Critical wave-packet dynamics in the power-law bond disordered Anderson model

R. P. A. Lima, F. A. B. F. de Moura, and M. L. Lyra
Departamento de Física, Universidade Federal de Alagoas, Maceió AL 57072-970, Brazil

H. N. Nazareno
ICCMP, Universidade de Brasília, Caixa Postal 04513, 70919-970, Brasília-DF, Brazil
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We investigate the wave-packet dynamics of the power-law bond disordered one-dimensional Anderson model with hopping amplitudes decreasing as $H_{nm} \propto |n-m|^{-\alpha}$. We consider the critical case ($\alpha=1$). Using an exact diagonalization scheme on finite chains, we compute the participation moments of all stationary energy eigenstates as well as the spreading of an initially localized wave packet. The eigenstates multifractality is characterized by the set of fractal dimensions of the participation moments. The wave packet shows a diffusivelike spread developing a power-law tail and achieves a stationary nonuniform profile after reflecting at the chain boundaries. As a consequence, the time-dependent participation moments exhibit two distinct scaling regimes. We formulate a finite-size scaling hypothesis for the participation moments relating their scaling exponents to the ones governing the return probability and wave-function power-law decays.

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I. INTRODUCTION

Noninteracting electron systems with uniformly distributed disorder usually show an Anderson transition from localized to extended states. In general, such a transition occurs only for spatial dimensions greater than $d=2$ in the case of systems with short-range hopping, a result supported by a single parameter scaling theory.[1,2] On the other hand, when long-range couplings are assumed, a transition from localized to delocalized electronic states can be found even in one-dimensional (1D) disordered systems.[3,4] In this case, one has an interplay between the hopping range and the degree of disorder. The former favors propagation while the later inhibits it. It is worthwhile to mention that propagation of carriers was also obtained in low-dimensional models with short-range hopping but presenting correlated disorder, such as random dimer chains[5–8] and in chains with scale-free disorder,[9–11] as well as in chains containing quasiperiodic structures, as for example Fibonacci, Thue-Morse, and Harper sequences.[12–14]

On the other hand, for an ordered 1D system with hopping terms decaying with a power law with exponent α, it was shown that for $\alpha>2$ one recovers the result for the tight-binding model.[15] More interesting is the behavior corresponding to $0<\alpha<1$. For $\alpha=0$ an initially localized wave packet presents *self-trapping*, i.e., the particle performs oscillations in a definite region of the lattice, visiting periodically the starting position. By increasing α the localization is lost. When the power exponent equals unity, and for sufficient short times, the packet diffuses with a diffusion coefficient that increases with the number of sites. This effect is absent in the model with only nearest-neighbor hopping.[15]

More recently, the dynamics of an electron in a one-dimensional Anderson model with nonrandom hopping terms falling off as some power α of the distance between sites was investigated.[16] It was found that the larger the hopping range, the more extended the wave packet becomes as time evolves. When the disorder is increased, the wave packet tends to remain more localized. For a low degree of disorder, the exponent $\alpha=1.5$ indicates the onset for fast propagation. Moreover, the inclusion of a dc electric field introduces the effect of dynamical localization. The fast propagation found for $\alpha<1.5$ is in agreement with the reported delocalization of states located close to one of the band edges.[17–19]

The power-law random band matrix (PRBM) model also exhibits a delocalization transition.[3,4] This model describes one-dimensional electronic systems with random long-range hopping amplitudes with standard deviation decaying as $1/r^{\alpha}$ for sites at a distance $r \gg b$, where b is a typical bandwidth. It was shown that at $\alpha=1$ it presents an Anderson-like transition with all states being localized for $\alpha>1$ and extended for $\alpha<1$. At the critical point $\alpha=1$, the inverse participation ratio distribution, the wave functions multifractal spectra, the level statistics, and the time evolution of the wave-packet size have been investigated both analytically and numerically.[3,4,20–23] Within the same spirit of the PRBM, a model for noninteracting electrons in a two-dimensional (2D) lattice with random on-site potentials and random power-law decaying transfer terms was numerically investigated by exploring the finite-size scaling properties of the fluctuations in the mean level spacing.[24] It was found that the one-electron eigenstates become extended for transfer terms decaying slower than $1/r^2$. Finally, the Anderson transition in a 1D chain with random power-law decaying hopping terms and nonrandom on-site energies was numerically characterized in Ref. 25.

