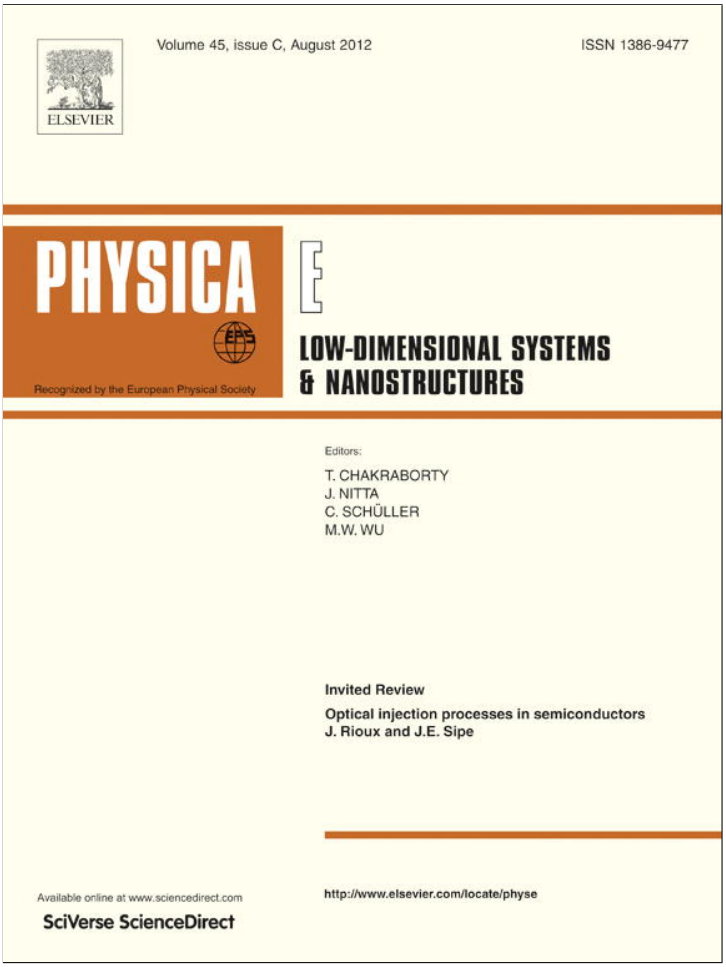

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Numerical study of the one-electron dynamics in one-dimensional systems with short-range correlated disorder

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HIGHLIGHTS

- Dynamics of one electron in 1*d* disordered systems.
- Effect of short-range exponential correlation on the diagonal disorder distribution.
- Scaling of localization length with correlation length.

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ABSTRACT

In this work, we numerically calculate the dynamics of an electron in one-dimensional disordered systems. Our formalism is based on the numerical solution of the time-dependent Schrödinger equation for the complete Hamiltonian combined with a finite-size scaling analysis. Our calculations were performed on chains with short-ranged exponential correlation on the diagonal disorder distribution. Our formalism provides an accurate estimate for the dependence of the localization length with the width of disorder. We also show here numerical calculations of the localization length by using a standard renormalization procedure. Our results agree within our numerical precision. We provide a detailed description of the role played by these short-range correlations within electronic transport. We numerically demonstrate the relationship between localization length, correlation length, and the strength of disorder.

1. Introduction

The time-dependent propagation of an initially localized one-electron wave-packet in a disordered system can reveals some detail about the insulator/metal properties of such system [1–4]. From the Anderson localization theory for $d \leq 2$ [3] it is well know that the width of the wave-packet saturates at a finite region around the initial position at limit of long time. However, during the last two decades, it has been shown that low-dimensional disordered systems can support extended states or a localization–delocalization transition in the presence of short or long-range correlations in the disorder distribution [5–31]. The absence of Anderson localization in the presence of spatial short-range correlations in disorder was theoretically pointed out by Flores [5] and Dunlap [6] at the end of eighties and the experimental confirmation was obtained by Domínguez-Adame and co-workers [14] in a semiconductor super lattice with intentional correlated disorder. The delocalization problem in one-dimensional (1d) systems with long-range correlated diagonal disorder have attracted attention since the end of the nineties. It has been reported [8,11,13,16] that these systems display an Anderson Metal–insulator transition (MIT) with mobility edges separating localized and extended states for sufficiently strong correlations. The effect of long-range correlated scatters on the transport properties of microwave guides was experimentally studied and corroborated the predicted presence of mobility edges [17]. Moreover, it was suggested that an appropriate algorithm for generating random correlated sequences with desired mobility edges could be used in the manufacture of filters for electronic or optical signals [11]. Furthermore, the theoretical prediction that is possible to *see* Anderson localization in a random multi layered filter[32] opened a wide field of investigations of effects of correlated disorder in optical systems.

