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The Landauer-Büttiker Formula and Resonant Quantum Transport

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We give a short presentation of two recent results. The first one is a rigorous proof of the Landauer-Büttiker formula, and the second one concerns resonant quantum transport. The detailed results are in [2]. In the last section we present the results of some numerical computations on a model system.

Concerning the literature, then see the starting point of our work, [6]. In [4] a related, but different, problem is studied. See also [5] and the recent work [1]

1 The Landauer-Büttiker Formula

We start by introducing the notation and the assumptions. The model used here describes a finite sample coupled to a finite number of leads. The leads may be finite or semi-infinite. We use a discrete model, i.e. the tight-binding approximation. The sample is modeled by a finite set $\Gamma \subset \mathbf{Z}^2$. Each lead is modeled by $\mathcal{N} = \{0, 1, \ldots, N\} \subseteq \mathbf{N}$. The case $\mathcal{N} = \mathbf{N}$ $(N = +\infty)$ is the semi-infinite lead. We assume that we have $M \geq 2$ leads. The one-particle Hilbert space is then

$$\mathcal{H} = \ell^2(\Gamma) \oplus \underbrace{\ell^2(\mathcal{N}) \oplus \cdots \oplus \ell^2(\mathcal{N})}_{M \text{ copies}}. \tag{1}$$

The Hamiltonian is denoted by H. It is the sum of the following components. For the sample we can take any selfadjoint operator H^S on $\ell^2(\Gamma)$. In each lead we take the discrete Laplacian with Dirichlet boundary conditions. The leads are numbered by $\alpha \in \{1, 2, \ldots, M\}$. Thus

$$H^L = \sum_{\alpha=1}^{M} H^L_\alpha, \quad H^L_\alpha = \sum_{n_\alpha \in \mathcal{N}} t_L(|n_\alpha\rangle\langle n_\alpha + 1| + |n_\alpha\rangle\langle n_\alpha - 1|) \tag{2}$$

Functions in $\ell^2(\mathcal{N})$ are by convention extended to be zero at -1 and $N + 1$. The parameter t_L is the hopping integral. The coupling between the leads and the sample is described by the tunneling Hamiltonian

$$H^T = H^{LS} + H^{SL}, \quad \text{where} \quad H^{LS} = \tau \sum_{\alpha=1}^{M} |0_\alpha\rangle\langle\mathcal{S}^\alpha|, \tag{3}$$

and H^{SL} is the adjoint of H^{LS}. Here $|0_\alpha\rangle$ denotes the first site on lead α, and $|\mathcal{S}^\alpha\rangle$ is the contact site on the sample. The parameter τ is the coupling constant. It is arbitrary in this section, but will be taken small in the next section. The total one-particle Hamiltonian is then

$$H = H^S + H^L + H^T \quad \text{on } \mathcal{H}. \tag{4}$$

First we consider electronic transport through the system. Initially the leads are finite, all of length N, with N arbitrary. We work exclusively in the grand canonical ensemble. Thus our system is in contact with a reservoir of energy and particles. We study the linear response of a system of non-interacting Fermions at temperature T and with chemical potential μ. The system is subjected adiabatically to a perturbation, defined as follows.

Let χ_η be a smooth switching function, i.e. $0 \le \chi_\eta(t) \le 2$, $\chi_\eta(t) = e^{\eta t}$ for $t \le 0$, while $\chi_\eta(t) = 1$ for $t > 1$. The time-dependent perturbation is then given by

$$V(N,t) = \chi_\eta(t) \sum_{\alpha=1}^{M} V_\alpha I_\alpha(N).$$

Here $I_\alpha(N) = \sum_{n_\alpha=0}^{N} |n_\alpha\rangle\langle n_\alpha|$ is the identity on the α-copy of $\ell^2(\mathcal{N})$. This perturbation models the adiabatic application of a constant voltage V_α on lead α, which will generate a charge transfer between the leads via the sample.

