PHYSICAL REVIEW B VOLUME 41, NUMBER 11 15 APRIL 1990-I

Conductance of a disordered linear chain including inelastic scattering events

Jorge L. D'Amato
Instituto de Desarrollo Tecnológico para la Industria Química, Güemes 3450, 3000 Santa Fe, Argentina

Horacio M. Pastawski
Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

(Received 6 July 1989; revised manuscript received 27 December 1989)

A study of the conductance in a disordered linear chain of finite length L including inelastic scattering processes is presented. Inelastic scatterers are introduced as defined by Büttiker and are assumed to be uniformly distributed along the system. This defines an inelastic scattering time τ_{in} plus a condition of charge conservation which in turn introduces incoherent electrons. The four-probe conductance of the system is then reduced to a Landauer-like behavior $G=2(e^2/h)T_{\text{eff}}/(1-T_{\text{eff}})$, where the effective transmission through the sample, T_{eff}, is the sum of two terms, one of which accounts for the phase-coherent electrons which have not suffered any inelastic collision and another for electrons which have suffered at least one inelastic collision in their journey. To show explicitly this point, the conductance of an ordered system is analyzed. Analytical and numerical results are presented for disordered chains, where resonances in the transmission present a width which is associated with the minimum between the escape time and the relaxation time. Because of the denominator in the Landauer formula, strong fluctuations on the conductance are present even in the weak-disordered situation in which the localization length $\lambda > L$, but we observed that they become of order e^2/h when the inelastic scattering length $L_{\text{in}}=L$. Further decrease of the inelastic length causes the fluctuations to reduce following similar laws to that of the metallic regime.

I. INTRODUCTION

Transport phenomena in small systems have shown a rich variety of effects when some external parameter is varied. Some examples are resonant tunneling, the Aharonov-Bohm effect, and conductance fluctuations in metals. In all these effects, the quantum-mechanical coherence plays a crucial role. Unlike macroscopic systems, where the ensemble average provides the right answer, the transport properties in mesoscopic systems are strongly dependent on the specific sample under consideration. In order to study the conductance of these systems, the Landauer approach[1] has been extensively used. In its most simple version, this gives the conductance in terms of the transmission coefficient between two one-dimensional perfect current leads attached to the sample. The formulation assumes very low temperatures and that the phase coherence length is larger than the dimensions of the sample. Finite temperature effects have been introduced only by taking into account the thermal population of the reservoirs connected to the perfect conductors,[2-4] and extension to multiple channel perfect leads has also been given.[4-6] However, all these formulations maintain the assumption that, within the sample, carriers only suffer elastic collisions. Recently, a generalization of the Landauer formalism has been proposed by Büttiker to include voltage probes explicitly.[7] Then he realized that any additional lead coupled to the sample and connected to an electron reservoir can be thought of as either a voltage probe or as an inelastic scatterer.[8] The method has the advantage that the quantum-mechanical coherence of the sample is not completely lost because averaging procedures are not used. In Ref. 8, a systematic study of the resistance of a sequence of elastic scatterers as a function of the number of inelastic scatterers between them was given, showing the transition from the coherent case to the completely incoherent one. In that work, the inelastic scatterers were modeled in terms of a scattering matrix with a coupling parameter that measures the strength of the incoherence introduced.

The aim of this paper is to present an alternative way to model the strength of the inelastic scatterers in order to examine, in particular, the conductance of a one-dimensional disordered chain. Unlike Ref. 8, we define each inelastic scatterer in terms of an electron reservoir coupled to the sample by only one perfect wire. Nearest-neighbor tight-binding Hamiltonians are employed to simulate both the sample and the perfect conductors attached to it. The basic idea is to use the tight-binding parameters of these lateral perfect leads to represent the coupling of the inelastic scatterers to the sample. It will be shown that an adequate choice of the site energies makes it possible for the hopping parameter to play this role. In this way the effect of the inelastic scatterers is to introduce an imaginary part to the energy levels at the sample sites to which they are connected. Besides, we adopt the Büttiker proposal of self-consistent calculation of the chemical potential in such a way that no net loss or gain of particles is produced. This condition introduces incoherent electrons to allow a steady-state current to flow along the sample.

To study the conductance of a disordered chain we introduce as many inelastic scatterers as the number of sites in the sample. Thus phase randomization processes are uniformly distributed along the system. We present both analytical and numerical results for different degrees of disorder and as a function of the inelastic scattering time.

II. OUR MODEL AND ITS SOLUTION

The model used to study the conductance of the disordered chain with inelastic scattering corresponds to the situation depicted in Fig. 1. The disordered chain and the perfect conductors which couple it to the reservoirs are both simulated by a nearest-neighbor tight-binding Hamiltonian H. The chain representing the sample extends from site 1 to N and a is the lattice parameter. The hopping parameter is V and the site energies take on random values within the interval $(-W/2, W/2)$ (Anderson disorder). At both left and right sides, the chain is connected by perfect leads (channels 0 and $N+1$) to electron reservoirs. The hopping parameter in both leads is also V and their site energies are all equal to zero. Therefore we have a perfect matching between these channels and the sample if no disorder is present in the latter. This is the most usual configuration in the Landauer formalism. Phase randomization processes are included by connecting inelastic scatterers to the sample. We represent an inelastic scatterer as an electron reservoir coupled to the chain through a perfect lead. Each site of the chain is connected to a different inelastic scatterer. We have used the same index for sites, channels, and reservoirs to avoid confusion. Unlike the other perfect leads, channels $i=1,2,\ldots,N$ have hopping parameter η and their site energies are all equal and different from zero. We call them E_r for the moment.

Let us briefly derive the conductance of the system for completeness. A very clear and detailed presentation of the approach is given in Ref. 8. Here we summarize the principal facts. It is assumed that the temperature is small enough and the effects of thermal population in the reservoirs are neglected. Then the net current in each channel is determined by the chemical potentials μ_L, μ_R, and μ_i; $i=1,2,\ldots,N$ if the transmission and reflection probabilities $T_{i,j}$ and $R_{i,i}$ are given. $T_{i,j}$ is the transmission probability from channel j to channel i and $R_{i,i}$ is the reflection probability at channel i. Taking $\mu_L > \mu_R$, the condition of no net current flow at each lateral reservoir i implies the following relations:

$$(1-R_{i,i})(\mu_i-\mu_R)-\sum_{j=1\,(j\neq i)}^{N} T_{i,j}(\mu_j-\mu_R) - T_{i,0}(\mu_L-\mu_R)=0, \quad \forall i=1,2,\ldots,N\,. \tag{2.1}$$

