Appearance of carrier propagations in the one-dimensional Anderson model with long-range hopping

P. E. de Brito,[1] E. S. Rodrigues,[1] and H. N. Nazareno[2]
[1]*Universidade Católica de Brasília, Departamento de Física, Campus Águas Claras, 72030-070 Brasília, Distrito Federal, Brazil*
[2]*International Center of Condensed Matter Physics, Universidade de Brasília, P.O. Box 04513, 70910-900 Brasília, Distrito Federal, Brazil*

(Received 15 December 2003; revised manuscript received 19 March 2004; published 30 June 2004)

We study the dynamics of an electron wave packet in a one-dimensional Anderson model with a *nonrandom* hopping falling off as some power α of the distance between sites. We have found that the larger the hopping range, the more extended the wave packet as time evolves. When the disorder is increased, the wave packet tends to be more and more localized in a finite region of the lattice. For a low degree of disorder, the exponent $\alpha=1.5$ indicates the onset for fast propagation of the wave packet. This value is in good agreement with previous results obtained by diagonalizing the systems Hamiltonian. The inclusion of a dc electric field introduces the effect of *dynamical localization*, i.e., the acting field produces the localization of the wave packet in a definite region of the lattice, irrespective of the degree of disorder and hopping range. By appropriately tuning the electric field we obtained the Bloch oscillations of the wave packet.

DOI: 10.1103/PhysRevB.69.214204 PACS number(s): 71.30.+h, 78.30.Ly, 73.20.Jc, 72.15.Rn

I. INTRODUCTION

The single parameter scaling theory predicts the absence of extended states in noninteracting disordered electronic systems, in one- (1D) and two-(2D) dimensions.[1] Thus the theory precludes the existence of a metallic phase and a true localization-delocalization transition (LDT) in low-dimensional systems.[2] Nevertheless there is experimental evidence that this general belief may be incomplete. Metallic behavior, i.e., resistivity that decreases with decreasing temperature, has been observed to the lowest accessible temperature (for a state of the art in this subject, we refer to the work by Abrahams, Kravehenko, and Sarachik[3]). Recently, experiments performed on disordered 2D electron gas in Si heterostructures show the existence of a different kind of metallic behavior.[4] On the other hand, extensive numerical analysis done on binary alloys also points towards the existence of a metallic phase in a 2D disordered system.[5,6]

It is worth mentioning the situation encountered in 1D tight-binding systems, i.e., where only hopping between nearest neighbors was considered. When the system is random the carriers cannot propagate through it. Nevertheless, there are exceptions to this rule. In fact, *deterministic* nonperiodic structures, such as Fibonacci, Thue-Morse, and Harper models, can even present superdiffusive propagation.[7–9] In addition, there exist low-dimensional disordered systems that cannot be described by the standard Anderson model. For instance, the unexpected high conductance of several doped quasi-1D polymers was explained by Dunlap, Wu, and Phillips.[10] Assuming pairwise correlations in the disorder since they cause delocalization of eigenstates.[11] Similarly, the absence of Anderson localization in the presence of spatial correlations was put forward to account for transport properties of semiconductor superlattices with intentional correlated disorder.[12]

In this paper we present a systematic analysis of the effect of long-range hopping on the wave packet dynamics in a random 1D system. We consider on-site (diagonal) energetic disorder, but with *nonrandom long-range* intersite coupling. It was argued recently[13–15] that low-dimensional systems with diagonal disorder and *nonrandom* intersite coupling, which falls according to a powerlike law, can support extended states at one of the band edges. Furthermore, in recent works[14,15] it was claimed that a LDT may occur in 1D and 2D random systems with nonrandom powerlike hopping. These results, besides their interest from a general point of view, are relevant in context of Frenkel excitons and magnons in the presence of diagonal disorder, where the long-range dipole-dipole coupling plays a major role.

