Transport properties of a ladder with two random dimer chains*

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We investigate the transport properties of a ladder with two random dimer (RD) chains. It is found that there are two extended states in the ladder with identical RD chains and a critical state regarded as an extended state in the ladder with pairing RD chains. Such a critical state is caused by the chiral symmetry. The ladder with identical RD chains can be decoupled into two isolated RD chains and the ladder with pairing RD chains can not. The analytic expressions of the extended states are presented for the ladder with identical RD chains.

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1. Introduction

According to the single-parameter scaling theory all states are localized in one-dimensional (1D) or 2D disordered systems.[1] However, the resonant states can appear in 1D disordered systems with short-range correlations such as the random dimer model (RDM) and its generalized models.[2−13] An extended state exists in a 1D RDM chain in which there are two types of atoms, A and B, randomly assigned with probability p and $(1-p)$, but atoms B always appear in pairs. The energy of extended state is just the on-site energy $\varepsilon_{\rm B}$ of atoms B.[2] Two and more extended states exist in random trimer model and random n-mer models, respectively.[7−9] The states at energies $\varepsilon_{\rm B}$ and $\varepsilon_{\rm A}$ are both extended if A and B are both in pairs.[10] There are $n+1$ discrete extended states in a 1D system, in which pairs of atoms B are intermediated by n atoms A.[11] RDM was also generalized into a quasi-1D structure, a ladder with two identical RD chains.[12,13] By numerically calculating the transmittance of the ladder Mitra and Thakur found that there are extended states in the system with only one type atom being pairwise in each chain.[12] The similar structure with atoms A and B being both pairwise in each chain was also investigated by Sedrakyan and Ossipov. It was shown that there is a point of delocalization at the band centre.[13] The amplitude of wave function exponentially decays in localized states. However, the special chiral state can be power law localized and be usually regarded as an extended state in bipartite lattices.[14] In this study, by numerical calculation and decoupling method, we find the expressions of the extended states in ladder with identical RD chains. There is a critical state with power law localization in the ladder with pairing RD chains, which is caused by the chiral symmetry.

2. The models and the basic formulae

By using the transfer-matrix technique we investigate the transport properties of a ladder with two RD chains, which is shown in Fig. 1. Figure 1(a) is a ladder with two identical RD chains, and Fig. 1(b) is a ladder with pairing RD chains. In each chain there are two types of atoms, A and B, and they are randomly assigned, but atoms B always appear doubly.

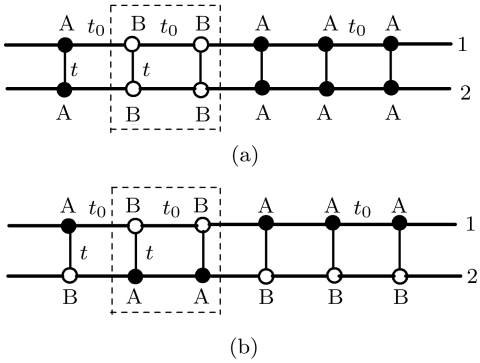


Fig. 1. Schematic representations of a ladder with (a) identical RD chains and (b) pairing RD chains, where A and B represent two different atoms, t_0 and t are intrachain hopping and interchain hopping, respectively.

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The Hamiltonian of the ladder can be written in a tight-binding form as

$$H = \sum_{l=1,i=1,2}^{L} [(t_0 c_{l+1,i}^{\dagger} c_{l,i} + t c_{l,1}^{\dagger} c_{l,2} + \text{H.c.}) + \varepsilon_{l,i} c_{l,i}^{\dagger} c_{l,i}], \tag{1}$$

where $c_{l,i}$ is an annihilation operator of an electron in the site l of the ith chain, and $\varepsilon_{l,i}$ is the on-site potential. t_0 and t are intrachain hopping and interchain hopping, respectively. The wave function of the ladder can be written as