In this paper we study the problem of one-electron localization in 1*d* systems with correlated disorder by using two numerical formalisms. The first one is a dynamics formalism based on the numerical solution of the time-dependent Schrödinger equation for the complete Hamiltonian. By considering the spread of the wave-function at the long-time limit we will estimate the bigger localization length inside the wave-packet. Moreover, we also

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apply a renormalization technique based on the Dyson equation for the Green's function elements to estimate the localization length at the band center. Our calculations were carried on chains with short-range exponential correlation on the disorder distribution. Our formalism provides an accurate estimate for the dependence of the localization length with the width of disorder. The results obtained using the two distinct formalisms used here are in agreements within our numerical precision. We numerically investigate the divergence of the large localization length with the correlation length. For weak disorder and small correlation length, the localization length increases cubically with the correlation length. However as the width of disorder is increased, the scaling relation between the localization length and the correlation function changes drastically. At the strong disorder limit, the localization length becomes almost a constant as the correlation length is increased. Our results have shown that there are a counterintuitive competition between the degree of correlations and the disorder strength. We will discuss in detail this competition by analyzing some local properties of the correlated disorder.

2. Model and formalism

The disordered Anderson model is defined by the one-electron Hamiltonian

$$H=\sum_{n=1}^{N}\epsilon_n|n\rangle\langle n|+V\sum_{\langle n,m\rangle}[|n\rangle\langle m|], \tag{1}$$

where $|n\rangle$ is a Wannier state localized at site n and $\sum_{\langle n,m\rangle}$ represents a sum over nearest-neighbor pairs. Here the hopping energy V is taken to be unitary ($V=1$). ϵ_n are the on-site disorder distribution. In our study we will consider systems with short-range correlated on-site disorder distribution. The on-site potential ϵ_n will be generated by using the following formalism: Initially we will calculate the sequence E_n defined by

$$E_n=\sum_m \eta_m * \exp(-|n-m|/\zeta), \quad n=1,\ldots,N, \tag{2}$$

where η_m are independent random number uniformly distributed in the interval $[-0.5,0.5]$ and ζ is the correlation length. We will take account to the sum of Eq. (2) the terms such that $|n-m|<50\zeta$. This cutoff speeds the numerical calculations and does not modify the statistical properties of sequence E_n. The on-site potential ϵ_n is obtained by using the formula

$$\epsilon_n=\Delta*[E_n-\langle E_n\rangle]/\sqrt{\langle E_n^2\rangle-\langle E_n\rangle^2}, \quad n=1,\ldots,N. \tag{3}$$

Therefore the on-site disorder distribution have null mean value ($\langle\epsilon_n\rangle=0$) and fixed standard deviation ($\Delta=\sqrt{\langle\epsilon_n^2\rangle-\langle\epsilon_n\rangle^2}$). The limit $\zeta\to 0$ recovers an uncorrelated disorder distribution. For $0<\zeta<\infty$ we generate a disorder distribution with short-range correlations. To characterized the degree of disorder we will use the standard deviation Δ of the disorder distribution as a tunable parameter. In Fig. 1(a) we plot on-site potentials generated by the preceding formalism. We can note the smoothening of the energy landscape as the localization length is increased. To compare some statistical properties of the above sequences, we compute the auto correlation function ($C(r)=[1/(N-r)]*\sum_{n=1}^{N-r}\epsilon_n\epsilon_{n+r}$) of the potential landscape of segments (see Fig. 1(b)). We can see clearly the exponential decay of the correlation function imposed in our numerical formalism to generate the diagonal potential.

