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Transport properties of a random binary side-coupled chain*

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We investigate the transport properties of a random binary side-coupled chain by using the transfer-matrix technique. It is found that there are resonant states in the systems with short-range correlations between the host chain atoms and the side-coupled atoms. The analytic expressions for the extended states are also presented in the systems with the side couplings between like atoms and between unlike atoms.

Keywords: localization in disordered structures, extended states, resonance
PACC: 7155J, 6320P

Since the pioneering work of Anderson,[1] the field of localized and delocalized states has attracted attention for a long time and experienced tremendous development. From the one-parameter scaling theory it follows that all states are localized by extremely weak disorder in systems with no more than two dimensions.[2] However, the delocalized states in 1D disordered systems can still be produced by the quantum interference. Extended states can exist in 1D Anderson disordered systems with long-range correlated disorder,[3,4] or in 1D Anderson disordered systems with long-range hopping.[5,6] A mobility edge was confirmed to separate extended states from localized states in such systems, which means that there exists a metal-insulator transition (MIT). The 1D model for the random binary alloy, where there are two types of atoms: A and B, shows that all wavefunctions are localized and the system behaves as an insulator.[7] When there are short-range correlations in a random binary system, an extended state can appear due to symmetries of resonant scattering in the structure, such as the well-known random-dimer model.[8] Many extended states can be obtained by generalizing the random-dimer model.[9−12] If the long-range correlations exist in a 1D random binary system, MIT also appears.[13] Generally, long-range correlations can result in extended states in an energy band and there are mobility edges which separate extended states from localized states in the framework of thermodynamics. However, there are some isolated extended states in the system with short-range correlations. Long-range or short-range correlations are diagonal in their Hamiltonians. Recently, off-diagonal correlations, hopping determined by the corresponding onsite potentials, have drawn attention. It is shown that there appears an extended state or fully extended states in the whole band.[14,15]

In the present paper, we investigate the random binary side-coupled chain, which is shown in Fig.1. It is found that there is no extended state in the chain with random side coupling, but there are two extended states in two cases, i.e. in the chain with the side coupling between unlike atoms and that between like atoms. We also present the analytical expressions of extended states, which are determined by the side hopping and the potentials of the corresponding atoms.

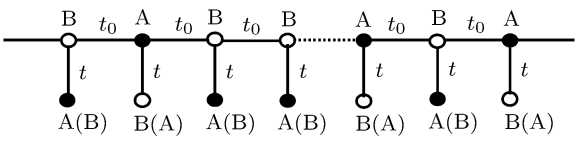


Fig.1. Schematic representation of the random binary side-coupled chain, where A and B represent two different atoms.

The Hamiltonian of the model can be written in

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a tight-binding form as

$$H = \sum_j [t_0(c_j^\dagger c_{j+1} + c_j^\dagger c_{j-1}) + t(c_j^\dagger c_{j'} + c_{j'}^\dagger c_j) + \varepsilon_j c_j^\dagger c_j + \varepsilon_{j'} c_{j'}^\dagger c_{j'}], \quad (1)$$

where c_j ($c_{j'}$) is an annihilation operator for an electron on the j-th atom of the host chain (on the j'-th side-coupled atom). t_0 (t) is the hopping in the host chain (the side-coupled hopping), and ε_j ($\varepsilon_{j'}$) is the on-site potential of the j-th atom in the chain (of the side atom). The wave function of the system can be written as

$$|\Psi\rangle = \sum_{i=j,j'} \varphi_i |i\rangle. \quad (2)$$

The Schrödinger equation can be used to determine the relations between the wave function coefficients in the adjacent atoms as follows:

$$(E - \varepsilon_j)\varphi_j = t_0\varphi_{j-1} + t_0\varphi_{j+1} + t\varphi_{j'} \quad (3)$$

and

$$(E - \varepsilon_{j'})\varphi_{j'} = t\varphi_j. \quad (4)$$

By solving Eqs.(3) and (4), one can obtain the following relation for the wave function coefficients in adjacent atoms in the transfer-matrix form:

$$\begin{pmatrix} \varphi_{j+1} \\ \varphi_j \end{pmatrix} = \hat{T}_j \begin{pmatrix} \varphi_j \\ \varphi_{j-1} \end{pmatrix}, \quad (5)$$

where

$$\hat{T}_j = \begin{pmatrix} E - \varepsilon_j - \dfrac{t^2}{E - \varepsilon_{j'}} & -1 \\ 1 & 0 \end{pmatrix}. \quad (6)$$

By using the recursion formula of wave function coefficients in adjacent atoms, the total transfer matrix can be written as

$$\hat{T} = \prod_{j=1}^{N} \hat{T}_{N+1-j} \quad (7)$$

and

$$\begin{pmatrix} \varphi_{N+1} \\ \varphi_N \end{pmatrix} = \hat{T} \begin{pmatrix} \varphi_0 \\ \varphi_{-1} \end{pmatrix}, \quad (8)$$

where N is the total number of the atoms in the chain.

