Electronic properties of one-dimensional systems with long-range correlated binary potentials*

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We study numerically the electronic properties of one-dimensional systems with long-range correlated binary potentials. The potentials are mapped from binary sequences with a power-law power spectrum over the entire frequency range, which is characterized by correlation exponent β. We find the localization length ξ increases with β. At system sizes $N \to \infty$, there are no extended states. However, there exists a transition at a threshold β_c. When $\beta > \beta_c$, we obtain $\xi > 0$. On the other hand, at finite system sizes, $\xi \geq N$ may happen at certain β, which makes the system "metallic", and the upper-bound system size $N^*(\beta)$ is given.

Keywords: electronic properties, long-range correlation, binary potentials, localization

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1. Introduction

The localization properties of disordered non-interacting electrons have been considered for more than fifty years.[1−4] For a long time, electronic properties (EPs) in systems, where the spatial correlation of disordered potentials remains unchanged, have been studied extensively, such as in the Anderson model,[1] the Harper model,[5−7] the random dimer model,[8] the Fibonacci model,[9] and the Thue–Morse model.[10] The electron properties in these models are mainly affected by the degree of potential strengths[1,5−7] or by the specific spatial correlation of disorder.[8−10]

Recently, electron properties in systems where the spatial correlation of disordered potentials changes with model parameters have attracted much attention.[11−20] The correlations of disordered potentials are comparable to the distance of the entire space, which can be characterized by a power-law power spectrum, $S(f) \propto 1/f^{\alpha}$, where α reflects the degree of correlation and changes with the model parameters. These potentials are called long-range correlated (LRC) random potentials. The value of potentials may be either continuous[11−16] or discrete.[17−20] For systems with continuous LRC random potentials, it is found that there exists a continuum of extended states[11−13,15,16] when α is greater than a certain value, i.e., Anderson-like metal–insulator transitions happen in these systems. However, for systems with discrete LRC random potentials, even for the simplest case, i.e., binary potentials (BPs), electron properties are not yet well understood today.[17−20]

In this article, we study numerically the electron properties in one-dimensional (1D) systems with LRC binary potentials. We find that the localization length ξ increases with β. At system sizes $N \to \infty$, there are no extended states and there exists a transition at a threshold correlation exponent β_c. On the other hand, at finite system sizes, there is an upper-bound $N^*(\beta)$, and the systems are "metallic" when $N \leq N^*(\beta)$.

2. Model

We consider single-particle electronic wave functions in the tight-binding approximation. In this approximation, the Schrödinger equation is written as

$$V_n\psi_n + t\psi_{n-1} + t\psi_{n+1} = E\psi_n, \tag{1}$$

where V_n is the on-site potential, t is a nearest-neighbour hopping integral, E is the eigenenergy and ψ_n is the wave function amplitude at the n-th site. We

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study LRC binary models of disordered alloys in 1D space, where there are two types of atoms, A and B, with $V_n = V_{\rm A}$ and $V_{\rm B}$, respectively. The arrangement of A and B atoms is based on LRC binary sequences $\{\varepsilon_n\}$, where $\varepsilon_n = 0$ or 1.

Below, we will introduce the method for generating 1D LRC binary sequences $\{\varepsilon_n\}$.[21] The algorithm consists of the following steps:

(i) Generate an uncorrelated 1D random sequence $\{u_n\}|_{n=1,2,...,N}$ for a Gaussian distribution with mean zero and variance 1.

(ii) Obtain the Fourier transform coefficients $\{u_f\}$ of the sequence $\{u_n\}$ using the fast Fourier transform (FFT).

(iii) Obtain a new sequence $\{\xi_f\}$ by $\xi_f = |f|^{-\beta/2}u_f$ for $1 < f < N/2$, and $\xi_f = |N-f|^{-\beta/2}u_f$ for $f > N/2$. If $f = 0$ or $f = N/2$, we set $\xi_f = 0$. Note that the parameter β can be preset.

(iv) Construct a new continuous random sequence $\{\xi_n\}$ from the sequence $\{\xi_f\}$ using the inverse FFT.

(v) Generate a binary sequence $\{\varepsilon_n\}$ from the sequence $\{\xi_n\}$ by the following coarse-grained rule

$$\varepsilon_n = \begin{cases} 1 & \text{if } E_n = \xi_{n+1} - \xi_n \geq 0, \\ 0 & \text{if } E_n = \xi_{n+1} - \xi_n < 0. \end{cases} \tag{2}$$

In the above algorithm, the (i)–(iv) steps are the standard method of the FFM to generate a continuous sequence $\{\xi_n\}$, and the step (v) is proposed in Ref. [22] to obtain binary sequences.

