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Localization-delocalization transition in one-dimensional system with long-range correlated diagonal disorder

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Abstract. We show that the electronic states in a one-dimensional (1D) Anderson model of diagonal disorder with long-range correlation proposed by de Moura and Lyra exhibit localization-delocalization phase transition in varying the energy of electrons. Using transfer matrix method, we calculate the average resistivity $\bar{\rho}$ and investigate how it changes with the size of the system N. For given value of α (> 2) we find critical energies E_{c1} and E_{c2} such that the resistivity decreases with N as a power law $\bar{\rho} \propto N^{-\gamma}$ for electron energies within the range of $[E_{c1}, E_{c2}]$, and exponentially grows with N outside this range. Such behaviors persist in approaching the transition points and the exponent γ is in the range from 0.92 to 0.96. The origin of the delocalization in this 1D model is discussed.

PACS. 73.20.Jc Delocalization processes – 72.15.Rn Localization effects – 05.40.-a Fluctuation phenomena, random processes, noise, and Brownian motion

1 Introduction

Since Anderson broached the renowned model of disorder and proved the existence of localized states in 1958 [1], the field of disordered systems and Anderson localization has attracted long-time attention among both theoretical and experimental researchers, and experienced a tremendous development. The localization is a result of quantum interference among waves scattered by the disorder with its intensity larger than a critical value. In the case of localization the wave functions of particles are localized in a range of space with an exponentially decaying envelope. If the states at Fermi energy are localized, the system exhibits insulating behavior at zero temperature. Thus, a metal-insulator transition (MIT) can be induced by introducing the disorder that changes the states from extended to localized. From the scale theory [2] it is commonly believed that in systems of dimensions not greater than 2 there does not exist MIT characterized by mobility edges which separate the extended and localized states in energy, and all the states are localized by extremely weak disorder.

In recent decades several low-dimensional models with correlated disorder which may have extended states were proposed. A one-dimensional (1D) tight-binding (TB) random dimer model is discussed in references [3–5]. In this model the impurity sites appear in dimers and there exists a single resonant energy level of extended state. Similar resonant levels of extended states are also found in 1D models with short-range correlated disorder [6–8]. Moreover, the extended states can appear in a Cantor-set-like manner and form a dilute conduction band if the randomness with the short-range correlation is specially constructed in a quasi-1D system [9]. A continuous band of extended states is also found in a 2D partially disordered system [10]. More recently, attention has been paid to the role played by the long-range correlations of disorder. In a recent paper de Moura and Lyra proposed a 1D TB model with diagonal disorder exhibiting long-range correlation where the sequences of site energies have an approximate spectral density of the form $s(k) \propto 1/k^{\alpha}$ with $s(k)$ being the Fourier transformation of the two-point correlation function of site energies $\langle \epsilon_i \epsilon_j \rangle$ and k the inverse of the wavelength λ of the undulation on the site-energy landscape [11]. It was shown that the extended states can exist in a range of energy for $\alpha > 2$. Similar conclusions were drawn for 1D models with long-range correlated disorder by using different methods [12,13]. The transition from localization to delocalization is experimentally observed in a waveguide with correlated disorder [14].

It is interesting to answer whether it is a continuous transition or not, and what is the critical properties near the transition in such 1D systems. In this paper, we consider the 1D TB model with long-range correlated diagonal disorder proposed in reference [11]. Using transfer matrix method, we calculate the average resistivity and investigate how it changes with the size of the system N.

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For given value of α (> 2), there exist critical energies E_{c1} and E_{c2}. For energy in the range $[E_{c1}, E_{c2}]$, the average resistivity decreases as a power law $\bar{\rho} \propto N^{-\gamma}$ with increasing the system size N, while outside this energy range it exponentially grows with N. The exponent γ on the delocalization side is in the range 0.92–0.96, a little smaller than one, the value corresponding to the 1D ballistic system, and slightly increased when approaching to the transition point. We also discuss the origin of the delocalization in this model.