In order to show the transport properties of systems, we calculate the transmission coefficient (TC). We suppose that the system is connected to two semi-infinite leads at the two ends and the leads are treated as pure chains. The wave functions in the two semi-infinite leads, with translational symmetry, can be expressed as plane waves. If an electron wave with unity amplitude is incident from the left lead, there will be a reflected wave to the left lead with amplitude r, and a transmitted wave to the right lead with amplitude s. The wave function at each site in the leads can be written as

$$\varphi_j = \begin{cases} \mathrm{e}^{\mathrm{i}kj} + r\mathrm{e}^{-\mathrm{i}kj}, & (j < 1), \\ s\mathrm{e}^{\mathrm{i}kj}, & (j > N). \end{cases} \quad (9)$$

Substituting expression (9) into equation (8) yields the following equation:

$$\begin{pmatrix} s \cdot \mathrm{e}^{\mathrm{i}k(N+1)} \\ s \cdot \mathrm{e}^{\mathrm{i}kN} \end{pmatrix} = \hat{T} \begin{pmatrix} 1 + r \\ \mathrm{e}^{-\mathrm{i}k} + r \cdot \mathrm{e}^{\mathrm{i}k} \end{pmatrix}. \quad (10)$$

TC of the system can be obtained by solving Eq.(10) as follows:

$$\mathrm{TC} = |s|^2 = \left| \frac{2t_0 \mathrm{i} \sin k \cdot (T_{12}T_{21} - T_{11}T_{22})}{(T_{11} - T_{21}\mathrm{e}^{\mathrm{i}k}) + (T_{12} - T_{22}\mathrm{e}^{\mathrm{i}k})\mathrm{e}^{\mathrm{i}k}} \right|^2. \quad (11)$$

The two types of atoms in the system are denoted by A and B, and the on-site potentials of A and B atoms are set to be 0 and 0.5, respectively. The hopping in the host chain is set to be 1, and the hopping of the side coupling is set to be 0.2. There are three cases for the side coupling: random coupling, dimeric coupling and paired coupling.

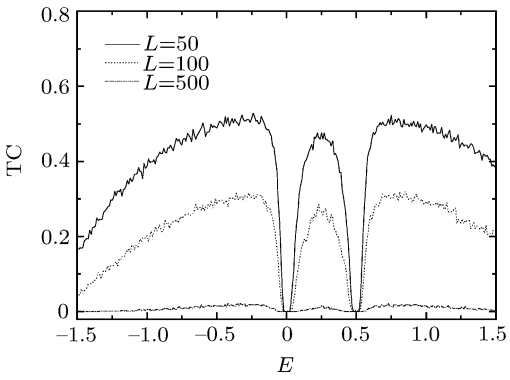


Fig.2. Dependences of TC on the energy of the electron in the random binary side-coupled chain with random coupling. The hopping between the nearest sites of the host chain (t_0) is set to be 1. The on-site energies of A and B atoms are set to be 0 and 0.5, respectively. The side coupling (t) is set to be 0.2. L is the length of the system. Each curve corresponds to an average over 1000 random configurations.

In the case of random coupling, each site of the side-coupled chain is arranged randomly by A or B atoms, and the probability for an A atom to occur at each site is equal to that for a B atom to be present at this site. The number of A atoms in the system should be equal to the number of B atoms. In this case, we

show the dependence of TC on the energy of the electron with an average over 1000 random configurations in Fig.2. As the system is disordered, TC decreases when the length of the system increases. Especially, there are two dips at $E = 0$ and 0.5 separately, which correspond to the on-site potentials of A and B atoms. In such a system there exists no extended state.

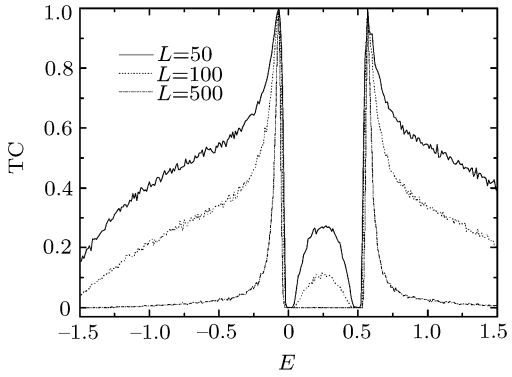


Fig.3. Dependences of TC on the energy of the electron in the random binary side-coupled chain with paired coupling. The other parameters are the same as those in Fig.2.

When the side coupling is paired coupling, each site of the host chain is arranged randomly by A or B atoms, and the probability for an A atom to occur at each site is still equal to that for a B atom to appear at the site, but the side-coupled atom is not random, which must always be different from the host chain. As each site of the host chain is occupied by A or B atoms with the same probability, the number of A atoms in such a system should be equal to the number of B atoms. We find that there exist two extended states in the system. In Fig.3. one can find that the two dips are still present at $E = 0$ and 0.5, and there are two resonant energies beside the on-site potentials of A and B atoms. In a recent paper, de Moura proposed a model of single strand deoxyribonucleic acid (DNA) with diluted base pairing.[16] It was shown that there was an extended state in poly (CT) DNA but no extended state in poly (CG) DNA. The disorder induced by the diluted base pairing promotes the exponential localization of all one-electron states for the poly (CG), but there is a resonant mode with on-site energy of thymine (T) which is not affected by the disorder and remains extended with a Bloch-like character. The poly (CG) or poly (CT) model and our model are both side-coupled and seem similar, whereas there is an essential difference between them. The translational symmetry of the host chain still exists in the poly models, but the random diluted side couplings completely destroy the translational symmetry in the poly (CG) model and the translational symmetry just in a state is not destroyed by the diluted side coupling. In our model there is no translational symmetry in the host chain, but the side coupling can change the structure of electrons, thereby leading to two extended states.