The moments of the position and those of the related probability density are known to exhibit different scaling behaviors.[26] This feature reflects the complexity of the scaling laws governing the dynamics of quantum systems.[27] In this paper, we investigate the critical dynamics of the power-law bond disordered Anderson model ($\alpha=1$) by looking at the moments of the wave-function probability distribution. Using an exact diagonalization scheme on finite chains, we compute the participation moments of all energy eigenstates and follow the time evolution of an initially localized wave

packet. After that, we perform an average of the participation moments over different configurations and energies, which allow us to compute the critical exponents D_q associated with the multifractal character of the critical eigenfunctions. Examining the time evolution of an initially localized wave packet, we obtain the decay exponent of the autocorrelation function $[C(t) \propto t^{-D_2}]$ and the size dependence of the asymptotic return probability $[R(t) \propto N^{-D_2^{\Psi}}]$. The exponent D_2^{Ψ} also governs the power-law decay of the wave packet.[27] We will employ a finite-size scaling analysis of the time dependent participation number moments, relating their scaling exponents with the power-law exponents of the evolving wave packet.

II. MODEL, FORMALISM, AND RESULTS

A. Model Hamiltonian

We consider a single electron in a 1D chain with open boundaries, described by the Anderson Hamiltonian

$$H = \sum_{n \neq m}^{N} H_{nm} |n\rangle\langle m|, \tag{1}$$

where $|n\rangle$ represents the state with the electron localized at site n. In the present random bond Anderson model, the on-site potentials ϵ_i are site independent and in Eq. (1) were taken to be $\epsilon_i = 0$ without any loss of generality. Long-range disorder is introduced by assuming the hopping amplitudes H_{ij} to be randomly distributed and also displaying a power-law decay. We will, hereafter, consider

$$H_{nm} = W_{nm} / |n - m|^{\alpha}, \tag{2}$$

where W_{nm} is a random variable with a uniform distribution in the interval $[-1, +1]$. As a function of the exponent α characterizing the decay of the hopping amplitudes, this model displays a localization-delocalization transition at $\alpha = 1$ (Ref. 25) in close connection with the PRBM.[3,4] For off-diagonal terms decaying slower than $1/|n-m|$, i.e., for $\alpha < 1$, all states become delocalized. At $\alpha = 1$ the states are critical and the level spacing statistics is between the Poison and Wigner surmises. In the limit of $\alpha \to \infty$ one recovers the 1D Anderson model with just first-neighbors random hopping amplitudes.

B. Eigenfunctions participation moments

We will be particularly interested in investigating the participation moments and the time evolution of an initially localized wave packet at the critical point $\alpha = 1$. The participation moments for a particular disorder configuration and eigenstate will be defined as the inverse of the moments of the probability density

$$P_q^j = \frac{1}{\sum_{n=1}^{N} |f_n^j|^{2q}}, \tag{3}$$

where $f_n^{(j)}$ is the amplitude at site n of the jth eigenstate obtained from an exact diagonalization scheme on finite chains with sizes ranging from $N = 400$ up to $N = 3200$ sites.