The paper is organized as follows: In the next section we describe the basic formalism in our calculations. In Section 3 we present the main results and their physical meaning. The last section is devoted to a brief summary of conclusions.

2 The basic formalism

The Hamiltonian of the 1D TB model is written as [11]

$$H = \sum_n \epsilon_n |n\rangle\langle n| + \sum_n t_0(|n\rangle\langle n-1| + |n\rangle\langle n+1|) \quad (1)$$

where ϵ_n is the energy level at site n, $|n\rangle$ is the corresponding Wannier function, and t_0 is the nearest-neighbor hopping amplitude. We will set energy units as $t_0 = 1$ throughout this paper. In this model the site energies ϵ_n ($n = 1, 2, \ldots, N$ with N being the total number of sites) are in a sequence, for which the Fourier transformation $s(k) \propto 1/k^\alpha$. For $\alpha = 0$, one obtains the traditional Anderson model with δ-correlated disorder $\langle \epsilon_n \epsilon_{n'} \rangle = \langle {\epsilon_n}^2 \rangle \delta_{n,n'}$. The power-law spectral density is imposed by constructing the site energies following the relation

$$\epsilon_i = \sum_{k=1}^{N/2} \left[k^{-\alpha} \left| \frac{2\pi}{N} \right|^{1-\alpha} \right]^{\frac{1}{2}} \cos\left(\frac{2\pi \mathrm{i} k}{N} + \phi_k \right), \quad (2)$$

where ϕ_k are $\frac{N}{2}$ independent random phases uniformly distributed in the interval $[0, 2\pi]$. Then this energy sequence is normalized to have zero mean $\langle \epsilon_n \rangle = 0$ and unity variance $\Delta\epsilon = \sqrt{\langle \epsilon^2 \rangle - \langle \epsilon \rangle^2} = 1$. The normalization factor is size dependent so that the distribution of site energies and the band widths are kept fixed in changing the size [15].

To investigate the properties of the one-electron states of the above model, we adopt the transfer matrix method to calculate the average resistivity [16] for systems with different sizes. A state $|\psi\rangle$ with energy E can be expressed as a linear combination of site orbitals

$$|\psi\rangle = \sum_{n=1}^{N} \mu_n |n\rangle, \quad (3)$$

where coefficients μ_n obey the Schrödinger equations

$$\epsilon_n \mu_n + \mu_{n-1} + \mu_{n+1} = E \mu_n. \quad (4)$$

Equation (4) can be rewritten as

$$\mu_{n+1} = E - \epsilon_n \mu_n - \mu_{n-1} \quad (5)$$

from which one has

$$\begin{pmatrix} \mu_{N+1} \\ \mu_N \end{pmatrix} = \hat{T}_N \begin{pmatrix} \mu_1 \\ \mu_0 \end{pmatrix} \quad (6)$$

with $\hat{T}_N$ being a 2×2 transfer matrix defined as

$$\hat{T}_N = \prod_{n=1}^{N} \begin{pmatrix} E - \epsilon_n & -1 \\ 1 & 0 \end{pmatrix}.$$

If the left and right ends of the system are connected to two semi-infinite perfect chains serving as leads, the coefficients of the wave function in the leads ($n < 1$ and $n > N$) can be expressed as those of plane waves. When a particle is injected into the system from the left lead with unit amplitude, it can be transmitted into the right with amplitude t_N, or be reflected to the left with amplitude r_N. Thus, we have

$$\mu_n = \begin{cases} \exp(\mathrm{i}k_n) + r_N \exp(-\mathrm{i}k_n), & n \le 1, \\ t_N \exp(\mathrm{i}k_n), & n \ge N. \end{cases} \quad (7)$$