For the case of dimeric coupling, the host chain is the same as those in the above cases, but the side-coupled atom must always be identical with the atom of the host chain. The fractions of A atoms and B atoms should be equal, too. There are also two resonant states in Fig.4. The two resonant states are present between the on-site potentials of A and B atoms.

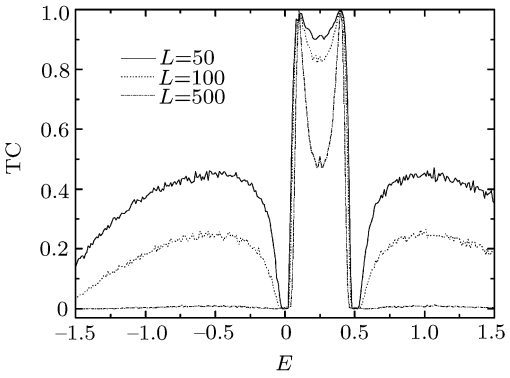


Fig.4. Dependences of TC on the energy of the electron in the random binary side-coupled chain with dimeric coupling. The other parameters are the same as those in Fig.2.

The most disorder arrangement in a system, which is composed of two kinds of atoms, is random arrangement with two kinds of atoms which have the same fractions. With the increase of fraction of one kind of atom and the decrease of that of another kind of atom, the disorder in elements will decrease, which means that the system tends to be ordered in elements. So when the difference in fraction between the A atom and the B atom increases, the transmission of the system will increase. But the positions of dips and resonant states will not shift. When the system is composed of only one kind of atom, the electrons in the whole band except electrons with on-site potential will transmit completely without reflection. In this paper we investigate only the transport properties of the random binary side-coupled chain, with the same fraction of each kind of atom.

In order to explain the above results, we obtain

the following equation from Eqs.(3) and (4):

$$\left(E-\varepsilon_j-\frac{t^2}{E-\varepsilon_{j'}}\right)\varphi_j=t_0\varphi_{j-1}+t_0\varphi_{j+1}. \quad (12)$$

Each side-coupled atom can be renormalized into an atom of the host chain,[17] and the renormalized atom of the chain with effective on-site potential V_j satisfies

$$V_j=\varepsilon_j+\frac{t^2}{E-\varepsilon_{j'}}. \quad (13)$$

If the effective on-site potentials of atoms are equal, electrons can transmit through the system without reflection because of the translational symmetry of the system. As there are only two kinds of atoms, A and B, the electrons will completely transmit through the system only when the following relation is satisfied in paired coupling:

$$V_{\text{eff}}=\varepsilon_{\text{A}}+\frac{t^2}{E-\varepsilon_{\text{B}}}=\varepsilon_{\text{B}}+\frac{t^2}{E-\varepsilon_{\text{A}}}. \quad (14)$$

From formula (14) we can obtain

$$E=\frac{\varepsilon_{\text{A}}+\varepsilon_{\text{B}}\pm\sqrt{(\varepsilon_{\text{A}}-\varepsilon_{\text{B}})^2+4t^2}}{2}, \quad (15)$$

which are the two resonant energies in this system.

For the dimeric coupling the resonant energies satisfy

$$E=\frac{\varepsilon_{\text{A}}+\varepsilon_{\text{B}}\pm\sqrt{(\varepsilon_{\text{A}}-\varepsilon_{\text{B}})^2-4t^2}}{2}. \quad (16)$$

In our systems with short-range correlations, there are two extended states, which are resonant states with no reflection. The results are similar to those obtained from the random-dimer model and its generalized models.[8−12] When the side coupling is random coupling, the effective on-site potentials cannot be identical. All states of this system in the case of random coupling are localized.

From formula (13) we can find that if the energy of electrons is equal to the potential of the side-coupled atom, the effective on-site potential V_{eff} will be infinite. Scattered by infinite potential the electrons with a finite energy will be reflected completely. The side-coupled atoms are only two kinds of atoms in the three kinds of couplings, so there are two anti-resonant energies in our system.

In summary, three cases of side couplings, i.e. random coupling, dimeric coupling and paired coupling, are discussed in this paper to investigate the transport properties of a random binary side-coupled chain. In the case of random coupling all states are localized. There are two resonant energies in each of the other cases. There are two anti-resonant energies in our system, which are equal to the on-site potentials of the A and B atoms, respectively. We also give the analytic expressions for the extended states in the systems with the side coupling between like atoms and between unlike atoms. It is expected that our results would be useful for explaining the transport properties of polymer and DNA.

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