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Electrochemical-potential variations across a constriction

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By means of the Keldysh-Green-function method, the electrochemical-potential variations across a constriction are analyzed. We discuss specifically the case of a one-dimensional chain joining two Bethe lattices of coordination four. Our results show that the total conductance of the system and its local chemical potential variations depend dramatically on the interference between the chain transmittivity and the reflectivity at the reservoir-chain contact. We show a case in which, with a transmittivity less than one, a zero chemical-potential drop is found along the inner linear chain.

With the advent of mesoscopic physics,[1,2] a lot of interest has arisen in the electrical transport and the corresponding resistance of small and low-dimensional systems. The scanning tunneling microscope[3] (STM) is an example of one of these cases, where the contact between two reservoirs takes place through a constriction, typically consisting of a few atoms. The resemblance and analogy between a low-dimensional conductor and the STM microscope can be easily understood by considering their conductance behavior. In a one-dimensional (1D) conductor, for example, with n channels for electron injection, it is a well-known result[4,5] that the conductance of the sample may be quantized in multiples of $2(e^2/h)$, depending on the number of open channels contributing to the conductance; likewise, it has been shown[6] recently that in the STM microscope the maximum conductance through a sample tip atom is also $2(e^2/h)$; this value increasing to $2n(e^2/h)$ for n atoms.

A long-standing debate has evolved recently about the value of the total resistance for the case of disordered low-dimensional systems.[1,2,4] Summarizing this debate, we can say, referring to a 1D system, that the two main points of view relate the conductance of a 1D channel to either (i) the transmission coefficient of the system T, or (ii) the factor[7] $T/(1-T)$. The realization that both results depend on the reservoir–low-dimensional-system link has directed people[8] to the assertion that "entire transit (through the low-dimensional system) from one reservoir to the other has to be viewed as a simple quantum-mechanically coherent event."[9]

It is also of interest to comment that the effect of disorder or impurities in the low-dimensional system has its counterpart in the STM microscope; in this case by changing the tip-sample distance one can control the transmission (the T parameter introduced above) of the constriction.

Since it has been argued[1,2,4] that self-consistency may be of primordial importance in the calculation of the conductance of low-dimensional systems (or the STM microscope), it could be in order to analyze the problem of how the electrochemical potential changes across a constriction.[10] As we shall find in this paper, this analysis is directly related to the conductance problem and shows in a very intuitive and transparent way the role played by the interference between the reservoirs and the low-dimensional system.

The model we have chosen to analyze this problem is shown in Fig. 1 and corresponds to a case simulating the interface of a STM microscope. Here we describe the tip and the sample (or the reservoirs) by two Bethe lattices, and assume that a one-dimensional chain joins the tip and the sample. A free ideal interface should be described by both Bethe lattices joined by a hopping parameter t'; the case of a long chain could represent the effect of a long molecule adsorbed between the tip and the sample. In order to analyze how the defects of the chain may modify the constriction conductance, we have assumed that one of the hopping parameters associated with a chain bond (see Fig. 1) may be t', different from all the other ones.

Our starting Hamiltonian (per spin) is the following:

$$\hat{\mathcal{H}}=\hat{\mathcal{H}}_{\mathrm{Bethe1}}+\hat{\mathcal{H}}_{\mathrm{Bethe2}}+\sum_{i=1}^{N}E_i\hat{n}_i+\sum_{i,j=1}^{N}t_{i,j}(c_i^\dagger c_j+c_j^\dagger c_i)+t_{0,1}(c_0^\dagger c_1+c_1^\dagger c_0)+t_{N,N+1}(c_N^\dagger c_{N+1}+c_{N+1}^\dagger c_N)\,, \tag{1}$$

where E_i represents the diagonal level of the single orbital of each chain atom, $t_{i,j}$ the hopping between nearest neighbors, $\hat{\mathcal{H}}_{\mathrm{Bethe}}$ the Hamiltonian of each Bethe lattice,[11] and $t_{0,1}$ and $t_{N,N+1}$ the couplings between the chain and the reservoirs. The Bethe lattice is assumed to have fourfold coordination, with the following Hamiltonian:

$$\hat{\mathcal{H}}_{\mathrm{Bethe}}=\sum_j E_j\hat{n}_j+\sum_{l,p}t_{l,p}(c_l^\dagger c_p+c_p^\dagger c_l)\,.$$

