde{E}_1(\tau)$. The third statement is also straightforward. □

6 Appendices

6.1 Appendix 1: The discrete Laplacian on the half-line

Denote by $\{|n\rangle\}_{n\geq 0}$ the standard basis in $l^2(\mathbb{N})$. For $t_L > 0$, consider the operator H_α^L which acts on $\psi \in l^2(\mathbb{N})$ as follows:

$$(H_\alpha^L\psi)(j) = t_L\psi(j+1) + t_L\psi(j-1), \quad j \geq 0,\ \psi(-1) := 0.$$

It is well-known that the spectrum of H_α^L is absolutely continuous and moreover $\sigma(H_\alpha^L) = [-2t, 2t]$. We are interested in the matrix elements for the resolvent of H_α^L; if $\Im(z) > 0$ one can easily compute

$$\langle m, R_\alpha^L(z)n\rangle = \frac{1}{t_L(\zeta_2-\zeta_1)}\left(\zeta_1(z)^{|m-n|} - \zeta_1(z)^{m+n+2}\right) \tag{6.1}$$

where $\zeta_{1,2}$ are solutions of the equation

$$t_L\zeta^2 - z\zeta + t = 0 \tag{6.2}$$

and ζ_1 is chosen such that $|\zeta_1| \sim 1/|z|$ at infinity (notice that $\zeta_1\zeta_2 = 1$).

Let us be more precise and give several explicit representations for ζ_1. By $\ln(x) = \ln(|x|) + i\arg(x)$ we understand the principal branch of the natural logarithm defined on $\mathbb{C}\setminus(-\infty, 0]$, and $\arg(x) \in (-\pi, \pi)$. Accordingly, we put $\sqrt{x} := e^{(1/2)\ln(x)} = \sqrt{|x|}e^{(i/2)\arg(x)}$.

Proposition 6.1. *We have the following properties:*
i. *Assume that* $z \notin [-2t_L, 2t_L]$. *Then*

$$\zeta_1(z) = \frac{z}{2t_L}\left(1 - \sqrt{1 - 4t_L^2/z^2}\right). \tag{6.3}$$

ii. *Consider the holomorphic functions*

$$\zeta_\pm(z) = \frac{z}{2t_L} \mp i\sqrt{1 - z^2/(4t_L^2)}, \quad z \notin ((-\infty, -2t_L] \cup [2t_L, \infty)). \tag{6.4}$$

Then $\zeta_1(z) = \zeta_+(z)$ *if* $\Im(z) > 0$, *and* $\zeta_1(z) = \zeta_-(z)$ *if* $\Im(z) < 0$.
iii. *We have* $\zeta_2(z) = 1/\zeta_1(z)$.

Proof. We see that ζ_1 in (6.3) solves the equation and behaves like $1/z$ for large $|z|$. Second, since ζ_1 and $\tilde{\zeta}_\pm$ are holomorphic, it is enough to verify their equality at points of the form $\pm i\alpha$ with $\alpha > 0$ which is trivial. □

6.2 Appendix 2: The second quantization of an ideal Fermi gas

Although these things are very well known (see for example [7]), we briefly present them here mostly for fixing notation.

Given a separable Hilbert space $\mathcal{H}$ we define an associated antisymmetric Fock space as

$$\mathcal{F}_a(\mathcal{H}) = \bigoplus_{n=0}^{\infty} \mathcal{H}^{\otimes_a n}, \quad \mathcal{H}^{\otimes_a 0} := \mathbb{C}.$$

Here the subscript a indicates the total antisymmetrization of the tensor products. Let $\mathcal{B} = \{e_k\}_{k\geq 1}$ be an orthonormal basis in $\mathcal{H}$. Then we can construct the "occupation number" basis in $\mathcal{F}_a(\mathcal{H})$ associated to $\mathcal{B}$; we denote a generic vector in it as $\Psi_{N_1,N_2,\dots}$, where the N_k's are numbers (either 0 or 1) showing how many times e_k appears in the tensor products defining Ψ. For example, $\Psi_{0,0,\dots} = 1 \in \mathbb{C}$ is the vacuum.

