Delocalization and conductance quantization in one-dimensional systems attached to leads

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We investigate the delocalization and conductance quantization in finite one-dimensional chains with only off-diagonal disorder coupled to leads. It is shown that the appearance of delocalized states at the middle of the band under correlated disorder is strongly dependent upon the even-odd parity of the number of sites in the system. In samples with inversion symmetry the conductance equals $2e^2/h$ for odd samples and is smaller for even parity. This result suggests that this even-odd behavior found previously in the presence of electron correlations may be unrelated to charging effects in the sample.

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Since the pioneering work of Anderson,[1] localization in disordered systems has become a key issue in solid-state physics. Mott and Twose[2] suggested that all the electronic eigenstates in less than two-dimensional (2D) disordered systems are localized. Borland[3] gave a rather general proof of this statement. Economou and Cohen[4] have reexamined the localization problem in the 1D tight-binding model, concluding that all states are localized if and only if the nearest-neighbor coupling is considered. However, Theodorou and Cohen[5] showed that the state at the middle of the band is extended, regardless of the randomness of the nearest-neighbor hopping matrix elements. Recently, it has also been argued that the delocalization transition exists in 1D systems with correlated diagonal and/or nondiagonal disorder, i.e., that at some particular energies the states are extended.[6] The delocalization transition has now been investigated in 1D random quantum Ising chains,[7] 1D random XY models,[8] weakly disordered quasi-1D tight-binding hopping models,[9] and dirty superconducting wires.[10]

On the other hand, Oguri[11] found an even-odd parity effect in the conductance characteristics of a finite Hubbard chain coupled with continuum states. He attributed such a parity effect to the many-body Kondo resonance and the presence of the reservoirs of continuum states, while Brouwer *et al.*[9] explained it by level repulsion of the transmission eigenmodes. Similar even-odd behavior in the conductance has been found in first-principles numerical calculations in monatomic molecular wires within the local-density-functional approximation and interpreted as arising from charge neutrality and resonant tunneling due to the sharp tip structure.[13]

Here we address the question of whether these effects are many-body effects or not. Our approach is to check if they arise in the absence of a Coulomb term in the Hamiltonian. Within a tight-binding model in the absence of electron-electron interactions we find that both delocalization in a sample with correlated disorder and the even-odd parity feature in symmetric strings are present, irrespective of any charging effects.

For the sake of simplicity, we consider only nondiagonal disorder keeping on-site energies the same at all sites. We derive an explicit delocalization condition to be satisfied by the parameters associated with hopping between sites and coupling to the reservoirs of continuum states. We find that it depends on the parity of the string, i.e., on whether the number of sites is even or odd. Applied to the molecular wire structure with inversion symmetry, we observe that the conductance in the odd case always equals $2e^2/h$ while it is smaller than this quantity if the number of sites is even.

The system considered here is a chain of N sites labeled $1,2,\ldots,N$ from left (L) to right (R), with its ends connected to reservoirs with chemical potential ϵ_F. The hamiltonian is

$$H=\sum_{i=1}^{N}\epsilon_0 a_i^\dagger a_i+\sum_{i=1}^{N-1}(t_i a_i^\dagger a_{i+1}+\text{H.c.})+\sum_{k,r=L,R}\epsilon_{kr}b_{kr}^\dagger b_{kr}+\sum_k (V_k^L b_{kL}^\dagger a_1+V_k^R b_{kR}^\dagger a_N+\text{H.c.}), \tag{1}$$

where a_i (b_k) is the annihilation operator of electron at site i (lead r), and the other terms have their usual meaning. We will characterize delocalization by perfect transmission at some particular energy, i.e., by a transmission coefficient that equals 1. The corresponding state is then extended.[5] Considering the sites to the right of site 1 as part of the right reservoir, the Keldysh formalism[12] yields for the transmission probability the expression

$$\mathcal{T}(\epsilon_F)=\frac{-2\Gamma^L|t_1|^2\,\mathrm{Im}\,G_{2R}^r}{(\epsilon_F-\epsilon_0-|t_1|^2\,\mathrm{Re}\,G_{2R}^r)^2+(\Gamma^L-2|t_1|^2\,\mathrm{Im}\,G_{2R}^r)^2/4}, \tag{2}$$

where

$$\Gamma^{L/R}=\sum_k 2\pi|V_k^{L/R}|^2\delta(\epsilon_F-\epsilon_{kL/R}),$$

$$G_{iR}^r(\epsilon_F)=\{[g_i^r(\epsilon_F)]^{-1}-|t_i|^2G_{i+1,R}^r(\epsilon_F)\}^{-1},$$

$$i=2,3,\ldots,N-1,$$

$$G_{NR}^r(\epsilon_F)=\left[[g(\epsilon_F)]^{-1}+\frac{i}{2}\Gamma^R\right]^{-1},$$

$$g_i^r(\epsilon_F)=(\epsilon_F-\epsilon_0+i0^+)^{-1},\quad i=1,2,\ldots,N,$$

and the usual notation for Green functions has been employed. The transmission probability depends in general on the position of the Fermi level at the reservoirs as well as on the disorder configuration of the hopping parameters $(t_1, t_2, \ldots, t_{N-1})$. Here we consider the most interesting case, when the Fermi level ϵ_F is pinned at the value of the independent site energy ϵ_0, the middle of the band, or level group of the 1D system.[6,9] The real part of all retarded Green functions becomes zero and the first term in the denominator of Eq. (2) vanishes. Perfect transmission through the 1D lattice is then obtained if