In our initial Hamiltonian all the levels, E_i and E_j, are taken to be equal to E_0 and $t_{l,p}=t_{i,j}=t$ except for the sin-

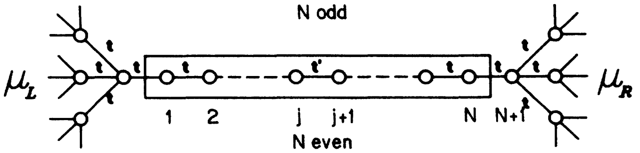

FIG. 1. Model used in the calculation of this paper. A linear chain with N sites is joining two Bethe lattices.

gle bond shown in Fig. 1. We are interested in obtaining the total current and the induced electrochemical potential along each site of the system, when both reservoirs have chemical potentials μ_L and μ_R.

In order to get the total intensity I and the local charge in each atom ρ_i from Hamiltonian (1), and the chemical potentials μ_L and μ_R (see Fig. 1), we follow the Keldysh-Green's-function method.[12] Our starting point is afforded by the two following matrix equations:[12,13]

$$\hat{G}^{+,-}=(\hat{I}+\hat{G}^R\hat{\Sigma}^R)\hat{G}_0^{+,-}(\hat{I}+\hat{\Sigma}^A\hat{G}^A)\,, \tag{2a}$$

$$\hat{G}^{R,A}=\hat{G}_0^{R,A}+\hat{G}^{R,A}\hat{\Sigma}^{R,A}\hat{G}_0^{R,A}\,, \tag{2b}$$

where the $\hat{G}^{+,-}$, $\hat{G}^R$, and $\hat{G}^A$ are the Keldish, retarded, and advanced Green's functions, respectively; $\hat{G}_0$ refers to the uncoupled system with $t'=0$. In this case we have local equilibrium, and we get the corresponding Green's functions using the well-known techniques for equilibrium systems.[11] Equations (2) yield the nonequilibrium Green's functions, $\hat{G}^R$ $\hat{G}^A$, and $\hat{G}^{+,-}$ by introducing the self-energy $\Sigma^R=\Sigma^A$ defined by the hopping parameter t'.

Once we calculate the different $\hat{G}^{+,-}$ Green's function, we obtain the total current and the local charges ρ_i using the following equations:[13]

$$I=2\frac{e}{h}\int_{-\infty}^{\infty}d\omega[t'_{j,j+1}G^{+,-}_{j,j+1}(\omega)-t'_{j+1,j}G^{+,-}_{j+1,j}(\omega)]\,, \tag{3a}$$

$$\rho_i=\frac{e}{\pi i}\int_{-\infty}^{\infty}d\omega\, G^{+,-}_{i,i}(\omega)\,, \tag{3b}$$

where j and $j+1$ refer to the atoms being connected by the hopping $t'(t_{j,j+1}=t')$. In our calculation we introduce potential self-consistency; this is achieved by allowing the level at site i, F_i, to change by a diagonal perturbation V_i, in order to fulfill the following charge-neutrality condition at site i:

$$\frac{e}{\pi i}\int_{-\infty}^{\infty}d\omega\, G^{+,-}_{i,i}(\omega)=\rho_i^0\,, \tag{4}$$

ρ_i^0 being the neutral charge of the ith atom. In practice, these perturbations V_i extend to the whole 1D chain and only to three or four atoms inside the Bethe lattice (or the reservoirs). Notice that the reservoirs play the role of taking the current crossing the chain to the infinities; in practice, what is relevant is that the local intensity in the reservoirs decreases exponentially as we move inside, due to the four coordination of the Bethe lattice.

