

Classical and quantum transport from generalized Landauer-Büttiker equations

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(Received 13 December 1990; revised manuscript received 13 May 1991)

The electronic transport in a finite-size sample under the presence of inelastic processes, such as electron-phonon interaction, can be described with the generalized Landauer-Büttiker equations (GLBE). These use the equivalence between the inelastic channels and a continuous distribution of voltage probes to establish a current balance. The essential parameters in the GLBE are the transmission probabilities, $T(\mathbf{r}_n, \mathbf{r}_m)$, from a channel at position \mathbf{r}_m to one at \mathbf{r}_n . A formal solution of the GLBE can be written as an effective transmittance $\tilde{T}(\mathbf{r}_n, \mathbf{r}_m)$ which satisfies $\tilde{T}(\mathbf{r}_n, \mathbf{r}_m) = T(\mathbf{r}_n, \mathbf{r}_m) + \int d\mathbf{r}_i T(\mathbf{r}_n, \mathbf{r}_i) g_i \tilde{T}(\mathbf{r}_i, \mathbf{r}_m)$, where $1/g_i = \int d\mathbf{r}_j T(\mathbf{r}_j, \mathbf{r}_i)$. The T 's are obtained from the Green's functions of a Hamiltonian which models the electronic structure of the sample (with density of states N_0 , Fermi velocity v , mean free path l , and localization length $\lambda \geq l$), the geometrical constraints, the measurement probes, and the electron-phonon interaction (providing the inelastic rate $1/\tau_{in}$). By using known results for the Green's functions of infinite systems in dimension d , we show that \tilde{T} defined in the above equation describes a conductivity of the form $\bar{\sigma}_d = 2e^2 \bar{D}_d N_0$. In the ballistic regime ($v\tau_{in} < l$) the conductance is limited by inelastic scattering and the diffusion coefficient is $\bar{D}_d = v^2 \tau_{in} / d$. In the metallic regime of weak disorder ($v\tau_{in} \ll \lambda$), we obtain $\bar{D}_d = D_d \equiv vl/d$. These results, derived from microscopic principles, formalize an earlier picture of Thouless. Hence, we obtain the weak-localization correction for a quasi-one-dimensional case as a factor $[1 - (D_1 \tau_{in})^{1/2} / \lambda]$ in the diffusion coefficient. For strong localization ($\lambda \ll D_1 \tau_{in}$) we get $\bar{D}_d = \lambda^2 / 3\tau_{in}$. The wide range of validity of the whole description gives further support to the GLBE which are then very appropriate to deal with transport not only in mesoscopic systems but also in macroscopic systems in the presence of inelastic processes.

I. INTRODUCTION

In the past decade, the continued drive toward miniaturization of electronic devices required the evaluation of the conductance of small samples.¹ Many authors opted for some of the variants² of the Landauer formula, which represent an alternative to the traditional Boltzmann and Kubo equations. This is because while the latter remained more appropriate to describe macroscopic samples,^{3,4} the former gives a very direct and intuitive way to deal with small samples. The original Landauer formula⁵ considers a sample with contacts to two perfect conductors (L and R), each connected to an electron reservoir. The difference between their chemical potentials (μ_L and μ_R) produces a current through the sample proportional to the transmission probability $T_{R,L}$ from conductor L to R . In order to evaluate the conductance associated with the sample region one needs to define the voltage drop in this region. Clearly it is not the voltage difference between the reservoirs connected to the current leads R and L , because some voltage must drop inside the leads. One possibility is to measure the chemical potentials associated with the charge pileup and charge depletion at the contact regions A and B where the current leads inject and extract current. These determine the voltage drop across the sample $V = (\mu_A - \mu_B) / e$. Landauer estimated their difference as $(\mu_A - \mu_B) = (1 - T_{L,R})(\mu_L - \mu_R)$. Considering the spin degeneracy, Landauer's conductance results:

$$G_L = 2 \frac{e^2}{h} \frac{T_{R,L}}{1 - T_{R,L}}. \quad (1.1)$$

In general, the transmission coefficient should include *all* the physical processes that affect an electron in its transit through the sample. However, since only coherent quantum tunneling can be evaluated from a simple model Hamiltonian, it is usual to require that complicated processes beyond the quantum coherent tunneling occur only in the reservoirs connected to the leads. In that case $T_{L,R}$ is the quantum transmittance for a particle with Fermi energy, $\epsilon_F = \mu^0$. Therefore there are two conditions which have been essential for the applicability of this formula: (a) The inelastic and phase-relaxation processes occur only in the reservoirs connected to the leads and (b) Eq. (1.1) implicitly requires the presence of two additional probes A and B (e.g., two other leads). These should have an interaction with the system which is weak enough to be considered noninvasive but still allow one to measure the chemical potential. Although the first of the requirements restricts the range of applicability of the formula, it can be conveniently achieved experimentally⁶ by controlling the sample size, temperature range, and impurity type. The second condition has been more polemic. From the theoretical side, early deductions⁷ of (1.1) from the Kubo formula found difficulties in the definition of the voltage drop inside the sample, with the consequent loss of the denominator in (1.1). Engquist and Anderson⁸ emphasized that this voltage drop inside

the sample should be measured through actual voltage probes which in turn introduce some phase randomization in the quantum states. From the experimental aspect, the common situation is that voltage probes are indeed invasive to some degree and hence should be considered as part of the system.

The decisive advance over the second limitation is due to Büttiker, who extended⁹ the Landauer and Engquist-Anderson ideas to the consideration of a sample with many (M) leads or channels, each connected to a reservoir characterized by a chemical potential $\mu_n = \mu^0 + \delta\mu_n$, with $n=1, 2, \dots, M$. As in the original Landauer approach, each reservoir is able to absorb any electron entering the lead, while it injects electrons back with a distribution of energies given by the Fermi occupation factor $f(\varepsilon - \mu_n)$. The net electric current at each channel n is determined by the balance between the “in” and “out” particle currents, $J_n^<$ and $J_n^>$, respectively. This can be expressed in terms of the chemical potentials and the quantum transmission probabilities $T_{n,m}$ from channel m to channel n and the reflection probability $R_{n,n} = 1 - \sum_{m(\neq n)} T_{m,n}$ for a particle coming from channel n :

$$I_n = 2e(J_n^< - J_n^>) \quad (n=1, 2, \dots, M)$$

$$= 2\frac{e}{h} \left[\sum_{m(m\neq n)} T_{n,m} \delta\mu_m - (1 - R_{n,n}) \delta\mu_n \right]. \quad (1.2)$$

At least two of the channels should act as current source and sink, and hence they have an externally fixed difference in their chemical potentials. The others, being voltage probes, present a cancellation in the net current and their chemical potentials $\delta\mu_n$ must be adjusted to fulfill this condition. Equation (1.2) together with these boundary conditions are the Landauer-Büttiker equations. Then the chemical potential in the voltage probes and the currents at the current leads must be determined using the system of equations (1.2). By using phenomenological guesses for the transmission coefficients, these equations were successfully used to describe a wide variety of experiments. Besides, Eq. (1.1) can be reobtained¹⁰ from Eq. (1.2) if some interferences are neglected.⁸

Of course, the most desirable situation is to evaluate the transmission probabilities using an electronic Hamiltonian which describes the sample with leads. This has the advantage that all the interferences are taken into account exactly. As a general rule it is more fundamental (and safe) to make physical approximations in the modeling of Hamiltonians rather than in the transmittances. However, we mentioned that in many experimental situations the electrons can spend enough time inside the sample to lose their phase coherence due to the collisions with phonons, magnetic impurities, or other electrons. Therefore a description limited to the coherent propagation through the sample may not be a good enough approximation. The author in collaboration with D'Amato¹⁰ and independently Datta,¹¹ have proposed a way to overcome this computational limitation of the

Landauer approach concerning the inelastic processes inside the sample. Our work exploited a seminal idea of Büttiker,¹² also advocated by other authors,¹³ according to which the voltage probes are equivalent to inelastic processes. In fact, we proved that both give a lifetime to the electron states, and in both cases no current leaves the sample. Therefore Eq. (1.2) remains valid with the boundary conditions of zero current in the inelastic channels. These are what we call the generalized Landauer-Büttiker equations (GLBE). It should be clear that this identification is not heuristic but based on a well-defined model Hamiltonian which describes the sample, the leads, and the electron-phonon interaction. Within this context Eq. (1.2) can be deduced¹¹ using the Keldysh technique¹⁴ in the linear response regime. We will show in the next section how the transmission coefficients are obtained from the Green's functions.