$$|\Psi\rangle = \sum_{l=1,i=1,2}^{L} \varphi_{l,i} |l,i\rangle. \tag{2}$$

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

$$(\boldsymbol{E}\hat{\boldsymbol{I}} - \hat{\boldsymbol{M}})\varphi_l = t_0(\varphi_{l-1} + \varphi_{l+1}), \tag{3}$$

where

$$\hat{\boldsymbol{I}} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{4}$$

$$\hat{\boldsymbol{M}} = \begin{pmatrix} \varepsilon_{l,1} & t \\ t & \varepsilon_{l,2} \end{pmatrix}, \tag{5}$$

$$\boldsymbol{\varphi}_l = \begin{pmatrix} \varphi_{l,1} \\ \varphi_{l,2} \end{pmatrix}. \tag{6}$$

The 4×4 total transfer matrix $\hat{\boldsymbol{T}}$ can be obtained by the transfer matrix method[15,16]

$$\hat{\boldsymbol{T}} = \prod_{j=1}^{L} \hat{T}_{L+1-j}, \tag{7}$$

where

$$\hat{\boldsymbol{T}}_j = \begin{pmatrix} \dfrac{E-\varepsilon_{j,1}}{t_0} & -\dfrac{t}{t_0} & 1 & 0 \\ -\dfrac{t}{t_0} & \dfrac{E-\varepsilon_{j,2}}{t_0} & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \tag{8}$$

The Hermitian matrix $(\hat{\boldsymbol{T}}^{\dagger}\hat{\boldsymbol{T}})^{1/2L}$ has four eigenvalues, which are positive and come in inverse pairs due to the unitarity of the matrix.[16,17] Two positive logarithms of eigenvalues, denoted as γ_1 and γ_2, are Lyapunov exponents reflecting the exponential decay of the wavefunction in corresponding channels. The conductance of the system with length L can be written as[16,17]

$$g = \frac{2e^2}{h} \sum_{i=1}^{2} \frac{1}{\cosh^2(\gamma_i L)}, \tag{9}$$

here the two spins are taken into account. Being two channels the maximal conductance may be $4e^2/h$ in the system.

3. Numerical results and discussion

When the system is the ladder with identical RD chains (as shown in Fig. 1(a), the extended states may be found by calculating the conductance with energy of electrons. Figure 2 is the conductance with energy of electrons for different lengths of the ladder. The intrachain hopping (t_0) is set to be 1, and the interchain hopping (t) is set to be $0.2t_0$. The on-site potential of atom B, which is dimer, is set to be $0.3t_0$, and that of atom A is set to be $0.4t_0$. When the length of the system is 10^4 or 10^5 atomic distance, there is no evidence about extended states. But when the length reaches 10^6 atomic distance, two peaks appear in the curve of the conductance, and they are very distinct when the length of the ladder is up to 10^7. The conductance at each peak descends with the length of the ladder increasing, but the locations of the peaks are fixed, which are at about $0.1t_0$ and $0.5t_0$, respectively. The locations of the two peaks are right at $\varepsilon_{\rm B} \pm t$.

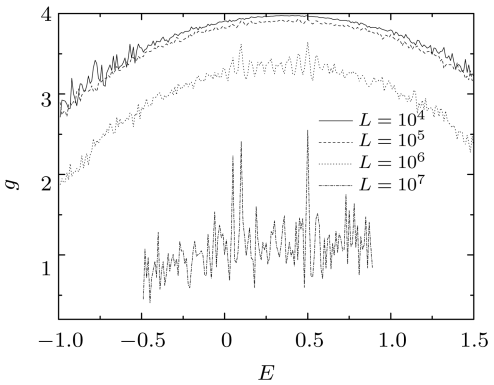


Fig. 2. The electron energy dependent conductance of the ladder with identical RD chains. The hopping between the nearest sites in each chain (t_0) is set to be 1, and the interchain hopping (t) is set to be $0.2t_0$. The on-site potential of atom A is set to be $0.4t_0$, and that of atom B, which is dimer, is set to be $0.3t_0$. The units of conductance and energy are e^2/h and t_0, respectively. Atoms A and B appear with the same probability. L is the length of the system. The curves correspond to average over 100 random configurations for the length of the ladder being 10^4, 10^5, and 10^6 atomic distance, and average over 10 random configurations for that of 10^7 atoms.