The power spectrum for the sequences is $S(f) = \langle (1/N)|\sum_{n=0}^{N-1} \varepsilon_n \, {\rm e}^{-{\rm i}2\pi(f/N)n}|^2 \rangle$, where $\langle \cdots \rangle$ denotes the average over disorder realizations based on different random sequence $\{u_m\}$ and $f = 0, 1, ..., N-1$. We plot the typical binary sequences and the corresponding $S(f)$ for one realization in Figs. 1(a) and 1(b), respectively. This shows $S(f) \propto 1/f^{\alpha}$ over the entire frequency f range, where α depends on β. We find that $S(f) \propto 1/f^{\alpha}$ is satisfied even for very small N. We have numerically given the relation between α and β[21]

$$\alpha = \begin{cases} 0.9288\beta - 1.8643 \text{ when } \beta \in [2.000, 3.082], \\ 0.5301\beta - 0.6356 \text{ when } \beta \in [3.082, 4.924], \\ 0.0354\beta + 1.8000 \text{ when } \beta \in [4.924, 6.000]. \end{cases} \tag{3}$$

The relation is visually shown in Fig. 1(c). We find there are three β regions, which correspond to $\alpha \in [0.0, 1.0]$, $\in [1.0, 2.0)$ and α are saturated to 2.0.

We use the map: $\varepsilon_n = 0 \mapsto$ A atom and $\varepsilon_n = 1 \mapsto$ B atom. Similar to that in Ref. [17], we choose the binary potentials $V_{\rm A} = -V_{\rm B} = 0.5t$. In this situation, there is a strong localization for electronic states in the case of pure disorder.

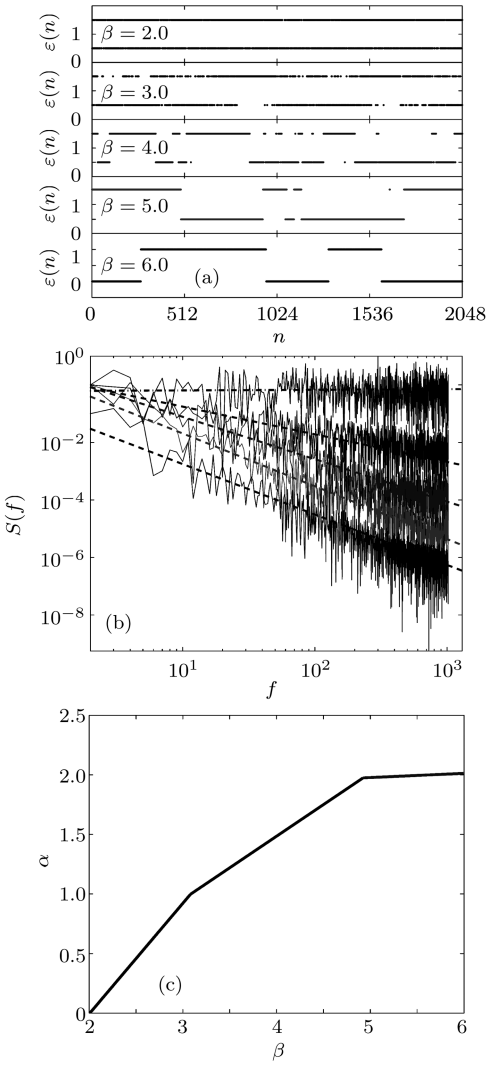


Fig. 1. (a) Binary sequences ε_n and (b) the corresponding power spectrum $S(f)$ for $\beta = 2.0, 3.0, ..., 6.0$. The lines are linear-fitted for corresponding data. The binary sequence length $N = 2^{11}$. (c) The relation between α and β in Eq. (3).

3. Numerical results

In what follows, we will analyse how LRC binary potentials affect the electron properties. We calculate the participation ratio[23] and the Lyapunov exponent,[2,24] which are quantities widely used to characterize the localization properties of electronic states.

3.1. Participation ratio

The participation ratio[23] is defined as

$$PR_{\rm E} = \left(N \sum_{n=1}^{N} |\psi_n^{\rm E}|^4 \right)^{-1}, \tag{4}$$

where $\psi_n^{\rm E}$ is the amplitude of the wave function with eigenenergy E in the n-th site, and N is the system size. Physically, $PR_{\rm E}$ gives the ratio of lattice sites occupied to all lattice sites at an eigenstate. Generally speaking, the larger the $PR_{\rm E}$, the more delocalized the eigenstate is. For 1D Bloch states at $N \to \infty$, the $PR_{\rm E}$ reaches 2/3.

