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Localization-delocalization transition in chains with long-range correlated disorder

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Abstract. We investigated numerically localization properties of electron eigenstates in a chain with long-range correlated diagonal disorder. A tight-binding one-dimensional model with on-site energies exhibiting long-range correlated disorder (LCD) was used with various disorder strength W. LCD was defined so that it gave a power-law spectral density of the form $S(k)\alpha k^{-p}$, where p determines the roughness of the potential landscape. Numerical results on the correlation length ξ of eigenstates shows the existence of the localization-delocalization transition at $p = 2$. It is found that the critical values for disorder strength W_c and also the critical exponent ν for localization length change with the values of p.

PACS. 05.60.Gg Quantum transport – 72.15.Rn Localization effects – 72.20.Ee Mobility edges; hopping transport – 64.60.Cn Order-disorder transformations; statistical mechanics of model systems

1 Introduction

Electronic wave functions in perfectly ordered crystal are extended Bloch's wave functions, implying that the probability density of an electron is the same over the entire crystal. But when the periodic structure is destroyed by introducing disorder in the crystal, the wave function can become localized. Although the exact treatment of the problem is cumbersome, there are model systems which contain the basic physical ingredients of the system. The simplest theoretical model for studying the nature of one electron states in disordered states was introduced by Anderson [1]. The model shows that if the disorder is very strong the wave function may become exponentially localized with a characteristic localization length ξ. From scaling arguments it is also well-known that electron states are exponentially localized in one and two dimensions in any amount of disorder. In three dimensional systems at zero temperature a localization-delocalization transition takes place at critical value W_c [2,3]. For a uniform disorder distribution, $W_c = 16.5$. For $W < W_c$ despite some degree of disorder, the electron wave function is extended, and the system behaves as a conductor, whereas when $W > W_c$, the wave function becomes localized, and the system behaves as an insulator. However, introducing correlation in the disorder can markedly change the physics.

The effects of long-range power-law correlated disorder or scale-free disorder are omnipotent in nature [4]. This is not only observed in physical systems [5,6] but also in many other diverse systems including biological and economical systems [7,8]. Of particular interest to us in this work, however, is the influence of long-range power-law correlated disorder in the neighborhood of a metal-insulator transition when the correlation length ξ becomes sufficiently large.

In recent years several low-dimensional models with correlated disorder have been proposed to investigate the localization properties of one-dimensional systems. A one-dimensional tight-binding random dimer model was studied in references [9–13]. The model shows that there exists single resonant energy levels of extended states. Similar resonant levels of extended states are even found in one-dimensional models with short-range correlated disorder [14,15]. The absence of localization has also been reported to occur in disordered chains with correlated off-diagonal interactions [16,17].

More recently, de Moura and Lyra [18] have also studied the localization properties of the one-dimensional Anderson model with long-range correlated disorder. The on-site energy landscape is generated by considering the potential as the trace of a fractional Brownian motion with a specified spectral density $S(k)\alpha k^{-p}$, namely power-law spectral density. It has been found that the localization length diverges for $p > 2$ within a finite range of energy values exhibiting an Anderson transition with mobility edges separating localized and extended states. In this work, the roughness of the potential landscape defined by the exponent of the power-law spectral density p was considered. But the effect of the disorder strength W characterized by the amplitude of the potential was unclarified. There are also several other works using the same power-law spectral density [19–22].

The effects of disorder strength W on the localization properties of eigenstates have also been investigated by

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using a sequence of long-range correlated disorder which is produced by the Fourier filtering method [23]. The main outcome of this work is that there is a critical disorder amplitude $W_c = 4$ independent of the values of p. In this work the amplitude of energy sequence or disorder strength $\{\varepsilon_i\}$ is controlled by imposing a normalization condition on the variance of energy sequence as $\triangle\varepsilon = \sqrt{\langle\varepsilon^2\rangle - \langle\varepsilon\rangle^2} = 1$. The relevance of this condition is going to be examined in the following section. But, it is worth mentioning from the outset that the true effect of W on the localization properties of eigenstates may disappear due to this condition. Therefore, a more relevant consideration is needed to present the effects of the disorder strength W on the long-range correlated systems. That is mainly what we are going to consider in this work.

This paper is organized as follows. In the following section we are going to define an on-site potential landscape to study the effect of disorder strength. In Section 3 we are going to present a brief description of Anderson tight binding model and finite-size scaling which are going to be used in our numerical calculations. In Section 4, we are going to present our numerical results and the calculated critical values of disorder strength W_c and critical exponent ν. Our conclusion will also be presented in the same section