We would like to stress that in Refs. [11,12,30,31] models with exponentially decaying correlations in the disorder distribution were investigated. Particularly, it was analytically studied for the first time in Ref. [11], the Anderson model with exponential correlations in the disorder distribution. The authors obtained, by using a perturbative approach at the weak disorder limit, an analytical expression for the energy-dependent localization length in terms of the intrinsic correlation function. Calculations indicate that for a finite correlation length all eigenstates remains localized [11,12,30]. Moreover, the Anderson model with dichotomic correlated diagonal disorder was investigated in Ref. [31]. The dichotomic or random telegraph process consist of a binary sequence defined by $\epsilon_n=\epsilon_0(-1)^{U_n}$. The initial dichotomic variable ϵ_0 can assume values W or $-W$ with same probability $p=0.5$. U_n denotes a Poisson process and n is the nth lattice site [31]. By using this formalism the authors generated a random process with zero mean ($\langle\epsilon_n\rangle=0$) and the two points correlation function $\langle\epsilon_n\epsilon_{nr}\rangle\propto\exp(-2r/\zeta)$. Calculations of the localization length were done by using a perturbative approach at the weak disorder limit. It was shown analytically the absence of the extended state in this limit [31]. In our manuscript we revisit the problem of one-electron moving in chains with exponentially decaying correlations in the disorder distribution on light of numerical formalisms based on the time-dependent Schrödinger equation and also renormalization group technique.

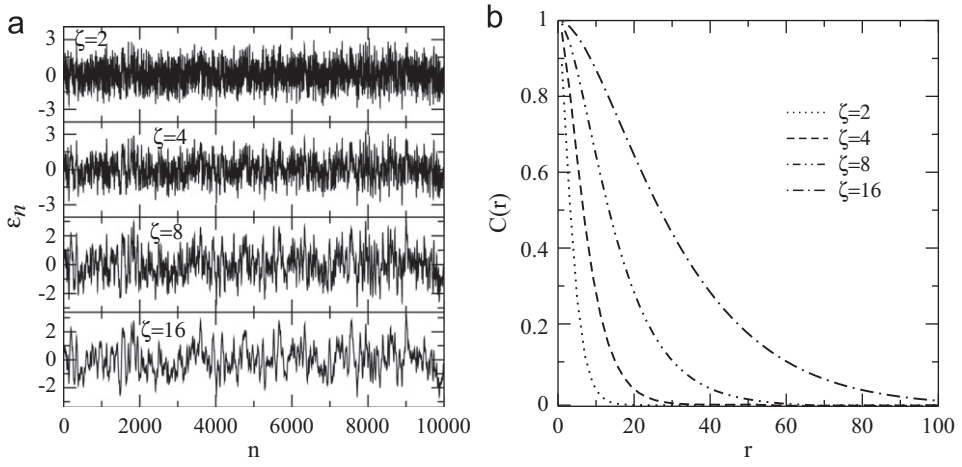

Fig. 1. (a) The on-site energy landscape with exponentially decaying correlations. Notice the smoothening of the energy landscape as the ζ is increased. (b) Numerical calculation of the two-point auto correlation function defined by $C(r)=[1/(N-r)]*\sum_{n=1}^{N-r}\epsilon_n\epsilon_{n+r}$.

3. Numerical calculation

We will follow the time evolution of an initially localized wave packet. The Wannier amplitudes evolve in time according to the time-dependent Schrödinger equation as ($\hbar = 1$)

$$i\frac{dc_n(t)}{dt} = \epsilon_n c_n(t) + \sum_{\langle m \rangle} c_m(t). \tag{4}$$

We consider a wave packet initially localized at site n_0, i.e. $|\Phi(t=0)\rangle = \sum_n c_n(t=0)|n\rangle$ where $c_n(t=0) = \delta_{n,n_0}$. The above set of equations were solved numerically by using a high-order method based on the Taylor expansion of the evolution operator $U(\Delta t)$

$$U(\Delta t) = \exp(-iH\Delta t) = 1 + \sum_{l=1}^{l_o} \frac{(-iH\Delta t)^l}{l!}, \tag{5}$$

where H is the Hamiltonian. The wave-function at time Δt is given by $|\Phi(\Delta t)\rangle = U(\Delta t)|\Phi(t=0)\rangle$. The method can be used recursively to obtain the wave-function at time t. To obtain $H^l|\Phi(t=0)\rangle$ we will use a recursive formula derived as follow. Let define $H^l|\Phi(t=0)\rangle = \sum_n C_n^l|n\rangle$. Using the Hamiltonian formula (Eq. (1)) we can compute $H^1|\Phi(t=0)\rangle$ and obtain C_n^1 as