We are interested in deriving the current response of the system due to the perturbation. In the grand canonical ensemble we need to look at the second quantized operators. We omit the details and state the result. The current at time $t = 0$ in lead α is given by

$$\mathcal{I}_\alpha(0) = \sum_{\beta=1}^{M} g_{\alpha\beta}(T,\mu,\eta,N) V_\beta + \mathcal{O}(V^2). \tag{5}$$

The $g_{\alpha\beta}(T,\mu,\eta,N)$ are the conductance coefficients [3]. It is clear from the above formula that we work in the linear response regime. Below we are going to take the limit $N \to \infty$, followed by the limit $\eta \to 0$. The limits have to be taken in this order, since the error term is in fact $\mathcal{O}(V^2/\eta^2)$.

The next step is to look at the transmittance, which is obtained from scattering theory, applied to the pair of operators (K, H_0), where $H_0 = H^L$ ($N = +\infty$ case) and $K = H_0 + H^S + H^T$. Properly formulated this is done in the two space scattering framework, see [7]. Since the perturbation $H^S + H^T$ is of finite rank, and since we have explicitly a diagonalization of the operator H_0, the stationary scattering theory gives an explicit formula for the scattering matrix, which is an $M \times M$ matrix, depending on the spectral parameter $\lambda = 2t_L \cos(k)$ of H_0. The T-operator is then given by an $M \times M$ matrix $t_{\alpha\beta}(\lambda)$, and the transmittance is given by

$$\mathcal{T}_{\alpha\beta}(\lambda) = |t_{\alpha\beta}(\lambda)|^2. \tag{6}$$

It follows from the explicit formulas that $\mathcal{T}_{\alpha\beta}(\lambda)$ is real analytic on $(-2t_L, 2t_L)$, and zero outside this interval.

With these preparations we can state the main result.

Theorem 1. *Consider $\alpha \neq \beta$, $T > 0$, $\mu \in (-2t_L, 2t_L)$, and $\eta > 0$. Assume that the point spectrum of K (corresponding to the $N = +\infty$ case) is disjoint from $\{-2t_L, 2t_L\}$. Then taking first the limit $N \to \infty$, and then $\eta \to 0$, we have*

$$\begin{aligned} g_{\alpha,\beta}(T, \mu) &= \lim_{\eta \to 0} \Big[\lim_{N \to \infty} g_{\alpha,\beta}(T, \mu, \eta, N) \Big] \\ &= -\frac{1}{2\pi} \int_{-2t_L}^{2t_L} \frac{\partial f_{\mathrm{F-D}}(\lambda)}{\partial \lambda} \mathcal{T}_{\alpha\beta}(\lambda) d\lambda. \end{aligned} \tag{7}$$

Here $f_{\mathrm{F-D}}(\lambda) = 1/(e^{(\lambda-\mu)/T} + 1)$ is the Fermi-Dirac function. If we finally take the limit $T \to 0$, we obtain the Landauer formula

$$g_{\alpha,\beta}(0_+, \mu) = \frac{1}{2\pi} \mathcal{T}_{\alpha\beta}(\mu). \tag{8}$$

The proof of this main result is quite long and technical. One has to study the two sides of the equality above. The scattering part (the transmittance) is quite straightforward, using the Feshbach formula. The conductance part is a fairly long chain of arguments, as is the proof of the equality statement in the theorem. We refer to [2] for the details.

2 Resonant Transport in a Quantum Dot

In the previous section we have allowed the coupling constant τ (see (3)) to be arbitrarily large. The only assumption was that $\{-2t_L, 2t_L\}$ was not in the point spectrum of K. We now look at the small coupling case, $\tau \to 0$. In this case we will assume that the sample Hamiltonian H^S does not have eigenvalues $\{-2t_L, 2t_L\}$. It then follows from a perturbation argument, using the Feshbach formula, that the same is true for K, provided τ is sufficiently small.

Since H^S is an operator on the finite dimensional space $\ell^2(\Gamma)$, is has a purely discrete spectrum. We enumerate the eigenvalues in the interval $(-2t_L, 2t_L)$:

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

Let $\beta \neq \gamma$ be two different leads. The conductance between these two is now denoted by $\mathcal{T}_{\beta,\gamma}(\lambda, \tau)$, making the dependence on the coupling constant explicit, see (6).