2 Long-range correlated potential sequence

In order to introduce long-range correlations in the disorder distribution, there are two main methods, the fractional Brownian motion consideration and the Fourier filtering method. In the fractional Brownian motion consideration [24–26], the site energies are considered to be in a sequence that describes the trace of a fractional Brownian motion with a specified spectral density $S(k)\alpha k^{-p}$. For $p = 0$ one recovers the traditional white noise of the Anderson model with δ-correlated disorder $\langle\varepsilon_i\varepsilon_j\rangle = \langle\varepsilon_i^2\rangle\delta_{i,j}$. The exponent p is directly related to the Hurst exponent H of the rescaled range analysis ($p = 2H + 1$) which describes the self-similar character of the energy sequence and persistent character of its increments. When $H > 1/2$ the process is said to have long-range correlation while $H < 1/2$ means that the process is uncorrelated. In the second method, a sequence of long-range correlated potential $\{\varepsilon_i\}$ is produced by the Fourier filtering method [27,28]. This method is based on a transformation of the Fourier components of a random number sequence. The outline of the model is: (i) a sequence $\{x_i\}$ of uncorrelated random numbers with a Gaussian distribution is prepared; (ii) its Fourier components $\{x_q\}$ are computed by the Fourier transformation; (iii) a new sequence is generated for a given p from the relation $\varepsilon_q = q^{-p/2}x_q$; (iv) finally, the desired potential sequence $\{\varepsilon_i\}$ having a power-law spectral density is obtained as the inverse Fourier transform of $\{\varepsilon_q\}$.

In the study of long-range correlated one-dimensional electron systems, the on-site potential produced by the first method has been employed by de Moura and Lyra without considering the effect of the disorder strength. In this work the on-site long-range correlated potential was produced by the following relation

$$\varepsilon_i = \sum_{k=1}^{N/2}\left[k^{-p}\left(\frac{2\pi}{N}\right)^{1-p}\right]^{1/2}\cos\left(\frac{2ik\pi}{N} + \phi_k\right) \qquad (1)$$

where N is the number of sites and ϕ_k are $N/2$ independent random phases uniformly distributed in the interval $[0, 2\pi]$.

Table 1. The constants C of equation (2).

L	$p=1$	$p=1.5$	$p=2$	$p=2.5$	$p=3$	$p=3.5$	$p=4$
4×10^4	2.3	10.2	73.7	586.6	4956	42822	374630
2×10^4	2.2	8.6	51.3	347.7	2471	17961	132171
1×10^4	2.1	7.1	36.1	206.2	1234	7552	46774

The effect of the disorder strength is considered in the work of Shima, Nomura, and Nakayama. In this work the on-site potential is produced using the Fourier filtering method. The effect of the disorder strength was related to the width of uncorrelated Gaussian distribution, the first step of the Fourier filtering method. Later, the obtained long-range correlated potential sequence was normalized with the relation $\triangle\varepsilon = \sqrt{\langle\varepsilon^2\rangle - \langle\varepsilon\rangle^2} = 1$. For short-range correlated disorder Anderson models, relating the disorder strength to the width of the Gaussian distribution is a relevant consideration since on-site potential is taken directly from the Gaussian distribution. However, if Fourier filtering method and the imposed renormalization condition are considered, the true effect of the disorder strength disappears. In other words, the amplitudes of on-site potential sequences $\{\varepsilon_i\}$ are set to be constant due to the imposed normalization condition. Furthermore it is well-known that the disorder strength is only related to the amplitude of the on-site potential energy sequence $\{\varepsilon_i\}$. Thus, relating disorder strength to the width of the Gaussian distribution in the study of long-range correlated disorder turns out to be an irrelevant consideration. Therefore, we think that the true effect of the disorder strength is absent in the work of Shima, Nomura, and Nakayama due to the imposed renormalization condition. In other words, studying the effect of the disorder strength in a long-range correlated disorder chain is still an important problem. To do so, one has to properly define a long-range correlated disordered potential sequence with the dependence of disorder strength. We think the following procedure is effective in keeping the true effect of the disorder strength in the long-range correlated energy sequence.

As a first step, the potential in equation (1) was normalized with the relation $\triangle\varepsilon = \sqrt{\langle\varepsilon^2\rangle - \langle\varepsilon\rangle^2} = 1$. The normalization coefficients denoted by C are given in Table 1. Thus the normalized energy sequence ε_i^n is equal to ε_i/C.

In order to present the effect of the disorder on the system, we are going to use a modified form of the above potential sequence in the following manner. If the disorder is totally uncorrelated ($p = 0$), it is easy to see from

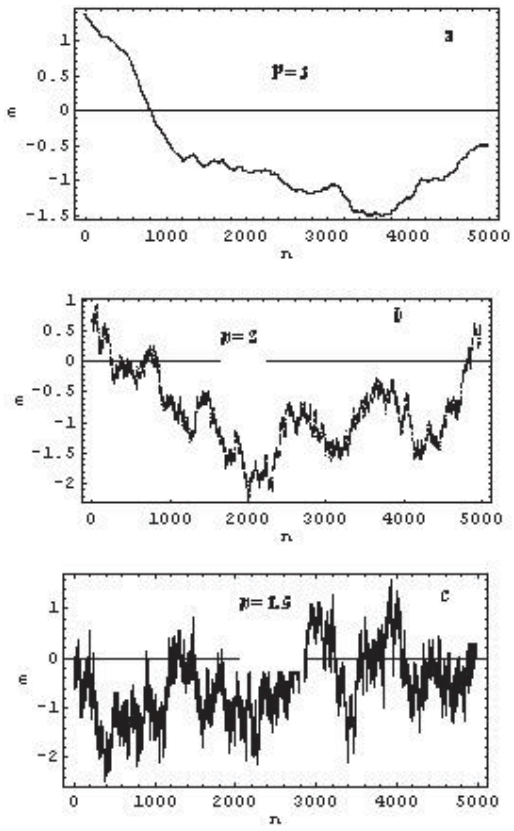

Fig. 1. The long-range correlated potential sequence obtained from equation (4) for $W = 3.4$. (a) Is plotted for $p = 3$, (b) is plotted for $p = 2$, and (c) is plotted for $p = 1.5$.