Here all contributions to current in the ith channel are summed: the first term on the left-hand side is the outgoing current, the second term involves the currents flowing from different lateral reservoirs to the ith channel, and the last term gives the contribution to the current of the left reservoir. Notice that this is completely equivalent to requiring current conservation along the sample, since the net current at each link between two consecutive sites in the sample becomes a constant. Chemical potentials μ_i, $i=1,2,\ldots,N$, are determined by imposing that Eq. (2.1) could be satisfied simultaneously. Therefore, they are given by

$$\mu_i-\mu_R=\left[\sum_{j=1}^{N} W^{-1}{}_{ij}T_{j,0}\right](\mu_L-\mu_R)\,, \quad \forall i=1,2,\ldots,N\,, \tag{2.2a}$$

where $\underline{W}^{-1}$ is the inverse matrix of the symmetrical matrix $\underline{W}$ given by

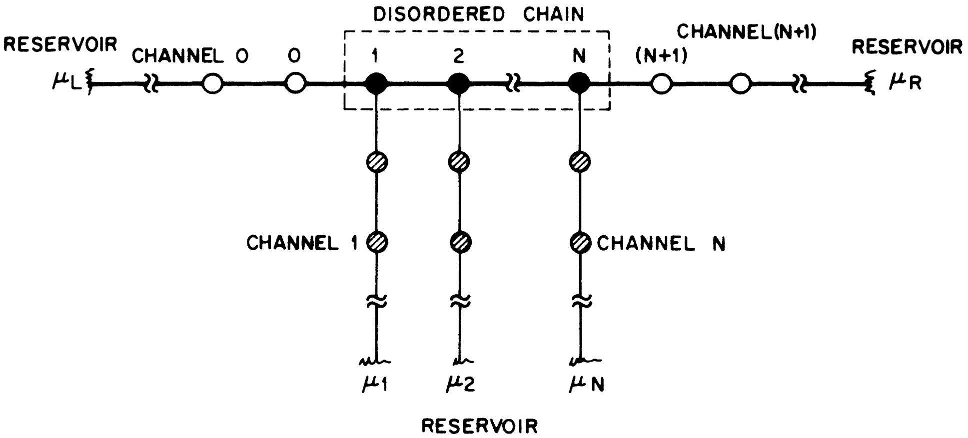

FIG. 1. Representation of the model. The chain extends from site 1 to site N and is connected by perfects leads (channels 0 and $N+1$) to electron reservoirs. To each site of the sample an inelastic scatterer is coupled.

$$\underline{W}=\begin{bmatrix}1-R_{1,1} & -T_{1,2} & \cdots & -T_{1,N}\\ -T_{2,1} & 1-R_{2,2} & \cdots & -T_{2,N}\\ \vdots & \vdots & \ddots & \vdots\\ -T_{N,1} & -T_{N,2} & \cdots & 1-R_{N,N}\end{bmatrix} . \tag{2.2b}$$

Using Eq. (2.1b), the current through the sample is only given in terms of the difference between the chemical potentials μ_L and μ_R:

$$I=\frac{2e}{h}T_{\rm eff}(\mu_L-\mu_R) , \tag{2.3a}$$

where

$$T_{\rm eff}=T_{N+1,0}+\sum_{i,j=1}^{N} T_{N+1,i}W^{-1}{}_{ij}T_{j,0} . \tag{2.3b}$$

This effective transmission has a clear physical interpretation. The first term is the probability of a coherent tunneling through the system, while the second term accounts for the electrons which have already suffered phase randomizing scatterings at the lateral reservoirs. Different perturbative orders in this process could be obtained in a series expansion of $\underline{W}^{-1}$. Therefore, Eq. (2.3a) defines the two probe conductance of the system in the presence of inelastic scattering:

$$G_{\rm TP}=\frac{2e^2}{h}T_{\rm eff} . \tag{2.4}$$

In order to obtain the four-probe conductance, the voltage across the sample should be obtained as the difference between the chemical potentials in two voltage probes: $eV=\mu_A-\mu_B$. We will follow Engquist and Anderson[2,9] defining two infinitesimally coupled voltage probes, A and B, attached at sites 0 and $N+1$, respectively. Therefore, the zero current condition, characteristic of voltmeter probes, can be obtained applying Eq. (2.1) to both channels. The corresponding transmission probabilities can be evaluated considering only the lowest order in ϵ, the transmission probability toward a lateral lead: $1-R_{A,A}=1-R_{B,B}=2\epsilon$; $T_{B,0}=\epsilon T_{\rm eff}$ and $T_{A,0}=\epsilon+\epsilon(1-T_{\rm eff})$. These give

$$\mu_A-\mu_R=\frac{2-T_{\rm eff}}{2}(\mu_L-\mu_R) , \tag{2.5a}$$

$$\mu_B-\mu_R=\frac{T_{\rm eff}}{2}(\mu_L-\mu_R) . \tag{2.5b}$$

Therefore, the final result for the four-probe conductance is

$$G=\frac{2e^2}{h}\frac{T_{\rm eff}}{1-T_{\rm eff}} . \tag{2.6}$$

The analogy of Eq. (2.6) with the Landauer formula is apparent from the discussion of Eq. (2.3b). Note that the spin degeneracy of the electrons has been included. Although the form of Eq. (2.6) is independent of the parameters that describe the current leads, this is not true for the transmission and reflection probabilities $T_{i,j}$ and $R_{i,i}$. Therefore the chemical potentials and the conductance are determined not only by the sample properties, but they also depend on the perfect leads that introduce current to the system.[7,8] This is just used to simulate the inelastic scattering in the sample. A further remark is convenient. The definition of $T_{A,0}$ used above assumes a random phase between the incident and reflected waves, which is not exact when evaluating the A contact. This is also the assumption of the evaluation of the chemical-potential difference through the piled-up charge[4,8] at incoming and outcoming channels. However, Büttiker[10] has recently pointed out that in the absence of phase-breaking processes this could be not quite accurate, because interference effects may increase slightly the conductance.

Now, let us return to the parameters of channels $i=1,2,..,N$. To compute Landauer's type formulas, the transmission and reflection probabilities are always calculated between plane-waves solutions in the channels at the Fermi energy $E=E_F$. This means that channels are assumed infinitely long. Under these conditions it becomes convenient to evaluate the transmission probabilities in terms of the matrix elements of the exact Green's function of the whole system, $G(E)=(E-H)^{-1}$, as given by Fisher and Lee:[6]

$$T_{i,j}=\frac{\hbar^2}{a^2}v_i v_j|G_{i,j}(E)|^2 , \tag{2.7}$$

where subscript i (j) indicates a site in the sample chain, and v_i (v_j) is the Fermi velocity at the corresponding lateral chain. A further simplification is possible because an exact decimation scheme allows us to include the effect of the leads through the self-energy corrections in the sample Green's function (see Ref. 11 and references therein). In this scheme the correction to the self-energy $\Sigma_B(E)$ of any site in the sample due to the presence of the lateral chain attached to it can be written in terms of correction Σ_1 at the first site of the lead due to the semi-infinite portion further away:

$$\Sigma_B=\frac{\eta^2}{E-E_r-\Sigma_1} . \tag{2.8}$$

Analogous expressions give Σ_1 in terms of Σ_2 and so on. Since the lateral leads are infinite and ordered, it is clear that a site on the sample sees attached from below (see Fig. 1) the same semi-infinite portion as any other site in the lead itself, therefore[12]