Once we know the transmission coefficients, the next step is to solve (1.2), obtain the local quasiequilibrium chemical potentials, and evaluate the currents. In Ref. 10 we have solved Eq. (1.2) with the condition that only channels m and n act as current source and drain. We found that the current between these channels results proportional to an effective transmission probability $\tilde{T}_{n,m}$. Then, $\tilde{T}_{n,m}$ represents a dimensionless conductance. In Ref. 10, this conductance was evaluated both analytically and numerically for various one-dimensional situations representing samples of finite size. Following that procedure, it is easy to show that \tilde{T} has a series expansion of the form

$$\tilde{T}_{n,m} = T_{n,m} + \sum_{(n\neq j\neq m)} T_{n,j} g_j T_{j,m}$$

$$+ \sum_{(n\neq j\neq m)} \sum_{(n\neq k\neq m)} T_{n,j} g_j T_{j,k} g_k T_{k,m} + \dots \quad (1.3)$$

Here $1/g_n = 1 - R_{n,n}$ and the summation index runs over inelastic channels and voltage probes. \tilde{T} can also be interpreted as a two-probe conductance in units of $2e^2/h$. Notice that the occupation factors do not appear explicitly because the self-consistent chemical potentials have been written in terms of the transmission coefficients. Each factor g_i indicates that, in its journey between current channels m and n , an electron has entered the intermediate channel i and then returned incoherently to the sample. The discussion of the physical meaning of this equation will be expanded throughout this paper.

Notice that the GLBE are well suited (but do not need) to use real space representation, while the traditional forms of the Kubo formula are evaluated in the momentum representation resorting to ensemble averages. This gives some advantage to the first method, because not using ensemble averages it describes exactly the quantum interferences of a particular mesoscopic device. However, one might think that this is also a limitation as it could not deal with macroscopic transport. The present paper intends to show that this is not the case. We will prove that Eq. (1.3) also describes most of the known situations of transport in macroscopic samples. For this, we will need to relate the transmission probabilities to

well-established properties of the Green's functions.

The results of this paper are presented as follows. In Sec. II we show how the transmittances are evaluated from a model Hamiltonian for the dissipative electronic system, emphasizing the results that hold for a macroscopic sample. Section III presents the main results of this paper. First we show that for a macroscopic sample with inelastic processes there is an inelastic channel associated with each point \mathbf{r}_n within the sample and the solution of Eq. (2.3) takes the form

$$\tilde{T}(\mathbf{r}_n, \mathbf{r}_m) = T(\mathbf{r}_n, \mathbf{r}_m) + \int d\mathbf{r}_i T(\mathbf{r}_n, \mathbf{r}_i) g_i \tilde{T}(\mathbf{r}_i, \mathbf{r}_m),$$

where $1/g_i = \int d\mathbf{r}_j T(\mathbf{r}_j, \mathbf{r}_i)$. By identifying T with a density propagator, we show that this equation represents a classical random walk of an excited electron. From this we sketch the evaluation of the corresponding diffusion constant \tilde{D} . In Sec. IV we perform some approximations which allow us to evaluate \tilde{D} in a wide range of transport regimes: ballistic, metallic, weakly localized, and strongly localized. This shows that the description of Sec. III is consistent with known results of transport. Finally, in Appendixes A and B, we present known results about Green's functions and their averages introducing a notation consistent with the present work.

II. THE GENERALIZED LANDAUER-BÜTTIKER EQUATIONS

Formulation in terms of Green's functions

In order to describe the quantum nature of transport we need to define a Hamiltonian. We describe the isolated sample by a tight-binding Hamiltonian with one orbital at each point \mathbf{r}_n (with $n = 1, \dots, M$) of a hypercubic lattice with spacing a .

$$\mathbf{H}^0 = \sum_{n=1}^M \left[E_n^0 c^\dagger(\mathbf{r}_n) c(\mathbf{r}_n) + \sum_{\substack{m \\ (\mathbf{r}_m \text{ nn, of } \mathbf{r}_n)}} V_{m,n}^0 c^\dagger(\mathbf{r}_m) c(\mathbf{r}_n) \right]. \quad (2.1)$$

The site energy E_n^0 represents the potential energy and hence should contain contributions due to the impurity potential $U(\mathbf{r}_n)$ as well as those arising from a self-consistent Hartree potential. The kinetic energy term is defined through the hopping parameter $V_{m,n}^0$. For simplicity, the sum is restricted to \mathbf{r}_m nearest neighbors of \mathbf{r}_n . In this case $V_{m,n}^0 = \hbar^2 / (2m^* a^2) \exp(i\phi_{m,n})$ is given in terms of the lattice constant, the effective mass, and a phase. The phase is determined by the path integral of the magnetic vector potential: $\phi_{m,n} = (e/c\hbar) \int_{\mathbf{r}_n}^{\mathbf{r}_m} \mathbf{A} \cdot d\mathbf{r}$. In the following calculations we assume $\mathbf{A} \equiv 0$. This model describes all the relevant parameters of the electronic structure: the local density of states per spin at the Fermi energy $N_0(\mathbf{r})$, the Fermi velocity v , the mean free path l and, if finite, the localization length $\lambda \geq l$. The specific geometry of the sample is imposed by restricting the domain of the points \mathbf{r} .

In the notation introduced above, the expression “ X^0 ”

indicates that a physical quantity X is evaluated in the closed system described by the Hamiltonian (2.1). Later, we will use \tilde{X} to indicate the self-consistent evaluation of X in a system with dissipative processes and open boundaries. An actual sample is in fact an open system and then requires the appropriate treatment. The idea is to partition the Hilbert space of the universe in two pieces: the subspace spanned by \mathbf{H}^0 , and its orthogonal complement. This breaks the total Hamiltonian in four blocks. The diagonal blocks are \mathbf{H}^0 (sample) and \mathbf{H}^1 (external world). The nondiagonal blocks correspond to their coupling. We must adopt some model for this external world by modeling the leads and the phonon bath, that is, $\mathbf{H}^1 \approx \mathbf{H}_{\text{esc}} + \mathbf{H}_{\text{in}}$. Then we perform a projection¹⁵ over the subspace of the “sample” and get an effective Hamiltonian^{16,10} of the form

$$\mathbf{H} = \mathbf{H}^0 + \Sigma_{\text{esc}} + \Sigma_{\text{in}}. \quad (2.2)$$

As a result, the Hamiltonian (2.1) is renormalized by the connection to the external world through the effects of the leads and the electron-phonon coupling.

The leads renormalize the Hamiltonian (2.1) with a self-energy operator Σ_{esc} . We will see below that as long as we deal with a macroscopic sample we will not need an explicit expression for Σ_{esc} . Therefore it is enough to conceive the leads as represented by a set of independent one-dimensional channels which can be assimilated to the propagating modes of real ordered leads. In that case their effect is the renormalization of the site energies at the boundaries with a complex (non-Hermitic) self-energy whose imaginary part represents the escape rate to the contacts.

