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Localization and topological disorder

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We analyze the electronic properties of a one-dimensional chain with a random distribution of linear side branches and loops. This model constitutes a first approach to the study of systems whose geometrical shape is highly irregular. The main new feature, not present in other models of disordered systems, is the exact vanishing of the transmission coefficient at the band center due to the existence of a local antiresonance. At this energy the density of states shows strong site dependence. (We show in an appendix that both linear side branches of arbitrary length and asymmetric loops of arbitrary size introduce antiresonances in the transmission coefficient.) Working in the dilute limit, we derive simple expressions for the conductance of long chains as a function of temperature and length. Our theory is extended to finite concentrations of defects using computer simulation. We think that the reported results are relevant to the study of transport in branched polymers and fractals (like percolation clusters). This mechanism could also play a role in explaining the experimental behavior of long dirty wires at very low temperatures.

I. INTRODUCTION

The role of substitutional disorder on the transport properties of metals, in the absence of many-body effects, is fairly well understood.[1,2] There is a wide variety of materials, however, which also exhibit intrinsic, topological disorder associated with the randomness in their geometrical shape. Among them, we can consider fractals, and in particular percolation clusters[3] and branched polymers, and it is not unlikely that experimental realizations of one-dimensional wires show similar properties.

In the present work we will consider the transport properties of the simplest system with this geometrical disorder, namely a one-dimensional tight-binding chain with a random distribution of side branches consisting of an extra single atom. There is one orbital per site, and all hopping energies are taken to be equal to a value V which defines the scale of energies. Diagonal site energies are set to zero. A schematic representation of the model is shown in Fig. 1.

As will be discussed below, this simple model already shows nontrivial features which cannot be explained within the standard one-parameter scaling theory of localization.[2] Also, a strong energy dependence is observed in most properties, more pronounced than in the case of the substitutional Anderson model. We think that these novel features can be relevant to the understanding of quantum transport properties in branched polymers, percolation networks,[4] and other highly ramified fractals, such as diffusion-limited aggregates,[5] and can also play a role in explaining the unusual properties of thin wires at low temperatures.[6]

In the next paragraph we present an extensive study of the single- and double-defect cases, in order to analyze its similarities and differences with the well-known substitutional impurity. Then, a numerical study of chains with different concentrations of these defects will be presented, and the main features of the data will be discussed and analyzed, as well as compared with results from other theories[7,8] which also predict strong energy dependence in the transport properties of disordered one-dimensional systems. Finally, the main conclusions of our work and an analysis of how the conductance of these chains depends on their length and temperature will be presented.

II. THE SINGLE- AND DOUBLE-DEFECT CASES

We will first consider the perturbation induced in an otherwise perfect chain by a single defect. The Hamiltonian, even in the presence of defects, has particle-hole symmetry, so that the distribution of its eigenenergies has to be symmetric around $E=0$. Thus, we need only to study the density of states or the transmission coefficient for half of the electronic band.

Site C interacts only with its adjacent site-within the chain (B, in Fig. 1). Its effects on the chain can be replaced by an energy-dependent self-energy acting only on sites B, $\Sigma_B(E)$:

$$\Sigma_B(E)=V^2/E \ . \tag{1}$$

This effective potential is distributed randomly along the chain, like in the standard Anderson model of substitutional impurities. The main difference is the energy dependence which this potential has and, in particular, the

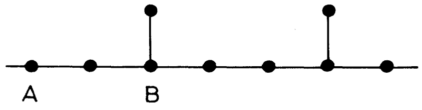

FIG. 1. Schematic representation of the model considered in the text.

pole at $E=0$. This pole arises from the existence of an extra electronic level at that energy in site C. It is easy to show (see Appendix) that a more complicated side branch leads to a richer distribution of poles in the associated self-energy, one for each level of the isolated branch. When we have one of these poles, the effective potential acting on sites B becomes infinite, and the amplitudes of the eigenstates with these energies tend to zero at sites B. Alternatively, we can say that sites C act like a resonance interacting with a continuum, defined by the band of the perfect chain. At sites B we have an antiresonance, and the local density of states vanishes at the corresponding energies.