$$C_n^1 = \epsilon_n c_n(t=0) + \sum_{\langle m \rangle} c_m(t=0), \tag{6}$$

where $\sum_{\langle m \rangle}$ represents a sum over nearest-neighbor pairs. Therefore, using that $H^l|\Phi(t=0)\rangle = H\sum_n C_n^{l-1}|n\rangle$, C_n^l can be obtained recursively as

$$C_n^l = \epsilon_n C_n^{l-1} + \sum_{\langle m \rangle} C_m^{l-1}. \tag{7}$$

The following results were taken by using $\Delta t = 0.5$ and the sum was truncated at $l_o = 15$. This cutoff was sufficient to keep the wave-function norm conservation along the entire time interval considered ($t_{max} \gg 10^5$). This formalism is faster than high order Runge–Kutta methods and it is easier to implement. We are particularly interested in calculating the wave packet mean-square displacement $\sigma(t)$ defined by [21]

$$\sigma(t) = \sqrt{\sum_n [(n-n_0)^2]|c_n(t)|^2}. \tag{8}$$

Note that $\sigma(t)$ varies from 0, for a wave function confined to a single site, to proportional to number of sites, for a wave uniformly extended over the whole system. We are interested in the long time behavior of mean square displacement $\Sigma = \lim_{t\to\infty}\sigma(t)$ in our calculation we will use $t_{max} > 10^6$. In addition we will estimate directly the localization length by using a general renormalization technique which is based on the particular form assumed by the Dyson equation [8]

$$(E-\epsilon_m^0)G_{m.n} = \delta_{m.0} + H_{m,m-1}G_{m-1,n} + H_{m,m+1}G_{m+1,n}, \tag{9}$$

where $G_{m,n} = \langle m|1/(E-H)|n\rangle$ is the Green's function elements and $H_{m,m\pm1} = V = 1$. After eliminating the elements associated with a given site, the remaining set of equations of motion can be expressed in the same form as the original one but with site energies and hopping amplitude renormalized. Therefore, we can remove iteratively the sites 1,2,3, ...,N of the lattice, obtaining the effective energies of the extremal sites and the effective hopping interaction between them through the following three iterative equations:

$$\epsilon_0^{N+1} = \epsilon_0^N + V_{0,N}^{eff}\frac{1}{E-\epsilon_N^{N-1}}, \tag{10}$$

$$\epsilon_{N+1}^N = \epsilon_N^0 + \frac{1}{E-\epsilon_N^{N-1}}, \tag{11}$$

$$V_{0,N+1}^{eff} = V_{0,N}^{eff}\frac{1}{E-\epsilon_N^{N-1}}, \tag{12}$$

where ϵ_0^N and ϵ_{N+1}^N are respectively the effective energy at sites 0 and $N+1$ after the decimation of the N internal sites. $V_{0,N+1}^{eff}$ is the effective hopping between sites 0 and $N+1$. The localization length is defined as [8]

$$\lambda = \left\{-\lim_{N\to\infty}\frac{1}{N}\log|V_{0,N+1}^{eff}|\right\}^{-1}. \tag{13}$$

In our calculations we compute the average localization length defined by $\Lambda = (1/N_f)\sum_{E=-0.01}^{E=0.01}\lambda(E))$ where N_f is the number of eigenstates within each interval $[-0.01,0.01]$. $\Lambda \propto N$ for extended states and it is finite for exponentially localized ones. From the point of view of time-dependent Schrödinger equation, the long lime electronic spread is dominated by the eigenvector with larger localization length, i.e. the localization length at the band center. Therefore, we expected that $\Sigma \approx \Lambda$.

4. Results

Initially, we numerically obtained the time evolution of a wave-packet initially localized at center of a self-expanding chain (i.e. $\{c_n(t=0) = \delta_{n,n_0}\}$). The self-expanding chain was used to minimize end effects;whenever the probability of finding the particle at the ends of the chain exceeded 10^{-30}, ten new sites were added to each end. The high-order method based on the Taylor expansion of the evolution operator is used to solve the set of time-dependent Schrödinger coupled equations (Eq. (4)). Numerical convergence was ensured by conservation of the norm of the wave-packet at every time step, i.e., $|1-\sum_n|c_n(t)|^2| < 10^{-10}$. All calculations were averaged over 30 disorder configurations. Calculations of localization length were done by using Green function method for chains with $N \approx 5\times10^7$. We will start our calculations by reproducing some previous results about electron localization in chains with uncorrelated disorder [1,30]. To simulate chains with uncorrelated disorder we will consider ϵ_n as independent random number with zero mean $\langle\epsilon_n\rangle = 0$ and fixed standard deviation ($\Delta = \sqrt{\langle\epsilon_n^2\rangle - \langle\epsilon_n\rangle^2}$). In Fig. 2 we plot