$$\Sigma_B=\Sigma_n,\quad \forall n=1,2,\ldots . \tag{2.9}$$

Hence, Eq. (2.8) has a solution:

$$\Sigma_B=\frac{E-E_r}{2}-i\left[\eta^2-\left[\frac{E-E_r}{2}\right]^2\right]^{1/2} , \tag{2.10}$$

where the sign in front of the square bracket corresponds to a retarded Green's function. This is the basic perturbation introduced by the inelastic scatterers to each site in the sample. The Fermi energy E is assumed to be inside the band, otherwise no current can flow through the channel. Site energies are corrected by the real part of the self-energy which only affects the energy levels of the system. Due to the damping introduced by the imaginary part of the self-energy, a portion of the current which flows through the sample goes away through that channel. The key point of the approach is that by including the reservoirs and imposing no net current flow into them the current is conserved along the sample. Phase coherence is lost because the reservoirs introduce a carrier with a random phase for each one "lost" in the reservoir. It is clear that phase randomization is more effective when more current flows into the leads toward the reservoirs, which happens when the damping is stronger. Our intention was to simulate all the inelastic scattering processes by a uniform damping in all the sites of the sample. Looking at Eq. (2.11), one immediately sees that adopting E_r equal to the Fermi energy E under study of the self-energy is purely imaginary: $\Sigma_B=-i\eta$; $\eta>0$. This is equivalent to requiring that the band center of the leads should coincide with the Fermi energy of the system. In this way the leads only introduce damping at the sites of the chain. With this criterion, the inelastic scattering strength is governed by the hopping parameter η, which is proportional to the bandwidth of the leads. However, observe the generality of the model in the sense that it can represent any interaction provided that it gives a finite lifetime to the electron state at each site.

In these conditions the transmission probabilities involved in (2.3a) become

$$\begin{aligned} &T_{0,N+1}=|G_{1,N}|^2 v'^2 , \\ &T_{0,i}=|G_{1,i}|^2 2\eta v', \quad T_{i,N+1}=|G_{i,N}|^2 2\eta v' , \\ &T_{i,j}=|G_{i,j}|^2 4\eta^2, \quad \forall i,j=1,2,\ldots,N , \end{aligned} \tag{2.11}$$

where $v'=2V\sin ka$ is proportional to the Fermi velocity $v=v'a/\hbar$ at the channels 0 and $N+1$, and 2η is proportional to the Fermi velocity $v_i=2\eta a/\hbar$ at the inelastic scatterers channels. The reflection coefficients $R_{i,i}$ verify $R_{i,i}=1-\sum_{j\,(\neq i)} T_{j,i}$ by current conservation.

Observe again that we have shown for our model that, in the evaluation of the Green's function, the presence of the lateral chains is taken into account by introducing an imaginary shift in the site energy. The identification of this parameter with the imaginary part added externally to the energy levels in the Kubo formulation[13] is straightforward. Therefore we could define an inelastic scattering time as $\tau_{\text{in}}=\hbar/(2\eta)$. In other words, the inelastic scattering in the sample is described in terms of an imaginary potential $-i\eta$ plus the condition of current conservation which fixes the chemical potential at each sample site. We have shown that this potential could also be interpreted either as the perturbation of a lead with appropriate parameters coupled to each site of the sample or originated in any relaxation process which provides a mean life to the electronic states. Therefore we are able to compute transmission coefficients and to empoly the Büttiker approach. For $\eta=0$, Eq. (2.6) reduces to the Landauer formula. In this limit, each term in the summation in Eq. (2.4) is zero and $T_{0,N+1}$ is the usual transmission coefficient T.

III. THEORETICAL RESULTS

A. Ordered chain

It is interesting to begin with the study of an ordered chain to show explicitly that the strength of the inelastic scatterers is well described in terms of an inelastic scattering time τ_{in}. As a first step, one needs to evaluate the transmission coefficients $T_{i,j}$. Due to the good matching between the channels 0 and $N+1$ with the sample, it is easy to evaluate (2.11) up to corrections of order a/L_{in}, where $L_{\text{in}}=v\tau_{\text{in}}$ is the inelastic scattering length. The Green's functions present an exponential decay because of the damping introduced by the complex self-energies. In an infinite system, the general behavior of this damping is given by the dispersion relation in terms of the wave vector k and its complex κ:

$$E-i\eta=2V\cos(k+i\kappa)a ,$$

which has a general solution[14]

$$\kappa=\frac{1}{a}\text{arccosh}\left\{\left[\left[\frac{E-2V}{4V}\right]^2+\left[\frac{\eta}{4V}\right]^2\right]^{1/2}+\left[\left[\frac{E+2V}{4V}\right]^2+\left[\frac{\eta}{4V}\right]^2\right]^{1/2}\right\};$$

but it reduces to

$$\kappa\approx\frac{\dfrac{\eta}{2Va}}{\left[1-\left[\dfrac{E}{2V}\right]^2\right]^{1/2}}=\frac{\eta}{\hbar v(E)}=\frac{1}{2L_{\text{in}}} \tag{3.1}$$

provided that $v/a \gg \tau_{\text{in}}$.

Therefore, the approximate transmission coefficients are

$$T_{N+1,0}\sim\exp[-(N-1)a/L_{\text{in}}] , \tag{3.2a}$$

$$T_{i,0}\sim\frac{a}{L_{\text{in}}}\exp[-(i-1)a/L_{\text{in}}] , \tag{3.2b}$$

$$T_{N+1,i}\sim\frac{a}{L_{\text{in}}}\exp[-(N-i)a/L_{\text{in}}] , \tag{3.2c}$$

$$T_{j,i}\sim\left[\frac{a}{L_{\text{in}}}\right]^2\exp[-|i-j|a/L_{\text{in}}] . \tag{3.2d}$$

It is useful to discuss the clear physical meaning of these terms. This comes from the observation that the factor a/L_{in} measures the probability of an inelastic collision a given site for an electron traveling with the Fermi velocity. Hence (3.2a) is the probability that an electron travels from the reservoir on the left to that on the right without any inelastic collision. (3.2b) is the probability that an electron emerging from the left reservoir travels without collisions but it suffers a collision at site i so it is absorbed by this reservoir. (3.2c) is the opposite of the latter; the inelastic collision picks up an electron from the reservoir at site i which travels towards the reservoir on the right without further inelastic collisions. Obviously, in (3.2d) a collision introduces an electron at i which travels to site j phase coherently, and there it suffers a new inelastic event.