In order to confirm whether the states at peaks are extended states or not, we calculate the conductance with length at these two energies and at other two energies. For an extended state the conductance is always finite in the limit of thermodynamics. However, it tends to be zero for a localized state. Figure 3 is the dependence of conductance on the length in the ladder with identical RD chains. When the energies of electrons are right at the peaks, the conductance is always greater than a finite value, which is just $2e^2/h$ in Figs. 3(a) and 3(b). The conductance tends to decay exponentially at the other energies (Figs. 3(c) and 3(d)). From this phenomenon we can conclude that the states at peaks are both extended states, and the others are all localized in this system.

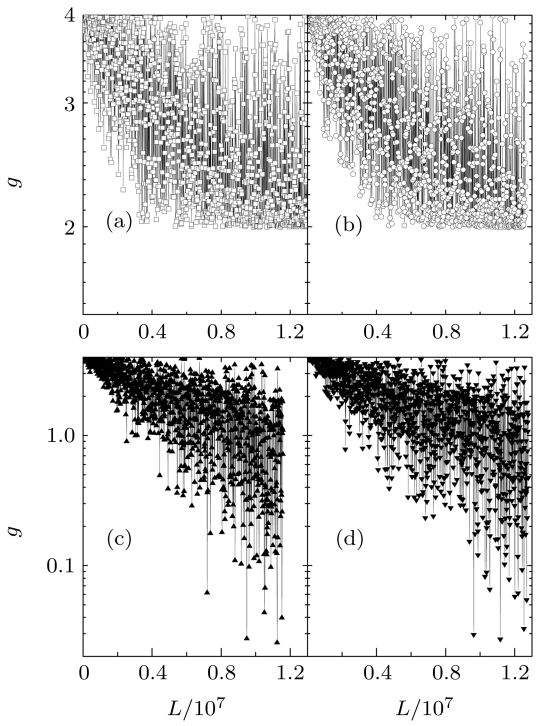


Fig. 3. The length dependent conductance of the ladder with identical RD chains in energy of 0.1 for (a), 0.5 for (b), 0.3 for (c), and 0.4 for (d). Here data a point is acquired every 10^4. There is just one configuration in each curve. The other parameters are the same as in Fig. 2.

We can decouple the ladder into two isolated chains to understand the two extended states. According to Refs. [18] and [19] the equation (3) can be decoupled into the following equation by diagonalizing the matrix $\hat{\boldsymbol{M}}$

$$(E-\varepsilon_{l,i}^{,})\phi_{l,i}=t_0(\phi_{l+1,i}+\phi_{l-1,i}), \qquad (10)$$

where $\phi_{l,i}$ is the wave function at l location in ith decoupled chain, which is the linear combination of coupling atoms in the ladder. $\varepsilon'_{l,i}$ is the effective on-site potential at l location of the ith decoupled chain, which is the eigenvalue of the matrix $\hat{\boldsymbol{M}}$ as follows

$$\varepsilon'_{l,1(2)}=\frac{(\varepsilon_{l,1}+\varepsilon_{l,2})\pm\sqrt{(\varepsilon_{l,1}-\varepsilon_{l,2})^2+4t^2}}{2}. \qquad (11)$$