Using standard tight-binding techniques, we can calculate the density of states at sites B and C, and the transmission coefficient $T(E)$ along the chain, for a single defect:

$$\rho_B(E)=\frac{1}{\pi}\frac{(4V^2-E^2)^{1/2}}{(V^4/E^2)+4V^2-E^2}\,,$$

$$\rho_C(E)=(V^2/E^2)\rho_B(E)\,, \tag{2}$$

$$T(E)=\frac{4V^2-E^2}{(V^4/E^2)+4V^2-E^2}$$

in the energy range defined by $|E|\le|2V|$. There are also localized states at $E_0=\pm V(\sqrt{5}+2)^{1/2}$. These states have their maximum weight on site $C\,[1/(10+4\sqrt{5})]$ and slowly decay as we move away from it, with a decay length

$$l=2a/\ln[(1+\sqrt{5})/2]\,.$$

As a consequence of the resonance mentioned before, $T(E)$ goes to zero as $E\rightarrow 0$. It is interesting to note, however, that the case analyzed here is not related to the resonance tunneling situation introduced in Refs. 8 and 9. In that phenomenon, a given distribution of impurities gives rise for certain energies to a localized state in the center of the chain, which greatly enhances the transmission coefficient. In our case, however, the resonances are intrinsic to the single defects under study. They occur at fixed energies for each type of defect, and they lead to the vanishing of the transport coefficient.

The calculation reported above can be generalized, after straightforward but tedious manipulations, to small clusters of impurities. To throw some light on the interference effects between two side branches, we give here analytical results for the density of states on sites C and the transmission coefficient of two side chains which are connected to sites on the main chain n positions apart:

$$\rho_C(E)=-\frac{1}{\pi}\,\mathrm{Im}\left[\frac{E-V^2G_D(E)}{[E-V^2G_D(E)]^2-V^4G_{\mathrm{ND}}(E)}\right], \tag{3}$$

$$T(E)=\left|\frac{E^2}{E^2+V^4[G_D(E)^2-G_{\mathrm{ND}}(E)^2]^2-2V^2EG_D(E)}\right|^2,$$

where both the diagonal $G_D(E)$ and nondiagonal $G_{\mathrm{ND}}(E)$ elements of the Green's function of a perfect chain are given in the Appendix. [See Eqs. (A9), (A6), and (A7).]

As $E\rightarrow 0$, the corresponding limits are

$$\rho_C(E)\rightarrow\begin{cases}\dfrac{1}{\pi V}, & n \text{ odd}\\[2ex] \dfrac{1}{2+(n/2)}\delta(E)+\dfrac{1}{\pi V}\dfrac{8+4n+n^2}{16+8n+n^2}, & n \text{ even}\end{cases}$$

$$T(E)\rightarrow\begin{cases}4E^4/V^4, & n \text{ odd}\\ 4E^2/\{[2+(n/2)]^2V^2\}, & n \text{ even}\,.\end{cases} \tag{4}$$

Thus, when n is even, there is a sharp peak in the local density of states at $E=0$ which corresponds to a state localized between the two impurities. This peak persists at a finite concentration of defects (see below). Finally, the transmission coefficient goes to zero as expected.

It is clear that the main features discussed above, the zero in the transmission coefficient and the local density of states at site B, should remain for any finite concentration of defects. It is also interesting to note that even when the distribution of impurities is regular, the transmission coefficient of such a chain is always zero when $E=0$. At this energy there is either a gap, when the number of sites per unit cell is even, or a set of localized states if it is odd.

This model is easily generalizable to other types of side branches and closed loops connected to the main chain. Calculations of the transmission coefficients of a variety of such defects are given in the Appendix, including linear side branches and bifurcations along the main chain. These two latter types constitute the basis of the most common model of a percolation cluster.[10]

All these imperfections show the existence of antiresonances of the type described above at various energies within the band of the perfect chain. As will become clear in the following, this is the crucial feature which explains the deviations from standard theories found in our analysis. Provided that there is only a finite number of such resonances associated with the defects scattered along the chain, the transport properties, when the Fermi energy lies close to one of them, will be independent of the existence of the others, at least for low temperatures and long enough chains. Thus, the analysis reported here should be very general, and applicable to more complex situations with no fundamental modifications.