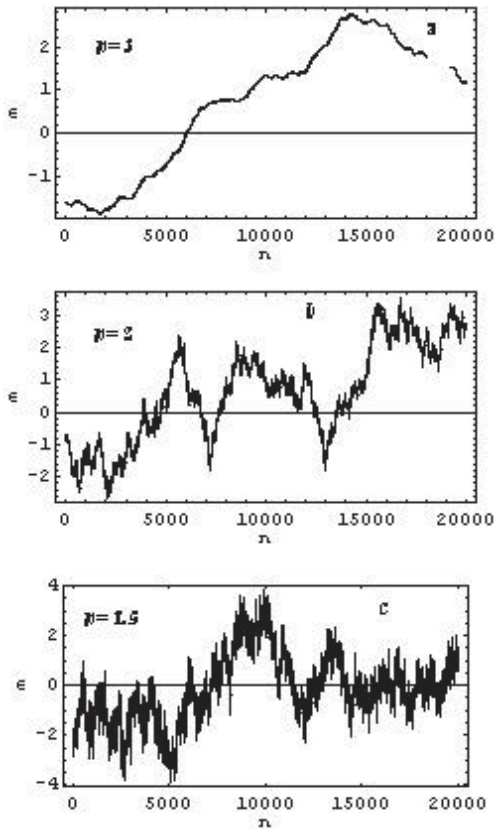

Fig. 2. The long-range correlated potential sequence obtained from equation (4) for $W = 5$. (a) Is plotted for $p = 3$, (b) is plotted for $p = 2$, and (c) is plotted for $p = 1.5$.

Anderson theory that an increase in W trivially induces a strongly localized wave function. Consequently, W can be related to the amplitude of the long-range correlated potential by the following relation

$$\varepsilon_i^n(W) = \frac{W}{\sqrt{12}}\varepsilon_i^n \tag{2}$$

where the modification term $W/\sqrt{12}$ is just the standard deviation of a Gaussian distribution. We are going to use this modified potential sequence throughout this work. We think this modified on-site potential sequence keeps the true effect of the disorder strength on the system since it is related to the amplitude of the energy sequence. In addition, when the disorder is sufficiently long-ranged to yield a conducting phase, the system may have a critical disorder strength W_c separating the conducting and insulating phases. The determination of W_c for different values of p leads to the phase diagram in the $W - p$ space, as well as providing a better understanding of the properties of long-range correlated systems.

3 Theoretical model

3.1 Correlation length

As a model system, we considered noninteracting electrons in a one-dimensional long-range correlated disordered system within a tight binding approximation. For a discrete lattice chain, the Schrödinger equation of the model is expressed as

$$\varepsilon_i\psi_i + t(\psi_{i+1} + \psi_{i-1}) = E\psi_i \tag{3}$$

where ψ_i is the amplitude of the wave function at the ith site of the lattice. The overlap integral parameter or the hopping energy t is going to be set unity in the following. A sequence of long-range correlated disorder potential is going to be produced by the modified energy sequence described in equation (2). The correlation length ξ of a state with energy E is given as [29]

$$\frac{1}{\xi_L} = -\frac{1}{2L}\langle \ln T_i \rangle \tag{4}$$

where L is the length of the chain, $\langle \dots \rangle$ denotes the average over possible realization of the system and T_i is the transmission eigenvalues of a matrix Q, defined as

$$Q = M^T M \tag{5}$$

where M is the the transfer matrix. For the discrete lattice model Hamiltonian, the propagation of the excitation along the system can be expressed in the following form:

$$\begin{pmatrix} \psi_{i+1} \\ \psi_i \end{pmatrix} = \begin{pmatrix} E - \varepsilon_i & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \psi_i \\ \psi_{i-1} \end{pmatrix} \tag{6}$$

where M_i is defined as

$$\begin{pmatrix} E-\varepsilon_i & -1 \\ 1 & 0 \end{pmatrix}. \quad (7)$$

The transfer matrix M describing the evaluation of the initial state vector across L sites can be readily expressed as the product of one-step matrices if the distance between adjacent sites is set to be unity, that is

$$M = \prod_i^L M_i. \quad (8)$$

The eigenvalues of Q are real positive numbers coming in inverse pairs. Expressing the eigenvalues as $q_{i,1} = e^{\nu_i}$ and $q_{i,2} = e^{-\nu_i}$, the transmission eigenvalues can be given by

$$T_i = \frac{2}{1+\cosh(\nu_i)}. \quad (9)$$

To obtain $\langle \ln T_i \rangle$ for a given L, we take the average over 10^2 realization of the system. Energy E is fixed at the band center $E = 0$ throughout this work.