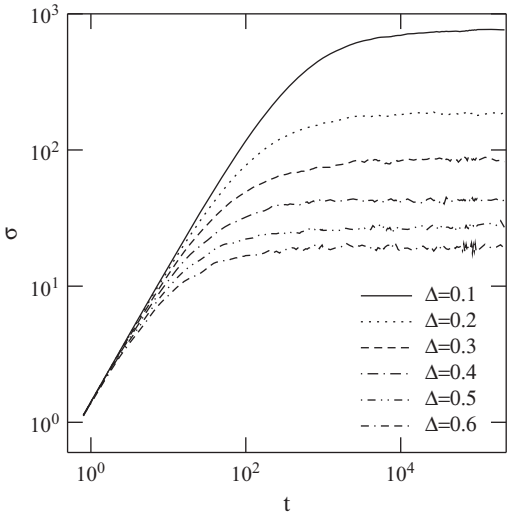

Fig. 2. Calculations of the wave packet mean-square displacement in a chain with uncorrelated diagonal disorder distribution with standard deviation $\Delta = 0.1$ up to 0.6. The initial condition was an initially localized one-electron wave-packet at the center 0 of the chain (i.e. $\{c_n(t=0) = \delta_{n,n_0}\}$). The spread of wave-function increases as the disorder degree Δ is decreased.

the wave packet mean-square displacement $\sigma(t)$ versus time t for a chain with uncorrelated diagonal disorder distribution with standard deviation $\Delta = 0.1$ up to 0.6. In good agreements with localization theory [1,30], the mean-square displacement is increasing as the disorder degree Δ is decreased. In Fig. 3 we collect the long time limit of the mean-square displacement $\Sigma = \lim_{t\to t_{max}} \sigma(t)$ versus the standard deviation of the on-site energy distribution Δ (see ($\triangleleft$) in Fig. 3). The best fit (dotted line) provide us $\Sigma \propto \Delta^{-2.00(5)}$. In Fig. 3 ($\diamond$) represent calculations of mean localization length at band center Λ versus Δ for the same chain with uncorrelated diagonal disorder. We can see that both results agree within numerical tolerance($\Lambda \propto \Delta^{-2.00(5)}$). Our results are in perfect agreements with previous prediction about degree of localization in 1d models with uncorrelated disorder [1,30]. Therefore, both formalisms provide accurate estimate of the degree of electronic localization in disordered systems. Now, we start our numerical analysis about the effect of short-range exponential correlation on the disorder distribution. We have generated the diagonal disorder by using the formalism described in Eqs. 2 and 3. Before show our results some words about numerical procedure and accuracy. The numerical calculation involving direct solution of Schrödinger equation, even using high order methods, require much computational time. Moreover, depending on the magnitude of largest localization length, the numerical precision obtained by using Green's function method is more interesting. As the correlation length is increased, the error bar obtained by using direct solution of Schrödinger equation becomes two or three times larger than the error bar obtained by using Green's function method. Therefore, from now we will show results obtained by using Green function formalism. However, we would like to stress that both calculations are in agreements within error bars. In Fig. 4(a) we show the log–log plot of the localization length Λ versus standard deviation Δ for several values of the correlation length ζ. Here we used $\Delta = 0.1$ up to 0.55. In general, Λ increases as ζ is increased. We can see also that, as was predicted in Ref. [30] even in the presence of short-range correlation $\Lambda \propto \Delta^{-2}$. However, about $\zeta > 7$ it seems that the localization length does not obey the power law tendency $\Lambda \propto \Delta^{-2}$ in the regime of disorder $\Delta > 0.45$. At the strong disorder limit (i.e. disorder width comparable with the band width) the effect of short range correlations within diagonal terms works in a counterintuitive way. This effect is analyzed in detail in Figs. 5 and 6. For a finite amount of disorder Δ the localization length becomes comparable to the size system.

