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Localization in the Anderson model with long-range correlated hopping and on-site disorders

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We study the metal–insulator transition in one-dimensional Anderson binary alloy with long-range disordered hopping integrals and on-site energies using the transfer matrix method. In this model, the on-site energies and hopping integrals are distributed randomly with long-range correlations characterized by power spectrum of the type $S(k) \propto 1/k^{(2\alpha-1)}$, with different exponents α_ε and α_t, respectively. We determine the critical value of long-range correlation exponent of hopping integral α_{t_c} in the presence of only off-diagonal disorder in which the transition from localized to extended states occurs in thermodynamic limit. When both of the on-site energies and hopping integrals are disordered, there are two parameters α_t and α_ε that control the metal–insulator transition in the system. We draw the phase diagram which separates the localized regime from extended one and it shows the critical values of α_t for a given value of α_ε.

1. Introduction

In a pure periodic system, the electronic eigenstates are extended.[1] Disorder originating from lattice imperfections drastically modifies the nature of the single electron eigenstates.[2] In a one-dimensional disordered system, Anderson localization is known to occur at any energy in thermodynamic limit when the disorder is uncorrelated and has white noise structure.[2,3] The interest for one-dimensional disordered models with correlated disorder has been started since 1990. It is found that spatial correlation of disorder can unexpectedly create extended states at some energies. For instance, if one introduces particular short-range correlations to the on-site disordered energies, e.g. in the random dimer model,[4] delocalization of a subset of the eigenstates can appear.

These observations attracted a great attention to investigate the existence of Metal–Insulator Transition (MIT) in low-dimensional disordered systems in the presence of correlated, especially *long-range* disorder.[5] Experimental evidence of delocalization caused by such short-range correlations has been found in semiconductor superlattices.[6] In this direction, De Moura and Lyra [7,8] considered the discrete Anderson model in which the diagonal energies of the hamiltonian were generated by considering the potential as the trace

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of a fractional Brownian motion and they imposed a normalization condition that kept fixed the variance of potentials for all system sizes (see also [9,10]). They showed how long-range correlated sequences of on-site energies could result in a continuum of extended states (see also [11,12]). Long-range correlations also affect the level statistics of the system, which can also experience a transition from Poissonian to non-Poissonian distribution.[13]

Several stochastic processes in nature are known to generate long-range correlated random sequences which have no characteristic scale, for example, in the nucleotide sequence of DNA molecules.[14] The relevance of the underlying long-range correlations for the electronic transport in DNA was firstly pointed out in [15], and then other researchers have confirmed this observation.[16,17] Indeed in DNA, the short- and long-range correlations between base pairs provide valuable information to distinguish between almost random distributions, and more complex sequences, whose long-range correlations might also be associated with some biological properties.[14,18–25] Furthermore, the variation of the temperature in the DNA induces structural disorder, and randomizes local hopping integral between the base pairs. Noting to the fact that timescale of charge transfer process is much faster than timescale of thermal fluctuations, then the disorder in hopping integral looks like a quenched disorder. A binary model used here, is the simplest model to approach this problem in the presence of randomness in hopping integrals and on-site energies for a quasi one-dimensional systems.

Analytically, to understand the effect of long-range correlations of the disorder on the MIT phase transition, Izrailev and Krokhin [26] derived perturbatively a relationship between localization length and two points correlation of potential. They showed how specific disorder with long-range correlations leads to the appearance of mobility edges in one-dimensional discrete models. An experimental confirmation of these findings was obtained by studying the transmission of microwaves in a single-mode waveguide with a random array of correlated scatterers.[27] In addition, there have been several theoretical and numerical studies of these problems in various systems.[28–47]

In this paper, we study one-dimensional Anderson model with long-range correlated quenched disorder chosen as a binary model. In this model, with some probability, both of the on-site energies and hopping integrals can have just two different values, for seeking simplicity. We create long-range correlated binary models by generating a correlated sequence of on-site energies and hopping integrals continuously distributed, which are mapped into two different values. At first, we turn off the on-site disorder and calculate the localization length of off-diagonal long-range correlated disordered system and show that there is a critical value of correlation exponent in which the metal–insulator transition occurs in the thermodynamic limit. When both of the on-site energies and hopping integrals fluctuate around their mean values, the two parameters α_t and α_v identify the phase diagram of the system. We plot a critical curve which separates the localized phase from extended one in the two-dimensional phase space.