Theorem 2. *Assume that the eigenvalues $\{E_1, \ldots, E_J\}$ are nondegenerate, and denote by $\phi_1, \ldots \phi_J$ the corresponding normalized eigenfunctions. We then have the following results:*

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

$$\lim_{\tau \to 0} \mathcal{T}_{\beta,\gamma}(\lambda, \tau) = 0. \tag{9}$$

(ii) *Let $\lambda = E_j$. If either $\langle \mathcal{S}^\beta, \phi_j \rangle = 0$ or $\langle \mathcal{S}^\gamma, \phi_j \rangle = 0$, then*

$$\lim_{\tau \to 0} \mathcal{T}_{\beta,\gamma}(E_j, \tau) = 0. \tag{10}$$

(iii) *Let $\lambda = E_j$. If both $\langle \mathcal{S}^\beta, \phi_j \rangle \neq 0$ and $\langle \mathcal{S}^\gamma, \phi_j \rangle \neq 0$, then there exist positive constants $C(E_j)$, such that*

$$\lim_{\tau \to 0} \mathcal{T}_{\beta,\gamma}(E_j, \tau) = C(E_j) \left| \frac{\langle \mathcal{S}^\beta, \phi_j \rangle \cdot \langle \mathcal{S}^\gamma, \phi_j \rangle}{\sum_{\alpha=1}^{M} |\langle \mathcal{S}^\alpha, \phi_j \rangle|^2} \right|^2 . \tag{11}$$

This result can be interpreted as follows. Case (i): If the energy of the incident electron is not close to the eigenvalues of H^S, it will not contribute to the current. Case (ii): If the incident energy is close to some eigenvalue of H^S, but the eigenfunction is not localized along both contact points $\mathcal{S}^\beta$ and $\mathcal{S}^\gamma$, again there is no current. Case (iii): In order to have a peak in the current it is necessary for H^S to have extended edge states, which couple to several leads.

3 A Numerical Example

We end this contribution with some numerical results on the transport through a noninteracting quantum dot described by a discrete lattice containing 20×20 sites and coupled to two leads connected to two opposite corners. The magnetic flux is fixed and measured in arbitrary units, while the lead-dot coupling was set to $\tau = 0.2$. The sample Hamiltonian H^S is given by the Dirichlet restriction to the above mentioned finite domain of

$$\begin{aligned} H^S(V_g) = \sum_{(m,n)\in \mathbf{Z}^2} \big((E_0 + V_g)|m,n\rangle\langle m,n| + t_1 (e^{-i\frac{Bm}{2}}|m,n\rangle\langle m,n+1| + h.c.) \\ + t_2 (e^{-i\frac{Bn}{2}}|m,n\rangle\langle m+1,n| + h.c.) \big). \end{aligned} \tag{12}$$

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.

The constant denoted V_g adds to the on-site energies E_0, simulating the so-called 'plunger gate voltage' in terms of which the conductance is measured in the physical literature. The variation of V_g has the role to 'move' the

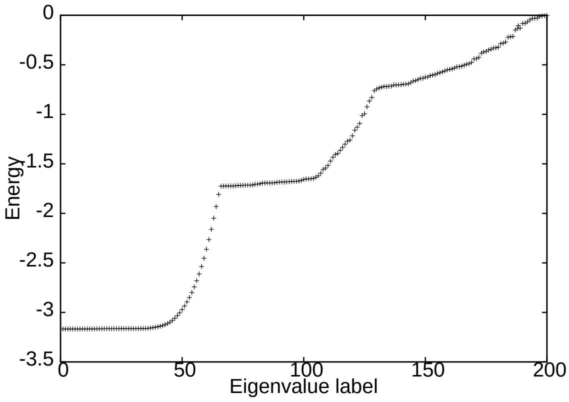

Fig. 1. The dot spectrum

dot levels across the *fixed* Fermi level of the system (recall that the latter is entirely controlled by the semi-infinite leads). Otherwise stated, the eigenvalues of $H^S(V_g)$ equal the ones of $H^S(V_g = 0)$ (we denote them by $\{E_i\}$), up to a global shift V_g. Using the Landauer-Büttiker formula (8), and the formulas (3.8) and (4.6) in [2], it turns out that the computation of the conductivity between the two leads (or equivalently, of $\mathcal{T}_{12}$) reduces to the inversion of an effective Hamiltonian.