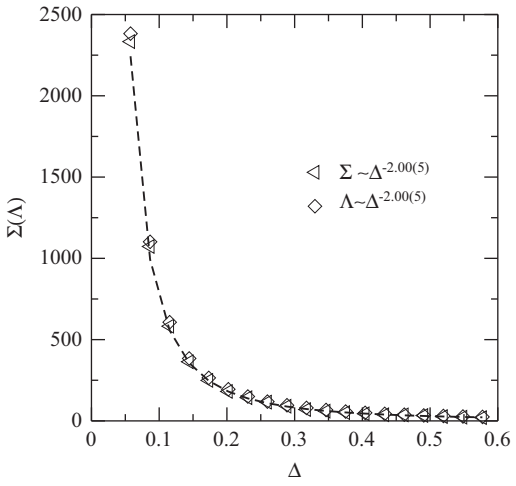

Fig. 3. ($\triangleleft$) The long-time limit of the mean-square displacement $\Sigma = \lim_{t\to t_{max}} \sigma(t)$ versus the standard deviation of the on-site energy distribution Δ. The best fit (dotted line) provide us $\Sigma \propto \Delta^{-2.00(5)}$. ($\diamond$) The same result obtained following localization length calculations at band center Λ.

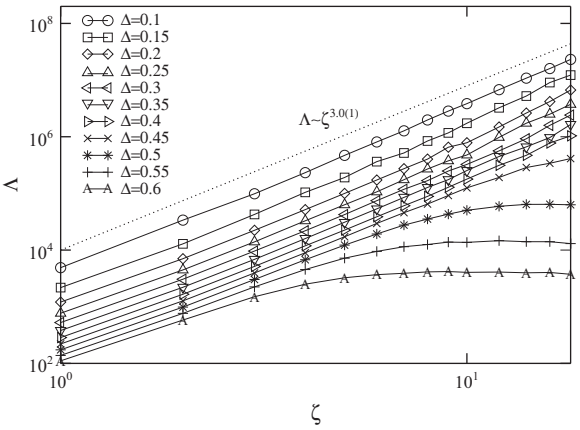

Fig. 5. Degree of localization versus ζ for $\Delta = 0.1$ up to 0.6. For weak disorder ($\Delta \ll 0.5$), the localization length scale is proportional to ζ^3. From another side, for large Δ short-range correlations are not sufficient to weaken the localization effects of a strong disorder distribution and Λ apparently saturates in a finite value as ζ is increased.

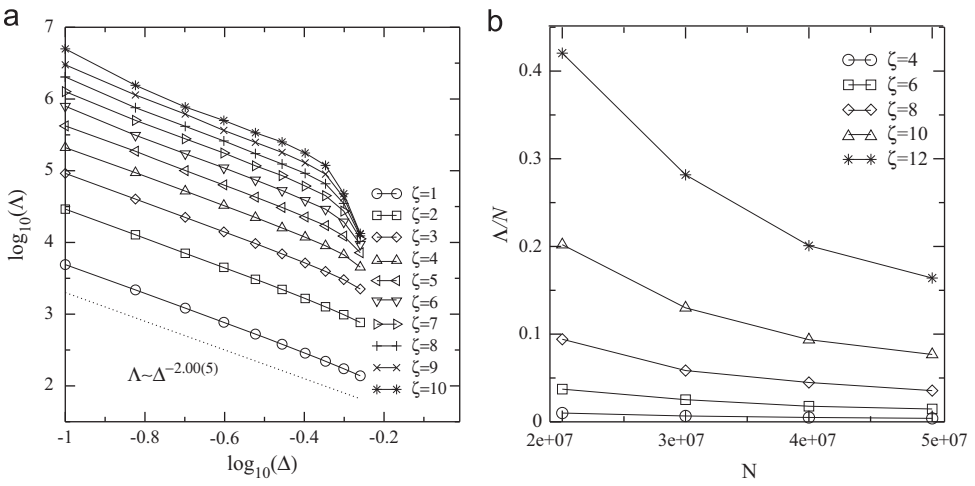

Fig. 4. (a) Localization length Λ versus standard deviation Δ for several values of the correlation length ζ. Λ increases as ζ is increased and the scaling behavior with Δ does not change qualitatively $\Lambda \propto \Delta^{-2}$. (b) Scaled localization length Λ/N versus system size for $\Delta = 0.1$ and $\zeta = 4$ up to 12. Finite size scaling suggest a finite localization length at the thermodynamic limit.