The dimensionless resistance $R(E, N)$ of the system can be calculated by the Landauer formula:

$$R(E, N) = \frac{|r_N|^2}{|t_N|^2}. \quad (8)$$

From the transfer matrix we can solve amplitudes t_N and r_N, from which the resistance can be expressed by an element of the transfer matrix

$$R(E, N) = |\left(\hat{T}_N\right)_{12}|^2. \quad (9)$$

In order to distinguish the delocalized and localized states, we use the average resistivity defined as [16]

$$\bar{\rho}(E, N) = \frac{1}{N} \sum_{i=1}^{N} R(E, i)/i. \quad (10)$$

For a delocalized state, the reflection coefficient is smaller than unity, so $R(E, i)$ is always finite and $R(E, i)/i \to 0$ when $i \to \infty$. As a result, $\bar{\rho}(E, N) \to 0$ when $N \to \infty$. On the contrary, for the localized states $\bar{\rho}(E, N)$ is non-zero at the thermodynamical limit because $\lim_{N\to\infty} |t_N|^2 = 0$. Thus, we can use this quantity as the order parameter to investigate the transition. It is interesting to see whether $\bar{\rho}(E, N \to \infty)$ continuously goes to zero from localized to delocalized states.

3 Numerical results

In this section we present our numerical results obtained by using the above method. We can perform calculations for systems with sizes up to 100 times larger than those

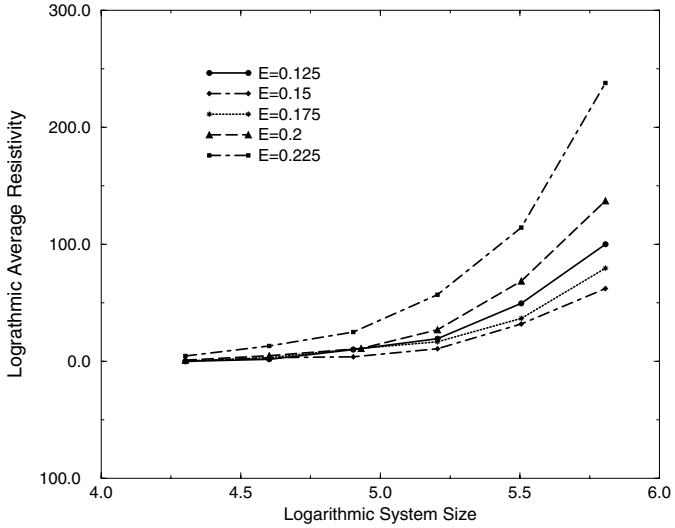

Fig. 1. Logarithmic average resistivity ($\log_{10}\bar{\rho}$) as a function of $\log_{10} N$ for various energies. Here $\alpha = 1.9$. The energy units are the hopping integral t_0.

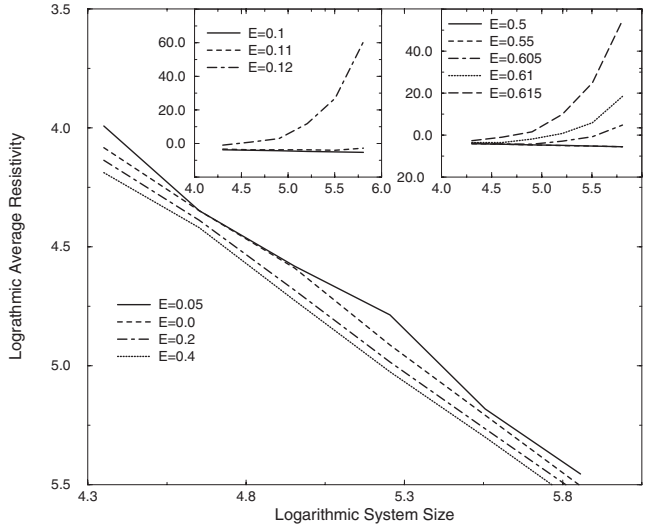

Fig. 2. Logarithmic average resistivity as a function of $\log_{10} N$ for various energies in the case $\alpha = 2.5$. Curves for $E \geq 0.5$ and $E \leq -0.1$ are shown in the insets.

adopted in reference [11], so we can carry out the scaling analysis more effectively.