$$\Gamma^L = -2|t_1|^2 \mathrm{Im}\, G^r_{2R}, \tag{3}$$

where now

$$\mathrm{Im}\, G^r_{2R} = -\frac{\Gamma^R}{2}\left|\frac{t_3 t_5 \cdots t_{N-2}}{t_2 t_4 \cdots t_{N-1}}\right|^2, \quad N \quad \text{odd}, \tag{4}$$

$$\mathrm{Im}\, G^r_{2R} = -\frac{2}{\Gamma^R}\left|\frac{t_3 t_5 \cdots t_{N-1}}{t_2 t_4 \cdots t_{N-2}}\right|^2, \quad N \quad \text{even}. \tag{5}$$

The condition for perfect transmission thus becomes

$$\left|\frac{t_1 t_3 \cdots t_{N-2}}{t_2 t_4 \cdots t_{N-1}}\right|^2 = \frac{\Gamma^L}{\Gamma^R}, \quad N \quad \text{odd}, \tag{6}$$

$$\left|\frac{t_1 t_3 \cdots t_{N-1}}{t_2 t_4 \cdots t_{N-2}}\right|^2 = \frac{\Gamma^L \Gamma^R}{4}, \quad N \quad \text{even}. \tag{7}$$

Equation (6) states that for a chain with an odd number of sites and mirror (inversion) symmetry ($\Gamma^L = \Gamma^R = \Gamma$, $t_1 = t_{N-1}$, $t_2 = t_{N-2}$, etc.) perfect transmission is automatically satisfied at the middle of the band or level group. From the Landauer-Büttiker formula $\mathcal{G} = 2e^2\mathcal{T}/h$ it follows that the conductance is then quantized to the value $2e^2/h$. This is not the case when N is even, however, as is apparent from the structure of Eqs. (7) and (2), yielding a transmission coefficient $4\lambda/(1+\lambda)^2$ less than unity, with

$$\lambda = \left|\frac{2 t_1 t_3 \cdots t_{N-1}}{\Gamma t_2 t_4 \cdots t_{N-2}}\right|^2,$$

and a conductance smaller than $2e^2/h$. We thus see that the even-odd feature appears in transport in the absence of any electron correlations. Our argument also proves that when the system is symmetric under inversion, the state at the middle of the band is always delocalized, regardless of the amount of disorder that respects such symmetry condition. This is a special kind of generic correlation in the disorder, defined by specular symmetry. Of course, Eq. (6) or (7) may be satisfied by a much broader set of parameter sequences, thus defining a class of correlated disorder constraints in which inversion symmetry is just a particular case. For example, the simple pairlike condition $t_1 = t_2, t_3 = t_4, \ldots, t_{N-2} = t_{N-1}, \Gamma^L = \Gamma^R$ would suffice to satisfy the even-odd rule, being one instance within such set. Notice that one may also find cases in which the rule is inverted, such as when $t_1 = t_2, t_3 = t_4, \ldots, |t_{N-1}|^2 = \Gamma^L\Gamma^R/4$ with $\Gamma^L \neq \Gamma^R$. But they are very special and difficult to achieve experimentally.

The above results show that the even-odd behavior found in symmetric Hubbard chains coupled to reservoirs[9,11] need not arise from Kondo-like or other type of electron correlations. The results are also relevant to the case of transport through a monatomic wire considered in the literature.[14] Then ϵ_0 is just the site energy of the *s* orbital of the noble- or alkali-like atoms, while the hopping elements t_i represent the overlap between the nearest-neighbor *s* orbitals and are all equal. Following our conclusions, if coupling to the left and right leads is the same, we then expect the conductance to be quantized, as long as the number of atoms in the chain is odd, again exhibiting the even-odd feature. For a wire with deformations perpendicular to its length the even-odd character of the conductance is preserved since the normal deformation just changes the inter-site couplings symmetrically.

The above results are valid for any finite N, no matter how long the chain is. Also, if the electron-electron interaction is added, we expect them to hold as well since the on-site Coulomb interaction introduces a self-energy term $\Sigma_{e\text{-}e}$ in the Green's function of each site. The influence of electron-electron interactions is then just to shift and split the resonance position[15] and Eq. (2) can also be formally used in their presence, with the formal replacement $g^r_i = (\epsilon_F - \epsilon_s - \mathrm{Re}\,\Sigma_{e-e})^{-1}$ and the new resonance condition $\epsilon_0 = \epsilon_F - \mathrm{Re}\,\Sigma_{e-e}$.

In summary, we have shown that in the absence of electron-electron interactions a broad class of off-diagonal correlated disordered 1D samples of finite length exhibit a state with transmission coefficient equal unity at the center of the band. The set includes all sequences with inversion symmetry, for which perfect transmission takes place if the number of sites is odd, while if it is even transmission is less than one, yielding a conductance equaling $2e^2/h$ in the first case, and smaller in the latter. In the case of general disorder, one expects the even-odd rule to be violated. Our results strongly suggest that previous interpretation of this even-odd effect in terms of electron correlations must be revised.

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