The paper is organized as follows. In Sec. II we describe the model we will be dealing with and summarize previous work, which is necessary for a better understanding of the present paper. The dynamics tools used to characterize the wave packet dynamics are introduced in Sec. III, namely the mean square displacement (MSD) and the participation function, at the same time that we presented 3D graphs of the wave packet evolution. In order to characterize the dynamic processes, we consider different values of the relevant parameters of the model, i.e., the exponent of the power law of the hopping term and the intensity of the disorder. The body of the paper is Sec. IV, where we present our results of the dynamics of initially localized wave packets, as well as relate the dynamical results to what is known from previous static study. Finally, in Sec. V, we discuss the inclusion of a dc electric field that produces dynamical localization.

II. MODEL HAMILTONIAN

In a previous work we have analyzed the effect of long-range hopping on the propagating properties of wave packets in regular (nondisordered) 1D systems.[16] The hopping was nonrandom and falling off as some *power* α of the distance between sites. We were able to show that different regimes of propagation arise for different values of α. Thus, for $\alpha=0$ we obtained the phenomenon of *self-trapping*, that is, starting with a well-localized packet, it remains localized around 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. For larger times, the packet propagates subdiffusively. The lattice subjected to a uniform applied electric field was also analyzed in our work, showing that the effect of *dynamical localization* takes place.

We now focus on the problem of long-range hopping in a *random* 1D system with diagonal disorder. The model Hamiltonian is the following:

$$\mathcal{H} = \sum_n \varepsilon_n a_n^\dagger a_n + \sum_n \sum_{r\neq 0} \left(\frac{V}{r^\alpha}\right)(a_n^\dagger a_{n+r} + a_{n+r}^\dagger a_n), \qquad (1)$$

where $a_n^\dagger$ creates an electron at site n, ε_n is the corresponding on-site energy which, following Anderson,[17] was taken from a uniform random distribution within an interval $[-\Delta/2,\Delta/2]$, and the parameter α determines the range of the nonrandom hopping. Therefore we consider a system with diagonal disorder and nonrandom power-law decaying hopping terms. We can characterize the strength of the disorder through the dimensionless parameter $\eta \equiv \Delta/V$, usually referred to as *degree of disorder*.

Recently, a very comprehensive study of the nature of the eigenfunctions of this Hamiltonian (1) was presented.[14,15] It was suggested that there exist delocalized states at the top of the band (for $V>0$) even for moderately large diagonal disorder, provided $1<\alpha<3/2$ in a 1D geometry. The system undergoes the LDT on further increasing the degree of disorder. For instance, for $\alpha=4/3$ it has been established that the critical degree of disorder for the LDT to occur is $\eta_c = 10.9\pm 0.2$.[18] The marginal case $(\alpha=3/2)$ is analogous to the standard 2D Anderson model[15] where the states are weakly localized, as predicted by Abrahams *et al.*[1]

In the present case it is expected that the influence of the long-range hopping, i.e., the α exponent, should produce different dynamical behaviors as compared to the ordered case. First of all, it is worth noticing that hopping is favored between sites degenerate in energy, while hopping between sites with different energies is inhibited. Our results show that, for a fixed V in (1), a decreasing MSD is obtained while increasing the exponent α. This can be understood by noticing that the greater the exponent, the lower the number of sites to which the electron can hop. On the other hand, smaller α values makes the hopping more extended and increase the possibility for the electron to jump to more distant sites. As a consequence, the smaller the exponent, the greater the MSD for a fixed V. This is in contrast to the behavior observed in ordered structures. On the other hand, the analysis of the participation function (to be defined below) is of great utility since it provides precise information on the extension of the wave packet.

III. DYNAMICAL PROPERTIES

In order to study the dynamical properties of our model, we expand the normalized wave function in the Wannier representation

$$|\psi(t)\rangle = \sum_n f_n(t)|n\rangle, \qquad (2a)$$

and the time-dependent Schrödinger equation for the Wannier amplitudes $f_n(t)$ reads

$$i\frac{df_n}{d\tau} = \epsilon_n f_n + \sum_{r>0} \frac{f_{n+r}+f_{n-r}}{r^\alpha} \qquad (2b)$$

in terms of the dimensionless variables $\tau = Vt/\hbar$ and $\epsilon_n = \varepsilon_n/V$. In the present simulations, we have assumed the following values: $V=25$ meV and the lattice parameter $d = 100$ Å.