In order to define a solvable electron-phonon interaction we assume, following Datta,¹¹ uncorrelated point scatterers in local thermodynamic equilibrium with a bath. This assumption produces, as a one-dimensional lead, a complex self-energy which is a δ function in real space and hence does not generate intersite interactions:

$$\Sigma_{\text{in}} = \sum_{n=1}^M \Sigma_{\text{in}}(\mathbf{r}_n) c^\dagger(\mathbf{r}_n) c(\mathbf{r}_n). \quad (2.3)$$

Details of the calculation of this self-energy in terms of the spectral density of the phonon field at a given temperature and the coupling constant may be found in Ref. 11. It is important to remark that by adopting this model for the electron-phonon interaction we may interchange the words inelastic channels and (one-dimensional) leads. In general, by independent channels we mean orthogonal sets of states, each set (channel) with infinite number of degrees of freedom. A complex part in the effective Hamiltonian means that density is not conserved within the subspace of the sample. One can include the real part of this self-energy as a homogeneous shift in the lattice potential and retain as a free parameter the site-independent imaginary part:

$$\text{Im} \Sigma_{\text{in}}^{R(A)}(\mathbf{r}_n) = \mp i\eta = \mp i \frac{\hbar}{2\tau_{\text{in}}}. \quad (2.4)$$

Here we used the label $R(A)$ denoting the retarded

(advanced) boundary condition on the self-energies, which determines that, given an initial state at time $t=0$, the electrons (holes) are lost in the quantum coherent description provided by the effective Hamiltonian because they escape toward the leads or mix with the phonon coordinates. These particles are recovered through boundary conditions on the occupation of the states which impose charge conservation at each later time. The “recovered” particles, however, do not have memory of the quantum phase of the previous state. As mentioned in the preceding section, this is just the physics described by Eqs. (1.2). These equations can also be ob-

tained¹¹ using the field-theoretical methods of nonequilibrium statistical mechanics.¹⁴ Hence Green’s-function techniques provide a formal way to describe this physics. From a practical point of view, the self-energies and transmission probabilities are more easily evaluated using the Green’s-function framework. Then, let us first consider the case of the isolated sample. We evaluate the retarded and advanced Green’s functions defined in terms of the electron field operator ψ at time t_n and position \mathbf{r}_n acting over the ground state $|\Psi_0\rangle$ of Eq. (2.1) or, equivalently, in terms of the one-particle eigenfunctions $\varphi_p(\mathbf{r}_n)$ as

$$\begin{aligned} G_{n,m}^{OR(A)}(t_n, t_m) &\equiv G^{OR(A)}(\mathbf{r}_n, t_n, \mathbf{r}_m, t_m) = \mp \frac{i}{\hbar} \Theta(\pm(t_n - t_m)) \langle \Psi_0 | \psi(\mathbf{r}_n, t_n) \psi^\dagger(\mathbf{r}_m, t_m) + \psi^\dagger(\mathbf{r}_m, t_m) \psi(\mathbf{r}_n, t_n) | \Psi_0 \rangle \\ &= \mp \frac{i}{\hbar} \Theta(\pm(t_n - t_m)) \sum_p \varphi_p(\mathbf{r}_n) \varphi_p^*(\mathbf{r}_m) \exp -iE_p^0(t_n - t_m)/\hbar. \end{aligned} \quad (2.5)$$

We often will use $G_{n,m}^0(\varepsilon) \equiv G^0(\mathbf{r}_n, \mathbf{r}_m, \varepsilon)$, the Fourier transform of Eq. (2.5) with respect to $t_n - t_m$. The Green’s function does not depend on $t = (t_n + t_m)/2$ and only the occupations might eventually depend on this variable if the system is not in a steady state.

We can include the inelastic processes and the escape toward the leads in the Green’s functions using the Dyson equation,

$$\mathbf{G} = \mathbf{G}^0 + \mathbf{G}^0(\Sigma_{\text{in}} + \Sigma_{\text{esc}})\mathbf{G}, \quad (2.6)$$

which is equivalent to Eq. (2.2). We will solve (2.6) exactly or use a perturbative approach suited to the specific system we need to deal with.

Let us assume that we have already evaluated the retarded (advanced) Green’s function. This is equivalent to knowing all the information about the spectral structure and the transition probabilities of our system. The first is given by the local density of states:

$$N_0(\mathbf{r}_n, \varepsilon) = \mp \frac{1}{\pi} \text{Im} G^{R(A)}(\mathbf{r}_n, \mathbf{r}_n, \varepsilon). \quad (2.7)$$

The transition probabilities are associated with the transmission coefficients, which are obtained in terms of the complex part of the self-energies in the corresponding channel and the Green’s functions using the expression obtained by Fisher and Lee:¹⁷

$$\begin{aligned} T_{n,m} &= T(\mathbf{r}_n, \mathbf{r}_m) \\ &= 2 \text{Im} \Sigma^R(\mathbf{r}_n) G^R(\mathbf{r}_n, \mathbf{r}_m, \varepsilon) G^A(\mathbf{r}_m, \mathbf{r}_n, \varepsilon) \\ &\quad \times 2 \text{Im} \Sigma^R(\mathbf{r}_m). \end{aligned} \quad (2.8)$$

The total transmission can also be written in a compact way as

$$1 - R_{n,n} = 4 \text{Im} \Sigma^R(\mathbf{r}_n) \text{Im} G^R(\mathbf{r}_n, \mathbf{r}_n, \varepsilon). \quad (2.9)$$

Notice that transmittances and self-energies in expres-

sions (2.8) and (2.9) would need an additional label to identify the nature of the channels connected with a given point of the sample (e.g., the electron-phonon, the lead channel, or any other process contributing with a self-energy correction). We did not write them to facilitate the notation. Besides, we will see that for a macroscopic sample described by our model Hamiltonian (2.2), only the inelastic channels are relevant. An obvious consequence of Eq. (2.8) is that channels which do not generate a complex self-energy have zero transmittance, even when they modify the Green’s function according to Eq. (2.6). This is the case of the evanescent modes of a lead.

III. GENERALIZED LANDAUER-BÜTTIKER EQUATIONS FOR MACROSCOPIC SYSTEMS

In order to deal with macroscopic samples we will take the limits of the sample size tending to infinity and the size of the mesh of the hypercubic lattice used to represent it tending to zero. We first observe that the effect of (2.3) is to shift the energy argument to the complex plane as $\varepsilon \rightarrow \varepsilon + i\eta$. The presence of the current leads and voltage probes is contained in Σ_{esc} which renormalizes strongly the site energies at sites in the contact regions. The effect is not trivial in the case of a finite sample. However, in a very large sample, the homogeneous complex part produced by the inelastic processes guarantees that those effects will be exponentially small¹⁸ far inside the sample. An upper bound is $\exp(-R/L_{\text{in}})$, where $L_{\text{in}} = v\tau_{\text{in}}$ is the inelastic length in the ballistic regime and R the distance to the surface. Therefore the Green’s-function solution of Eq. (2.6) is

$$G^{R(A)}(\mathbf{r}_n, \mathbf{r}_m, \varepsilon) = G^{OR(A)}(\mathbf{r}_n, \mathbf{r}_m, \varepsilon \pm i\eta). \quad (3.1)$$

In general, we know the main properties of the Green’s functions in the macroscopic limit. This allows us to

evaluate the transmittance using Eq. (2.8). Then, we must proceed with the solution of the GLBE, which has the form of Eq. (1.3). At this point, one realizes that in very large systems one can neglect the restrictions in the summations in (1.3). These restrictions are important when considering the contact regions, but because of the inelastic processes their effects cannot propagate far inside the sample. Besides, in the internal region of the sample the only channels are the inelastic ones which, in the model used, have a one-to-one correspondence with the lattice sites. This allows the conversion of the sums in Eq. (1.3) into integrals, giving

$$\tilde{T}(\mathbf{r}_n, \mathbf{r}_m) = T(\mathbf{r}_n, \mathbf{r}_m) + \int d\mathbf{r}_i T(\mathbf{r}_n, \mathbf{r}_i) g(\mathbf{r}_i) \tilde{T}(\mathbf{r}_i, \mathbf{r}_m). \quad (3.2)$$

This equation is central to the present work. It expresses that, in the steady state, the effective transmittance between the inelastic channels associated to two points is related to the transmittances between all the other channels. However, only those sites within a length L_{in} are relevant. The physical meaning is simple: The propagation of an electron from site \mathbf{r}_m to site \mathbf{r}_n can be done in two alternative ways: (a) With complete quantum coherence, which is represented by the first term on the right side; this term also contains the leak from the coherent state toward the inelastic channels and (b) having inelastic collisions on its journey with the last of them occurring at point \mathbf{r}_i , as represented by the integral. This term is essential to assure charge conservation and hence unitarity in \tilde{T} .