In Figure 1 we plot the logarithmic average resistivity as a function of the energy for various system sizes in the case $\alpha = 1.9$. It can be seen that $\bar{\rho}(E, N)$ rapidly increases with increasing the system size in the whole investigated energy range. Thus, we can conclude that in this case the resistivity goes to infinity at the thermodynamical limit and the states are localized. Since α characterizes the strength of the correlation of the disorder, the results in Figure 1 show that the states are localized if the correlation is not strong enough, in consistence with the other investigations.

The calculated results for $\alpha = 2.5$ are displayed in Figure 2. The remarkable feature is the existence of an energy interval $E_{c1} < E < E_{c2}$ with $E_{c1} = -0.1$ and $E_{c2} = 0.6$ where $\bar{\rho}(E, N)$ decreases with increasing N. This means that in this energy range the states are extended at the thermodynamical limit, and E_{c1} and E_{c2} are the transition points which separate the extended and localized regimes. Moreover, the transition is very sharp and the order parameter $\bar{\rho}$ is discontinuous at the transition points. This discontinuity becomes more pronounced with increasing the size. If the system size is not large enough, *e.g.*, $N \sim 5000$, the curves seem much more smooth. This implies that the discontinuity behavior of the transition can only be seen in numerical calculations with quite large system sizes.

In order to perform further scaling analysis, in Figure 3 we show the dependence of $\bar{\rho}$ on the size N for both extended and localized states with different α. We can see that for the extended states $\bar{\rho}$ exhibits a power-law dependence on N $\bar{\rho} \propto N^{-\gamma}$ with exponent $\gamma \sim 0.95$, except fluctuations for $\alpha = 2.1$ near the transition point. For the localized states, on the contrary, $\bar{\rho}$ exponentially grows with increase of N, $\bar{\rho} \propto \exp(\beta N)$, as can be seen in the inset. Following these scaling behaviors the order parameter $\bar{\rho}$ and its inverse are obviously discontinuous at the transition points.

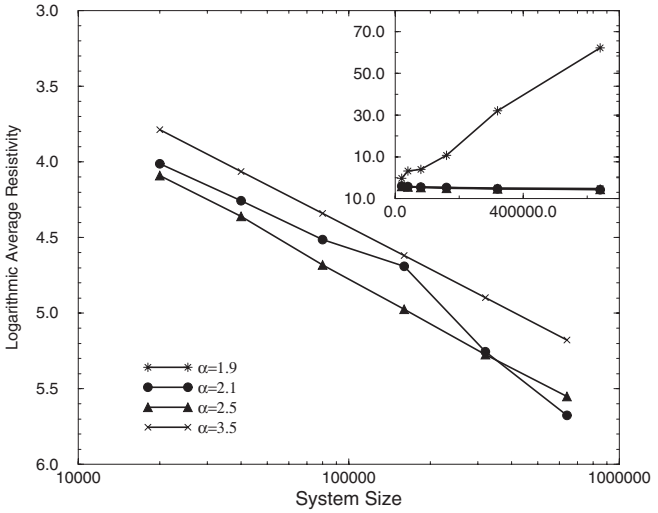

Fig. 3. Logarithmic average resistivity as a function of the system size for different values of α. The energy $E = 0.15$. The curves for the extended states ($\alpha = 2.1$, 2.5, 3.5) are shown in the main panel, where the system size is in logarithmic scale. The curve for localized state ($\alpha = 1.9$) is displayed in the inset, where the system size is in linear scale.

In Figure 4 we plot the scaling behavior of $\bar{\rho}$ for states with energies near the transition point E_{c1} for $\alpha = 3.5$. E_{c1} is numerically determined to be -0.337 ± 0.005. More precise power-law dependence is seen for all the investigated states on the delocalization side. The values of exponent γ and its errors estimated from the fitting is given in Table 1. It can be seen that γ is in the range of 0.92–0.96 and slightly increased with approaching to the transition point. In the inset of Figure 4 it is also shown that on the localization side the average resistivity exponentially

Table 1. The values and errors of exponent γ estimated from the fitting of the numerical data of $\bar{\rho}$ for the delocalized states in the case $\alpha = 3.5$.