Now, we are required to obtain the chemical potentials in a way such that the current is conserved along the sample. If the length of the chain goes to infinity the problem simplifies considerably. In this case, only the transmission coefficients $T_{i,j}$ between the inelastic scatterers channels appear in the problem and it is straightforward to verify that a linear solution $\mu_i=-\beta ia$ satisfies the requirement of current conservation. We will see that this solution is also valid for a finite chain. However, some care is needed with the chemicals potentials μ_L and μ_R, for these do not follow the linear dependence introduced above. A finite jump should be included between μ_L and μ_1 (μ_N and μ_R) in order to account for the contact resistance that appears between the reservoirs and the channels 0 and $N+1$.[9]

Therefore we consider

$$\begin{aligned} &\mu_i=-\beta ia, \forall i=1,2,\ldots,N\ , \\ &\mu_L=\Delta\ , \\ &\mu_R=-\beta(N+1)a-\Delta\ . \end{aligned} \tag{3.3}$$

Current conservation requires

$$\begin{aligned} 0=&\sum_{j=1\ (j\neq i)}^{N} T_{i,j}(\mu_j-\mu_i)+T_{i,0}(\mu_L-\mu_i) \\ &+T_{i,\ N+1}(\mu_R-\mu_i),\quad \forall i=1,2,\ldots,N\ . \end{aligned} \tag{3.4}$$

Inserting Eqs. (3.2) and (3.3) into Eq. (3.4), the equality is valid for all i as long as

$$\Delta=\beta L_{\text{in}} \tag{3.5}$$

up to corrections of order a/L_{in}, which are neglected. Now the current flowing along the sample can be obtained either at any link between two consecutive sites within the sample or at the channels 0 and $N+1$. Of course, the result will not depend on which one. In particular, it can be evaluated at the channel $N+1$,

$$I=\frac{2e}{h}\sum_{i=1}^{N} T_{N+1,i}(\mu_i-\mu_R)+T_{N+1,0}(\mu_L-\mu_R)\ . \tag{3.6}$$

Inserting Eqs. (3.2) and (3.3) into Eq. (3.6) and using Eq. (3.5) we obtain after some algebra

$$I=\frac{2e}{h}2\beta L_{\text{in}}\ , \tag{3.7}$$

where, as before, corrections of order a/L_{in} have been neglected. The current can now be written in terms of the difference $\mu_L-\mu_R$ obtaining in this way T_{eff}:

$$T_{\text{eff}}=\frac{1}{1+L/2L_{\text{in}}} \tag{3.8}$$

with $L=(N+1)a$. Since μ_A and μ_B are given by

$$\begin{aligned} &\mu_A=0\ , \\ &\mu_B=-(N+1)\beta a\ . \end{aligned}$$

Finally, the four-probe conductance becomes

$$G=\frac{2e^2}{h}\frac{2L_{\text{in}}}{L}\ . \tag{3.9}$$

Hence, the conductance of the sample corresponds to the Drude formula in terms of an inelastic scattering time.[11] Notice also that μ_A and μ_B, unlike μ_L and μ_R, follow the same linear behavior as the chemical potentials μ_i of the inelastic scatterers reservoirs. In fact, one can define the four-probe conductance between two arbitrary sites within the sample by employing these chemical potentials. These values will be the same as those measured by an infinitesimally coupled voltage probe to the same site of the sample, which is the same assumption used to obtain μ_A and μ_B. Therefore, the four-probe conductance between site i and site j is

$$G_{ij}=\frac{2e^2}{h}\frac{2L_{\text{in}}}{L_{ij}},\quad L_{ij}=|i-j|a\ . \tag{3.10}$$

It should be remarked that these results are strongly dependent on the assumption of weakly coupled voltage probes which could be defined, for instance, as the inelastic scatterers introduced with an η parameter infinitesimally small. If a pair of strongly coupled voltage probes to the sample is attached, these results will not be valid in general. The importance of this feature has been emphasized recently in several works dealing with conductance fluctuations in metals.[10,15–18] They are valid only when the voltage probes are separated a distance $L_v \gg L_{\text{in}}$. In order to show this point we introduced a pair of voltage probes in which their perfect leads were identical to channels 0 and $N+1$ and the chemical potentials μ_i were evaluated numerically. These are plotted in Fig. 2 for a chain with $N=200$, where $L_{\text{in}}=15a$. The chemical potentials at sites 30 and 100 correspond to the voltage probes, whereas all others correspond to the inelastic scatterers. It is clearly observed that the chemical potentials are perturbed due to the probes. At both sides of the probes there appear oscillations, with a period π/k as the Friedel oscillations, whose amplitude decays exponentially over length scales of order L_{in}. Therefore, for regions apart some L_{in} of the probes the chemical potentials will follow the linear dependence. Hence, Eq. (3.10) will be corrected approximately by a factor $(1+bL_{\text{in}}/L_v)$, where b is a number of order unity. For $L_v \gg L_{\text{in}}$ this factor becomes negligible but it is very important when $L_{\text{in}} \geq L_v$.

Another important point in the evaluation of the conductance was the perfect matching between channels 0 and $N+1$ and the sample. This feature makes possible that the self-consistent μ_i's follow a linear variation through the whole sample. Of course, if arbitrary leads were employed they should affect the result. As in Fig. 2, oscillations appear at both sides of the chain whose amplitude also decays exponentially. Therefore, the linear dependence is recovered after some lengths L_{in} from the contacts (sites 1 and N). This shows that the specific leads used to introduce the current are unimportant as long as the voltage is measured between points placed some L_{in} apart from the sample ends.

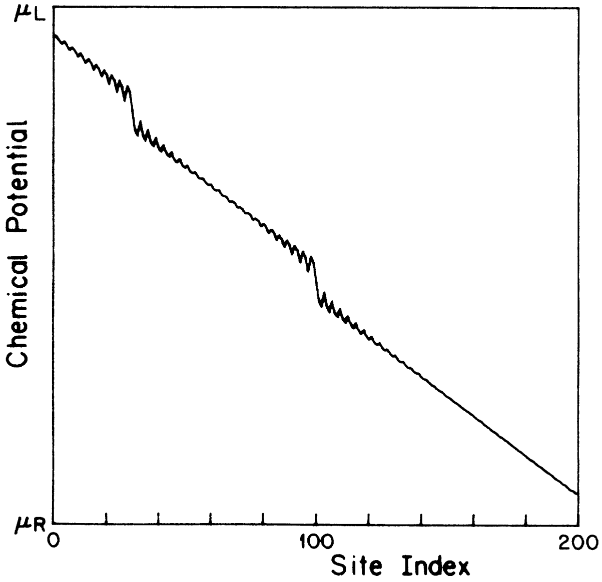

FIG. 2. Chemical potentials μ_i along the sample for a chain with $N=200$ and $L_{\text{in}}=15a$. Chemical potentials at sites 30 and 100 correspond to a pair of strongly coupled voltage probes.