In order to get a deeper interpretation of Eq. (3.2) it is convenient to come back to the connection to the Green's functions. According to the results in Appendix A we see that, apart from constant factors, Eq. (2.8) represents a density propagator. Therefore Eq. (2.8) is a particular case of a more general expression:

$$T(\mathbf{r}_n, \mathbf{r}_m) = T(\mathbf{r}_n, \mathbf{r}_m, \omega)|_{\omega=0} \quad (3.3a)$$

with

$$\begin{aligned} T(\mathbf{r}_n, \mathbf{r}_m, \omega) &= 2 \operatorname{Im} \Sigma^R(\mathbf{r}_n) G^R(\mathbf{r}_n, \mathbf{r}_m, \varepsilon^+) \\ &\quad \times (G^A(\mathbf{r}_m, \mathbf{r}_n, \varepsilon^-) 2 \operatorname{Im} \Sigma^R(\mathbf{r}_m)) \\ &= 2 \operatorname{Im} \Sigma^R(\mathbf{r}_n) \frac{2\pi}{\hbar} P_\varepsilon(\mathbf{r}_n, \mathbf{r}_m, \omega) N_0(\mathbf{r}_m, \varepsilon) \\ &\quad \times 2 \operatorname{Im} \Sigma^R(\mathbf{r}_m) \end{aligned} \quad (3.3b)$$

where $G^{R(A)}$ is given by Eq. (3.1) and we have defined $\varepsilon^\pm = \varepsilon \pm \frac{1}{2} \hbar \omega$. With this notation, Eq. (3.1) becomes

$$P_\varepsilon(\omega) = P_{\varepsilon+i\eta}^0(\omega) = P_\varepsilon^0 \left[\omega + i \frac{2}{\hbar} \eta \right], \quad (3.4)$$

according to the notation used in Appendix A, $P_\varepsilon^0(\mathbf{r}_n, \mathbf{r}_m, \omega)$, the Fourier transform, for a frequency ω , of $P_\varepsilon^0(\mathbf{r}_n, t_n, \mathbf{r}_m, t_m)$. The last gives the probability of propagation for an excitation, injected with an energy ε_m , from point \mathbf{r}_m to point \mathbf{r}_n in a time $t_n - t_m$. Since P^0 is evaluated in the absence of interactions, it conserves both energy and particle number.

Since the effective transmission coefficient \tilde{T} in Eq. (3.2) describes the self-consistent propagation of an excitation, we define a self-consistent density propagator \tilde{P} in analogy with Eq. (3.3).

$$\tilde{T}(\mathbf{r}_n, \mathbf{r}_m) = \tilde{T}(\mathbf{r}_n, \mathbf{r}_m, \omega)|_{\omega=0} \quad (3.5a)$$

and

$$\begin{aligned} \tilde{P}_{\varepsilon_m}(\mathbf{r}_n, \mathbf{r}_m, \omega) &= \int d\varepsilon_n \tilde{P}_{\varepsilon_n, \varepsilon_m}(\mathbf{r}_n, \mathbf{r}_m, \omega) \\ &= \frac{1}{2 \operatorname{Im} \Sigma(\mathbf{r}_n)} \tilde{T}(\mathbf{r}_n, \mathbf{r}_m, \omega) \frac{1}{2 \operatorname{Im} \Sigma(\mathbf{r}_m)} \\ &\quad \times \frac{1}{N_0(\mathbf{r}_m, \varepsilon_m)} \end{aligned} \quad (3.5b)$$

where the initial and final energies ε_m and ε_n are both very close to the Fermi energy ε_F . The essential idea is that Eq. (3.2) represents an equation for this density propagator. In fact, using this new notation we see that the solution of the generalized Landauer-Büttiker equation can be written as

$$\begin{aligned} \int d\varepsilon_n \tilde{P}_{\varepsilon_n, \varepsilon_m}(\mathbf{r}_n, \mathbf{r}_m, \omega) &= \frac{\hbar}{2\pi} G^{OR}(\mathbf{r}_n, \mathbf{r}_m, \varepsilon_m^+ + i\eta) G^{OA}(\mathbf{r}_m, \mathbf{r}_n, \varepsilon_m^- - i\eta) \frac{1}{N_0(\mathbf{r}_m, \varepsilon_m)} \\ &\quad + \int d\mathbf{r}_i \int d\varepsilon_i \frac{\hbar}{2\pi} G^{OR}(\mathbf{r}_n, \mathbf{r}_i, \varepsilon_i^+ + i\eta) G^{OA}(\mathbf{r}_i, \mathbf{r}_n, \varepsilon_i^- - i\eta) \frac{1}{N_0(\mathbf{r}_i, \varepsilon_i)} \frac{1}{\tau_{in}} \tilde{P}_{\varepsilon_i, \varepsilon_m}(\mathbf{r}_i, \mathbf{r}_m, \omega), \end{aligned} \quad (3.6)$$

for $\omega=0$, and $\varepsilon_m = \varepsilon_F$. We assume that this can be extended for all $\omega \neq 0$ but small enough so that densities of states and self-energies do not change appreciably in a range $\hbar\omega$ around the Fermi energy. We observe that the first term in the right-hand side of Eq. (3.6) is $P_\varepsilon^0(\mathbf{r}_n, \mathbf{r}_m, \omega + i2\eta/\hbar)$, the Fourier transform for a complex frequency. $\omega + i2\eta/\hbar$ of $P_\varepsilon^0(\mathbf{r}_n, t_n, \mathbf{r}_m, t_m)$. If we come back to the time variable we get

$$\tilde{P}_{\varepsilon_F}(\mathbf{r}_n, t_n, \mathbf{r}_m, t_m) = P_{\varepsilon_F}^0(\mathbf{r}_n, t_n, \mathbf{r}_m, t_m) \exp \left[\frac{t_n - t_m}{-\tau_{in}} \right] + \int d\mathbf{r}_i \int P_{\varepsilon_F}^0(\mathbf{r}_n, t_n, \mathbf{r}_i, t_i) \exp \left[\frac{t_n - t_i}{-\tau_{in}} \right] \frac{dt_i}{\tau_{in}} \tilde{P}_{\varepsilon_F}(\mathbf{r}_i, t_i, \mathbf{r}_m, t_m). \quad (3.7)$$

This is the basic equation we solve in this work. Its physical meaning is related to that already discussed in reference to Eq. (3.2). Observe that the first term in the right-hand side of Eq. (3.7), which describes the coherent beam, does not conserve the particle number. However, the second term, which considers all the incoherent paths, assures the total conservation. We often call $P_{\epsilon_F}^0$ the *quantum* probability of propagation because it represents the propagation in absence of phase breaking processes. When those processes are present \tilde{P}_{ϵ_F} is the total probability, which is composed of a *coherent* part $P_{\epsilon_F} = P_{\epsilon_F}^0 + i\eta$ and a *sequential* or *incoherent* part $\tilde{P}_{\epsilon_F} - P_{\epsilon_F}$. This nomenclature recognizes an antecedent in a discussion of dissipative tunneling process by Büttiker.¹² When a long-time scale is considered, \tilde{P}_{ϵ_F} becomes a *classical* probability of propagation due to the complete attenuation of its quantum (coherent) component. In fact, Eq. (3.7) represents a classical non-Markovian process,¹⁹ which describes a random walk of the excitation in a d -dimensional real space. Therefore, in the long-time and large distances regime, its behavior is characterized by a diffusion coefficient \tilde{D}_d . In this classical regime, the application of the fluctuation-dissipation theorem relates \tilde{D}_d to the conductivity through the Einstein relation:

$$\tilde{\sigma}_d = 2e^2 \tilde{D}_d N_0. \quad (3.8)$$

We will show in the next section that \tilde{D}_d evaluated from (3.7) describes the expected results for quantum transport.