Our main aim is to explore the (α,η) plane in order to characterize the different regions of propagation and localization. To accomplish the task, we analyze the following magnitudes, namely the MSD, which in units of the lattice parameter reads

$$\langle r^2\rangle(t) = \sum_n |f_n(t)|^2 n^2, \qquad (3a)$$

and the participation function[19]

$$P(t) = \left\{\sum_n |f_n(t)|^4\right\}^{-1}. \qquad (3b)$$

To complete the analysis we show plots of the wave packet taken at different times.

The dynamical behavior of the wave packet for a given random configuration deserves further comment. In fact, it could happen that for a particular configuration, sites very close together can be degenerated. In such a situation we should observe oscillations between these two sites, where the Wannier amplitudes will be much greater than in any other site of the lattice. The shorter the range of the hopping, the more pronounced this oscillatory movement will be. On the other hand, if the degenerate sites are far from each other, as it was said above, the amplitude of the wave at the distant site will grow in time. In other words, the kind of propagation one obtains in a random lattice could depend on the particular configuration assumed. Consequently, it is mandatory to perform an average over several configurations in order to mimic the behavior of real systems. In the next section we present the statistics obtained over a significative number of configurations.

IV. NUMERICAL RESULTS

Since the hopping considered is long range, we expect that initial wave packets of different extensions will evolve in time in a different way. Thus, we shall present the result of calculations where an initial Gaussian wave packet is centered at the middle of the lattice with N sites, and the standard deviation takes on three possible values, namely $\sigma = 0, 1$, and 3. The $\sigma=0$ case corresponds to a particle localized in a single site. By taking the more extended initial packet $(\sigma=3)$, we shall see that the corresponding MSD and participation function are greater than those in a more confined situation, $\sigma=1$. In Fig. 1 we show the MSD and participation function as functions of time for $\eta=1$, $\sigma=3$ and