3.2 Finite-size scaling analysis

In order to study the critical properties of the system, we are going to develop a scaling relation for a pure 1D system from the standard one parameter scaling analysis [30–33] obtained for quasi-1D bar of cross section $M \times M$ and a length L. For quasi-1D bar, the normalized correlation length $\Lambda = \xi/M$ was found to obey a scaling theory such that

$$\frac{d\ln\Lambda}{d\ln M} = \beta(\ln\Lambda) \quad (10)$$

which has a solution of the form

$$\ln\Lambda = f\left(\frac{M}{\xi_\infty}\right), \quad (11)$$

where ξ_∞ is a characteristic length or correlation length in the thermodynamic limit. It was also a common procedures to produce numerical data by keeping L constant and M as a variable in those works.

In this work, however, we study a pure 1D chain with a length L. We simply assume that the normalized correlation length $\Lambda = \xi/L$ obeys the following relation

$$\frac{d\ln\Lambda}{d\ln L} = \beta(\ln\Lambda) \quad (12)$$

which also has a solution of the form $\Lambda = g(L/\xi_\infty)$ or equivalently $\ln\Lambda = f(L/\xi_\infty)$. This final relation was used as a scaling relation in reference [23] from the outset. Here, ξ_∞ is also a characteristic length or correlation length, which can be identified with the localization length of the insulator, and which scales as the reciprocal of the resistivity of the metallic phase. The localization length of an infinite system obeys the following relation near the critical point $W = W_c$,

$$\xi_\infty \alpha |W - W_c|^{-\nu}. \quad (13)$$

But in practice only finite, and still relatively small, systems are numerically accessible. In order to determine the critical strength W_c and the critical exponent ν, one can only use the finite size data for Λ and the scaling function $f(L|W-W_c|^\nu)$. One can always find an equivalent function for the scaling function in the form of $F(L^{1/\nu}|W-W_c|)$. Thus the scaling equation becomes, $\ln\Lambda = F(L^{1/\nu}|W-W_c|)$. This final relation allows expansion of the scaling function around the critical point as

$$\ln\Lambda = a_0 + a_1|W-W_c|L^{1/\nu} + a_2|W-W_c|^2 L^{2/\nu} + \dots \quad (14)$$

We use this expansion of the scaling function to obtain the critical disorder strength W_c and the critical exponent ν by terminating the expansion at the third order.

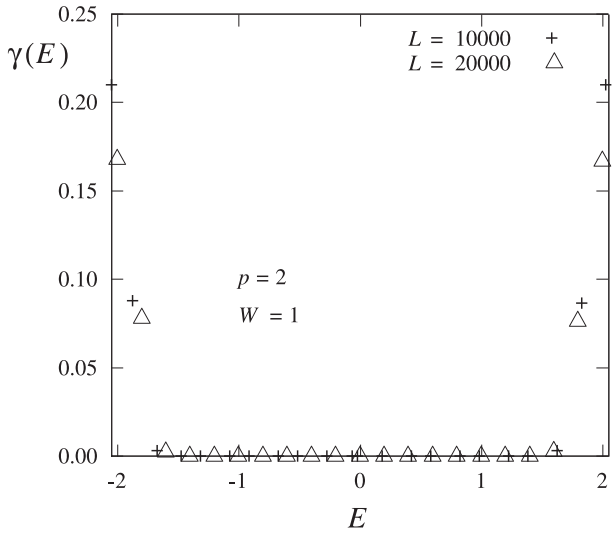

Fig. 3. The energy dependence of the Lyapunov exponent for $p = 2$ and $W = 1$.

4 Numerical results and conclusions

4.1 Existence of extended states

In this section, we are going to investigate the nature of electron states by computing three different physical quantities. The first quantity going to be considered is the average Lyapunov exponent, defined as the inverse of the correlation length $\gamma = 1/\xi$ [34]. In Figure 3 we show plots of γ versus E for the various values of the system size at $p = 2$ and $W = 1$. Both data for $L = 10^4$ and $L = 2 \times 10^4$ show that the Lyapunov exponents vanish within a finite range of energy values revealing the presence of extended states within this energy interval. More importantly, $\gamma(E)$ data for these two system sizes appears to be the same within this energy interval, meaning that the extended phases are

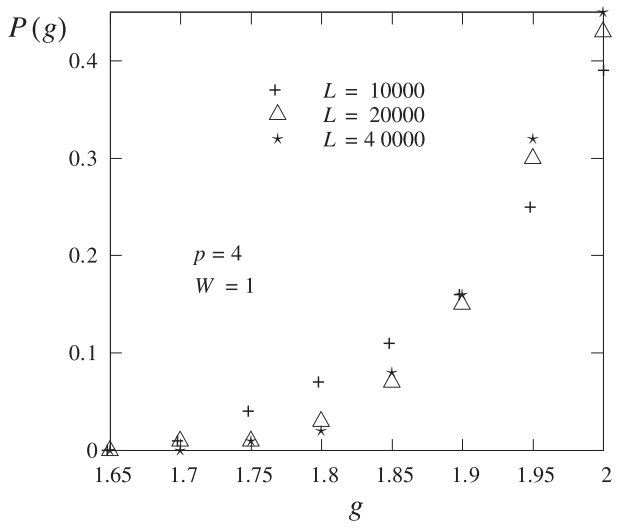

Fig. 4. The conductance distribution for $p = 4$ and $W = 1$.