On the other hand, if there is a continuous spectrum of such antiresonances, they will interfere with each other for any temperature or concentration, leading to more complex behavior. This latter case is under study and results will be presented elsewhere.

III. RESULTS FOR FINITE CONCENTRATIONS OF DEFECTS

We will now study numerically the transport properties of the chain for different concentrations of the defects described above. We have chosen a low-concentration case, 2% of defects, to make comparisons with the results in the preceding paragraph, and an intermediate case, 20% of defects. It will be shown that the main qualitative features do not change appreciably.

The local density of states, shown in Fig. 2, have been obtained by averaging over chains of fixed length, matched at both ends to perfect coherent-potential-approximation (CPA) systems in which each atom in them is perturbed by the CPA self-energy corresponding to that given concentration. In this way, the δ-function peaks of the density of states of a finite chain are rounded in a natural way. The A sites are defined as any of the sites not connected to a side branch.

For low concentrations, the results are rather similar to the single-impurity case discussed before. There is a well-defined peak on the C sites at $E=0$, which shows a tail extending into the A sites. It is also easy to observe the extra localized level outside the band of the perfect chain [the new bands go from $-V(\sqrt{2}+1)$ to $V(\sqrt{2}+1)$]. There are some extra sharp peaks associated with clusters of impurities, in a similar way to the case of substitutional disorder. Finally, the local density of states on B atoms goes to zero when $E=0$, as expected.

As we raise the concentration, the number of peaks increases, as the different clusters of impurities become more numerous (see Fig. 3). Also, the band edges of the perfect chain are no longer well defined. However, the main features associated with the resonance around $E=0$ remain. There is a peak on C sites, with an appreciable take on A sites, and the corresponding antiresonance on B sites. The main new effect is that now the concentration of resonances is large enough to influence the average density of states on A sites. (There is a gap around $E=0$.) Outside the region around $E=0$, the structure presented here does not differ qualitatively from the standard substitutional disorder.

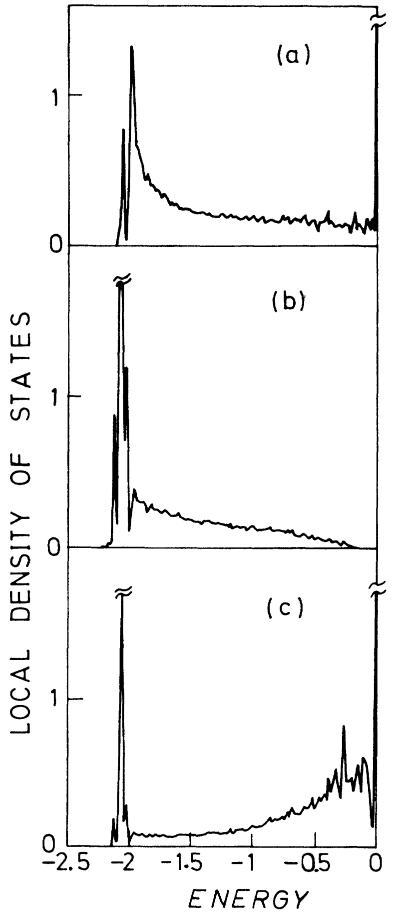

FIG. 2. Averaged densities of states at sites A, B, and C (from top to bottom). The curves are normalized to one and the energy is given in units of the hopping energy V. The concentration of defects is 2%.