Moreover, when V_g is fixed such that there exists an eigenvalue E_i of $H^S(V_g = 0)$ obeying $E_i + V_g = E_F$, the transmittance behavior is described by (11). Thus one expects to see a series of peaks as V_g is varied. Here the Fermi level was fixed to $E_F = 0.0$ and the hopping constants in the lattice $t_1 = 1.01$ and $t_2 = 0.99$. Then the resonances appear, whenever $V_g = -E_i$ (since the spectrum of our discrete operator $H^S(0)$ is a subset of $[-4, 4]$, the suitable interval for varying V_g is the same).

Before discussing the resonant transport let us analyze the spectrum of our dot at $V_g = 0$, in order to emphasize the role of the magnetic field. We recall that we used Dirichlet boundary conditions (DBC) and the magnetic field appears in the Peierls phases of H^S (see (12)). In Figure 1 we plot the first 200 eigenvalues (this suffices since the spectrum is symmetrically located with respect to 0, i.e both E_i and $-E_i$ belong to $\sigma(H_S(0))$). One notices two things. First, there are two narrow energy intervals ($[-3.17, -3.16]$ and $[-1.75, 1.65]$) covered by many eigenvalues ($\sim$ 33 and 45 respectively). Secondly, the much larger ranges $[-3.16, -1.72]$ and $[-1.65, -0.8]$ contain only 25 and 30 eigenvalues. This particular structure of the spectrum is due to both the magnetic field and the DBC. The dense regions are reminescences of the Landau levels of the infinite system while the largely spaced eigenvalues appear *between* the Landau levels due to the DBC. As we shall see below their corresponding eigenfunctions are mostly located on the edge of the sample. As the energy approaches zero, the distinction between edge and bulk states is not anymore clear and one can have quite complex topologies for eigenfunctions. We point out that the 'clarity', the length, and the number of edge states regions intercalated in the Landau gaps, increase as the sample gets bigger.

Now let us again comment on (11). Here E_i must be replaced by $E_i + V_g$, where E_i are eigenvalues of $H^S(0)$. Remember that we took $\mu = 0$. The number of leads is $M = 2$. By inspecting formula (4.6) in [2], one can show that the constant $C(E_i + V_g)$ will always equal 4 (we have $k_\mu = \pi/2$ and $t_L = 1$). Therefore, each time we fulfill the condition $V_g = -E_i$, we obtain a peak in the transmittance, which for small τ should be close to

$$4 \left| \frac{\langle \mathcal{S}^1, \phi_j \rangle \cdot \langle \mathcal{S}^2, \phi_j \rangle}{\sum_{\alpha=1}^{2} |\langle \mathcal{S}^\alpha, \phi_j \rangle|^2} \right|^2 \leq 1. \tag{13}$$

We have equality with 1, if and only if $|\langle \mathcal{S}^1, \phi_j \rangle| = |\langle \mathcal{S}^2, \phi_j \rangle|$, and this does not depend on the magnitude of these quantities. Therefore, even for weakly coupled, but completely symmetric eigenfunctions, we can expect to have a strong signal. In fact, in this case the relevant parameter is

$$\min \left\{ \frac{|\langle \mathcal{S}^1, \phi_j \rangle|}{|\langle \mathcal{S}^2, \phi_j \rangle|}, \frac{|\langle \mathcal{S}^2, \phi_j \rangle|}{|\langle \mathcal{S}^1, \phi_j \rangle|} \right\}. \tag{14}$$

Now let us investigate how the transmittance behaves, when V_g is varied. Figure 2a shows the peaks corresponding to the first six (negative) eigenvalues of $H^S(V_g = 0)$. Their amplitude is very small because the associated eigenvectors are (exponentially) small at the contact sites, and not completely symmetric (since $t_1 \neq t_2$). In fact, a few eigenvectors with more symmetry do generate some small peaks. The spatial localisation of the second and the sixth eigenvector is shown in Figs. 2b,c.

The peak aspect changes drastically at lower gate potentials as the Fermi level encounters levels whose eigenstates have a strong component on the contact subspace (see Figs. 3b and 3c for the spatial localisation of the 38^{th} and the 49^{th} eigenstate). The transmittance is close to unity in this regime, since the parameter in (14) is also nearly one. This is explained by the fact that t_1 and t_2 have very close values, and the relative perturbation induced by the lack of symmetry is much smaller than for the bulk states. One notices that the width of the peaks increases as V_g is decreased as well as their separation. In Figs. 3b,c we have plotted the 38^{th} eigenfunction, which gives the first peak on the right of Fig. 3a, and the 49^{th} eigenfunction associated to the peak around $V_g = 3.06$.