We diagonalize the Hamiltonian [Eq. (1)] numerically with the periodic boundary condition to find all eigenenergies E and the corresponding wave functions $\psi_n^{\rm E}$. As an example, figure 2(a) shows the $PR_{\rm E}$ as a function of E for $N = 2048$ at $\beta = 2.0, 3.0, 4.0,$ and 5.0, respectively. We find that on the whole, the $PR_{\rm E}$ for eigenstates near the band centre is larger than that for eigenstates near band edges. For small β (2.0 and 3.0), all $PR_{\rm E}$ are relatively small. For large β (4.0 and 5.0), $PR_{\rm E}$ are relatively large in the region $E \in [-1.5, +1.5]$ and some $PR_{\rm E}$ approach 2/3 in some discrete E, which correspond to delocalized states; all $PR_{\rm E}$ are relatively small in other E regions.

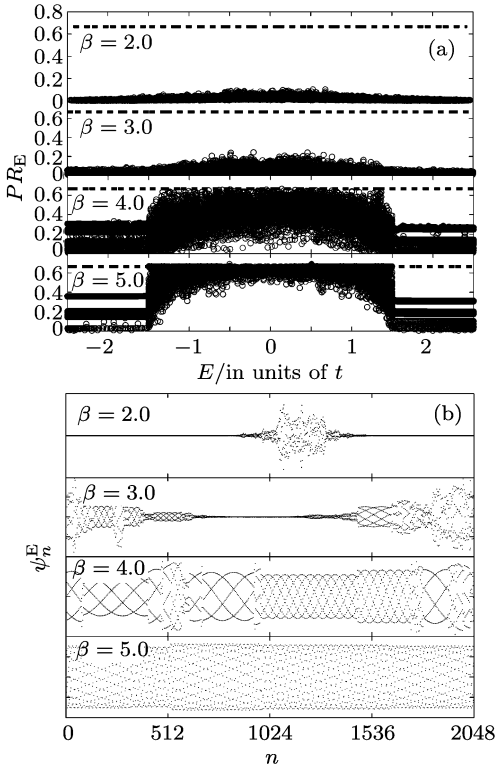


Fig. 2. (a) The participation ratio $PR_{\rm E}$ versus E at $\beta = 2.0, 3.0, 4.0,$ and 5.0 for six independent realizations, respectively. The dashed lines are $PR_{\rm E} = 2/3$. (b) Five typical wave functions for eigenstates near band centres, with $(E, PR_{\rm E}^{\max}) = (0.0257, 0.0595)$, $(0.0333, 0.1674)$, $(0.0966, 0.5934)$, $(0.0138, 0.6643)$ for $\beta = 2.0, 3.0, 4.0,$ and 5.0, respectively.

In fact, the energy region $E \in [-1.5, +1.5] = [V_{\rm A} - 2t, V_{\rm A} + 2t] \cap [V_{\rm B} - 2t, V_{\rm B} + 2t]$ is precisely the overlap of the energy bands corresponding to ordered chains formed only by A atoms and only by B atoms, i.e., delocalized states happen in the overlap region.

To demonstrate the localization properties of these states with relatively larger $PR_{\rm E}$ intuitively, we denote $PR_{\rm E}^{\max}$ to the local maximal participation ratio near the band centre. Figure 2(b) shows four typical wave function amplitude distributions at $\beta = 2.0, 3.0, 4.0$ and 5.0, respectively. As illustrated in the caption of Fig. 2, the values of $PR_{\rm E}^{\max}$ are relatively small ($\beta = 2.0$ and 3.0) for localized states and relatively large for delocalized states ($\beta = 4.0$ and 5.0). In particular, these delocalized states almost spread over the entire space, but they are uniform, which is different from those for Bloch states. What are the localization properties of these delocalized states at $N \to \infty$? Let us see another quantity to reflect the localization properties of electronic states, i.e., the Lyapunov exponent γ.[2]

3.2. Lyapunov exponent

We use the transfer matrix method to calculate the Lyapunov exponent γ. Equation (1) can be written in a recursive form,

$$\begin{pmatrix} \psi_{n+1} \\ \psi_n \end{pmatrix} = M_n \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix} = \begin{pmatrix} E - V_n & -1 \\ 1 & 0 \end{pmatrix}. \quad (5)$$

We obtain the transfer-matrix equation $\begin{pmatrix} \psi_{N+1} \\ \psi_N \end{pmatrix} = T_N \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix}$, with $T_N = \prod_{n=1}^{N} M_n$. The Lyapunov exponent $\gamma_{\rm E}$ is then the largest eigenvalue of the matrix $\lim_{N\to\infty} \ln(T_N T_N^{\dagger})^{1/2N}$. In calculations, we use the re-orthogonalization method.[24]