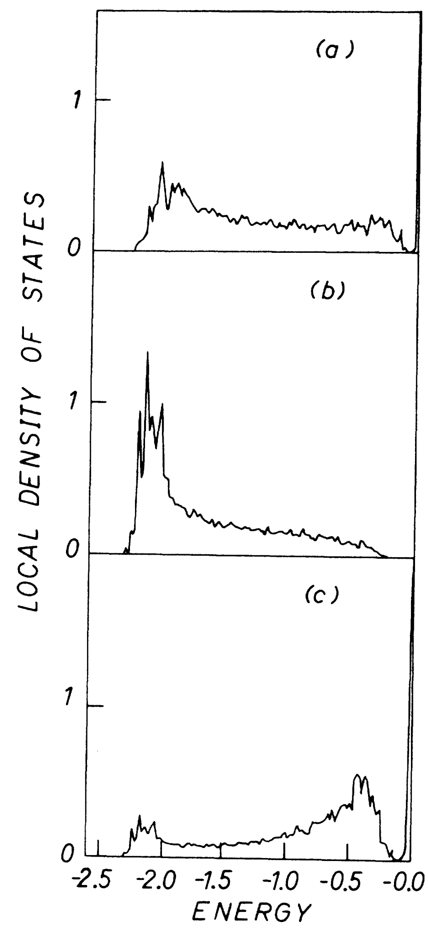

FIG. 3. Same as Fig. 2. The concentration of defects is 20%.

In order to analyze the transport properties of the chain, we have calculated the transmission coefficients of chains of different lengths.[11] We have matched chains with random distribution of impurities, and the same concentrations as before, to perfect chains of only A atoms at both ends, and studied the propagation of a running wave which reaches the disordered systems. From the transmission coefficient we have obtained the localization length, defined as

$$L(E)=-2L/\ln T_{\mathrm{chain}}(E)\ , \qquad (5)$$

where L is the length of the chain. From the way $T_{\mathrm{chain}}(E)$ is calculated, it is clear that it can only be defined for energies within the band of the perfect chains in contact with the disordered sample.

Values of $L(E)$ for chains of different lengths and different concentrations are shown in Figs. 4 and 5. In this case we have not averaged over different chains of the same length and concentration, i.e., the results presented in Figs. 4 and 5 correspond to single chains. In this way we can also reproduce, at least for short chains, the effects of resonant tunneling from Refs. 8 and 9. Those are the sharp peaks in $L(E)$ observed for short chains, which correspond to values of $T_{\text{chain}}(E)$ close to one. The positions of these peaks are strongly sample dependent, and would be wiped out by any averaging process. As the length of the chain increases, the width of these peaks is expected to decrease exponentially, and for the longest chains depicted in the figures it is well below the resolution of the graphs.

The structure in the energy dependence of $L(E)$ disappears as the size of the chains is increased, except for the extremely narrow resonances mentioned before. This behavior is different from that of the density of states, where the fluctuations persist even after averaging over many chains. For low concentrations, we can neglect coherent multiple scattering[12] and use the results for the single-defect case to estimate $L(E)$.[13] As a function of $T(E)$ for a single defect, Eq. (2), we have

$$T_{\text{chain}}=[T(E)]^{cL/a}\,,$$
$$L(E)=-2a/\{c\ln[T(E)]\}\,, \tag{6}$$

where c is the concentration of defects and a is the lattice constant. This curve is also shown in the lower panel of Figs. 4 and 5. It can be seen to be a very good approximation to the numerical results for $c=0.02$, and to reproduce the main features of the data when $c=0.2$, although with a clear tendency to underestimate $L(E)$.

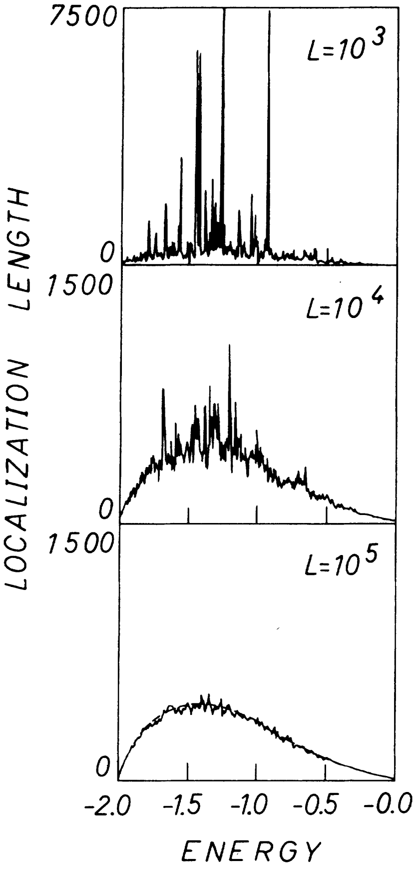

FIG. 4. Localization length (in units of the lattice constant a) as a function of energy (in units of the hopping energy V) for three chains of increasing length L (which is given in units of a). The concentrations of defects is 2%. On the bottom panel the analytical approximation given by Eq. (4) is also shown (dashed curve).