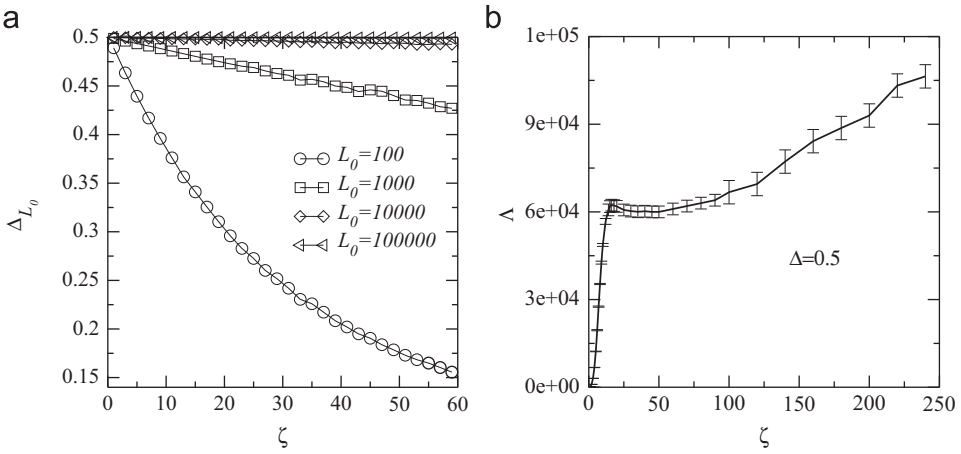

Fig. 6. (a) Δ_{L_0} versus ζ computed in on-site disordered sequences with standard deviation $\Delta = 0.5$, $N = 10^7$ and distinct values of L_0. In general lines in good agreements with usual theory of correlated random process, we observe the decreasing of the local disorder as the correlation length is increased. Moreover, for a fixed value of ζ, the local disorder degree increases as L_0 is increased. (b) Localization length Λ versus ζ computed in a chain with standard deviation $\Delta = 0.5$ and $N = 10^7$ sites. We can see the counterintuitive dependence of Λ with ζ. For small correlation length our results indicate a cubic increase. For an intermediate range of correlation length, the effect of the local disorder is majoritary thus stabilizing the localization length in a constant. For a large correlation length, the local disorder will decrease substantially and the localization length return to increase.

However, as was reported in Ref. [30], that this model does not contain extended states. In Fig. 4(b) we can see a finite size scaling analysis of the scaled localization length Λ/N versus system size $N = 2 \times 10^7$ up to 5×10^7. We have considered weak disorder $\Delta = 0.1$ and several values of the correlation length ($\zeta = 4$ up to 12). We have obtained $\Lambda/N \propto 1/N$ that indicate a finite localization length at the thermodynamic limit in good agreements with Ref. [30]. In Fig. 5 we study the scaling of the degree of localization with the correlation length ζ. We plot Λ versus ζ for $\Delta = 0.1$ up to 0.6. For weak disorder ($\Delta \leq 0.45$), the localization length scale proportional to ζ^3 within range of correlation length used here ($\zeta = 1$ up to 18). For strong disorder($\Delta > 0.45$), Λ increases cubically with ζ within range $1 \leq \zeta < 10$ however apparently saturates in a finite value smaller than the system size when $\zeta > 10$. Therefore, there are a counterintuitive competition between the degree of correlations and the disorder strength. We now discuss in detail this competition by analyzing some local properties of the on-site short-range correlated disorder. Let us compute the local standard deviation Δ_{L_0} of the on-site energies of a segment with L_0 sites. The local standard deviation Δ_{L_0} is defined by

$$\Delta_{L_0} = \left(\sum_{k=1}^{M} \Delta_{k,L_0} \right) \Big/ M, \tag{14}$$

where

$$\Delta_{k,L_0} = \sqrt{\sum_{i=(k-1)L_0+1}^{i=kL_0} (\epsilon_i)^2 / L_0 - \left(\sum_{i=(k-1)L_0+1}^{kL_0} \epsilon_i / L_0 \right)^2}, \tag{15}$$