E	-0.1	-0.15	-0.2	-0.25	-0.3	-0.325	-0.33	-0.335
γ	0.925	0.926	0.927	0.928	0.932	0.937	0.937	0.96
error	0.002	0.002	0.002	0.002	0.001	0.002	0.004	0.02

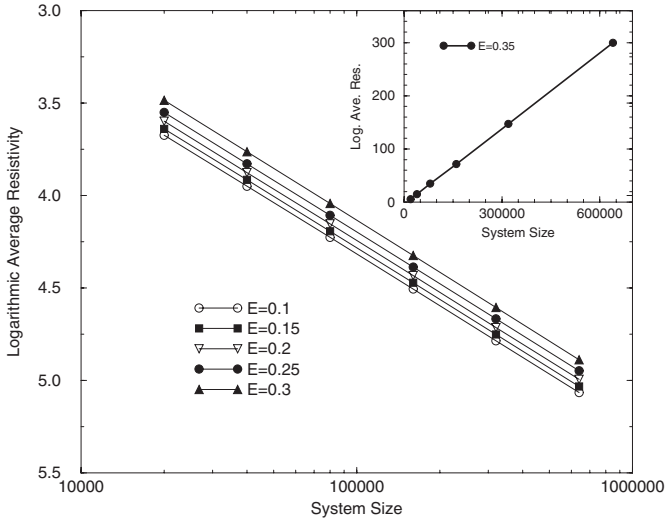

Fig. 4. The same as Figure 3 but for different energies near the transition point E_{c1}. $\alpha = 3.5$.

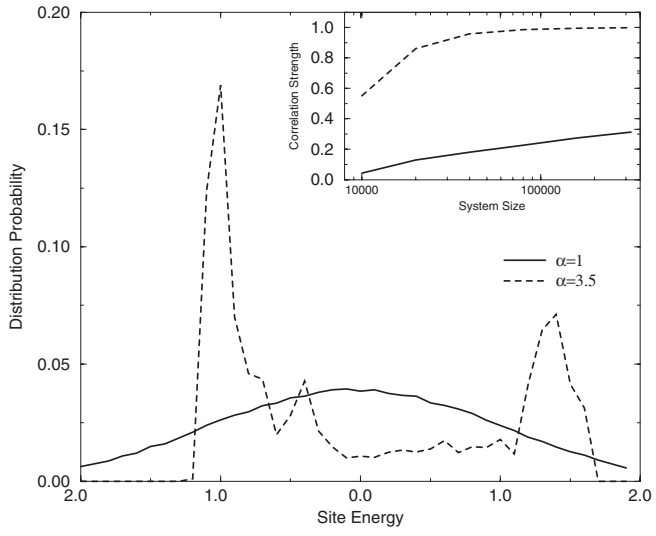

Fig. 5. The site-energy distribution of the model in cases $\alpha = 1$ and $\alpha = 3.5$. The curves for different sizes coincide with each other. Inset: the correlation strength at fixed distance $l = 1000$ as a function of the system size for $\alpha = 1$ and $\alpha = 3.5$.

grows with the size for a state near the transition point. This further confirms the discontinuity of the transition.

It was commented that the origin of the delocalization in this model is in the size-dependent features of the disorder [17]. In Figure 5 we plot the distribution probabilities of the site energies for the cases $\alpha = 1$ and $\alpha = 3.5$. They