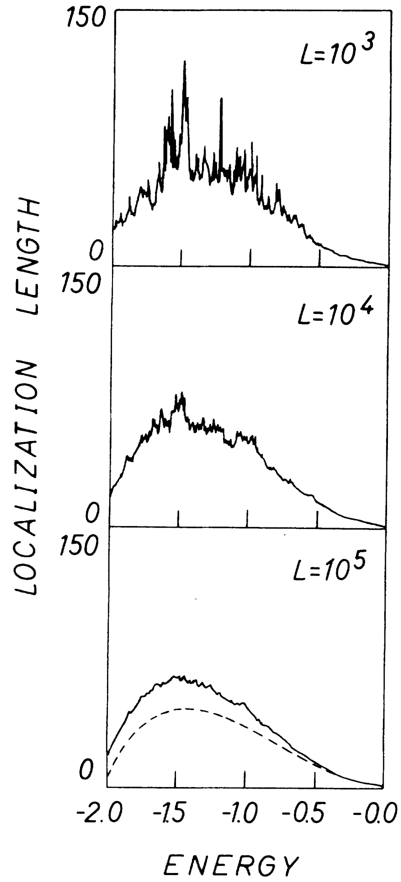

FIG. 5. Same as Fig. 4. The concentration of defects is 20%.

In both cases the fit is better near the region around $E=0$, when $L(E)$ goes to zero. This is expected, since when the localization length is very short, multiple-scattering processes are less important.

IV. TRANSPORT PROPERTIES

As discussed before, the novel features of our model with respect to substitutional disorder occur when $E\simeq0$, that is, for energies close to the energies of the eigenstates of the side branches. Thus, we will assume that the Fermi energy of the chains lies in that region and calculate their conductance in the absence of many-body effects. The transmission coefficient of the system goes to zero as $E \rightarrow 0$, and from Landauer's formula, the conductance has the same behavior. In order to derive analytical expressions, we will use the single impurity formula, Eq. (6), to estimate the dependence of $L(E)$ on E in this region. As already discussed, we expect this approximation to be valid for small concentrations and/or small localization lengths. We have for the transmission coefficient of the entire chain:

$$T_{\text{chain}}(E) \sim (2|E|/V)^{2cL/a} , \tag{7a}$$

and for the localization length [given by Eq. (5)] when $E \ll V$,

$$L(E) \sim -a/[c \ln(2|E|/V)] . \tag{7b}$$

At a given temperature T, we have to average these values over a range of energies proportional to $k_B T$. Thus, we obtain for the conductance of long wires:

$$g(T) \sim (k_B T/V)^{2cL/a} . \tag{8}$$

This strong dependence of g on T arises from the disorder only, and should be easily distinguishable from other possible mechanisms. Note that this behavior is only related to the presence of defects, and not to inelastic scattering events, which are the cause of most features in the temperature dependence of the resistance of wires. In fact, inelastic processes will blur this effect, which can only be observed at very low temperatures.

The average level spacing in a chain is proportional to V/N, where $N = L/a$ is the number of sites in the chain. When $k_B T \ll V/N$, the uncertainty in energies associated with this effect dominates, and we have to average $T_{\text{chain}}(E)$ or $L(E)$ over this range of energies in order to obtain the conductance. This means that for very low temperatures we have

$$g(L) \sim \exp[-(cL/a)\ln(L/a)] . \tag{9}$$

This length dependence is different from the expected behavior in the localized regime, where it is a simple exponential. This dependence, moreover, violates the simple scaling law derived for standard disordered systems. This law states that the conductance of a sample of length L can be expressed in terms only of the conductances of samples whose length is a fraction of the original L. In our case, we can calculate the function:

$$\beta = d \ln g / d \ln L = -(cL/a)\ln(L/a) - cL/a ,$$

which, if scaling holds, should be a function of g only. If the second term on the right-hand side is not negligible, as compared with the first, this is not true, and the scaling laws not only depend on g but also on other parameters of the chains, like the concentration c. We ascribe this effect to the nontrivial way in which the length of the chain appears in the calculation of the average conductance, via the separation of the energy levels of the system.