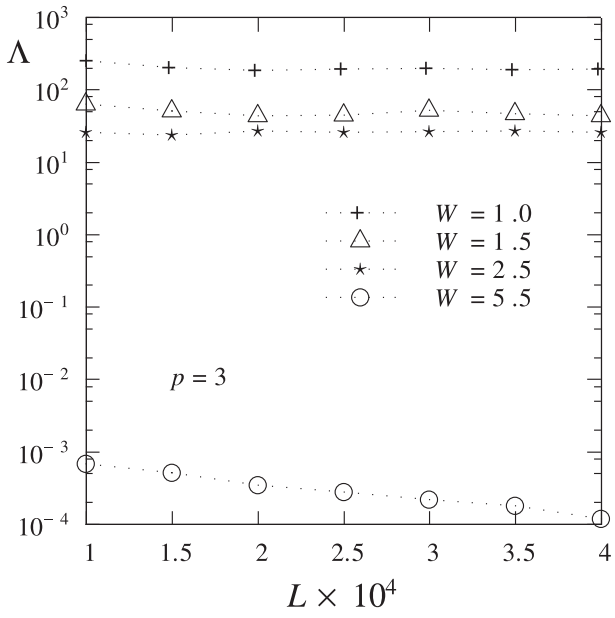

Fig. 5. The normalized correlation length $\Lambda = \xi/L$ as a function of L for various values of W for the case of $p = 3$.

stable as L grows larger. This is a good indication of the existence of extended states as $L \to \infty$ or in the thermodynamic limit. As a second consideration in the search for the existence of extended states we find that computing conductance distribution $P(g)$ is a relevant perspective. The conductance g is defined with the Landuer formula as $2T$ for a single channel transport, here T is defined by equation (9). The factor of 2 in the definition of the conductance is due to the electron spin degeneracy.

The nature of conductance distribution by itself is a really important subject in the treatment of localization problems, especially in the discussion of the validity of single parameter scaling theory. It is now well-known that single parameter scaling theory is valid if $P(g)$ is fully determined by a single parameter [35,36]. But, in this paper $P(g)$ is going to be computed in terms of its possible indication of the presence of the conducting states in the thermodynamic limit.

In Figure 4, $P(g)$ is plotted for various values of L at $p = 4$, $W = 1$ and $E = 0$. From the figure it is apparent that there are only slight changes in $P(g)$ compared with the changes in the system size. These conductance distributions produce an average conductance $\langle g \rangle$ having almost the same values for each system size. In other words, $\langle g \rangle$ is almost independent of system size L at these particular parameters of the system. This result is also a relevant indication of the presence of the conducting phase in the thermodynamics limit.

The last consideration in the study of the existence of extended states in this paper is going to be investigated by computing the normalized localization length $\Lambda = \xi/L$. In Figure 5, we show plots of Λ versus L at various values of W for $p = 3$. For values of $W = 1, 1.5$, and 2.5, the values of $\Lambda(L)$ oscillate around constant lines. Whereas, for $W = 5.5$, $\Lambda(L)$ decreases as L increases. The former is also another good indication of the existence of conducting states in the thermodynamic limit, while the latter indicates that the system becomes more localized as L increases. Thus one can conclude that the system is deeply localized in the thermodynamic limit at $W = 5.5$. From the results of Figure 5, one can also infer that there might be metal-insulator transition at a particular value of disorder strength W. Actually, a similar procedure was employed in the determination of the critical energy levels in reference [18]. The critical exponent ν, was also calculated for $p = 2$ from the Lyapunov exponent $\gamma(E)$ in the same work.

Before terminating this section we want to stress once more that there exist extended states in the long-range correlated Anderson model in the thermodynamic limit. The evaluation of the critical disorder strengths and critical exponents corresponding to various potential sequences are going to be worked out in the following section. In doing so we are going to consider finite-size scaling analysis due to its greater feasibility and its higher possibility of relevance.

4.2 Determination of the critical values

In this section we present our numerical result obtained by using the finite size scaling methods. We have performed calculations for systems with sizes approximately equal to those adopted in reference [23], so we have carried out scaling analysis with the same resolution. However, due to our computer time limitation, we have to take the averages over 10^2 realization of the systems in the following calculations except for the last three figures, in which the averages are taken over a 10^3 realization. Due to the same reason, we have to work with less data points than the data points in the cited reference.