2. Model and method

We consider noninteracting electrons in one-dimensional disordered system within a nearest-neighbor tight-binding formalism. In this model, we consider a single electron on a lattice with N sites described by the following Hamiltonian [13]:

$$H = \sum_{i \neq j}^{N} t_{ij} |i\rangle\langle j| + \sum_{i}^{N} \varepsilon_i |i\rangle\langle i|, \tag{1}$$

where $|i\rangle$ denotes the Wannier state at site i. The Schrödinger equation projected on site i becomes

$$\varepsilon_i \psi_i + t_{i,i+1}\psi_{i+1} + t_{i-1,i}\psi_{i-1} = E\psi_i \tag{2}$$

where E is the energy of the incoming electron. The norm $|\psi_\mathbf{i}|^2$ is the probability of finding an electron at site i, ε_i is the potential at site i and $t_{i-1,i} = t_{i,i+1}$ represents the hopping element connecting the ith to the $(i-1)$th site.

In this work, the disorder is applied both on the on-site energies $\{\varepsilon_i\}$ and the hopping terms $\{t_{i-1,i}\}$. A binary disorder is introduced for the on-site energies and the hopping terms. Therefore, two potential energies are possible in any site, for instance: $\varepsilon_i = +0.1$ and -0.1 (with zero mean) and hopping terms between nearest sites will be $t_{i-1,i} = 0.9$ and 1.1 (with unit mean).

The Equation (2) can be easily expressed using the conventional transfer matrix method as the following recursive matrix form [48]:

$$\begin{pmatrix} \psi_{i+1} \\ \psi_i \end{pmatrix} = \begin{pmatrix} t_{i,i+1}^{-1}(E - \varepsilon_i) & -t_{i,i+1}^{-1}t_{i-1,i} \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \psi_i \\ \psi_{i-1} \end{pmatrix}. \tag{3}$$

The wave functions of the two ends can be related together by calculating a product of matrices as $P_{N,1} = \prod_{i=1}^{N} P_{i,i-1}$. In this equation, $N = L/a$ where L is the sample size, a is the lattice constant and $P_{i,i-1}$ is the transfer matrix which connects the wave functions of sites i and $i-1$ as follows:

$$P_{i,i-1} = \begin{pmatrix} t_{i,i+1}^{-1}(E - \varepsilon_i) & -t_{i,i+1}^{-1}t_{i-1,i} \\ 1 & 0 \end{pmatrix}. \tag{4}$$

According to the component of this matrix, the Lyapunov Exponent is defined as:

$$\gamma = \lim_{N\to\infty} \frac{1}{N} < \ln \parallel P_{N,1} \parallel > . \tag{5}$$

The localization length corresponds to the inverse of Lyapunov Exponent ($\xi \propto 1/\gamma$).

Now, let us study the localization properties of the binary model with long-range correlated disorder. Thus, we need to first generate long-range correlated sequences of site energies and hopping integrals. A sequence of long-range correlated sequence is produced by the Fourier filtering method.[49] This method is based on a transformation of the Fourier components $\{u_k\}$ of a random number sequence $\{u_i\}$, which is uncorrelated random number with a Gaussian distribution. A sequence of $\{\eta_k\}$ is generated for a given α using the relation: $\eta_k = k^{-(2\alpha-1)/2}u_k$. Inverse Fourier transformation of sequence $\{\eta_k\}$ leads to the sequence of interest $\{\eta_i\}$. The resulting sequence of data is spatially correlated with spectral density

$$S(k) \propto k^{-(2\alpha-1)} \tag{6}$$

and the constructed data follow a Gaussian distribution. The exponent α is called correlation exponent, and it quantifies the degree of correlation imposed in the system. Now the sequences of $\{\varepsilon_i\}$ and $\{t_i\}$ in the binary alloy are produced by applying a map on the correlated sequences $\{\eta_i\}$. Every positive and negative values of $\{\eta_i\}$ are mapped into $\varepsilon_i = +0.1$ and $\varepsilon_i = -0.1$, respectively. In the same way, for generating the set of hopping integrals $\{t_i\}$,