V. CONCLUSIONS

We have analyzed a simple disordered model in which the irregularities are in the geometrical structure of the system rather than being produced by additional impurities. Systems such as branched polymers, percolation networks, and other types of fractals should show similar features, and it is not unlikely that experimental realizations of dirty conductors have similar properties.

Analytical and numerical results are given, and it has been shown that a strong energy dependence in most electronic properties arises in a direct way, unlike the case of other types of disorder. The irregularities in the geometrical structure lead to resonances at certain energies which block the transmission of waves along the chain. In our case, with a single conducting channel, this effect leads to the vanishing of the conductance at certain energies. For realistic models of wires, where a large number of channels are available, the conductance is not likely to go to zero, although a strong energy dependence should remain. Further research in this direction will be reported elsewhere. Unlike for resonant tunneling, this effect does not depend on the global distribution of impurities, and should not be sample dependent.

Finally, it has been shown that the transport properties of long chains are strongly altered when the Fermi energy lies in the vicinity of the resonance energies discussed before. This leads to a strong temperature dependence of the conductance, even in the absence of inelastic processes. The dependence of the conductance on the length of the sample is also anomalous, and differs from the exponential law expected in the localized regime typical of one-dimensional systems. This leads to a violation of the one-parameter scaling theory generally valid for standard models of disorder.

APPENDIX: SCATTERING DUE TO SIDE CHAINS AND LOOPS

The purpose of this appendix is to obtain the transmission coefficients through two different kinds of topological defects: (i) side chains of arbitrary but finite length, and (ii) asymmetric loops of arbitrary size. They constitute the simplest examples of dead ends and redundant loops that can appear on a conducting chain. As we are only interested in the effect of topological disorder on the conducting properties of the chain, we exclude both the possibility of different atoms forming part of the defect (standard diagonal disorder) and the appearance of interaction energies different from the interaction energy V between nearest-neighbor orbitals on the main chain (standard nondiagonal disorder).

We shall obtain the transmission coefficient through the defect from the transmission amplitude that is given by

$$t = \langle \alpha | G | \alpha' \rangle / \langle \alpha | G_0 | \alpha' \rangle , \tag{A1}$$

where G_0 and G are the Green's functions of the chain without and with defect, respectively, and $|\alpha\rangle$ and $|\alpha'\rangle$ are orbitals that are far from the defect and on different sides. The physical meaning of Eq. (A1) is very clear: the matrix element $\langle \alpha | G | \alpha' \rangle$ describes the propagation of an electron from one side to the other of the defect. The relation between the propagation from $|\alpha\rangle$ to $|\alpha'\rangle$ in the presence of the defect and the same propagation when the defect is absent gives just the transmission amplitude.

We first consider the scattering due to a side chain formed by N atoms (1 to N) and connected to atom 0 belonging to the main chain [see Fig. 6(a)]. We compute $\langle \alpha | G | \alpha' \rangle$ from Dyson equation

$$G = G_0 + G_0 \hat{V} G \,, \tag{A2}$$

where the perturbation potential $\hat{V}$ is given in this case by

$$\hat{V} = V(|0\rangle\langle 1| + |1\rangle\langle 0|) \,. \tag{A3}$$

Taking matrix elements in Dyson equation, the following set of equations is obtained:

$$\begin{aligned}
&\langle \alpha | G | \alpha' \rangle = \langle \alpha | G_0 | \alpha' \rangle + \langle \alpha | G_0 | 0 \rangle V \langle 1 | G | \alpha' \rangle \,, \\
&\quad \langle 1 | G | \alpha' \rangle = 0 + \langle 1 | G_0 | 1 \rangle V \langle 0 | G | \alpha' \rangle \,, \\
&\quad \langle 0 | G | \alpha' \rangle = \langle 0 | G_0 | \alpha' \rangle + \langle 0 | G_0 | 0 \rangle V \langle 1 | G | \alpha' \rangle \,,
\end{aligned} \tag{A4}$$

which can be solved for $\langle \alpha | G | \alpha' \rangle$,

$$\begin{aligned}
\langle \alpha | G | \alpha' \rangle &= \langle \alpha | G_0 | \alpha' \rangle \\
&\quad + \frac{\langle \alpha | G_0 | 0 \rangle V \langle 1 | G_0 | 1 \rangle V \langle 0 | G_0 | \alpha' \rangle}{1 - V^2 \langle 0 | G_0 | 0 \rangle \langle 1 | G_0 | 1 \rangle} \,.
\end{aligned} \tag{A5}$$