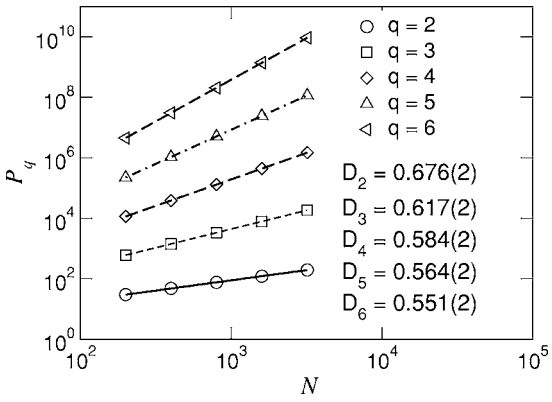

FIG. 1. The average participation moment (P_q) as a function of the chain size (N) for several values of q ranging from 2 to 6. The distinct fractal dimensions ($P_q \propto N^{D_q(q-1)}$) exhibited by the participation moments reflect the multifractality of the critical eigenstates.

Here we used 32×10^3 states for each chain size in order to average over distinct disorder configurations and energies

$$P_q = \left\langle \frac{\sum_{j=1}^{N} P_q^j}{N} \right\rangle, \tag{4}$$

where $\langle\rangle$ stands for configuration average. Therefore, P_q probes the average qth moment of the critical stationary states. In Fig. 1 we show the finite-size scaling of different moments ranging from $q = 2$ up to $q = 6$. As it has been shown by Wegner,[28] all moments show a power-law dependence on the form $[P_q \propto N^{D_q(q-1)}]$. Each moment has its characteristic exponent D_q as indicated in Fig. 1, which reflects the multifractality of the critical eigenstates. Our results indicate that the fractal dimension D_q slowly decreases from $D_2 = 0.676$ towards the asymptotic value $D_\infty = 0.5$.

C. Wave-packet dynamics

In order to obtain the time evolution of an initially localized wave packet $[|\Phi(t=0)\rangle]$, we expand the wave function in the Wannier representation

$$|\Phi(t)\rangle = \sum_n f_n(t) |n\rangle. \tag{5}$$

We solve the time-dependent Schrödinger equation for the wave-function components $f_n(t)$ $(\hbar = 1)$

$$i \frac{df_n(t)}{dt} = \sum_{n \neq m}^{N} \frac{W_{nm}}{|n-m|^{\alpha}} f_n(t), \tag{6}$$

using the numerical formalism proposed in Ref. 29

$$|\Phi(t)\rangle = \mathbf{U}^{\dagger} \exp(-i\mathbf{D}t)\mathbf{U}|\Phi(t=0)\rangle, \tag{7}$$

where $\mathbf{D}$ is the diagonal form of the Hamiltonian and $\mathbf{U}$ is a unitary matrix. An advantage of the above method in comparison with those employing numerical solutions of the time-dependent Schrodinger equation is the fact that it is free of the propagation of errors. As the method is based on the complete diagonalization of the Hamiltonian, the size of the

system is limited by the computational capability of dealing with large matrices. However, the wave-packet dynamics in the limit of infinite chains can be extrapolated using finite-size scaling arguments. In what follows we consider the electron initially localized in a single site, i.e., $|\Phi(t=0)\rangle=|n_0\rangle$. We start by discussing the behavior of the autocorrelation function

$$C(t)=\frac{1}{t}\int_0^t R(t')dt', \tag{8}$$

where $R(t)=|f_{n_0}(t)|^2$ denotes the return probability.[30] The time-dependent autocorrelation function provides information about localization of the wave packet as well as of its fractal character. In fact, after an initial waiting time, the autocorrelation function shall behave as

$$C(t)\propto t^{-D_2}, \tag{9}$$

for one-dimensional systems, which by definition is the same power-law decay presented by the return probability. In Fig. 2(a) we plot the return probability for $t\to\infty$ as a function of the number of sites. After the initial decay due to the wave-function spread, it saturates at a size-dependent plateau, which decreases as $1/N^{D_2^{\Psi}}$. In Fig. 2(b), the autocorrelation function versus time t is shown for different chain sizes. It exhibits a power dependence for intermediate times whose exponent is in good agreement with the previous estimate for D_2. Its saturation for $t\to\infty$ has the same finite-size origin presented by the return probability.