In Figure 6, we plotted the normalized correlation length $\Lambda = \xi/L$ as a function of disorder strength for the case $p = 1$. It can be seen from the figure that Λ rapidly decreases while the disorder strength increases for every

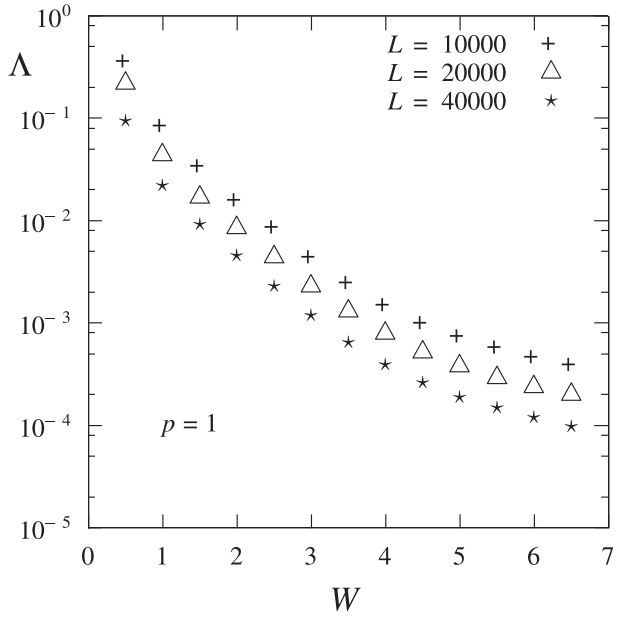

Fig. 6. The normalized localization length $\Lambda = \xi/L$ as a function of disorder strength for the case $p = 1$.

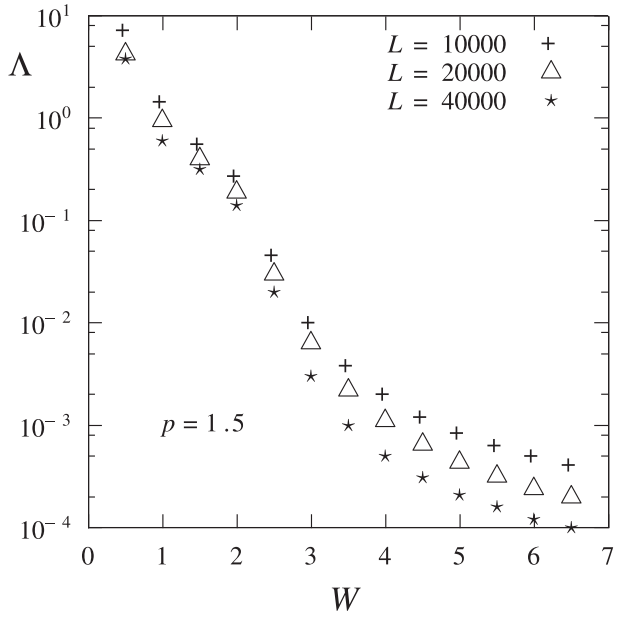

Fig. 7. The normalized localization length $\Lambda = \xi/L$ as a function of disorder strength for the case $p = 1.5$.

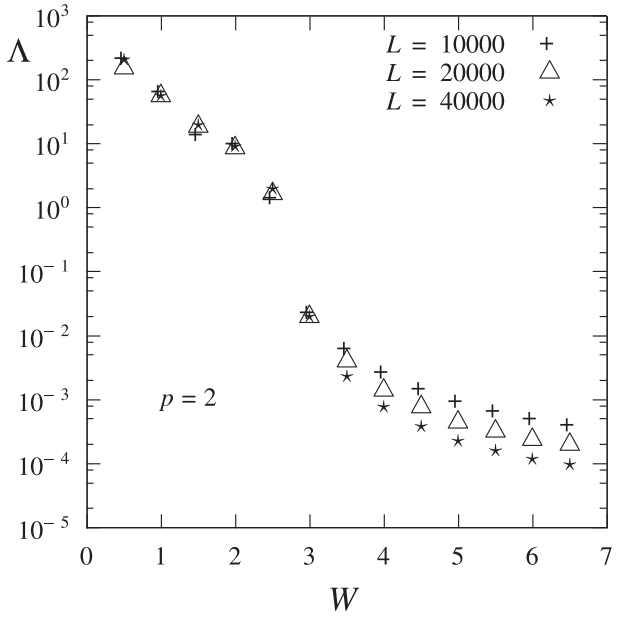

Fig. 8. The normalized localization length $\Lambda = \xi/L$ as a function of disorder strength for the case $p = 2$.

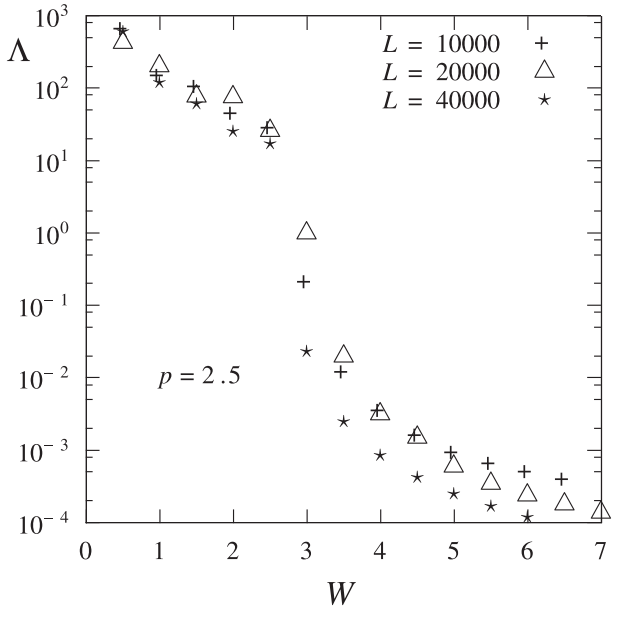

Fig. 9. The normalized localization length $\Lambda = \xi/L$ as a function of disorder strength for the case $p = 2.5$.