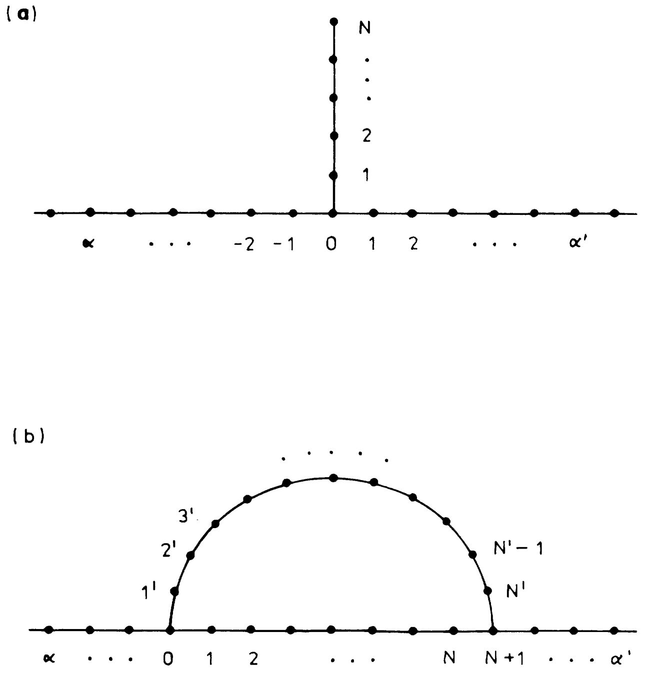

FIG. 6. (a) Schematic representation of a side chain formed by N atoms. (b) Sketch of a (N,N') loop inserted in the main chain.

Now, we use the general formula giving the matrix elements of the Green's function of an infinite chain,[14] i.e.,

$$\langle n | G_0 | n' \rangle = \langle 0 | G_0 | 0 \rangle e^{i|n'-n|\theta} \,, \tag{A6}$$

where the angle θ is related to the energy E through the relationship

$$E = 2V\cos\theta \,. \tag{A7}$$

Using Eq. (A6) repeatedly, Eq. (A5) reduces to

$$\langle \alpha | G | \alpha' \rangle = \langle \alpha | G_0 | \alpha' \rangle \frac{1}{1 - V^2 \langle 0 | G_0 | 0 \rangle \langle 1 | G_0 | 1 \rangle} \,. \tag{A8}$$

The transmission amplitude is computed directly from Eq. (A8) once the value of the diagonal element of the Green's function of the infinite chain

$$\langle 0 | G_0 | 0 \rangle = \frac{1}{E - 2Ve^{i\theta}} = \frac{i}{2V\sin\theta} \,, \tag{A9}$$

and the diagonal element at the extreme of the finite chain of N atoms

$$\langle 1 | G_0 | 1 \rangle = \frac{\sin(N\theta)}{V\sin[(N+1)\theta]} \tag{A10}$$

are used. Finally,

$$\begin{aligned}
t = \frac{\langle \alpha | G | \alpha' \rangle}{\langle \alpha | G_0 | \alpha' \rangle} &= \left[1 - V^2 \frac{i}{2V\sin\theta} \frac{\sin N\theta}{V\sin[(N+1)\theta]} \right]^{-1} \\
&= \left[1 - \frac{i}{2} \frac{\sin(N\theta)}{\sin\theta \sin[(N+1)\theta]} \right]^{-1}
\end{aligned} \tag{A11}$$

and the transmission coefficient is given by

$$T_N(E) = tt^* = \left[1 + \tfrac{1}{4} \left[\frac{\sin N\theta}{\sin\theta \sin[(N+1)\theta]} \right]^2 \right]^{-1} \,. \tag{A12}$$