The asymptotic return probability decaying slower than $1/N$ indicates that the statistically stationary wave function does not assume a uniform profile. In Fig. 3 we plot the average stationary wave-function profile achieved long after the wave-function reflection at the chain boundaries. It develops a power-law decaying tail with $|f_n(t\to\infty)|^2\propto 1/(n-n_0)^{1-D_2^{\Psi}}$ (see inset), as expected according to the wave-function normalization constraint. Before reaching the chain boundaries, the average wave-function envelope can be well described by

$$|f(n,t)|^2=R(t)(n-n_0+1)^{-(1-D_2^{\Psi})} \tag{10}$$

for $n-n_0<N^*(t)$, where $N^*(t)$ is a time-dependent cutoff after which the wave function decays exponentially and, therefore, can be considered as having a vanishing amplitude. The return probability decays as $R(t)\propto t^{-D_2}$. It is straightforward to show, using the normalization criterium, that the cutoff shall scale as $N^*(t)\propto t^{D_2/D_2^{\Psi}}$. The above asymptotic power-law shape of the wave function is in agreement with the previous prediction for the wave-packet spreading in quantum systems with fractal energy spectra and eigenfunctions.[27] For distances larger than the cutoff $N^*(t)$, numerical data as well as analytical results based on the memory function formalism have shown that the tail of a diffusing wave packet actually assume a stretched exponential form whose characteristic exponent is related to the diffusion exponent D_2/D_2^{Ψ}.[31] We further calculated the time-dependent participation moments

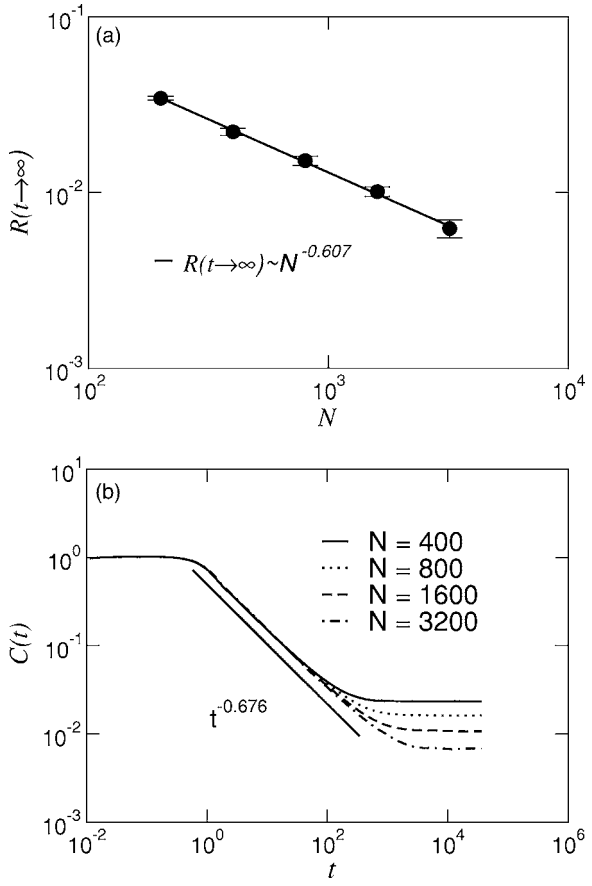

FIG. 2. (a) The return probability function for $t\to\infty$ as a function of the number of sites. The small power-law decay exponent $R(t\to\infty)\propto N^{-D_2^{\Psi}}$, with $D_2^{\Psi}=0.607(10)$, is consistent with a wave function with a slowly decaying envelope. (b) Autocorrelation function vs time t for chains with $N=400$ up to $N=3200$ sites. The power-law decay for intermediate times with an exponent $D_2=0.676$ is in good agreement with the previous numerical estimate for D_2.