The annihilation operators associated to this particular basis are defined as

$$a_\alpha \Psi_{N_1,N_2,\dots,N_\alpha=0,\dots} = 0,\ a_\alpha \Psi_{N_1,N_2,\dots,N_\alpha=1,\dots} = (-1)^{\sum_{\beta<\alpha} N_\beta} \Psi_{N_1,N_2,\dots,N_\alpha=0,\dots},$$

while their adjoints (the creation operators) are

$$a_\alpha^+ \Psi_{N_1,N_2,\dots,N_\alpha=1,\dots} = 0,\ a_\alpha^+ \Psi_{N_1,N_2,\dots,N_\alpha=0,\dots} = (-1)^{\sum_{\beta<\alpha} N_\beta} \Psi_{N_1,N_2,\dots,N_\alpha=1,\dots}.$$

If A is a bounded linear operator in $\mathcal{H}$, we define its second quantization $\mathbf{A} = d\Gamma(A)$ as the operator on $\mathcal{F}_a$ whose restriction to $\mathcal{H}^{\otimes_a n}$ is

$$A \otimes \mathrm{Id} \otimes \ldots \mathrm{Id} + \cdots + \mathrm{Id} \otimes \ldots \mathrm{Id} \otimes A,$$

where the above sum has n terms. Using the particular basis $\mathcal{B}$ we have

$$\mathbf{A} = d\Gamma(A) = \sum_{k,j\geq 1} \langle e_k, Ae_j \rangle a_k^+ a_j. \tag{6.5}$$

For example, the total Hamiltonian is $\mathbf{H} = d\Gamma(H)$, and the number operator is $\mathbf{N} = d\Gamma(\mathrm{Id})$.

Now assume that $\mathcal{H}$ has finite but arbitrarily large dimension; define the grand-canonical partition function Ξ and the density matrix operator in the grand-canonical ensemble $\hat{\rho}_0$ as

$$\Xi := \mathrm{Tr}_{\mathcal{F}_a} e^{-\beta(\mathbf{H}-\mu\mathbf{N})}, \quad \hat{\rho}_0 := \frac{1}{\Xi} e^{-\beta(\mathbf{H}-\mu\mathbf{N})}. \tag{6.6}$$

Finally, define

$$f_{F-D}(x) = \frac{1}{e^{\beta(x-\mu)}+1}, \quad \rho_0 := f_{F-D}(H). \tag{6.7}$$

The following proposition will be extensively used in Section 3:

Proposition 6.2. *Let A and B be bounded operators in $\mathcal{H}$. Denote by $[A, B] = AB - BA$ their commutator. Then*

$$d\Gamma([A, B]) = [\mathbf{A}, \mathbf{B}], \tag{6.8}$$

$$e^{\mathbf{A}} \mathbf{B} e^{-\mathbf{A}} = d\Gamma(e^A B e^{-A}). \tag{6.9}$$

and

$$\mathrm{Tr}_{\mathcal{F}_a} \left(\hat{\rho}_0 \mathbf{A}\right) = \mathrm{Tr}_{\mathcal{H}} \left(\rho_0 A\right). \tag{6.10}$$

Proof. The first identity is easily proven using the anticommutation relations

$$\begin{aligned}
[\mathbf{A}, \mathbf{B}] &= \sum_{k,j,m,n} \langle e_k, Ae_j \rangle \langle e_m, Be_n \rangle [a_k^+ a_j a_m^+ a_n - a_m^+ a_n a_k^+ a_j] \\
&= \sum_{k,j,m,n} \langle e_k, Ae_j \rangle \langle e_m, Be_n \rangle [a_k^+ a_n \delta_{jm} - a_m^+ a_n \delta_{kn}] \\
&= \sum_{k,j} \langle e_k, (AB - BA) e_j \rangle = d\Gamma([A, B]),
\end{aligned}$$

while the second one is implied by the first equality, the Baker-Haussdorf formula

$$e^{\mathbf{A}}\mathbf{B}e^{-\mathbf{A}} = \mathbf{B} + [\mathbf{A},\mathbf{B}] + \frac{1}{2}[\mathbf{B},[\mathbf{B},\mathbf{A}]] + \dots,$$

and the linearity of $d\Gamma(\cdot)$.

We give more details for the third identity (see also Proposition 5.2.23 in [7]). Since the trace is invariant with respect to the basis we use, we may assume that the basis $\mathcal{B} = \{e_k\}$ is the set of eigenvectors of H, and we consider the occupation number basis derived from $\mathcal{B}$. Also denote the eigenvalues of H with $\{\lambda_k\}$.