In the particular case of a side branch formed by only one atom, Eq. (A12) reduces to

$$\begin{aligned}
T_1(E) = \left[1 + \tfrac{1}{4} \frac{1}{\sin^2(2\theta)} \right]^{-1} &= \left[1 + \frac{1}{16\sin^2\theta\cos^2\theta} \right]^{-1} \\
&= \frac{4V^2 - E^2}{4V^2 - E^2 + V^4/E^2} \,.
\end{aligned} \tag{A13}$$

Equation (A13) has been used repeatedly in the main text of this paper. On the other hand, general equation (A12) shows that the transmission coefficient $T_N(E)$ vanishes for

$$E = 2V\cos\left[n\frac{\pi}{N+1} \right] \quad \text{with } n = 0,1,2,\ldots,N+1 \,, \tag{A14}$$

proving that the vanishing of the transmission coefficient is a very common result when topological disorder is considered.

Next, we shall consider the scattering due to a loop inserted in the infinite chain. A sketch of the defect is given in Fig. 6(b). In this case, the perturbation potential is

$$\hat{V}=V(\,|0\rangle\langle 1'|+|1'\rangle\langle 0|+|N+1\rangle\langle N'|+|N'\rangle\langle N+1|\,)\,. \tag{A15}$$

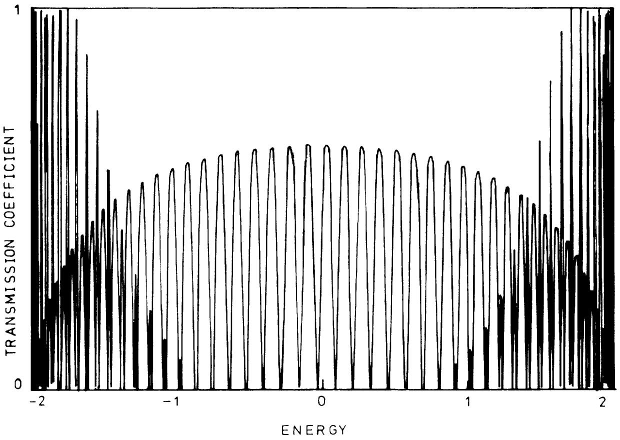

FIG. 7. Transmission coefficient corresponding to a (0,101) loop inserted in the main chain. Formulas (A20) and (A21) give the energies at which the transmission coefficient vanishes.

Straightforward, but very tedious, algebraic manipulations along the lines followed in the study of side chains yields the result for the transmission coefficient $T_{N,N'}(E)$ through the (N,N') loop,

$$T_{N,N'}(E)=4\sin^2\alpha\cos^2\beta\{[\sin(2\alpha)+\cot\theta(\sin^2\beta-\sin^2\alpha)]^2+[\cot\theta\sin(2\alpha)+3\sin^2\alpha-\sin^2\beta+\tfrac{1}{2}(\sin^2\beta-\sin^2\alpha)/\sin^2\theta]^2\}^{-1}\,, \tag{A16}$$

where

$$\alpha=\frac{N+N'+2}{2}\theta\,, \tag{A17}$$

and

$$\beta=\frac{N'-N}{2}\theta\,. \tag{A18}$$

The result for the symmetric loop is more simple. The transmission coefficient is

$$T_{N,N}(E)=\frac{4}{(2\cos\alpha-\cot\theta\sin\alpha)^2+(2\cot\theta\cos\alpha+3\sin\alpha-\frac{1}{2}\sin\alpha/\sin^2\theta)^2}\,. \tag{A19}$$

Equation (A19) shows that the transmission through the symmetric loop never vanishes. On the other hand, the general result given by Eq. (A16) proves that for every pair of values (N,N') with $N'\neq N$, there are many energies for which $T_{N,N'}(E)$ vanishes. In particular, for $N=0$ and $N'>0$, there is no transmission at the following energies:

$$E=2V\cos\left[n\frac{2\pi}{N'+2}\right] \tag{A20}$$

and

$$E=2V\cos\left[(2n+1)\frac{\pi}{N'}\right]\,, \tag{A21}$$

where n is an arbitrary integer and the angle is bound by $-\pi\leqq\theta\leqq\pi$. An example of the behavior of $T_{0,N'}(E)$ is given in Fig. 7.

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