B. Disordered chain

It is well known that the coherent transmission coefficient through a disordered region consists of a superposition of resonances as a function of the Fermi energy.[19,20] We are interested in how are they affected by the presence of inelastic scattering. As in the preceding section, the exact retarded Green's function in the sample should be obtained in order to compute the transmission coefficients, which requires us to include the perturbation due to all the channels. If they were uncoupled, the Green's function would be that of the isolated disordered chain

$$G^0_{i,j}=\sum_{v}\frac{a_i^v a_j^v}{E-E^v}\ , \tag{3.11}$$

where a_i^v is the amplitude of the wave function with an eigenvalue E^v at site i. The inelastic scatterers only introduce an imaginary potential $-i\eta$ independent of the site. Thus their effect is trivial and the corrected Green's function is

$$G^{0'}_{i,j}=\sum_{v}\frac{a_i^v a_j^v}{E-E^v+i\eta}\ . \tag{3.12}$$

Finally, we must include the self-energy corrections introduced by channels 0 and $N+1$ at sites 1 and N, respectively. This perturbation has the form

$$\underline{\Sigma}=\Sigma_L|1\rangle\langle 1|+\Sigma_R|N\rangle\langle N|\ , \tag{3.13}$$

where Σ_R (Σ_L) is the self-energy correction of the first (last) in the sample due to the presence of the semi-infinite lateral chain at the left (right) representing the current lead. It is given by an expression similar to (2.10) with η replaced by V. For the case considered here this is

$$\Sigma_R=\Sigma_L=\Delta/2-i\Gamma/2=E/2-iv'/2\ .$$

The exact Green's function can be obtained in terms of $\underline{G}^{0'}$ by using the Dyson equation $\underline{G}=\underline{G}^{0'}+\underline{G}^{0'}\underline{\Sigma}\,\underline{G}$. As we are interested in the resonances associated with the eigenstates of the isolated chain, instead of the exact $\underline{G}^{0'}$ we will take approximately

$$G^{0'}_{i,j}\sim\frac{a_i^v a_j^v}{E-E^v+i\eta}\ , \tag{3.14}$$

which is valid for E near to the eigenvalue E^v provided η is small in comparison to the level separation. Otherwise, the importance of the neighbors levels is not negligible. By using the Dyson equation and Eq. (3.14) one finally arrives at

$$G_{i,j}\sim\frac{a_i^v a_j^v}{(E-E^v-\Delta^v)+i(\eta+\Gamma_v)} \tag{3.15}$$

with

$$\Delta^v=\Delta(a_1^{v2}+a_N^{v2})/2\ ,$$

$$\Gamma_v=\Gamma(a_1^{v2}+a_N^{v2})/2\ ,$$

where $\hbar/\Gamma_v$ is the time for a particle in the state v to escape through the boundaries of the sample. The $T_{i,j}$'s can now be evaluated using Eqs. (2.11) and the condition of current conservation is satisfied if $(\mu_i-\mu_R)=[a_1^{v2}/(a_N^{v2}+a_1^{v2})](\mu_L-\mu_R)$. Finally, we can compute the current

$$\begin{aligned}I&=\frac{2e}{h}\left[T_{N+1,0}(\mu_L-\mu_R)+\sum_{i=1}^{N}T_{N+1,i}(\mu_i-\mu_R)\right]\\&=\frac{2e}{h}T_{\text{eff}}(\mu_L-\mu_R)\ ,\end{aligned} \tag{3.16}$$

which gives

$$T_{\text{eff}}=T_0\frac{\Gamma_v(\Gamma_v+\eta)}{(E-E^v-\Delta^v)^2+(\Gamma_v+\eta)^2}\ , \tag{3.17}$$

where

$$T_0=\frac{4a_1^{v2}a_N^{v2}}{(a_1^{v2}+a_N^{v2})^2}\ .$$

This extends a previous result in which inelastic scattering events in the sample were not included.[21] By using the Breit and Wigner formulas, a similar result was obtained by Büttiker[22] for the total transmission through a double barrier. Let us point out that Eq. (3.7) is also valid if many-channel perfect leads are used to introduce the current instead of strictly one-dimensional leads. The evaluation is similar to that presented here. The only difference is that Γ_v and Δ^v should be computed using the self-energy contribution of these many-channel leads to the sites 1 and N. This is a crucial point, because in this case the use of the two-probes conductance remains valid. T_0 is the peak value at the resonance for $\eta=0$ and is related to a generalized symmetry of the wave function at both sides of the sample. If the magnitudes of a_1^ν and a_N^ν are equal, $T_0=1$. Γ_ν is the half-width of the resonance for $\eta=0$ and is entirely due to the coupling of the sample to the channels 0 and $N+1$. This coupling also shifts the center of the resonance in Δ^ν from the exact eigenvalue E^ν. In the presence of inelastic scattering events, both the half-width and the peak amplitude are corrected:

$$T_p=T_0\frac{\Gamma_\nu}{\Gamma_\nu+\eta}\ ,\qquad \Gamma=\Gamma_\nu+\eta\ . \tag{3.18}$$

Therefore, in the presence of inelastic events, the new characteristic time associated with the resonance width is the shorter of the escape time and the inelastic one. The effective transmission T_{eff} decreases near to the resonance center and increases for energies situated away from the resonance center. Let us emphasize that Eq. (3.17) is independent of the specific nature of the disorder and is valid as long as the shift Δ^ν and η are small in comparison to the level separation. The first condition is obeyed, for example, in strongly disordered system as the amplitudes of the wave function at both sides are exponentially small. When η, which is a temperature-dependent parameter, becomes comparable or larger than the level separation, Eq. (3.4) is no longer valid. In this case, all the states situated in a range 2η around the Fermi energy will contribute to the total effective transmission. In the next section, a numerical study is presented for this regime.

IV. NUMERICAL RESULTS

The computation of Eq. (2.6) involves two basic steps. One of them is to evaluate the retarded Green's function. This can be done by employing a recursive technique[13] which also has been extended for many-channel systems.[23] The other step is to evaluate T_{eff}. We have used a decimation scheme which does not require the computation of the inverse matrix of $\underline{W}$. The procedure consists of eliminating one by one all chemical potentials by using the equation of current conservation. This renormalizes the transmission coefficients between all the remaining channels and, by iteration, all the chemical potentials of the inelastic reservoirs are finally eliminated and T_{eff} is obtained. In addition, the same method provides the chemical potentials by using T_{eff} and the renormalized transmission coefficients. The associated problems are the large storage area needed and the number of arithmetic operations involved. Hence we have used chains no longer than 500 sites.