While Eq. (3.5) involves a continuous time distribution for the inelastic processes, which might be difficult to solve in the general case, we get a Markovian approximation considering a discrete time process. This involves the replacement $\exp(-t/\tau_{in}) \rightarrow \tau_{in} \delta(t - \tau_{in})$ in Eq. (3.7). In physical terms this corresponds to a process in which the loss of coherence occurs with probability one at a characteristic clock's tick, with a period τ_{in} . At that time the quantum probability of propagation is sampled and a new quantum evolution starts with the new initial value until the next clock's tick. Therefore, at τ_{in} the quantum probabilities are the transition probabilities of the Markovian process. In this condition Eq. (3.7) becomes

$$\begin{aligned} \tilde{P}_{\epsilon_F}(\mathbf{r}_n, \tau_{in}, \mathbf{r}_m, 0) &= P_{\epsilon_F}^0(\mathbf{r}_n, \tau_{in}, \mathbf{r}_m, 0) \\ &\equiv P(\mathbf{r}_n, \mathbf{r}_m). \end{aligned} \quad (3.9)$$

which can be interpreted as a matching condition between the quantum and classical regimes of the probability of propagation. This equation also defines $P(\mathbf{r}_n, \mathbf{r}_m)$, the transition probability in a classical Markov process, which can be used to estimate the kinetic constants involved in the solutions of Eq. (3.7). For example, the evaluation of the mean square displacement between inelastic collisions gives

$$2d\tilde{D}_d\tau_{in} = \langle [\mathbf{r}_m(\tau_{in}) - \mathbf{r}_n(0)]^2 \rangle^0. \quad (3.10)$$

Here the mean value of the right-hand side is evaluated

with the quantum probability in the absence of inelastic processes, while the left-hand side corresponds to a classical diffusive process.

IV. EVALUATION OF THE TRANSPORT COEFFICIENT

A. Ballistic regime

In this case the electrons propagate ballistically until they suffer a phase randomizing collision in a characteristic time τ_{in} . The quantum propagation is associated with the product of Green's functions.

$$G^{0R}(\mathbf{r}, \mathbf{r}_0, \epsilon_F) G^{0A}(\mathbf{r}_0, \mathbf{r}, \epsilon_F) \sim \frac{1}{|\mathbf{r} - \mathbf{r}_0|^{d-1}}, \quad (4.1)$$

which reflects the fact that quantum mechanics gives a propagation probability $P_{\epsilon_F}^0(\mathbf{r}, t, \mathbf{r}_0, 0)$ with a mean at $|\mathbf{r} - \mathbf{r}_0| = vt$ in correspondence with the classical ballistic behavior. Therefore Eq. (3.7) describes a classical diffusive transport with a diffusive constant given by

$$\tilde{D}_d = \frac{v^2}{d} \tau_{in}, \quad (4.2)$$

the same value that we would obtain using (3.10). The same value of $\tilde{\sigma}_1$ has been obtained in a previous paper¹⁰ by solving directly Eqs. (1.2).

B. Weakly disordered systems

This regime corresponds to the metallic limit in which the resistance is linear on the concentration of impurities. In order to perform analytic evaluations of Eq. (3.7) we may resort to ensemble averages which restore the homogeneity of the space. Performing the Fourier transform of spatial coordinates in Eq. (3.6) we get

$$\begin{aligned} \tilde{P}_{\epsilon_F}(\mathbf{q}, \omega) &= P_{\epsilon_F}^0(\mathbf{q}, \omega + i2\eta) \\ &+ P_{\epsilon_F}^0(\mathbf{q}, \omega + i2\eta) 2\eta \tilde{P}_{\epsilon_F}(\mathbf{q}, \omega). \end{aligned} \quad (4.3)$$

The input in this equation is the averaged density propagator in the absence of phase randomizing processes, that is, the product of Green's functions $\langle G^{0R} G^{0A} \rangle$. This, in turn, can be expressed as a Bethe-Salpeter equation (see Appendix B) in terms of $\langle G^{0R} \rangle \langle G^{0A} \rangle$, the product of the ensemble averaged Green's functions of the form (B2). In the limit of long distances it gives

$$\begin{aligned} \langle G^{0R}(\mathbf{r}, \mathbf{r}_0, \epsilon_F) \rangle \langle G^{0A}(\mathbf{r}_0, \mathbf{r}, \epsilon_F) \rangle \\ \sim \frac{1}{|\mathbf{r} - \mathbf{r}_0|^{d-1}} \exp \left[-\frac{|\mathbf{r} - \mathbf{r}_0|}{l} \right] \end{aligned} \quad (4.4)$$

which resembles the product of Green's function in the ordered system but with an exponential decay with a characteristic length $l = v\tau_{el}$.

As shown in Appendix B, the quantum density propagator can be evaluated in terms of the expression (4.4) in an approximation in which only ladder diagrams are retained. This is expressed by Eq. (B4). The solution for times $t > \tau_{el} = l/v$ is a diffusive behavior described by Eq.

(B6) that is,

$$P_{\varepsilon_F}^0(\mathbf{q}, \omega) = \frac{1}{D_d q^2 - i\omega}, \quad (4.5)$$

with $D_d = vl/d$. We replace (4.5) in the expression (4.3), obtaining

$$\tilde{P}_{\varepsilon_F}(\mathbf{q}, \omega) = \frac{1}{\tilde{D}_d q^2 - i\omega}, \quad (4.6)$$

with $\tilde{D}_d = D_d$. This is a remarkable result, which could be expected on physical grounds. This means that as long as the quantum evolution is well described by a diffusive process, the inelastic time does not appear explicitly in the transport coefficient. However, this approximation breaks down in two opposite regimes.

(a) When τ_{in} is small as compared with τ_{el} , the mean time between elastic collisions. In fact, observe that we do not recover the ordered regime for the propagator defined in Eq. (A6) if we use the approximation to the mean value given by Eq. (B7). This approximation, which gives a diffusive behavior (4.5) for the quantum evolution, is not good for short times where the transport is still ballistic.

(b) When τ_{in} becomes comparable to the time in which quantum interferences start to contribute. These interferences arise from multiple scattering between impurities, a process which is neglected when only the ladder diagrams are considered. An improvement is to evaluate the density propagator including also the ‘‘fan’’ diagrams.²⁰ In this regime the inelastic time is a necessary ‘‘cutoff’’ to avoid divergences of the integrals and therefore the quantum corrections depend on its value. These corrections, however, are not enough to deal with the strongly localized regime, in the usual conductivity calculations. The GLBE, instead, describe also the localized regime provided that the behavior of $P_{\varepsilon_F}^0(\mathbf{r}_n, t_n, \mathbf{r}_m, t_m)$ is known in this regime.