We know then that

$$\Xi = \Pi_k(1 + e^{-\beta(\lambda_k - \mu)}) < \infty \tag{6.11}$$

and we write

$$\mathrm{Tr}_{\mathcal{F}_a}(\hat{\rho}_0\mathbf{A}) = \sum_{N_1,N_2,\dots\in\{0,1\}} \langle \Psi_{N_1,N_2,\dots}, \hat{\rho}_0\mathbf{A}\Psi_{N_1,N_2,\dots}\rangle.$$

Since

$$\hat{\rho}_0\Psi_{N_1,N_2,\dots} = \frac{1}{\Xi}e^{-\beta\sum_j N_j(\lambda_j-\mu)}\Psi_{N_1,N_2,\dots} = \frac{1}{\Xi}\Pi_j e^{-\beta N_j(\lambda_j-\mu)}\Psi_{N_1,N_2,\dots},$$

and

$$\langle \Psi_{N_1,N_2,\dots}, \mathbf{A}\Psi_{N_1,N_2,\dots}\rangle = \sum_{k,m}\langle e_k, Ae_m\rangle \delta_{N_k,1}\delta_{N_m,1}\delta_{k,m},$$

we have

$$\mathrm{Tr}_{\mathcal{F}_a}(\hat{\rho}_0\mathbf{A}) = \sum_k \langle e_k, Ae_k\rangle \frac{1}{\Xi}\sum_{N_1,N_2,\dots\in\{0,1\}} \Pi_j e^{-\beta N_j(\lambda_j-\mu)}\delta_{N_k,1}.$$

Notice that

$$\begin{aligned}\sum_{N_1,N_2,\dots\in\{0,1\}} \Pi_j e^{-\beta N_j(\lambda_j-\mu)}\delta_{N_k,1} &= (1 + e^{-\beta(\lambda_1-\mu)}) \\ \cdot \quad (1 + e^{-\beta(\lambda_2-\mu)})\dots e^{-\beta(\lambda_k-\mu)}&\dots(1 + e^{-\beta(\lambda_j-\mu)})\dots,\end{aligned} \tag{6.12}$$

hence

$$\frac{1}{\Xi}\sum_{N_1,N_2,\dots\in\{0,1\}} \Pi_j e^{-\beta N_j(\lambda_j-\mu)}\delta_{N_k,1} = f_{F-D}(\lambda_k)$$

and therefore

$$\mathrm{Tr}_{\mathcal{F}_a}(\hat{\rho}_0 \mathbf{A}) = \sum_k \langle e_k, Ae_k \rangle f_{F-D}(\lambda_k) = \mathrm{Tr}_{\mathcal{H}}(\rho_0 A).$$

□

6.3 Appendix 3: A discrete Krein formula and exponential decay

We now give a formula relating the resolvent of the discrete Laplacian defined on $l^2(\mathcal{N})$, $\mathcal{N} := \{0, 1, \ldots, N\}$, with the resolvent of the Laplacian defined on $l^2(\mathbb{N})$; both operators are with Dirichlet boundary conditions. We denote with $r^L(N, z)$ the resolvent on the finite segment, and with $r^L(z)$ the resolvent on the semi-infinite lead; we use small letters for emphasising that we model only one lead. The operator itself is denoted by $h^L(N)$ when restricted to a segment, and by h^L on $l^2(\mathbb{N})$.

We need some more notation. By δ_m we understand the vector in $l^2(\mathcal{N})$ having 1 on the m-th position and 0 elsewhere. Define for every $z \in \mathbb{C} \setminus \mathbb{R}$ the "integral kernels":

$$g_{m,n}(N, z) = \langle \delta_m, r^L(N, z)\delta_n \rangle, \quad g_{m,n}(z) = \langle \delta_m, r^L(z)\delta_n \rangle. \tag{6.13}$$

The Dirichlet boundary condition means:

$$g_{-1,n}(N, z) = g_{N+1,n}(N, z) = g_{-1,n}(z) = 0, \tag{6.14}$$

and similar equalities for the second argument due to the symmetry property $g_{m,n}(N, z) = \overline{g_{n,m}}(N, \overline{z})$.