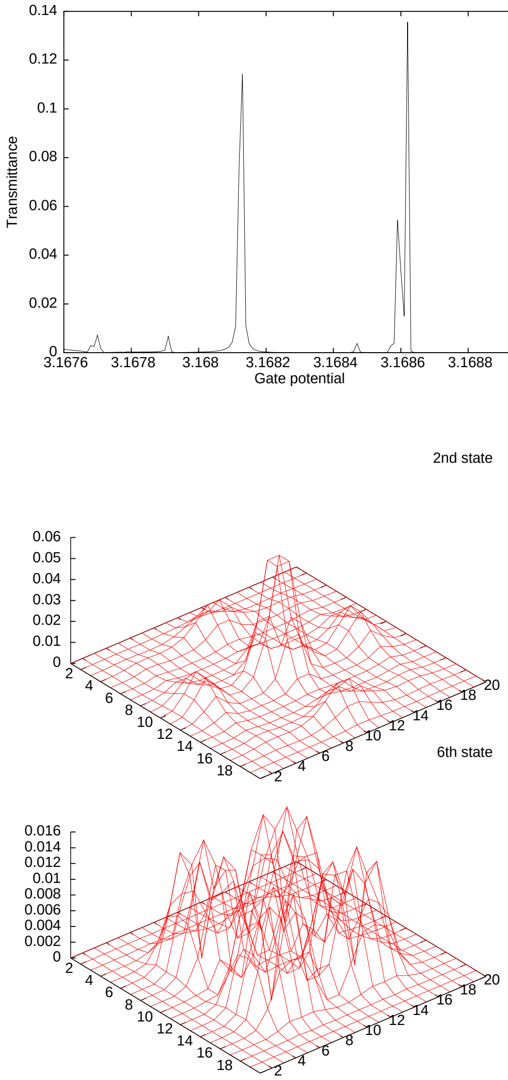

Fig. 2. Top to bottom: parts a, b, c

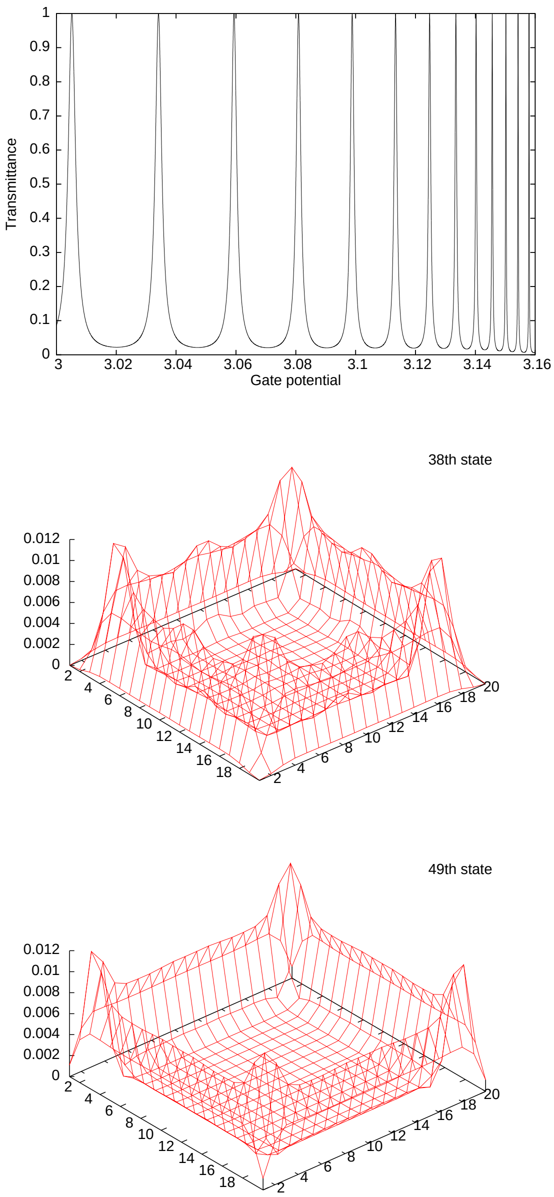

Fig. 3. Top to bottom: parts a, b, c

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