system size investigated. From the same figure it is easily seen that Λ is a monotonous function of W for all system sizes. Furthermore, there is no intersection point, indicating that the system undergoes no phase transition. Thus we can conclude that the states are localized at $p = 1$, in consistence with other investigations. In Figures 7 and 8, we also plotted Λ with respect to W for the values of $p = 1.5$ and $p = 2$. As seen from the figures, the values oféΛ are almost the same at around $W = 2.5$. However, Λ turns out to be a monotonous function for $W > 2.5$. This is an indication of phase transition. But, our further scaling analysis around $W = 2.5$ shows that there is no critical transition at around that point for $p = 1.5$. From these three figures we can conclude that there might be possible phase transition for larger values of $p \geq 2$.

Figures 9–11 also illustrate the behavior of Λ as a function of W for $p = 2.5$, $p = 3$, and $p = 4$ respectively. All of these figures show two common striking features. The first is of course the kinks around some particular values of W. For instance, in Figure 9 at around $W = 2.8$ there is a sharp decrease. The same features can be seen at around $W = 3$ in Figure 10 and at around $W = 3.95$ in Figure 11.

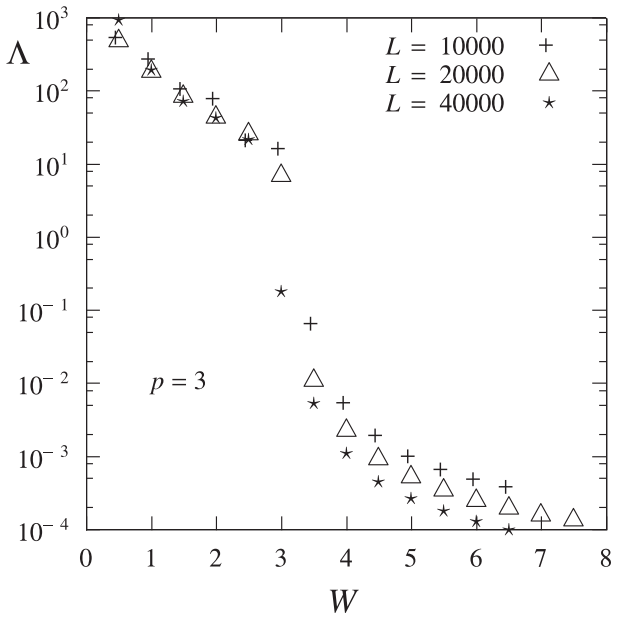

Fig. 10. The normalized localization length $\Lambda = \xi/L$ as a function of disorder strength for the case $p = 3$.

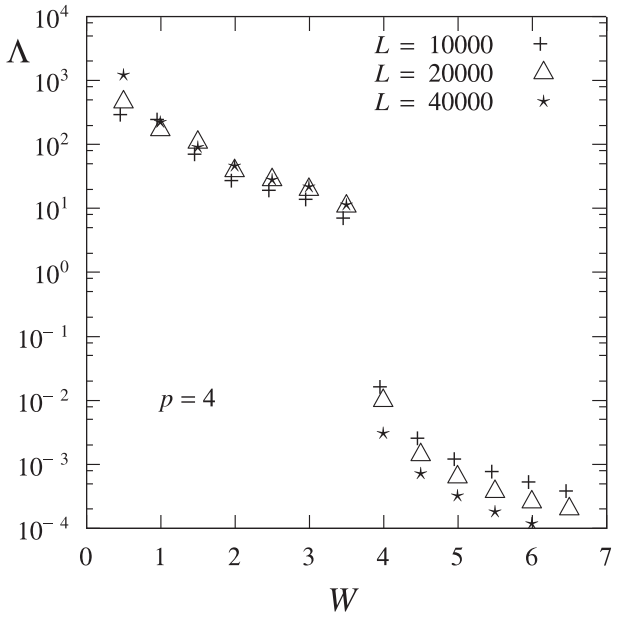

Fig. 11. The normalized localization length $\Lambda = \xi/L$ as a function of disorder strength for the case $p = 4$.

The second observation that can be made concern is the values of Λ with respect to p. For W less than cited values, the values of Λ rise as p increases indicating that the growth of p for W less than cited values causes an increase in the correlation length of eigenstates. In contrast, the values of Λ for W larger than cited values decrease as p increases. Thus, for W larger than cited values, larger values of p produce strongly-localized eigenstates.