As mainly the delocalized states in the system concern us, we study the minimal $\gamma_{\rm E}$ for $E - \Delta/2 < E < E + \Delta/2$, where Δ is a small quantity, denoted as $\gamma_{\rm E}^{\min}$. Since states near the band centre are more sensitive to model parameters, we only study the case $E = 0$. In practice, we choose $\Delta = 0.1$, which ensures enough states in the interval Δ. Based on $\gamma_{E=0}^{\min}$, we also define a localization length $\xi = 1/\langle\gamma_{E=0}^{\min}\rangle$ and a reduced localization length $\Lambda_N = \xi/N$, where $\langle\cdots\rangle$ denotes the average over disorder realizations of V_n in Eq. (1). In our studies, the number of realizations is 10×10^3 for $N = 2^{12}, 2^{13}, 2^{14}$, and 2^{15}; and 5×10^3 for $N = 2^{16}, 2^{17}, 2^{18}$, and 2^{19}, and more realizations give similar results. It is known that Λ_N decreases (increases) with N for localized (extended) states, and

Λ_N does not change with N at the phase transition from localized to extended states.[12]

Figure 3(a) shows Λ_N versus correlation exponents β for different system sizes N. We find that at the same N, Λ_N increases with β, which reflects the delocalized effects of β. At the same β, Λ_N decreases with N for $\beta < 5.0$ and Λ_N is almost independent of N for $\beta \geq 5.0$. In detail, as examples, figure 3(b) shows Λ_N as a function of N for $\beta = 2.0, 3.8$, and 5.0. We find that $\lg(\Lambda_N)$ is almost linearly dependent on $\lg(N)$ for all N at $\beta = 2.0$ and 5.0, but it does not for all N at $\beta = 3.8$. Therefore, we try a piecewise linear-fit line to the relation between $\lg(\Lambda_N)$ and $\lg(N)$. One piecewise line is for data at $N = 2^{12}$ to 2^{15}, and the other is for data at $N = 2^{16}$ to 2^{19}, i.e., $\Lambda_N = A_1 N^{\nu_1}$ and $\Lambda_N = A_2 N^{\nu_2}$, respectively. For comparison, we also apply a linear fit for all N, i.e., $\Lambda_N = AN^{\nu}$. Here ν_1, ν_2, and ν are just slopes of corresponding fitted lines shown in Fig. 3(b) and these parameters, ν_1, A_1, ..., in general depend on β. Figure 3(c) shows the dependences of ν, ν_1, and ν_2 on β. We find $\nu < 0$ and $\nu \sim 0$ at $\beta < 5.0$ and $\beta \geq 5.0$, respectively. This indicates $\Lambda_N(\beta) \to 0$ or $\Lambda_N(\beta) = A(\beta)$ as $N \to \infty$, which means that there are no extended states in the model. All these are similar to those for ν_1 and ν_2.

On the other hand, we find that as $N \to \infty$, $\xi = \Lambda_N N = AN^{1+v} \to 0$ at $\nu < -1$, and $\xi > 0$ at $\nu \geq -1$. The localization lengths are significantly different when ν is below and above -1. As shown in Fig. 3(c), the values of ν, ν_1, and ν_2 are all equal to or greater than -1 at $\beta >= \beta_c \approx 4.25$, which corresponds to $\alpha_c = 1.62$ according to Eq. (3). The β_c is a threshold value. When β is above β_c, $\xi > 0$ as $N \to \infty$. More interestingly, $\xi \geq N$ may happen for finite system sizes N when N is less than a certain $N^*(\beta)$. As shown in Fig. 3(a), the states above the dashed line satisfy the condition. Based on ν, ν_1, and ν_2, we plot the up-bound system sizes N^* versus β in Fig. 3(d). At $N < N^*(\beta)$, the wave functions for these states will almost occupy the whole space, and thus the system is "metallic", which will determine the electronic transport for finite system sizes.