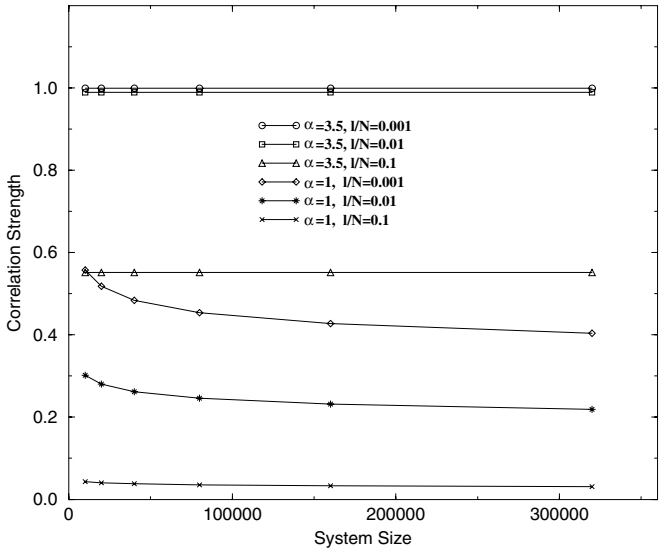

Fig. 6. The correlation strength at various reduced distances l/N as a function of the system size for $\alpha = 1$ and $\alpha = 3.5$.

are almost size independent due to the normalization procedure [15]. The shapes of the probabilities are quite different for $\alpha = 1$ and $\alpha = 3.5$, the former is Gaussian-like, and the latter has two peaks at the ends. Since $\alpha = 1$ corresponds to the localization and $\alpha = 3.5$ is for the case of delocalization, one may argue that this difference in the site-energy distribution may provide partial origin of the delocalization. However, the independence of this distribution on the system size is only from the viewpoint of the uncorrelated disorder. If we look at the correlation strength of the disorder defined as $S(l) = \langle \epsilon_{i+l}\epsilon_i \rangle - \langle \epsilon_{i+l} \rangle \langle \epsilon_i \rangle$ at a given distance l, it is really size-dependent for both $\alpha = 1$ and $\alpha = 3.5$, as shown in the inset of Figure 5. In the case $\alpha = 3.5$ the correlation strength grows more rapidly with increasing the system size, and then saturates to its maximum value (~ 1). This implies that the existence of the delocalized states in the case of larger α is related to the size dependence of the correlation in disorder. To explore this more clearly, in Figure 6 we plot the size dependence of the correlation strength at given reduced distance l/N. In this calculation the distance l in the correlation is proportional to the size to keep l/N constant. As shown in Figure 6, under this definition the correlation strength is size-independent for $\alpha = 3.5$, and is reduced with increasing N in the case $\alpha = 1$. This indicates that in the scaling transformation the reduced correlation length, defined as l/N at which the correlation has

a constant strength, is invariant for $\alpha = 3.5$, but decreased with increasing N for $\alpha = 1$. From this we can conclude that the origin of the existence of the delocalized states is just in the scaling invariance of the reduced correlation length that, together with the scaling invariance of the site-energy distribution, keeps the effective strength of the disorder in the reduced landscape (with all the distances divided by N) unchanged in the scaling transformation.

4 Conclusions

We show that the electronic states in a one-dimensional Anderson model of diagonal disorder with long-range correlation proposed by de Moura and Lyra exhibit localization-delocalization phase transition in varying the energy of electrons. In this system the sequences of site energies have an approximate spectral density of the form $s(k) \propto 1/k^{\alpha}$. Using transfer matrix method, we calculate the average resistivity and investigate how it changes with the size of the system N. For given value of α (> 2) we find critical energies E_{c1} and E_{c2} which separate the extended and localized regimes. In the extended regime, the average resistivity exhibits a power-law dependence on the system size, $\bar{\rho} \propto N^{-\gamma}$, with exponent $\gamma \sim 0.96$ independent of the energy and α. On the contrary, in the localized regime $\bar{\rho}$ exponentially grows with N as can be expected from the envelopes of localized states. Since these behaviors persist in approaching the transition points, both $\bar{\rho}$ and its inverse are discontinuous in the transition at the thermodynamical limit. As γ is smaller than 1 but very near 1, the extended states are not completely ballistic but behave like the ballistic ones. From the scaling analysis of the site-energy distribution and the correlation strength of the disorder we conclude that the existence of the delocalized states stems from the scaling invariance of the reduced correlation length.

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