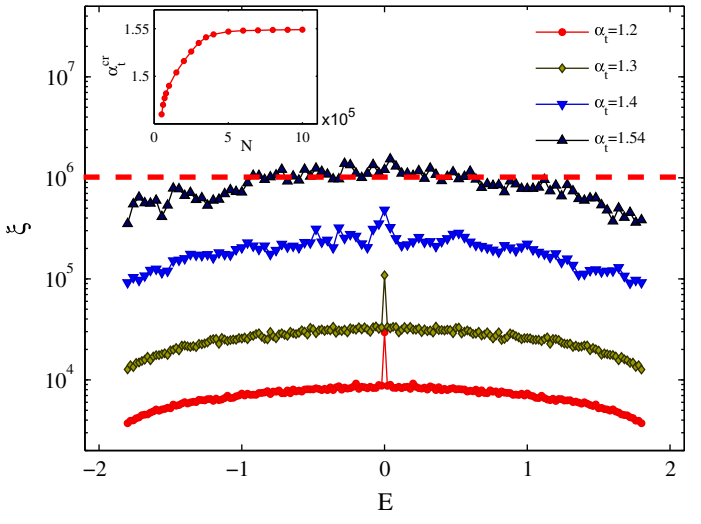

Figure 1. Localization length of off-diagonal correlated disordered as a function of electron energy for different values of correlation exponents. The system size is fixed to $N = 10^6$. The averages are obtained using 5000 realizations of randomness. Inset shows the critical value of off-diagonal correlation exponent as a function of system size N.

we map every positive and negative values of $\{\eta_i\}$ into $t_i = 0.9$ and $t_i = 1.1$, respectively. Such a mapping of course can change the correlation properties of the series; and therefore, the correlations are not properly quantified by the power-law exponents as the original correlated series. To quantify the correlations in the final binary sequence, we calculate the scaling exponent α using detrended fluctuation analysis, which is one of the most widely used method to quantify long-range correlations.[50–52] We note that the exponent $\alpha = 0.5$ corresponds to uncorrelated disorder (white noise), while the case $\alpha > 0.5$ indicates positive correlations. Once the sequence of numbers is generated, we normalize them so that the mean value $\langle \eta_i \rangle$ is set to zero, and the variance is set to unity. This choice is maintained in all the numerical calculations in this paper.

3. Numerical results

In the numerical calculations, the localization properties and the possibility of the existence of a phase transition from localized to extended states are investigated in the band center. For a given system size N, there are two parameters which control the localization length of the system, the on-site potential correlation exponent α_ε and the hopping integrals correlation exponent α_t. In all the cases considered below, we calculate the localization length ξ as a function of energy E for the finite system size N and for different values of the correlation exponents imposed in the system. When the localization length starts to be greater than the system size $\xi \geq N$, we say that a transition from localized states (insulator) to extended states (metal) is observed for the finite system size. The α value at which the transition is detected for a fixed N is called $\alpha_c(N)$.

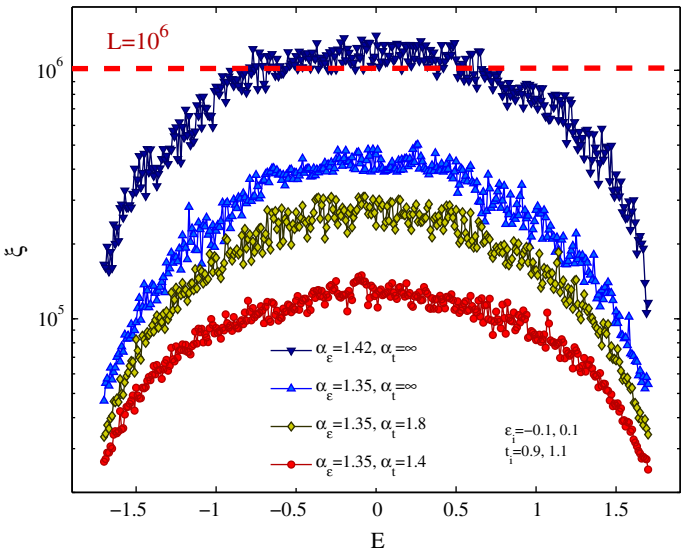

Figure 2. Localization length of the system as a function of energy for different values of on-site and hopping correlation exponents. The size of the system is fixed to $N = 10^6$. The averages are obtained using 10,000 realizations.

Let us first turn off the disorder in on-site energies. Figure 1 shows the localization length of the system with size $N = 10^6$ as a function of the energy E for different values of α_t. In this figure, the on-site energies have the same values and fixed to $\varepsilon_i = 0$. So only the off diagonal disorder is imposed in the system with different correlation exponents. As shown in this figure, the localization length increases with increasing the correlation exponent α_t and the metal–insulator transition occurs for $\alpha_t^{cr} \simeq 1.54$.

In order to find the critical value of the correlation exponent hopping integrals α_t^{cr} in thermodynamic limit, we plot α_t^{cr} as a function of system size N in the inset of Figure 1. According to this figure, the higher size of system needs the larger correlation exponent α_t^{cr} to experience a phase transition. Also, as shown in this figure, α_t^{cr} has an asymptotic value at large N and converge to $\lim_{N\to\infty} \alpha_t^{cr} \approx 1.58$. Similar result has been found for critical exponent of on-site energies correlation (with ordered hoping integrals) in [15], where the exponent converges to $\lim_{N\to\infty} \alpha_\varepsilon^{cr} = 1.45$ in the thermodynamic limit.