A. Strongly disordered chain

We first consider a chain with Anderson disorder when $\lambda<L$. Here, λ is the localization length of the square of the wave function. In this case, the coherent transmission coefficient is exponentially small for almost every energy. Only for energies near to a resonance center will its value be appreciable,[19–21] because the resonances are very sharp due to the fact that Γ_ν depends on the amplitudes of the wave function at both sides of the sample and these are exponentially small. We will consider the effect of the inelastic scattering in both extreme cases. That is, for E at a resonance peak and just at the bottom of the valley between the resonance and another neighbor to it. Typical numerical simulations are showed in Fig. 3 for G as a function of L_{in}/L. Note that $L_{\mathrm{in}}=v\tau_{\mathrm{in}}$ is no longer, in general, the mean length over which the carriers propagate between successive inelastic collisions, because the chain is disordered. The sample contains $N=100$ sites and $\lambda\sim 12a$. This value has been obtained by using the scaling law for a tight-binding chain.[13] Let us consider the numerical data. It can be seen that when $\eta<\Gamma_\nu$, the resonance peak [Fig. 3(a)] takes on its asymptotic value T_0. The same happens for the valley (Fig. 3) where G is exponentially small. Only when η becomes comparable to Γ_ν do both curves begin to be affected. The resonance peak decreases, as was shown in the preceding section, whereas at the valley the conductance increases. This point can be understood because the width of the two neighbor resonances is larger than before, increasing the effective transmission. The theoretical result Eq. (3.18) for the resonance peak was plotted with a dashed line by using the values of Γ_ν and T_0 measured from the resonance shape for $\eta=0$. Note that the fitting is extremely good for the range of validity of the approximation. When η becomes comparable to the level separation (which means $L_{\mathrm{in}}\sim L$ if the density of states of an or-

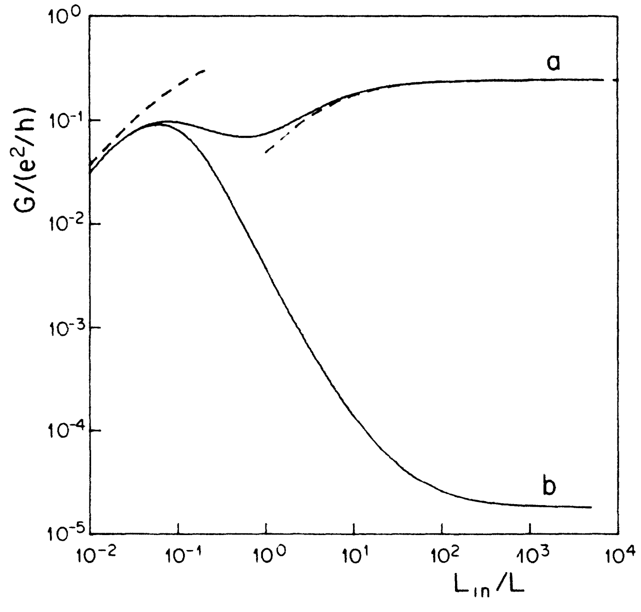

FIG. 3. Conductance in a strongly disordered chain ($\lambda<L$) as a function of L_{in}/L: curve a is just at the peak of a resonance and curve b is at the bottom of a valley near to the resonance. The dashed line at the right corresponds to the theoretical result for the conductance in a resonant situation. The dashed line at the left corresponds to the Drude formula, Eq. (4.1).

dered chain is employed to estimate the separation) the theoretical estimation fails. At this stage the resonance peak decreases more slowly and after that it begins to increase again. A qualitative explanation could be given in terms of the neighboring resonances. The tails of the resonances situated in an interval 2η around the peak become an important contribution. This contribution grows as the inelastic scattering increases, causing the resonance peak to decay more slowly and finally the peak starts increasing again. On the other hand, the conductance at the valley has been enhanced considerably by the same effect. A point is reached where both curves overlap. This happens when $L_{\text{in}} \sim \lambda$, where the conductance takes on a maximum value. For shorter L_{in}, both the peak and valley conductance follows the same curve. Here, the wave functions are extended over length scales of order L_{in}. Therefore, the conductance should tend to that of an ordered system (3.9), following approximately the Drude formula in the presence of both elastic and inelastic scattering:

$$G = \frac{2e^2}{h}\frac{2L_\phi}{L}; \quad \frac{1}{L_\phi} = \frac{1}{L_{\text{in}}} + \frac{1}{\lambda} . \tag{4.1}$$

This equation has been plotted at the left of the figure with a dashed line using the value of λ given by the scaling law. This expression gives values a bit larger than the numerical ones but having the same functional dependence. The discrepancy can be understood as we have not performed ensemble averages and therefore λ is not a well-defined parameter. Another important point is that our samples are too short. Thus to have $L_{\text{in}} < \lambda \sim 12a$, L_{in} takes on values near to a where approximation (3.1) fails. Then, even Eq. (3.9) for an ordered system is not exactly valid, and so (4.1) fails. For a better study of this limit, longer chains should be used. Therefore we see a diversity of well-known phenomena using the same formalism. When $\lambda < L \ll L_{\text{in}}$, the conductance presents the Azbel picture of resonant tunneling with exponentially sharp resonances over a background where G is exponentially small. As the inelastic scattering increases, it begins to smooth the fluctuations until L_{in} becomes comparable to the localization length. For $L_{\text{in}} < \lambda < L$ the classical result of Drude is recovered.

B. Weakly disordered chain

Let us consider the case in which $\lambda > L$. As in strongly disordered systems, the coherent transmission consists of a superposition of resonances as a function of the Fermi energy. However, here the nearly extended character of the wave function is important. This causes the half-width Γ_v to become comparable to the level separation. Besides, the peak transmission T_0 could take values close to unity because the magnitudes of the wave function at both sides does not differ appreciably. Therefore, the dimensionless Landauer formula $g = 2T/(1-T)$ could take values much larger than unity for energies close to the resonance center. In contrast, g is of order unity for energies situated between resonances. This shows that g is a strongly fluctuating function of the Fermi energy. Of course, in the absence of disorder no resonances show up at all unless the sample presents a considerable mismatch with the current leads.

Our intention was to examine how these fluctuations are affected by inelastic scattering. To see this point, let us consider Fig. 4(a). There, the conductance is plotted as a function of the Fermi energy (E_F) for $L_{\text{in}} = \infty$ for a chain with $\lambda \sim 400a$ at $E=0$ and $N=100$. The localization length does not vary appreciably over the range of energy in the figure. It is clearly seen that the resonance peaks whose transmission is $T_0 \sim 1$ gives enormous values for G. Therefore the fluctuations δG also are much bigger than e^2/h. However, when inelastic scattering is introduced, these peaks are reduced drastically as one sees in Fig. 4(b), where $L_{\text{in}} \sim L$ (this is exact for $E=0$) and the resulting fluctuations are smooth. The peaks cannot be greater than the conductance of an ordered system with the same energy and the same inelastic scattering length. This value is an upper bound for the peaks, which in this case correspond to $G = 4e^2/h$. Notice that here every eigenstate manifests itself in a resonance of the same order of magnitude. Besides, the reso-