It is worth mentioning that within a linear-response theory, the above condition [Eq. (4)] implies

$$\Delta\mu_i=V_i\,,$$

where $\Delta\mu_i$ defines the electrochemical potential of an i site.

Next, we discuss the results of our calculation. Let us consider, first of all, the total current I given by Eq. (3a). The first point to notice is that, in this case, the total current is independent of the final consistency in the charges or, in other words, of the local potentials V_i. Indeed, $G^{+,-}$ depends on $\mu_L-\mu_R$ and V_i, but the effect of V_i within linear theory is to induce charges in the atoms but no current through the chain, as can be understood by realizing that

$$\delta G^{+,-}[(\mu_L-\mu_R),V_i]\simeq\frac{\partial G^{+,-}}{\partial\mu}(\mu_L-\mu_R)+\frac{\partial G^{+,-}}{\partial V_i}V_i \tag{5}$$

and that $\partial G^{+,-}/\partial V_i$ is calculated for $\mu_L=\mu_R$.

Then, the intensity can be obtained as explained in Ref. 6, yielding the following result (for $\mu_L=\mu_R$ small):

$$I=2\frac{e^2}{h}(\mu_L-\mu_R)\frac{t'^2\,\mathrm{Im}[G^R_{0;j,j}(E_F)]\,\mathrm{Im}[G^R_{0;j+1,j+1}(E_F)]}{|1-t'^2\,\mathrm{Im}[G^R_{0;j,j}(E_F)]\,\mathrm{Im}[G^R_{0;j+1,j+1}(E_F)]\,|^2}\,. \tag{6}$$

Figure 2 shows the total conductance of the chain for $t'=t$ in units of $2(e^2/h)$, as a function of the Fermi-level position and the different number of chain atoms. The conductance has a maximum value of $2(e^2/h)$ due to the two channels for transport (one per spin), and shows oscillations depending on the numbers of atoms in the chain. These oscillations obviously reflect the interference between the standing waves of the chain and the reflection at the reservoir contacts. It is also worth mentioning that there is a common envelope for the minimum conductance of the different N-atom cases (see Fig. 2), which in the particular case considered in this paper takes the value $\frac{3}{4}$ for $\omega=0$ (in this case the Fermi energy is located at the midband of the 1D chain). This means that for the ideal chain, $N=$even and the Fermi energy at the middle of the chain band, the conductance is $\frac{3}{2}(e^2/h)$.

We now discuss the more interesting case of how the electrochemical-potential changes along the Bethe lattices and the 1D chain; let us comment that, as shown by Eq. (5), we define the electrochemical potential at each site by the local external potential V_i induced at each point in order to have local neutral conditions. Figure 3 shows the electrochemical potential along the chain for different chain lengths and different hopping parameters t'. The main results that come out of our calculation are the following:

(i) In all the cases, for t' very small, the total potential drop appears between the atoms limiting the t' bond.

(ii) As t' grows, the total potential drop is redistributed along the atoms of the linear chain and the contacts of the two reservoirs. For t' substantially smaller than t (say, less than $0.3t$-$0.4t$) the potential drop is concentrated in the four central atoms distributed around the t' bond. For larger values of t', the potential drop starts to concentrate in the reservoir contacts.

(iii) As far as t' varies between $t/\sqrt{3}$ and $t\sqrt{3}$, we find several facts depending on the number N of chain atoms. Thus, for N odd (say 5 in Fig. 3) and $t'=t$, all potential drop is localized across the reservoir's contact (a kind of Sharvin's resistance[14]), in such a way that the potential