Proposition 6.3. *For every $0 \leq m, n \leq N$ we have the following Krein formula:*

$$g_{m,n}(N, z) - g_{m,n}(z) = t_L g_{m,N}(N, z) g_{N+1,n}(z). \tag{6.15}$$

Proof. We only sketch the proof, and do not give all technical details. For every fixed n, the vectors $g_{\cdot,n}(N, z)$ and $g_{\cdot,n}(z)$ are in $l^2(\mathcal{N})$ and $l^2(\mathbb{N})$ respectively. Then

$$\begin{aligned} &\left[(h^L(N) - z)g_{\cdot,n}(N, z)\right](m) = \delta_{m,n}, \\ &\left[(h^L - z)g_{\cdot,n}(z)\right](m) = \delta_{m,n}. \end{aligned} \tag{6.16}$$

Then we have after "summation by parts" the identity (the scalar products are on $l^2(\mathcal{N})$)

$$\begin{aligned} \left\langle \left[(h^L(N) - \overline{z})g_{\cdot,m}(N,\overline{z})\right], g_{\cdot,n}(z)\right\rangle &= \left\langle g_{\cdot,m}(N,\overline{z}), (h^L - z)g_{\cdot,n}(z)\right\rangle \\ &- t_L g_{m,N}(N,z)g_{N+1,n}(z) \end{aligned} \tag{6.17}$$

where we employed various symmetry properties of the kernels, together with (6.14). The use of (6.16) finishes the proof. □

Finally, we need an exponential decay estimate for the resolvents, given next:

Proposition 6.4. *There exist two positive constants c and C (the first one small enough, the second one large enough) such that uniformly on N and z with $0 < |\Im(z)| < 1$ we have*

$$|g_{m,n}(N,z)| \leq \frac{C}{|\Im(z)|} \exp\left(-c|\Im(z)|\,|m-n|\right), \quad \forall m,n \in \mathcal{N}. \tag{6.18}$$

The same remains true when $N = \infty$.

Proof. This proposition is nothing but a discrete (and simpler) version of the usual Combes-Thomas argument (see [10]) which leads to boundedness for resolvents between spaces with exponential weights. Define the discrete dilation for $\alpha > 0$

$$(W_\alpha \psi)(n) = e^{\alpha n}\psi(n) \tag{6.19}$$

Then by direct computation the dilated Hamiltonian $H(\alpha) = W_\alpha H W_{-\alpha}$ acts like

$$\begin{aligned} (H(\alpha)\psi)(n) &= e^{-\alpha}\psi(n+1) + e^{\alpha}\psi(n-1) \\ &= (H\psi)(n) + (e^{-\alpha} - 1)\psi(n+1) + (e^{\alpha} - 1)\psi(n-1) \\ &= ((H + V(\alpha))\psi)(n) \end{aligned}$$

where the 'perturbation' $V(\alpha) := (e^{-\alpha} - 1)T_1 + (e^{\alpha} - 1)T_{-1}$, $T_{\pm 1}$ being the shift operators. Noticing that $V(\alpha)$ is roughly of $\mathcal{O}(\alpha)$, and if $\alpha \leq c|\Im(z)|$ where c is a small enough positive constant, we can write

$$(H(\alpha) - z)^{-1} = (H - z)^{-1}\left(1 + V(\alpha)(H - z)^{-1}\right)^{-1} \tag{6.20}$$

where the second part is invertible and its norm is less than a chosen constant (2 say). Hence,

$$\|(H(\alpha)-z)^{-1}\| \leq \|(H-z)^{-1}\|\cdot\| \left(1+V(\alpha)(H-z)^{-1}\right)^{-1} \| \leq \frac{2}{|\Im(z)|}. \quad (6.21)$$

Define the following vectors in $l^2(\mathcal{N})$ (the exponential is on the m-th position):

$$\Psi_{mn} = (0,0,...,e^{i\arg(g_{mn}(N,z))},...,0,0), \quad m \geq n. \quad (6.22)$$

Then

$$\begin{aligned}\langle \Psi_{mn}, W_\alpha (H-z)^{-1} W_{-\alpha}\delta_n\rangle &= e^{\alpha(m-n)}|g_{mn}(N,z)| \\ &= \langle \Psi_{mn}, (H(\alpha)-z)^{-1}\delta_n\rangle \leq \frac{C}{|\Im(z)|},\end{aligned}$$

from where the claimed estimate follows. □

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