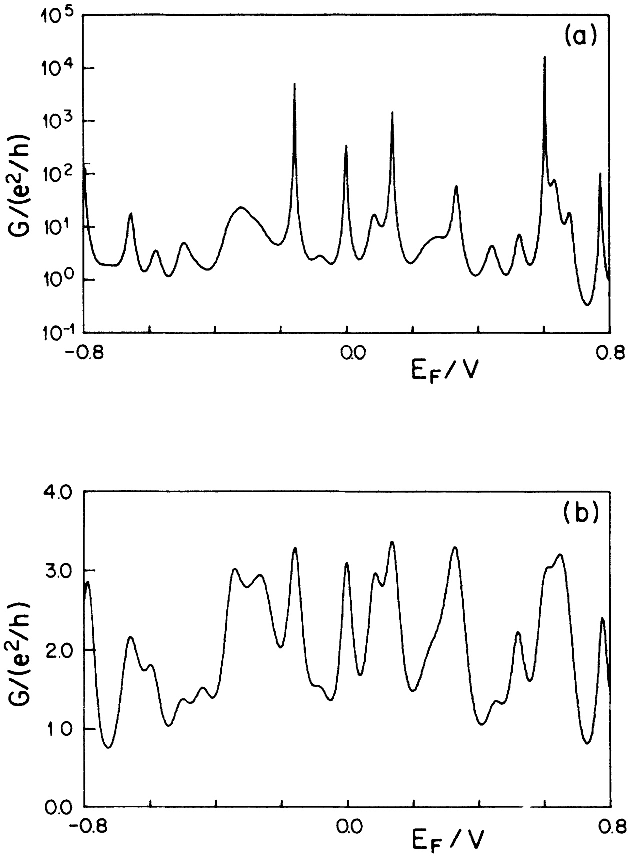

FIG. 4. Conductance as a function of the Fermi energy (in units of the hopping parameter V) in a weakly disordered chain ($\lambda > L$) with $N=100$ and $\lambda \sim 400a$ at $E=0$. (a) In the absence of inelastic scattering; (b) when $L_{\text{in}} = L$ at $E=0$.

nances become wider and this also reduces the fluctuations. For $L_{\text{in}} \sim L$ both facts make the conductance fluctuations δG be of order e^2/h, as it is seen in Fig. 4(b).

It would be interesting to see how the observed behavior compares with that of metallic systems. In these, it has been shown[24] that the fluctuations δG are of order e^2/h as long as L_{in} is of order of the sample length L and the disorder is weak ($\lambda > L$). The inelastic or phase-breaking length is given by $L_{\text{in}} = (D\tau_{\text{in}})^{1/2}$ because the electron motion in these systems is diffusive[24] (D is the diffusion constant). When $L_{\text{in}} < L$, δG decreases proportionally to $(L_{\text{in}}/L)^{3/2}$ for quasi-one-dimensional strip geometries. This result has been interpreted[24] in terms of the classical addition of L/L_{in} series resistors, each one with an uncorrelated fluctuation of order e^2/h which has been confirmed experimentally.[25] We have found that strictly one-dimensional systems also show this behavior, but in terms of $L_{\text{in}} = v\tau_{\text{in}}$. This is because in one dimension the electron motion is either ballistic or localized[14,24,26] and $\lambda > L$ corresponds to the ballistic regime.

To obtain a qualitative estimation of δG we employ the ergodic hypothesis of Lee *et al.*[24] and compute the mean $\langle g \rangle$ $[g = G/(e^2/h)]$ and the root-mean-square deviation $\delta g = (\langle g^2 \rangle - \langle g \rangle^2)^{1/2}$ over an ensemble of 500 systems. These values are

$$\langle g_\phi \rangle \sim 2.81, \quad \delta g_\phi \sim 0.74; \quad L_{\text{in}} = L = \lambda/4$$

just at the center of the band. We have also computed δg for $L_{\text{in}} < L$ for the same energy and with an ensemble as before. These values are plotted in Fig. 5, where δg has been normalized to the value δg_ϕ (open circles). In the same figure the theoretical dependence $\delta g = \delta g_\phi (L_{\text{in}}/L)^{3/2}$ has been plotted for comparison with a dashed line. The agreement is quite good. Based on these results, one could be tempted to study δg for $L_{\text{in}} > L$, taking into account that recent experiments show that this increases as $(L_{\text{in}}/L)^2$ approximately for diffusive transport.[16,17] It is clear that δg will increase in the model because the resonances are less influenced by the inelastic scattering. Finally, we also have compared our results with the perturbative theory of Ref. 18. They showed that the fluctuations follow $\delta G = (e^2/h)(\langle G \rangle / G_\phi)^2 t(\ )$, where $\langle G \rangle$ is the average conductance of the sample, G_ϕ is the average conductance of a sample of length L_{in}, and $t(\ )$ is a dimensionless function of order unity. Adopting $t(\ ) = \delta g_\phi$, this relation was also plotted using the numerical results for $\langle G \rangle$ in Fig. 5 (solid circles). Good agreement between the perturbative prediction and the numerical data (open circles) is obtained.

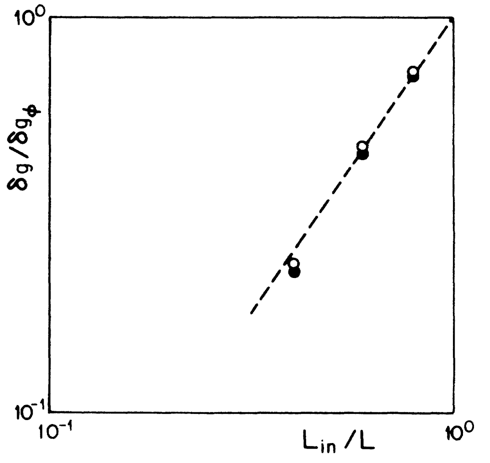

FIG. 5. Conductance fluctuations $\delta g/\delta g_\phi$ (open circles) evaluated over an ensemble of 500 systems ($E=0$, $\lambda=4L$), as a function of L_{in}/L. The dashed line corresponds to the equation $\delta g/\delta g_\phi = (L_{\text{in}}/L)^{3/2}$. The solid circles represent the values $(\langle G \rangle / G_\phi)^2$.

We should remark once again that strong values of the conductance fluctuations observed in our weak disordered systems are a consequence of the smallness of the denominator in the generalized Landauer's formula (2.6). The expression (2.4) would present much weaker fluctuations instead. Therefore, the manifestation of this behavior in real experiments would depend on which description is more appropriate. Even for a four-probe measurement, notice that the conductance given by Eq. (2.6), although it corresponds to a four-probe measurement, assumes that the voltage probes are infinitesimally coupled to the ideal perfect leads. As we mention before, numerous recent papers[27,15–18] remarked the importance of the voltage probes, which in a real experiment are not only strongly coupled to the sample, but also are disordered and should include inelastic scattering processes. These features turn out to be very important when the separation between the voltage probes verifies $L_v < L_{\text{in}}$. Therefore a complete description of the conductance fluctuations in this regime would require a correct modeling of these probes. In order to study adequately this situation, a system like that described in the perturbative theory of Ref. 18 should be used. Four disordered leads of length L_p should be coupled to a disordered chain of length L (two at each side). Two of them are used as current leads and the other two as voltage probes. Including an inelastic scattering length as we have proposed, these leads can be coupled to ideal ones after some L_{in} from the point of contacts.[18] In this way the problem to be solved is a finite one. This can be extended to many-channel systems, but we believe that it is numerically tractable in one dimension, at least as was solved by us. The fact is that L_p should include some L_{in}, while for the most favorable situation, which is at the center of the band, the condition $L_{\text{in}} \gg a$ would require even in one dimension a higher computational effort than that done here.