The effective on-site potentials of each decoupled chain are still dimeric because the coupling atoms between chains in the ladder are identical. The on-site potential of effective dimer atom is $\varepsilon_{\rm B}+t$ and the other is $\varepsilon_{\rm A}+t$ in one decoupled chain, while $\varepsilon_{\rm B}-t$ and $\varepsilon_{\rm A}-t$ in the other. The on-site potentials of each decoupled chain fit RDM. There is an extended state at $\varepsilon_{\rm B}+t$ with the conductance being $2e^2/h$ in one decoupled chain, and the other is at $\varepsilon_{\rm B}-t$ in the other decoupled chain. In fact the double-chain system and the two decoupled chains are the identical system in different representations. So the conductance of the ladder is still the sum of the conductance of the decoupled chains. The conductance at the extended state of RDM is always $2e^2/h$ in spite of the length being infinite or not, so the conductance at $\varepsilon_{\rm B}\pm t$ is never less than $2e^2/h$, which means that there are two extended states in the system. The two energies are just corresponding to the bond and anti-bond energy levels.

If the atoms A and B are both in pairs in each chain of the ladder, the two types of effective atoms are both dimers in each decoupled chain. There are two extended states in each decoupled chain, $\varepsilon_{\rm B}+t$ and $\varepsilon_{\rm A}+t$ for one decoupled chain, $\varepsilon_{\rm B}-t$ and $\varepsilon_{\rm A}-t$ for the other. Usually, there are four extended states in such system. If $\varepsilon_{\rm A}=-\varepsilon_{\rm B}=t$, one can find that there are only three extended states, which are $2t$, 0, and $-2t$, respectively. Sedrakyan *et al.* found a point of delocalization at the band centre in such system,[13] but they neglected the other delocalized states.

When the system is the ladder with pairing RD chains (as shown in Fig. 1(b)), we calculate the conductance with energy of electrons for different lengths of the pairing ladder in Fig. 4. It is found that when the length of the system increases up to 10^7 there appears a peak of conductance, which is in the middle of the potentials of atoms A and B.

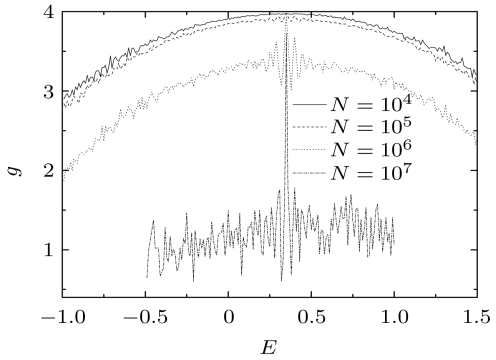


Fig. 4. The electron energy dependent conductance of a ladder with pairing RD chains. The other parameters are the same as those in Fig. 2.

In order to confirm whether the energy $0.35t_0$ is an extended state, we calculate the conductance with length at the energy and at others (in Fig. 5). When the energy is $0.35t_0$, the conductance decreases more slowly than the others (in Fig. 5). A special state with chiral symmetry exists in bipartite lattice, which is power law localized instead of exponential localized.[14] Such state is usually regarded as an extended state. The others are exponentially localized. The chiral symmetry exists in the system with pairing RD chains. The band centre is $(\varepsilon_{\rm A}+\varepsilon_{\rm B})/2$, $\varepsilon_{\rm A} = 0.4t_0$ and $\varepsilon_{\rm B} = 0.3t_0$, so the band centre is $0.35t_0$. According to Ref. [14] the state at $0.35t_0$ is the special state, which is power law localized. The results of calculations (in Figs. 4 and 5(b)) show that the state at $0.35t_0$ should be power law localized instead of exponentially localized. It can be regarded as an extended state.