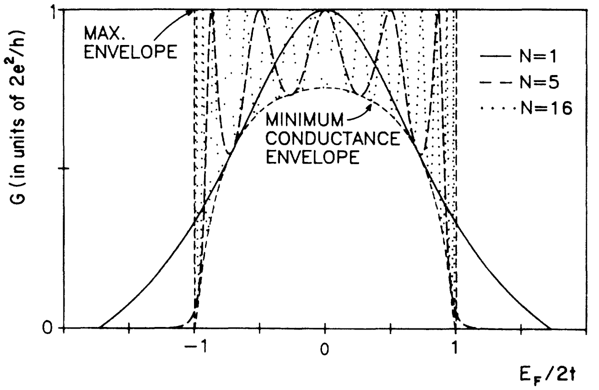

FIG. 2. Total conductance G of the chain in units of $2(e^2/h)$ as a function of the Fermi-level position. The zero of energy represents the middle of the one-dimensional conduction band of the chain.

drop along the chain is zero, with the electrochemical potential constant; for this case, we find that the total conductance is $2(e^2/h)$, the maximum one.

For an even number of atoms (say, $N=4$ or 6 in Fig. 3) and $t'=t$, although we also find that the total potential drop is mainly localized in the reservoir contacts, the electrochemical potential along the chain oscillates around a zero mean value. This is related to the interference between the chain standing waves and the reflections at the reservoir contacts; due to this fact, the chain conductance is smaller than $2(e^2/h)$, namely $\frac{3}{2}(e^2/h)$. Moreover, for N even we find different results depending on whether the number $N/2$ is either even or odd. For $N/2$ even we find that if $t'=\sqrt{3}t$, the total conductance is $2(e^2/h)$ and, then, the potential drop along the chain is zero with a constant electrochemical potential in the chain atoms; the total potential drop is then localized around the reservoir contacts. We find similar results for $N/2$ odd, if we take $t'=t/\sqrt{3}$ instead of $\sqrt{3}t$.

We should mention that the qualitative results found in this paper are independent of the reservoir-contact details. Although we have used two Bethe lattice as reservoirs, little differences appear if we assume to have a cubic lattice or some other appropriate reservoirs that play the role of taking the chain intensity along many different channels to infinity. For other reservoirs and n even, the value of t' giving the maximum conductance is different from $t/\sqrt{3}$ or $\sqrt{3}t$, otherwise the results of this paper are the same.

The main conclusion coming out of the results shown in Fig. 3 is that the interference between the chain transmittivity and the reflection of the reservoirs is of primordial importance to define the total conductance of the system.