V. DISCUSSION

We have proposed a new way to consider the strength of the inelastic scatterers which are described in terms of an imaginary potential plus the Büttiker condition of current conservation. We have shown that this potential at a given site could be interpreted as the self-energy contribution of an adequate perfect lead coupled to it or any interaction producing a complex self-energy. Very recently, this scheme has obtained fundamental support since it has been deduced[28] as a steady-state condition for the time evolution of the Wigner distribution function within the Keldish formalism. In this treatment a complex self-energy appears as the electron mean life in a local phonon model for the electron-phonon interaction.

Therefore, for a homogeneous distribution of inelastic processes, the transmission coefficients can be evaluated in terms of the analytic continuation to the complex plane of the corresponding Green's functions in the absence of inelastic scattering. This allows us to evaluate the transport properties by using a generalized Landauer equation in which the effective transmission probability (which now has a contribution from the incoherent electrons) accounts for the locally self-consistent chemical potential according to the current conservation prescriptions. Besides, we have also shown explicitly the effect of the voltage probes when their coupling with the sample is not weak.

The consequences of our approach have been shown by considering a linear chain, at both ordered and disordered situations. In the strong disorder regime the conductance presents a resonant behavior at the "symmetric" eigenstates of the system. However, the characteristic time associated with the resonance width is shorter between the escape time and the relaxation time. In the weak disorder regime, we have found that the oscillations of the conductance in a strictly one-dimensional sample follow a similar behavior to that of a metallic system as long as $L_{\text{in}} < L < \lambda$.

A remarkable success of our method is a description of the temperature- ($T \sim \eta^{-p}$) dependent conductance at resonances or valleys, which is in qualitative agreement with experimental results.[29] When $L_{\text{in}} \sim L$ almost any eigenstate manifests itself as a peak in the conductance. Therefore, a treatment of the inelastic processes in a similar way to that presented here should be an important ingredient in the understanding of these experiments.

ACKNOWLEDGMENTS

We acknowledge M. Passeggi for his critical reading of the manuscript. One of the authors (H.M.P.) is very grateful to M. Büttiker for illuminating correspondence and B. L. Altshuler and P. A. Lee for useful comments.

---

[1] R. Landauer, Philos. Mag. **21**, 863 (1970).

[2] H. L. Engquist and P. W. Anderson, Phys. Rev. B **24**, 1151 (1981).

[3] M. Ya. Azbel, Solid State Commun. **45**, 527 (1983).

[4] M. Büttiker, Y. Imry, R. Landauer, and S. Pinhas, Phys. Rev. B **31**, 6207 (1985).

[5] D. C. Langreth and E. Abrahams, Phys. Rev. B **24**, 2978 (1981); P. W. Anderson, *ibid.* **23**, 4828 (1981); M. Ya Azbel, J. Phys. C **14**, L225 (1981).

[6] D. S. Fisher and P. A. Lee, Phys. Rev. B **23**, 6851 (1981).

[7] M. Büttiker, Phys. Rev. Lett. **57**, 1761 (1986).

[8] M. Büttiker, Phys. Rev. B **32**, 1846 (1985); **33**, 3020 (1986); IBM J. Res. Dev. **32**, 317 (1988).

[9] O. Entin-Wohlman, C. Hartztein, and Y. Imry, Phys. Rev. B **34**, 921 (1986); U. Sivan and Y. Imry, *ibid.* **33**, 551 (1986).

[10] M. Büttiker, Phys. Rev. B **40**, 3409 (1989).

[11] P. R. Levstein, H. M. Pastawski, and J. L. D'Amato, J. Phys. Condens. Matter (to be published).

[12] J. F. Weisz and H. M. Pastawski, Phys. Lett. **105A**, 421 (1984); H. M. Pastawski, C. M. Slutzky, and J. F. Weisz, Phys. Rev. B **32**, 3642 (1985).

[13] D. J. Thouless and S. Kirkpatrick, J. Phys. C **14**, 235 (1981); see also G. Czycholl and B. Kramer, Solid State Commun. **32**, 945 (1979).

[14] D. E. Rodrigues, H. M. Pastawski, and J. F. Weisz, Phys. Rev. B **34**, 8545 (1986).

[15] S. Maekawa, Y. Isawa, and H. Ebisawa, J. Phys. Soc. Jpn. **56**, 25 (1987); M. Büttiker, Phys. Rev. B **35**, 4123 (1987); C. L. Kane, P. A. Lee, and D. P. DiVincenzo, *ibid.* **38**, 2995 (1988).

[16] A. Benoit, C. P. Umbach, R. B. Laibowitz, and R. A. Webb, Phys. Rev. Lett. **58**, 2343 (1987).

[17] W. J. Skocpol, P. M. Mankiewick, R. E. Howard, L. D. Jackel, D. M. Tennant, and A. D. Stone, Phys. Rev. Lett. **58**, 2347 (1987).

[18] D. P. DiVincenzo and C. L. Kane, Phys. Rev. B **38**, 3006 (1988), and references therein.

[19] I. M. Lifshits and V. Ya. Kirpichenkov, Zh. Eksp. Teor. Fiz. **77**, 989 (1979) [Sov. Phys.—JETP **50**, 499 (1979)].

[20] M. Ya. Azbel, Phys. Rev. B **28**, 4106 (1983); M. Ya. Azbel and D. P. DiVincenzo, *ibid.* **30**, 6877 (1984).

[21] J. L. D'Amato, H. M. Pastawski, and J. F. Weisz, Phys. Rev. B **39**, 3554 (1989).

[22] M. Büttiker, IBM J. Res. Dev. **32**, 63 (1988).

[23] A. D. Stone, Phys. Rev. Lett. **54**, 2692 (1985); A. D. Stone and Y. Imry, *ibid.* **56**, 189 (1986).

[24] P. A. Lee and A. D. Stone, Phys. Rev. Lett. **55**, 1622 (1985); P. A. Lee, A. D. Stone, and H. Fukuyama, Phys. Rev. B **35**, 1039 (1987); B. L. Al'tshuler, Pis'ma Zh. Eksp. Teor. Fiz. **42**, 291 (1985) [JETP Lett. **41**, 648 (1985)]; Y. Imry, Europhys. Lett. **1**, 249 (1986).

[25] W. J. Skocpol, P. M. Mankiewick, R. E. Howard, L. D. Jackel, D. M. Tennant, and A. D. Stone, Phys. Rev. Lett. **56**, 2865 (1986).

[26] D. J. Thouless, J. Phys. C **6**, 149 (1973).

[27] H. U. Baranger, A. D. Stone, and D. P. DiVincenzo, Phys. Rev. B **37**, 6521 (1988).

[28] S. Datta, Phys. Rev. B **40**, 5830 (1989).

[29] J. H. F. Scott-Thomas, S. B. Field, M. A. Kastner, H. I. Smith, and D. A. Antoniadis, Phys. Rev. Lett. **62**, 583 (1989).