The ladder with pairing RD chains can not be decoupled into two isolated chains. According to formula (11), when atom A is in the first chain and the coupling atom B is in the second chain, the effective on-site potential in one decoupled chain will be always $\varepsilon'_{l,1} = ((\varepsilon_{\rm A}+\varepsilon_{\rm B}) + \sqrt{(\varepsilon_{\rm A}-\varepsilon_{\rm B})^2+4t^2}\,)/2$, and that in another one will be always $\varepsilon'_{l,2} = ((\varepsilon_{\rm A}+\varepsilon_{\rm B}) - \sqrt{(\varepsilon_{\rm A}-\varepsilon_{\rm B})^2+4t^2}\,)/2$ if it could be decoupled. But the linear combinations $\phi_{l,1}$ are different for atom A and atom B in 1th chain of the ladder. For atom A $\boldsymbol{\phi}_{l,1} = \begin{pmatrix}\sqrt{b}\\ \sqrt{a}\end{pmatrix}$ and for atom B $\boldsymbol{\phi}_{l,1} = \begin{pmatrix}\sqrt{a}\\ \sqrt{b}\end{pmatrix}$. Here $a = ((\varepsilon_{\rm B}-\varepsilon_{\rm A}) + \sqrt{(\varepsilon_{\rm B}-\varepsilon_{\rm A})^2+4t^2}\,)/2$ and $b = ((\varepsilon_{\rm A}-\varepsilon_{\rm B}) + \sqrt{(\varepsilon_{\rm A}-\varepsilon_{\rm B})^2+4t^2}\,)/2$. For the ladder being decoupled into two isolated chains, linear combinations at every locations must be identical. As the linear combinations are different for atom A and atom B in one chain of the pairing ladder, the ladder can not be decoupled into two isolated chains. However, the ladder with identical chains can be decoupled into two isolated chains. Because they are the same atom in lth site of the ladder with identical chains, $a = b$, then $\boldsymbol{\phi}_{l,1} = \begin{pmatrix}1\\ 1\end{pmatrix}$ is the same in each site. Therefore, the ladder with identical RD chains can be decoupled into two isolated RD chains.

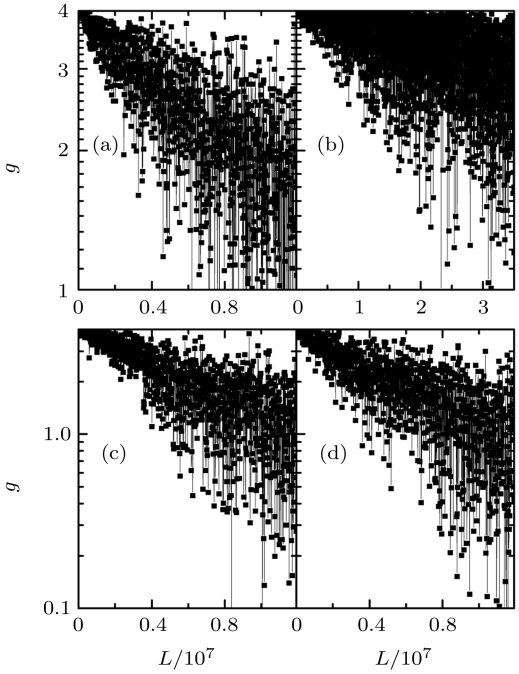


Fig. 5. The length dependent conductance of the ladder with pairing RD chains in energy of 0.3 for (a), 0.35 for (b), 0.4 for (c), and 0.5 for (d). The other parameters are the same as in Fig. 3.

4. Conclusion

We have investigated the transport properties of the ladder with two RD chains. It is shown that there are two extended states in the ladder with two identical RD chains and a critical state regarded as an extended state in the ladder with pairing RD chains because of the chiral symmetry. The former can be decoupled into two isolated RD chains and the latter can not. The analytical expressions of the extended states can be written as $E_{\rm ex} = \varepsilon_{\rm B} \pm t$ in the ladder with identical RD chains in which only atom B in pairs, and $E_{\rm ex} = \varepsilon_{\rm A} \pm t$ and $E_{ex} = \varepsilon_{\rm B} \pm t$ in the ladder with identical RD chains in which both atoms A and B in pairs. There is a critical state in the band centre of the ladder with pairing RD chains, which is power law localized and can be regarded as an extended state. The results may be useful to explain the transport properties of the polymers and DNA.

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