C. Localized regime

When we need to consider the regime where the localization is important we recall that the asymptotic behavior of the average of the products of Green’s functions is

$$\langle G^{OR}(\mathbf{r}, \mathbf{r}_0, \varepsilon_F) G^{OA}(\mathbf{r}_0, \mathbf{r}, \varepsilon_F) \rangle \sim \frac{1}{|\mathbf{r} - \mathbf{r}_0|^{d-1}} \exp\left[-\frac{|\mathbf{r} - \mathbf{r}_0|}{\lambda}\right]. \quad (4.7)$$

Here the localization length satisfies $\lambda \geq l$, with the equality only valid in strictly one-dimensional systems. This result cannot be obtained diagrammatically. A complete summation of diagrams would be necessary to include a dependence of D_d on ω and \mathbf{q} which describes the localization effects. However, Eq. (3.7) does not contradict (4.4), which is still valid. Besides, for times shorter than that required to reach the boundaries of the localization regions, $t_{loc} = \lambda^2/2D_d$, the diffusive behavior should be a good approximation of the quantum evolution. Therefore we can use an early idea of Thouless,²¹ who approximated the localized behavior of $P_{\varepsilon_F}^0(\mathbf{r}_n, t_n, \mathbf{r}_m, t_m)$ as the

solution of the diffusion equation within a spherical box of radius λ and surface S which contains \mathbf{r}_0 as an interior point. Then the particle diffuses limited by this constraint, represented as a boundary condition requiring that at every time the current vanishes at the surface of the localization sphere, that is,

$$\mathbf{n} \cdot \nabla P_{\varepsilon_F}^0(\mathbf{r}, t, \mathbf{r}_0, 0)|_{\mathbf{r} \in S} = 0 \quad (4.8)$$

where \mathbf{n} is the normal to S . When an inelastic process occurs at a given point \mathbf{r} a new evolution starts in a sphere enclosing this point. This observation leads to an interpretation of the function:

$$P(\mathbf{r}, \mathbf{r}_0) = \frac{1}{\tau_{in}} P_{\varepsilon_F}(\mathbf{r}, \mathbf{r}_0, \omega)|_{\omega=0} = \int_0^\infty \frac{dt}{\tau_{in}} \exp(-t/\tau_{in}) P_{\varepsilon_F}^0(\mathbf{r}, t, \mathbf{r}_0, 0) \quad (4.9)$$

as the probability distribution for an inelastic collision at position \mathbf{r} after an inelastic collision at time 0 at position \mathbf{r}_0 . This also gives a physical interpretation for the zero-frequency limit of $P(\mathbf{r}, \mathbf{r}_0, \omega)$. This is also the same physical meaning as the probability defined in Eq. (3.9). However, in that case it was evaluated as a discrete time process. Introducing (B7) in (4.9) we get

$$P(\mathbf{r}, \mathbf{r}_0) - D_d \tau_{in} \nabla^2 P(\mathbf{r}, \mathbf{r}_0) = \delta(\mathbf{r} - \mathbf{r}_0). \quad (4.10)$$

The boundary condition (4.8) translates in an equivalent condition for $P(\mathbf{r}, \mathbf{r}_0)$. Apart from the boundary condition and a normalization factor, Eq. (4.10) expresses that $P(\mathbf{r}, \mathbf{r}_0)$ is itself a Green’s function and hence its asymptotic square modules is given by (4.7). The energy variable is replaced by $-\varepsilon = \hbar^2/(2m^* L_{in}^{*2})$. This gives a new attenuation length $L_{in}^* = (D_d \tau_{in})^{1/2}$, which is the inelastic length in the disordered regime. In one dimension (4.10) can be solved exactly by considering that the initial point x_0 may be anywhere in the range $[-\lambda, \lambda]$. This gives the probability distribution:

$$P(\mathbf{r}, \mathbf{r}_0) = \frac{1}{L_{in}^*} \frac{\cosh[(x_0 \pm \lambda)/L_{in}^*]}{\sinh(2\lambda/L_{in}^*)} \cosh[(x \mp \lambda)/L_{in}^*] \quad \text{for } \pm(x - x_0) > 0. \quad (4.11)$$

As in the discrete time process of Eq. (3.10), this solution can be used to evaluate the mean square displacement $\langle (x - x_0)^2 \rangle$ and from this we get the diffusion constant that includes the inelastic processes:

$$\tilde{D}_1 = \frac{\langle (x - x_0)^2 \rangle}{2\tau_{in}} = D_1 \left[1 - \left[\frac{L_{in}^*}{\lambda} \right] \tanh \left[\frac{\lambda}{L_{in}^*} \right] \right]. \quad (4.12)$$

This result contains the quantum correction due to weak localization when the inelastic time is relatively short:

$$\tilde{D}_1 \simeq D_1 \left[1 - \frac{L_{in}^*}{\lambda} \right] \quad (4.13)$$

in agreement with the diagrammatic calculations.²⁰ No-

tice that the localization length appears explicitly in this expression. For very weak inelastic events, the localization will manifest itself, preventing the diffusion beyond the limits of the localization “sphere.” The asymptotic value given by (4.11) is a uniform distribution inside S , and we get

$$\bar{D}_1 = \frac{\lambda^2}{3\tau_{\text{in}}} . \quad (4.14)$$

We should remark that we have described the right physics of the transport phenomena, using a rough estimate of the shape and eccentricity of the localization region. The fluctuation of this last is very important to determine the form of the weak-localization correction. A symmetric approximation would give a correction of the order $D_1 2(\lambda/L_{\text{in}}^*) \exp(-\lambda/L_{\text{in}}^*)$, which is weaker than that in Eq. (4.13). Therefore this model also sheds some light on the physics of the weak-localization correction.

V. FINAL REMARKS

In the present work we present the analytical proof that the generalized Landauer-Büttiker equations, originally devised to describe transport in small samples in the presence of measurement probes and dissipative processes, also contain the most important results of quantum transport in macroscopic systems. The explicit account of the inelastic processes constitutes an essential ingredient in our derivation. Currently, numerical solutions of GLBE for mesoscopic devices in the presence of dissipative processes are becoming an exciting topic of solid-state physics and an important tool to proceed toward the development of a new generation of electronic devices. However, while the GLBE are well suited for numerical implementation in small samples, actual codes^{10,22} cannot be easily applied to the macroscopic limits because of the huge computational time required. We expect that those methods could be improved to take advantage of the physics discussed in this paper.

In addition, our work clarifies the physics involved in transport processes. It supports a vision within which the coupling with the external world is fundamental to obtain the real relaxation, and hence determines the dissipative nature of the transport processes. We have discussed how, if we only consider the collisions with the impurities, the diffusion of an excitation is an approximation, within certain limits, to the exact quantum evolution of the closed system. Only the interaction with a system open to the external world (e.g., phonons) is able to transform this “almost” diffusive evolution in a true irreversible diffusive process. In the Boltzmann and Kubo equations, dissipation is somewhat subtly introduced by assigning statistical occupation factors which describe the conservation of the average current. That is why, when the inelastic processes are introduced explicitly in the Kubo equations as in Ref. 23, the local currents are not conserved.²⁴ In the linear response regime of the quantum Boltzmann equation, presented in the form of the generalized Landauer-Büttiker equations, the conservation of current is imposed at every point of the system

and hence it determines self-consistently the local occupation of the energy states. This self-consistency is contained in Eq. (3.2), which is the cornerstone of this work.