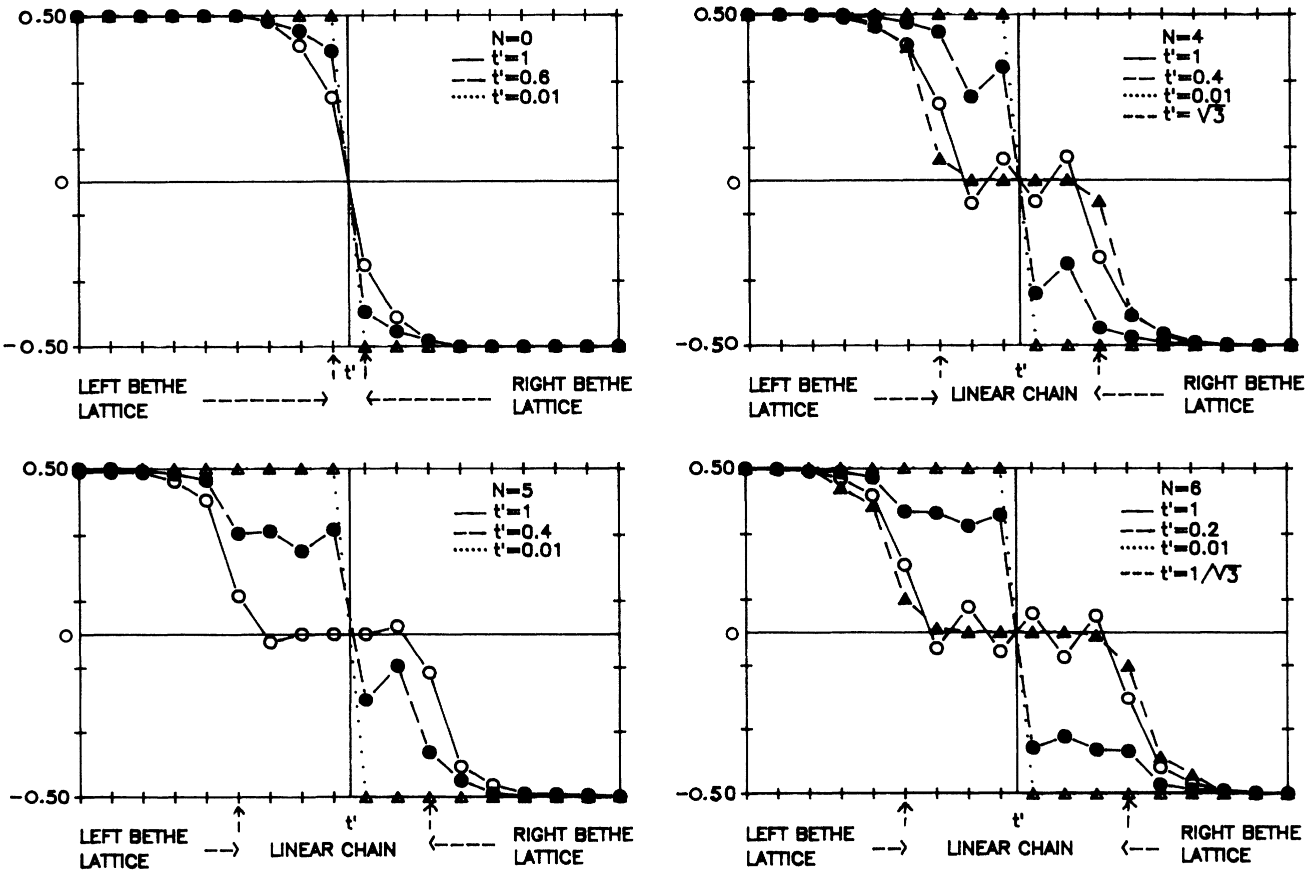

FIG. 3. Electrochemical-potential values along the Bethe lattices and the chain sites in units of $\mu_L-\mu_R$ for different numbers of chain atoms (a) $N=0$, (b) $N=4$, (c) $N=5$, and (d) $N=6$. It has been assumed for the sake of simplicity that $\mu_L=-\mu_R$.

In particular, we find two very interesting results:

(a) For a perfect 1D chain (transmittivity equal to one), the electrochemical potential oscillates around a zero mean value along the chain, with a wavelength related to the Fermi wavelength of the conducting electrons[10] (in the particular case considered in Fig. 3, two chain atoms define the wavelength).

(b) A nonperfect 1D chain (with transmittivity less than one) can show a constant electrochemical potential. In this case the interference between the chain transmittivity and the reflection of the resevoir contacts can yield a zero chain resistance, with the potential drop localized around the reservoir contacts.

It is worth mentioning at this point that these results also show that the total chain conductance is not necessarily proportional[8] to either T (its transmittivity) or $T/(1-T)$. These results depend on the particular conditions taken for the reservoir-chain contacts: only if the reservoir is assumed to give no reflected wave into the chain (for the waves outgoing from the chain itself) can one relate the chain conductance to T or $T/(1-T)$ (these two different results only depend on taking the total voltage drop either across the total system including the reservoirs or the individual chain). As mentioned above, these single results for the 1D conductance have to be modified when the transit process is viewed as a single quantum-mechanically coherent event between the reservoirs and the chain.[1,9]

The cases discussed in this paper show that the conductance of one-dimensional systems can be very much dependent on the reservoir-chain contacts. In particular, when the contact is such that the total conductance coincides with the maximum value associated with the number of open channels, one can expect that the voltage drop along the chain is zero and that the total voltage drop is localized at the reservoir contacts.

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