Moreover, we find that the difference between ν_1 and ν_2 is relatively small for $\beta < 3$ and $\beta > 5$, and relatively large for other β. The three regions for β are consistent with that shown in Fig. 1(c). Perhaps this is related to the fact that binary potentials correspond to stationary sequences when $\beta < 3$ ($\alpha < 1$) and to non-stationary sequences when $\beta > 3$ ($\alpha > 1$). The binary potentials become almost ordered sequences when $\beta > 5$ ($\alpha \approx 2$).[21]

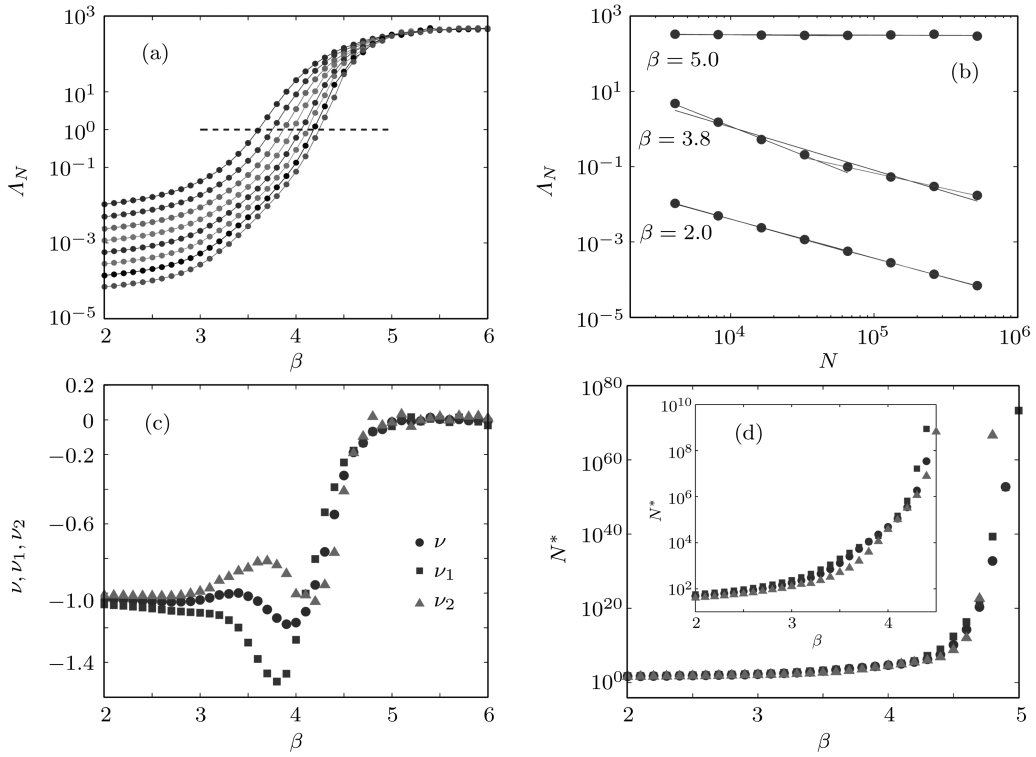


Fig. 3. (a) Reduced localization length Λ_N versus β for $N = 2^{12}, 2^{13}, \ldots, 2^{19}$ (from top to bottom). The dashed line is the one for $\Lambda_N = 1$. (b) Λ_N versus N for $\beta = 2.0, 3.8$, and 5.0. The lines are linear-fitted for corresponding data, which are explained in the text. (c) ν, ν_1, and ν_2 versus β. (d) The up-bound system sizes N^* versus β.

4. Discussion and summary

In other studies of 1D systems with LRC binary potentials,[19,20] there were also non-extended states, with critical exponent α limited to the interval $[0.0, 1.5]$[19] or only equal to 2.0.[20] In Refs. [17] and [18], a transition from disordered system to ordered system was described, which was consistent with our results that α is saturated at 2.0 when $\beta > 5.0$ and the corresponding sequences are almost ordered. At the same time, in systems with LRC continuous potentials, Carpena *et al.*[14] found that there was a transition in the distribution of energy levels at $\tilde{\alpha_c} = 1.55 \pm 0.05$. We found a transition at the threshold $\beta_c \approx 4.25$ ($\alpha_c = 1.62$). Therefore, the two transitions are consistent with each other and may be correlated. In practice, long-range correlations exist in real materials, such as in DNA molecules.[25] In experiments, DNA molecules are found to be insulating, semiconducting, or conducting.[26−28] Our finding that there is an upper-bound in system sizes $N^*(\beta)$ will be helpful to understand these LRC and length-related conduction properties.

In summary, with the help of the participation ratio and the Lyapunov exponent, we have investigated numerically the electron properties in 1D systems with LRC binary potentials. We found that there were no extended states and there existed a transition at the threshold β_c for system sizes as $N \to \infty$. When β is above β_c, we have $\xi > 0$. Interestingly, for finite system sizes, $\xi \geq N$ may happen at certain β, which makes the system "metallic", and we gave the upper-bound system size $N^*(\beta)$. These findings can be used in the creations of electron nano-devices, optic fibres, rough surfaces, and acoustic and electromagnetic waveguides with selective transport properties.

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