Our formal description could also help to clarify other phenomena. An old problem is the variable range hopping regime for the conductance. In this extremely localized limit, the essential physics has been pointed out many years ago by Mott and Davies.²⁵ However, a description from a model Hamiltonian without further adjustable parameters²⁶ and consistent with the other regimes has been elusive. Our numerical simulations and some analytical results seem to show that the GLBE provide again the right track toward this objective. Another area in which the GLBE could be used in the treatment of magnetotransport in the presence of dissipation for the different regimes. Finally another problem of fundamental interest in the transport phenomena is to account for the electron-electron interaction. From a formal point of view the problem becomes much more complex; however, it is this complexity which drives the quantum evolution of the system close to irreversibility. Therefore, as discussed with reference to Eqs. (3.7) and (3.9), there is a characteristic collision time τ_ϕ , at which the one-body description breaks down and becomes so complex that it can be approximated by a diffusive process. Therefore τ_ϕ plays a role similar to τ_{el} in the description of Sec. III B. The true irreversibility is assured by the interaction with a bath in characteristic time τ_{in} which, however, does not appear explicitly in the diffusion constant provided that it is much larger than τ_ϕ . This is the regime of the recent experiments²⁷ of electrostatic focusing of electron beam, in solid-state devices in which the coherence of the ballistic propagation is broken by the electron-electron interactions. In a different context, we have recently reported²⁸ results on experimental kinetic constants in the regime of strongly interacting electrons. There, we used a set of crystals in which the dimensionality of the dynamics can be engineered to take values between one and two. The analysis of the data showed consistency with the above point of view.

ACKNOWLEDGMENTS

It is a pleasure to acknowledge Boris Altshuler for discussions on the Keldysh technique and the transport problem as well as discussions with Patrick Lee. Conversations with R. Landauer, M. Büttiker, and A. Szafer have been of great benefit to the author. This work was partially supported by the Organization of American States. The author is a member of the Consejo Nacional de Investigaciones Científicas y Técnicas with a leave of absence from the Instituto de Desarrollo Tecnológico para la Industria Química (Santa Fe, Argentina).

APPENDIX A: DENSITY PROPAGATOR

Here we review results³ on the connection between the Green’s functions and the propagation in real space of a density excitation. That relation has been exploited by a number of Soviet authors.²⁹ First, we remember that the probability of finding a particle at point \mathbf{r}_2 and time t_2 ,

provided that it was injected at an earlier time t_1 at position \mathbf{r}_1 , is given by

$$P^0(\mathbf{r}_2, \mathbf{r}_1, t_2 - t_1) = \hbar^2 G^{OR}(\mathbf{r}_2, t_2, \mathbf{r}_1, t_1) \times G^{OA}(\mathbf{r}_1, t_1, \mathbf{r}_2, t_2). \quad (\text{A1})$$

However, we are interested in adding a particle with a

given energy close to the Fermi energy. Besides, this energy dependence would enable one to deal with the exclusion principle. For this we should allow an uncertainty in the initial and final times compatible with that energy. That is, we are seeking a propagation for particles which are placed with energy ε_1 and found with energy ε_2 , both very close to the Fermi surface. Hence we define the more general function:

$$G^{OR}(\mathbf{r}_2, t_2^R, \mathbf{r}_1, t_1^R) G^{OA}(\mathbf{r}_1, t_1^A, \mathbf{r}_2, t_2^A) = \int \frac{d\varepsilon_R}{2\pi\hbar} \int \frac{d\varepsilon_A}{2\pi\hbar} \exp[-i\varepsilon_R(t_2^R - t_1^R)/\hbar] \exp[-i\varepsilon_A(t_1^A - t_2^A)/\hbar] \times G^{OR}(\mathbf{r}_2, \mathbf{r}_1, \varepsilon_R) G^{OA}(\mathbf{r}_1, \mathbf{r}_2, \varepsilon_A). \quad (\text{A2})$$

Here, the initial and final times are $t_1 = (t_1^R + t_1^A)/2$ and $t_2 = (t_2^R + t_2^A)/2$, while the uncertainties are given by $\delta t_1 = t_1^R - t_1^A$ and $\delta t_2 = t_2^R - t_2^A$. We will be interested in a situation in which $\delta t_{1(2)} \ll |t_2 - t_1|$. Now we rewrite the above expression in terms of new energy and frequency variables $\varepsilon_1 = (\varepsilon_R + \varepsilon_A)/2$ and $\omega = (\varepsilon_R - \varepsilon_A)/\hbar$. Using the shorthand notation $\varepsilon^\pm = (\varepsilon \pm \frac{1}{2}\hbar\omega)$, we get

$$\int \frac{d\varepsilon_1}{2\pi\hbar} \int \frac{d\omega}{2\pi} \exp[-i\varepsilon_1(\delta t_2 - \delta t_1)/\hbar] \exp[-i\omega(t_2 - t_1)] G^{OR}(\mathbf{r}_2, \mathbf{r}_1, \varepsilon_1^+) G^{OA}(\mathbf{r}_1, \mathbf{r}_2, \varepsilon_1^-). \quad (\text{A3})$$

We introduce a further integral over a ‘‘final’’ energy ε_2 and a δ function to compensate it, so we get

$$\int d\varepsilon_1 \int d\varepsilon_2 \exp[-i(\varepsilon_2 \delta t_2 - \varepsilon_1 \delta t_1)/\hbar] \frac{1}{\hbar^2} \left[\frac{\hbar}{2\pi} \delta(\varepsilon_2 - \varepsilon_1) \int \frac{d\omega}{2\pi} e^{-i\omega(t_2 - t_1)} G^{OR}(\mathbf{r}_2, \mathbf{r}_1, \varepsilon_1^+) G^{OA}(\mathbf{r}_1, \mathbf{r}_2, \varepsilon_1^-) \right]. \quad (\text{A4})$$

When we allow the δt 's to take the smallest value compatible with the energy, the whole expression approaches Eq. (A1). In that condition the exponential functions in the energy integration take a unitary value in the range of interest. Therefore we identify the term inside the parentheses as the probability of propagation for a single particle. The δ function imposes the energy conservation $\varepsilon_2 = \varepsilon_1$; and (A1) becomes the integral over the initial energy of

$$\int d\varepsilon_2 P_{\varepsilon_2, \varepsilon_1}^0(\mathbf{r}_2, t_2, \mathbf{r}_1, t_1) N_0(\mathbf{r}_1, \varepsilon_1) = P_{\varepsilon_1}^0(\mathbf{r}_2, t_2, \mathbf{r}_1, t_1) N_0(\mathbf{r}_1, \varepsilon_1) = \frac{\hbar}{2\pi} \int \frac{d\omega}{2\pi} e^{-i\omega(t_2 - t_1)} G^{OR}(\mathbf{r}_2, \mathbf{r}_1, \varepsilon_1^+) G^{OA}(\mathbf{r}_1, \mathbf{r}_2, \varepsilon_1^-). \quad (\text{A5})$$

A comparison with Eq. (A1) shows that $P_{\varepsilon_F}^0$ measures the probability of propagation of a particle injected with energy ε_1 from the initial to the final point. Setting $\varepsilon_1 \approx \varepsilon_F$, the Fourier transform of Eq. (A5) is just

$$P_{\varepsilon_F}^0(\mathbf{r}_2, \mathbf{r}_1, \omega) N_0 = \int d\varepsilon P_{\varepsilon, \varepsilon_F}^0(\mathbf{r}_2, \mathbf{r}_1, \omega) N_0 = \frac{\hbar}{2\pi} G^{OR}(\mathbf{r}_2, \mathbf{r}_1, \varepsilon_F^+) G^{OA}(\mathbf{r}_1, \mathbf{r}_2, \varepsilon_F^-). \quad (\text{A6})$$

If we were dealing with a homogeneous system it might be convenient to transform these results to the momentum representation to describe a density fluctuation with wave vector \mathbf{q} . The procedure is analogous to that used with the time variable. We allow for an uncertainty in the initial and final position, in a d -dimensional space, in order to have a defined momentum \mathbf{p} . Using the shorthand notation $\mathbf{p}^\pm = \mathbf{p} \pm \frac{1}{2}\hbar\mathbf{q}$, we get

$$P_{\varepsilon_F}^0(\mathbf{q}, \omega) N_0 = \frac{\hbar}{2\pi} \int G^{OR}(\mathbf{p}^+, \varepsilon_F^+) G^{OA}(\mathbf{p}^-, \varepsilon_F^-) \frac{d\mathbf{p}}{(2\pi\hbar)^d}. \quad (\text{A7})$$

This expression will be used in Appendix B.