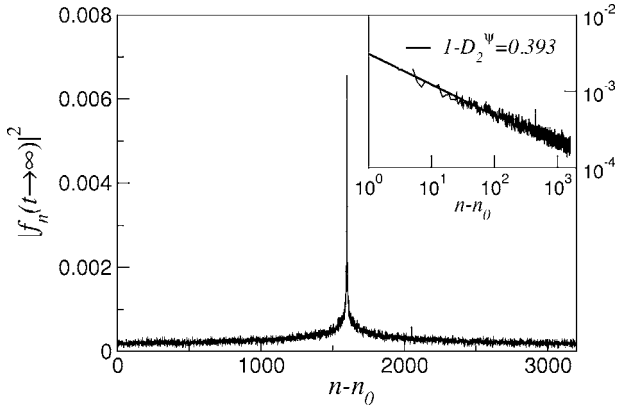

FIG. 3. Average wave-function profile after a very long evolution time ($t\to\infty$). In the inset, we note that the envelope displays a power-law decay with an exponent $1-D_2^{\Psi}=0.393$, is agreement with the measure exponent of the asymptotic return probability.

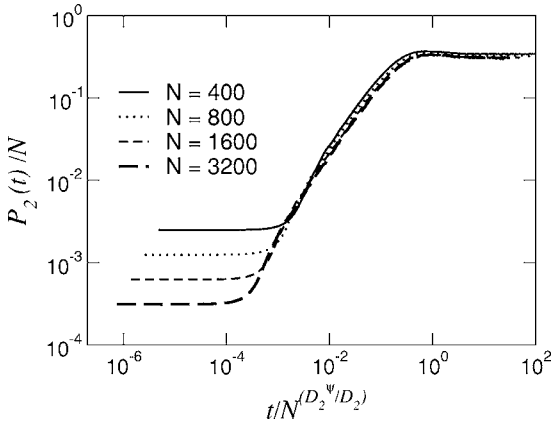

FIG. 4. The normalized average participation number P_2/N as a function of the scaled time $(t/N^{D_2^\Psi/D_2})$. After a short transient time, the data collapse indicates that the participation number grows as t^{D_2/D_2^Ψ} and saturates after the wave-function reflection at the chain boundaries. The destructive interference that sets up during the reflection at the boundaries is signaled by a maximum in P_2. The data collapse corroborates the scaling hypothesis in Eq. (12).

$$P_q(t) = \left\langle \frac{1}{\sum_n^N |f_n(t)|^{2q}} \right\rangle. \tag{11}$$

The second moment (P_2) has been commonly used as a measurement of the number of sites that participate in the wave function. For a wave packet fully localized at a single site, $P_2=1$, while for a uniform distribution of the wave function, P_2 reaches the maximum value N. In general, P_2 is size independent in the localized phase and scales linearly with the system size for extended states.

In the present case, for which the wave function develops the power-law form given by Eq. (10), the participation moments present a nontrivial scaling. Two distinct behaviors can be anticipated. For $q<1/(1-D_2^\Psi)$, the participation moment shall display a power-law growth (after a short waiting time) on the form $P_q(t) \propto t^{(q-1)D_2/D_2^\Psi}$, followed by a saturation after reaching the chain boundaries. The saturation plateau is predicted to scale as $P(N,t\to\infty) \propto N^{(q-1)}$. Both time regimes can be represented by a single finite-size scaling hypothesis for the participation moment which can be written as