Up to now, we have described the transition from localized to extended states in the presence of long-range correlated off-diagonal disorder in the system. When also the diagonal disorders are turned on, we observe that the localization length decreases and the transition from extended states to localized states occurs; therefore, the system will be an insulator as shown in Figure 2. Figure 2 shows that, for example, with $\alpha_t (= 1.8) > \alpha_t^{cr} (\approx 1.58)$ and for $\alpha_\varepsilon = 1.35$, where all the stats are localized. Also, for a fixed α_t, localization length increases with increasing α_ε and vice versa. Therefore, there are two parameters α_t and α_ε that control the metal–insulator transition in the system.

In Figure 3, we plot the critical values of α_t as a function of α_ε. As shown in this figure, there is a critical curve which separates the localized regime from extended one. For all of the calculations in this figure, the average of the localization length is obtained in the

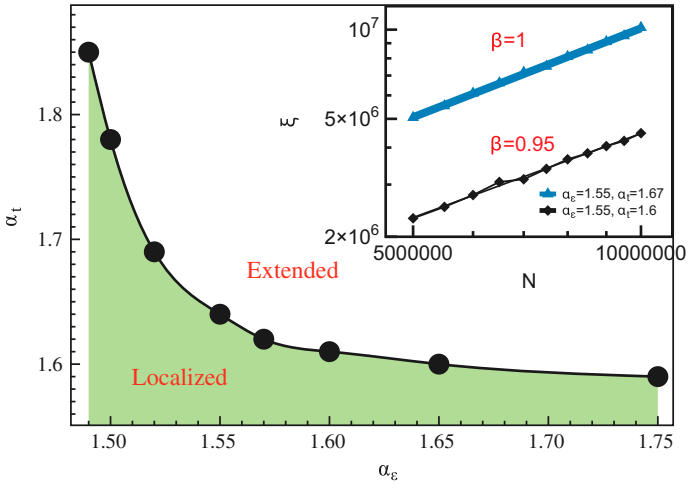

Figure 3. Phase diagram separating localized from extended states is shown in terms of the hopping integral correlation exponents α_t and on-site correlation exponents α_ε. The system size set to $N = 5 \times 10^6$. The inset shows the finite size scaling of localization length with system size N. For extended states, the localization length scales with system size as $\xi(E \in \text{extended} - \text{states}) \sim N$.

energy region $-\Delta \leq E \leq \Delta$ with finite and small Δ (with $\Delta = 0.1$) and for the system size $N = 5 \times 10^6$.

Finally, we would like to point out that the phase transition condition should be generally defined as $\xi \propto N^\beta$, where $\beta = 1$ and $\beta < 1$ correspond to extended and localized states, respectively. Therefore, we guarantee that in the thermodynamic limit, the localization length diverges with system size. As shown in the inset of Figure 3, we plot the localization length of the system as a function of N for two distinct points in phase space, i.e. $\alpha_\epsilon = 1.55$ and $\alpha_t = 1.62$, within the extended and localized regions as shown in the phase diagram. In the case of $\alpha_\epsilon = 1.55$ and $\alpha_t = 1.6$, the point inside the localized phase, we find $\beta \approx 0.95 < 1$. However, for $\alpha_\epsilon = 1.55$ and $\alpha_t = 1.67$, the point inside the extended phase, we find $\beta \approx 1$. Consequently, the finite size scaling confirm the extended nature of exponents belong to the extended area in phase space.

We note that the phase diagram can change with the values of on-site energies ε_i and hopping terms between nearest sites $t_{i-1,i}$. The general rule is that, for higher values of binary difference (which we have chosen $\Delta\varepsilon_i = 0.2$ and $\Delta t_i = 0.2$), one needs to have larger values for the exponents. In other words, to have higher probability to cross the barriers with $\Delta\varepsilon_i$ in on-site energies and Δt_i in hopping integral, the lager exponents that are more correlated are needed.

4. Conclusion

In summary, we have studied a one-dimensional Anderson model with long-range correlated disorder when disorder has been imposed in hopping integrals and on-site energies. The model is a binary alloy in which on-site energies and nearest sites hopping integrals are mapped into two values. The localization length of this system increases with increasing

the correlation exponents of both on-site and hopping integrals. We show that there is a metal–insulator transition when the correlation exponent increases, and there is a phase diagram which separates the localized regime from the extended one in terms of the two correlation exponents of the system.

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