APPENDIX B: DENSITY EVOLUTION IN A DISORDERED SYSTEM

Here we review the results^{29,3} of the evaluation of the density propagator in an infinite disordered system. As a model for the potential due to the impurities placed at random sites \mathbf{R}_i , we consider $U(\mathbf{r}) = \sum_i u(\mathbf{r} - \mathbf{R}_i)$. It is usual to retain only the lowest-order correlations and shift the energy origin in order to get a white-noise character for the potential:

$$\langle U \rangle = 0 \quad \text{and} \quad \langle U(\mathbf{r})U(\mathbf{r}') \rangle = u^2 \delta(\mathbf{r} - \mathbf{r}'), \quad (\text{B1})$$

where $u^2 = c_{\text{imp}} \int |u(\mathbf{r}) d\mathbf{r}|^2$ and c_{imp} is the concentration of impurities. Here $\langle X \rangle$ denotes the average of the quantity X over an ensemble of impurity configurations. The retarded (advanced) Green's function can also be averaged and we get

$$\langle G^{0R(A)}(\mathbf{p}, \varepsilon) \rangle = \frac{1}{\varepsilon - E_{\mathbf{p}} \pm i\hbar/2\tau_{\text{el}}} . \quad (\text{B2})$$

The elastic scattering rate can be calculated in the Born approximation which also defines a mean free path:

$$\frac{1}{\tau_{\text{el}}} = \frac{2\pi}{\hbar} u^2 N_0 \quad \text{and} \quad l = v\tau_{\text{el}} . \quad (\text{B3})$$

We need to evaluate $\langle G^R G^A \rangle$, the ensemble average of the product of Green's functions (A7) at the Fermi energy $\varepsilon = \varepsilon_F$. Because of the statistical correlation this is not equivalent to $\langle G^R \rangle \langle G^A \rangle$, the product of averaged Green's functions. However, we can perform a series expansion of the first in terms of the last. As usual in a conductance calculation, up to a precision $\hbar/\tau_{\text{el}}\varepsilon_F$, we only consider the ladder diagrams. In this approximation we get

$$\begin{aligned} P_{\varepsilon_F}^0(\mathbf{q}, \omega) &= \int \frac{d\mathbf{p}}{(2\pi\hbar)^d} \left[\frac{\hbar}{2\pi} \langle G^{0R}(\mathbf{p}^+, \varepsilon_F^+) \rangle \langle G^{0A}(\mathbf{p}^-, \varepsilon_F^-) \rangle \frac{1}{N_0} + \frac{\hbar}{2\pi} \langle G^{0R}(\mathbf{p}^+, \varepsilon_F^+) \rangle \langle G^{0A}(\mathbf{p}^-, \varepsilon_F^-) \rangle \frac{1}{N_0} \frac{1}{\tau_{\text{el}}} P_{\varepsilon_F}^0(\mathbf{q}, \omega) \right] \\ &= \frac{\hbar}{2\pi u^2 N_0} \frac{\zeta(\mathbf{q}, \omega)}{1 - \zeta(\mathbf{q}, \omega)} , \end{aligned} \quad (\text{B4})$$

where the function ζ is

$$\begin{aligned} \zeta(\mathbf{q}, \omega) &= u^2 \int \langle G^{0R}(\mathbf{p} + \frac{1}{2}\hbar\mathbf{q}, \varepsilon_F + \frac{1}{2}\hbar\omega) \rangle \langle G^{0A}(\mathbf{p} - \frac{1}{2}\hbar\mathbf{q}, \varepsilon_F - \frac{1}{2}\hbar\omega) \rangle \frac{d\mathbf{p}}{(2\pi\hbar)^d} \\ &= \int \frac{d\Omega}{S_d} \frac{1}{1 - i(\omega + \mathbf{v} \cdot \mathbf{q})\tau_{\text{el}}} \approx 1 + i\omega\tau_{\text{el}} - \frac{(lq)^2}{d} . \end{aligned} \quad (\text{B5})$$

Here the momentum integration was performed transforming as usual

$$\int \frac{d\mathbf{p}}{(2\pi\hbar)^d} \rightarrow \int \frac{d\Omega}{S} \int N_0(E_p) dE_p .$$

then the energy integral is evaluated by residues considering $q \ll p_F/\hbar$, and finally, the solid angle integration is evaluated in the limit $ql \ll 1$ and $\omega\tau_{\text{el}} \ll 1$. Using the ζ in (B4) we get the density propagator:

$$P_{\varepsilon_F}^0(\mathbf{q}, \omega) = \frac{1}{D_d q^2 - i\omega} , \quad (\text{B6})$$

with a diffusion constant defined as $D_d = v^2\tau_{\text{el}}/d$. The fact that the mean time between collisions is just the transport time is a consequence of the isotropic scattering against the impurity potential. Coming back to position and time variables, we find that the density propagator P^0 is indeed the Green's function of a diffusion equation:

$$\left[\frac{\partial}{\partial t_2} - D_d \nabla_2^2 \right] \langle P_{\varepsilon_F}^0(\mathbf{r}_2, t_2, \mathbf{r}_1, t_1) \rangle = \delta(t_2 - t_1) \delta(\mathbf{r}_2 - \mathbf{r}_1) . \quad (\text{B7})$$

which is interpreted as a probability of propagation for a density excitation in the hydrodynamic limit.

It is worthwhile to recall³⁰ the relation between the usual density-density response function χ and the density propagator defined above. In the linear response theory χ is defined in terms of the commutator of the density operator. $\delta\rho(\mathbf{r}, t) = \psi^\dagger(\mathbf{r}, t)\psi(\mathbf{r}, t) - \psi^\dagger(\mathbf{r})\psi(\mathbf{r})$, and it has the form

$$\chi(\mathbf{r}_2, \mathbf{r}_1, \omega) = \frac{i}{\hbar} \int_0^\infty d(t_2 - t_1) \exp[i\omega(t_2 - t_1)] \langle \Psi_0 | [\delta\rho(\mathbf{r}_2, t_2), \delta\rho(\mathbf{r}_1, t_1)] | \Psi_0 \rangle . \quad (\text{B8})$$

The commutator can be decomposed in three terms. Each one corresponds to the integral in energy of an expression of the form of (A6) in which any of the combinations $G^R G^A$, $G^R G^R$, and $G^A G^A$ appear multiplied by the corresponding occupation factors: $f(\epsilon^- - \mu^0) - f(\epsilon^+ - \mu^0)$, $-f(\epsilon^- - \mu^0)$, and $f(\epsilon^+ - \mu^0)$. Performing an average over impurity configurations, χ can be transformed to the \mathbf{q} space. The result (B6) holds for the $\langle G^R G^A \rangle$ term with an additional factor ω due to integration in energy. The terms with $\langle G^R G^R \rangle$ and $\langle G^A G^A \rangle$ combine to give, after integration, a contribution proportional to N_0 . In consequence, a simple expression for χ

in terms of P^0 can be obtained:

$$\chi(\mathbf{q}, \omega) = i\omega N_0 P_{\epsilon_F}^0(\mathbf{q}, \omega) + N_0 = \frac{N_0 D_d q^2}{D_d q^2 - i\omega}. \quad (\text{B9})$$

Including a factor of 2 to account for the spin degeneracy, the static conductivity can be evaluated as

$$\sigma_d = \lim_{\omega \rightarrow 0} \lim_{q \rightarrow 0} \left[-\frac{i\omega}{q^2} 2e^2 \chi(\mathbf{q}, \omega) \right] = 2e^2 N_0 D_d. \quad (\text{B10})$$

which is the Einstein formula.

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