$$P_q(t,N) = N^{(q-1)} g(t/N^{D_2^\Psi/D_2}), \tag{12}$$

with $g(x\to\infty)$ being a constant due to the wave-packet reflection at the chain boundaries and $g(x\to 0) \propto x^{(q-1)D_2/D_2^\Psi}$ in order to leave the participation moment size independent at intermediate times prior to the reflection. In Fig. 4, we show our numerical results for the scaled second moment (P_2/N) vs scaled time $(t/N^{D_2^\Psi/D_2})$, which falls in the above regime of $q<1/(1-D_2^\Psi)$. These data were averaged over 100 time histories considering distinct disorder configurations. The second moment remains constant during a very short initial waiting time before the spread effectively starts to take place. After that, we found that the above scaling hypothesis reproduces very well the participation time evolution as data from distinct chain sizes could be collapsed in the same curve. As anticipated, the participation moment has a power-law growth followed by a saturation. The slight deviation from perfect collapse is due to corrections to scaling that are more pronounced for the smaller system sizes. The maximum displayed by the participation number reflects the destructive interference between the incident and reflected waves near the chain boundaries.

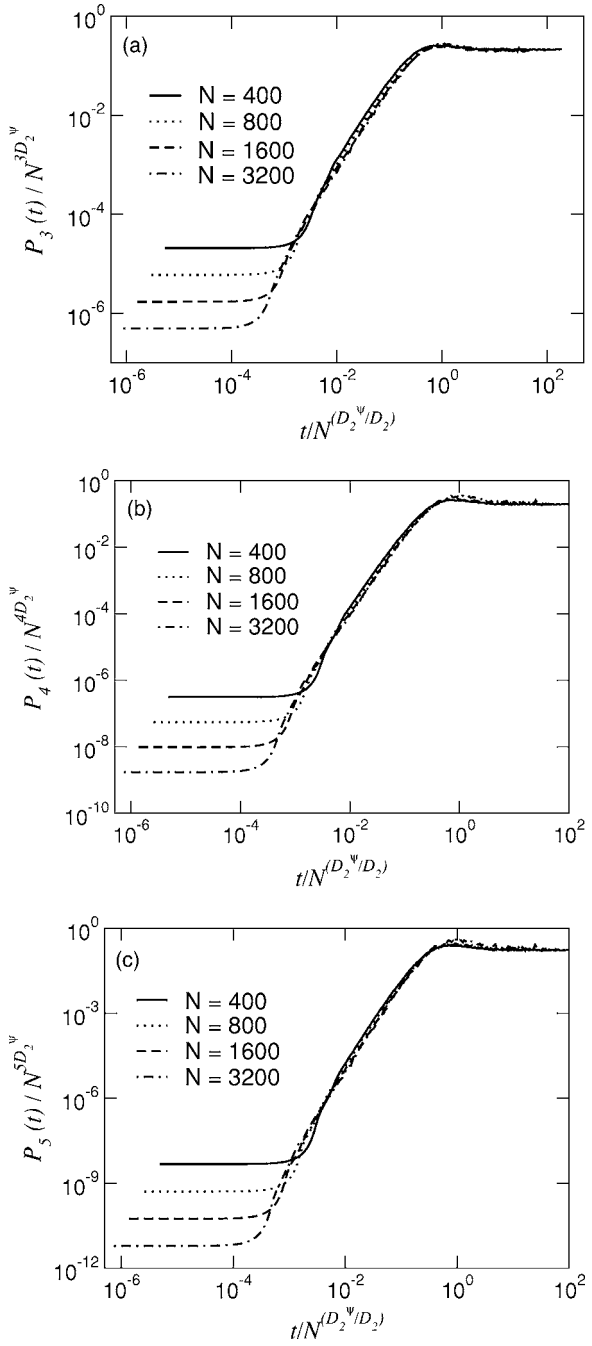

FIG. 5. Scaled participation moments $P_q(N,t)/N^{qD_2^\Psi}$ as a function of the scaled time $(t/N^{D_2^\Psi/D_2})$ for $q=3,4,5$. The data collapse corroborates the scaling hypothesis in Eq. (15). The maximum, also appearing in Fig. 4, signals the destructive interference between the incident and reflected waves near the chain boundaries.