We have performed further scaling analysis in Figure 12 in order to find out the critical value of disorder strength W_c and the critical exponent ν for $p = 4$. From

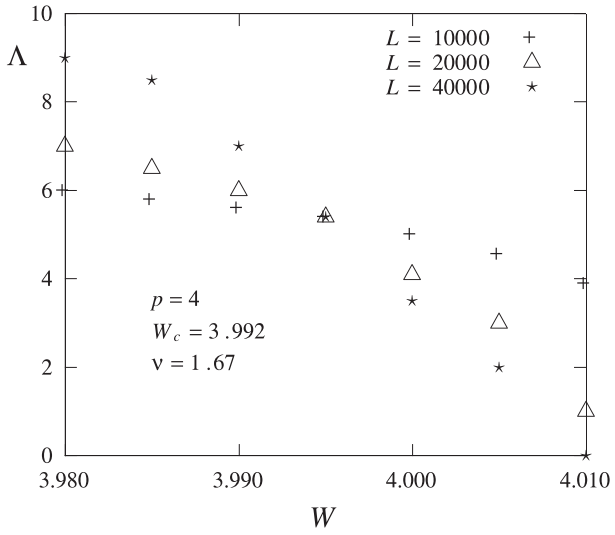

Fig. 12. The normalized correlation length $\Lambda = \xi/L$ as a function of disorder strength for the case $p = 4$. Plotted to find the critical value of W_c.

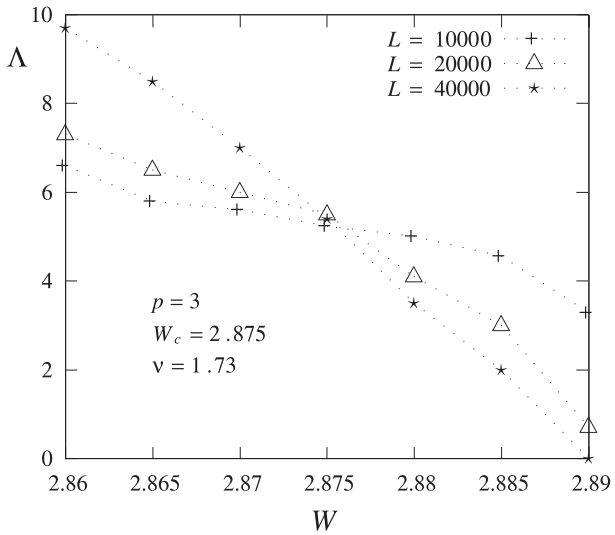

Fig. 13. The normalized correlation length $\Lambda = \xi/L$ as a function of disorder strength for the case $p = 3$. Plotted to find the critical value of W_c.

the figure it is apparent that W_c is equal to 3.992 since all curves in this figure intersect at this value. This is a good indication of the presence of the Anderson transition at $W = W_c$. Fitting the data of $\ln \Lambda$ for various L to equation (14), we obtain $\nu = 1.67$. Following the same procedure, we have also determined the critical value of disorder strength W_c and the critical exponent ν for $p = 2.5$ and $p = 3$. It was found from Figure 13 that $W_c = 2.875$ and $\nu = 1.73$ for $p = 3$. For $p = 2.5$, it was found from Figure 14 that $W_c = 2.746$ and $\nu = 1.82$. From these analysis we can conclude that the critical values of the systems depend on the long-range correlation parameter p. Intriguingly, all data of $\Lambda(W)$ for $p > 2$ indicates that W_c increases when p increases, while ν decreases when p increases.

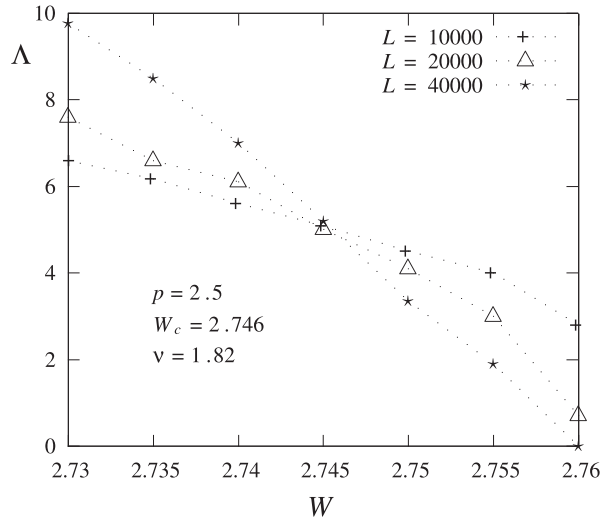

Fig. 14. The normalized correlation length $\Lambda = \xi/L$ as a function of disorder strength for the case $p = 2.5$. Plotted to find the critical value of W_c.

5 Conclusions

In this work we investigated the combined effects of disorder strength and the order of the long-range correlation or the potential roughness characterized by p. We have shown that the electronic states in a one-dimensional Anderson model of on-site potential with the long-range correlation proposed by de Moura and Lyra exhibit a localization-delocalization phase transition in varying the amplitude of the long-range correlated energy sequence. For values of $p < 2$, we have found no metal-insulator type phase transition. Whereas, for values $p > 2$, we have obtained critical disorder strength W_c which separates extended and localized regimes. We have also put considerable effort into relating the critical disorder strength with the order of long-range correlation p. In general we observed that W_c increases with increasing p. In other words, the value of W_c depends on the value of p. This prediction is in complete contrast to the result found in the work of Shima, Nomura, and Nakayama, where the value of $W_c = 4$ is independent of p. We think this independence is due to the constant amplitude of potential sequence used in their work. On the contrary, we have found that the critical exponent ν decreases with increasing p. This result is in agreement with the result found in the work of Shima, Nomura, and Nakayama.

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