and $M = N/L_0$. Δ_{L_0} is a measurement of the local disorder strength in a segment with L_0 sites. In Fig. 6(a) we plot Δ_{L_0} versus ζ computed by using Eqs. (14) and (15) in on-site potential sequences with standard deviation $\Delta = 0.5$ and $N = 10^7$. Calculations were done for $L_0 = 100, 1000, 10\,000, 100\,000$. We can see initially that for $L_0 = 100$ and 1000, Δ_{L_0} decreases substantially as the correlation length is increased. For $L_0 = 10\,000$ and $100\,000$ we observe also a decreasing with ζ however much slower. In general lines the decreasing of the local disorder as the correlation length is increased is in good agreements with usual theory of correlated random process. Our best fit indicate that the local disorder goes to zero as $\Delta_{L_0} \propto \exp[-B(L_0)\zeta]$. The exponential decay of the local disorder with ζ is related with kind of correlated disorder we have used. Let us return to discuss the data of Fig. 6(a) for distinct values of L_0. We observe that, for a fixed ζ, the local disorder degree increases as L_0 is increased. This behavior is the key ingredient behind the apparent saturation of localization length found in Fig. 5. Let us focus on the strong disorder case ($\Delta \geq 0.45$): When the correlation length increases the localization length increases up to 10^4 or 10^5 sites. Therefore, the wave-function is trapped in a finite segment with about 10^4 or 10^5 sites. As we saw in Fig. 6(a), for the range of ζ used in our calculation, the strength of the disorder within a segment with 10^4 or 10^5 sites is comparable to the standard deviation of disorder Δ. Therefore, in this case, the strong local disorder will compete with the correlation effect slowing the increasing of the localization length. For a large correlation length, the local disorder will decrease substantially and the localization length will return to increase. We can see this behavior in Fig. 6(b). However, the large computational times needed at the limit of high correlation, force us to decrease the number of samples thus decreasing the accuracy. Therefore, we have obtained a big error bar for our date and the scaling behavior of the localization length with the correlation length was not obtained in this case.

5. Summary and conclusions

In this work, we studied the localization aspects of a one-dimensional system with a diagonal disorder distribution containing an exponential correlation function. The degree of correlations was controlled by the correlation length ζ. For $\zeta = 0$, we recovered the Anderson model with an uncorrelated diagonal disorder distribution. For $0 < \zeta < \infty$, we generated a disorder distribution with short-range correlations. By considering the spread of a wave-function at long-time, we calculated the largest localization length inside the wave-packet. Moreover, we also applied a renormalization technique based on the Dyson equation for Green's function elements to estimate the localization length at the band center. The results obtained using the two distinct formalisms are in agreement within our numerical precision. We would like to stress that the estimation of larger localization lengths based on long-time behavior of the wave-packet, in spite of being more expensive computationally, is a good technique for studying localization length aspects of high dimensional systems. Within the context of models having an exponentially correlated

disorder distribution, our results indicate that these correlations do not drastically modify the divergence of localization length with degree of disorder ($1/\Delta^2$). Moreover, by using a finite size scaling analysis, we predicted that the localization length, in spite of being large, is finite at the thermodynamic limit. Both results are in good agreement with previous works [30,31]. In addition, we investigated the divergence of the localization length with the correlation length. For weak disorder ($\Delta < 0.5$), the localization length is proportional to ζ^3. Our calculations for weak disorder were limited to small correlation length limit $\zeta < 20$. To analyze in detail the range $\zeta \gg 20$ within the weak disorder framework, we would need to consider a system size N that is much larger than our computational limit ($N \gg 10^8$ sites). A one-dimensional model with short-range correlated diagonal disorder similar to that was considered here was investigated in Ref. [30]. By using a Hamiltonian map approach, it was demonstrated that the localization length increases linearly with the correlation length [30]. The authors used perturbation theory at the weak disorder limit and large correlation length [30]. We believe that is difficult to compare our results with previous one since we cannot consider with good accuracy the range of large correlation length. For strong disorder and a small correlation length, the degree of localization increases also cubically with ζ. However, for an intermediate range of correlation length, due to the drastic effects of local disorder, the localization length apparently saturates in a finite value smaller than the system size. For a large correlation length, the local disorder will decrease substantially, and the localization length will return to increase. Our results show a relation between the local properties of the disorder distribution and the localization aspects. The presence of correlation in the disorder distribution can be understood as a smoothing of the disorder in a finite segment of the sample. This smoothing can be directly measured by monitoring the strength of the local disorder. We hope that our paper can stimulate discussion along this line.

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