For $q > 1/(1-D_2^{\Psi})$, the presence of a cutoff does not influence the initial spread of the participation moments. Therefore, the initial growth is completely determined by the return probability decay and results in $P_q(t) \propto t^{qD_2}$. On the other hand, the scaling of the asymptotic plateau only depends on the wave-function decay exponent, being given by $P(N, t \to \infty) \propto N^{qD_2^{\Psi}}$. For this regime, the proper scaling form of the participation moment reads

$$P_q(t,N) = N^{qD_2^{\Psi}} g'(t/N^{D_2^{\Psi}/D_2}), \tag{13}$$

with $g'(\infty) = cte$ and $g'(x \to 0) \propto x^{qD_2}$. In Fig. 5 we show the scaling analysis of participation moments for this regime ($q=3$, 4, and 5). The trends are mainly the same as that presented by P_2, namely data collapse with saturation for long times and a power-law growth for intermediate times preceded by a size-independent initial waiting time. However, the participation moment scaling exponent now depends on the wave-function decay exponent as predicted by Eq. (13).

In both regimes, the characteristic time scale after that finite-size effects starts to take place scales as $t^* \propto N^{D_2^{\Psi}/D_2}$, with $D_2^{\Psi}/D_2 = 0.90(2)$. The fact that this scaling exponent is smaller than unity (and therefore corresponds to a faster than ballistic dynamics) is related to the nonlocal nature of the long-range couplings. Finally, for exponentially localized wave functions, $[P_q]^{1/(q-1)}$ is proportional to the localization length for any q. Using N^* as a measure of the characteristic size of the present power-law decaying wave packet, this feature is only true for $q < 1/(1-D_2^{\Psi})$. For higher moments it displays a sublinear size dependence whose exponent continuously decreases towards D_2^{Ψ} as $q \to \infty$.

III. CONCLUSIONS

We investigated the one-dimensional Anderson model with off-diagonal disorder and matrix elements H_{ij} decaying as $1/|i-j|^{\alpha}$ for $\alpha = 1$ (critical regime). Using an exact diagonalization scheme on finite chains, we computed the participation moments of all energy eigenstates and reported the critical exponents D_q associated with the multifractal character of the stationary states. Examining the time evolution of an initially localized wave packet, we observed that the wave function develops a power-law tail in the form $|\Psi(n-n_0)|^2 \propto (n-n_0)^{-(1-D_2^{\Psi})}$ with $D_2^{\Psi} = 0.607(10)$. It achieves a stationary nonuniform profile after reflecting at the chain boundaries. As a consequence, the time-dependent participation moments $P_q(t)$ exhibit a nontrivial finite-size scaling. For $q < 1/(1-D_2^{\Psi})$, the participation moments grow in time as $P_q \propto t^{(q-1)D_2/D_2^{\Psi}}$, where the exponent $D_2 = 0.676(2)$ governs the decay of the return probability as well as the one of the autocorrelation function. It saturates in a plateau proportional to N^{q-1}. Therefore, the usual participation number P_2 reaches a value proportional to the chain size as occurs with a uniformly distributed state. Higher order participation moments with $q > 1/(1-D_2^{\Psi})$ grow in time as t^{qD_2} and saturate at a plateau proportional to $N^{qD_2^{\Psi}}$. We used a finite-size scaling hypothesis to put the participation moments in a universal form as a function of the reduced variable $t/N^{D_2^{\Psi}/D_2}$. As such, the characteristic size of the wave packet grows in time as $N^* \propto t^{D_2/D_2^{\Psi}}$, which for the present model with long-range couplings results in a faster than ballistic spread. The proposed dynamic scaling relations are expected to remain valid for general model systems of waves spreading in a power-law fashion over a random medium.[27] The special character of the present model, with all energy eigenstates being multifractal, provides a clear picture of the complex dynamic scaling, that takes place at the vicinity of the Anderson transition.

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