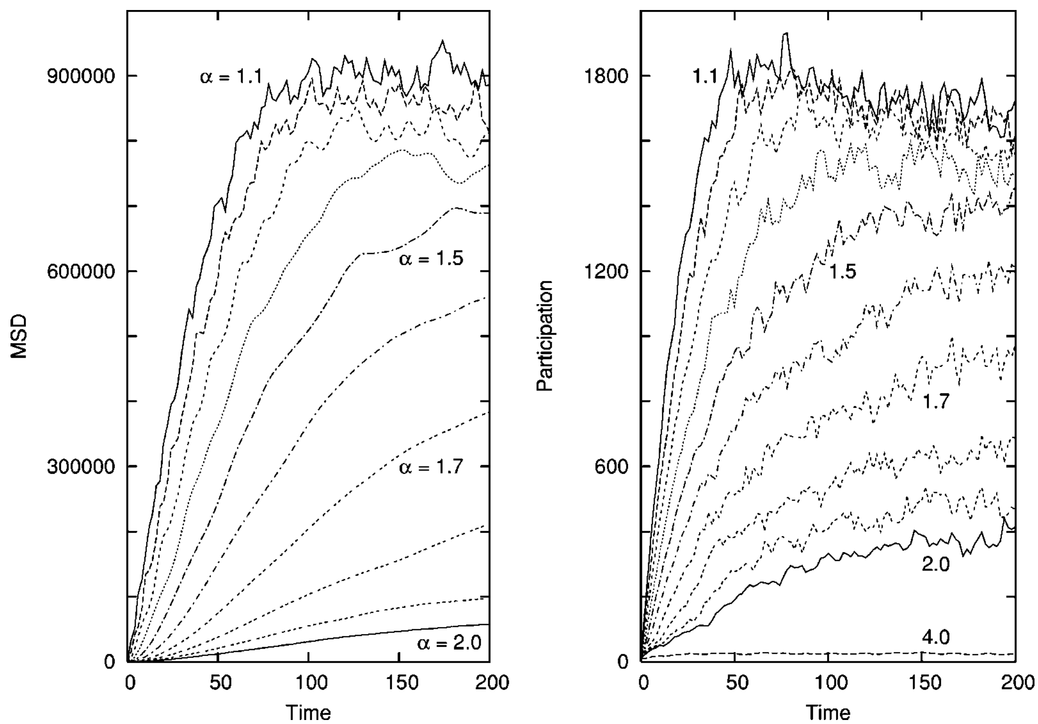

FIG. 1. Mean square displacement MSD (left panel) and participation function (right panel) for $\eta=1$ and several values of α from 1.1 to 4.0; note that in the left panel the $\alpha=4.0$ case is out of scale. From $\alpha=1.7$ on, we note a tendency to localization of the wave.

several values of α. Starting with $\alpha=1.1$ (extended hopping) and ending with $\alpha=4.0$, one notes that the wave packet clearly propagates until for α slightly larger than 1.7 starts to show a tendency to localization. This conclusion can be understood as follows. Saturation together with strong fluctuations around maximum values for the MSD and participation are indications that the tail of the wave packet has reached the boundary. For $\eta=1$ and α greater than 1.7 we note that saturation with *absence* of fluctuation occurs at the same time that the MSD values are smaller than that corresponding for smaller α, as shown in Fig. 1. The same trend is observed in Fig. 2 for $\eta=2$ but, in this case, the tendency to localization occurs for α greater than 1.5 instead. Finally, for $\alpha=4$ we note strong localization of the wave packet, as expected, since we are close to the nearest neighbors Anderson regime.

To shed more light into the interplay between the degree of disorder and the hopping range we show in Fig. 3 the MSD for $\alpha=1.3$, 1.5, and 1.7, while varying the degree of disorder η from 1 to 4 in the three cases, i.e., we illustrate situations for low to moderate disorder. One notes in Fig. 3 the MSD values for any given η increase rapidly when the hopping range is enlarged, that is for α going from 1.7 to 1.3. It is worth noticing that for all α considered, the MSD values corresponding to $\eta=1$ and $\eta=2$ are very different. It is evident from the obtained curves that for low enough disorder ($\eta=1.0$), the case of $\alpha=1.5$ is a kind of threshold since for lower values of α propagation is very fast, while for values larger than 1.5 the packet starts to slow down. The interplay we are discussing is evident in the plots we show in Figs. 4 and 5. In fact, in Fig. 4 we display the evolution in time of the wave packet for the two degrees of disorder, namely $\eta=1$ and 2 and for $\alpha=1.3$. We note that the spread of the packet is larger in the case $\eta=1$, while for $\eta=2$ one notes a much more localized wave. In Fig. 5 we show the time evolution for the same two degrees of disorder, but for $\alpha=1.6$. In both cases the spreading becomes evident, but for $\eta=2$ one notes a tendency to localization, which is absent for $\eta=1$.

Another feature that emerges from our model of long-range hopping is that the dynamical quantities evaluated depend much on the number of sites considered in the calculations, especially at low α, as well as on the structure of the initial wave packet. To illustrate this phenomenon we show in Fig. 6 the participation function for two degrees of disorder $\eta=1$ and 2, when the initial wave packet was taken for $\sigma=1$ (more localized) and the number of sites considered varies from 2000 up to 4000. We can clearly see that both functions increase with the number of sites and, at the same time, it is evident the different situations appearing for $\eta=1$ and $\eta=2$. Localization is evident in the latter case. Next we treat the initial wave packet corresponding to $\sigma=3$ (more extended) and the same other parameters than before. Now the dispersion of values when considering different site numbers is greater than in the previous case, and the participation function takes larger values than for the case $\sigma=1$ (see Fig. 7).

We have performed simulations with 100 different configurations and took the average values between them, at each time, for the MSD and participation functions. At the same time, we evaluated the standard deviation that could attain, at most, 10% of the average value, and this for large times. We show in Fig. 8 the results corresponding to the case: $\sigma=3$, $\eta=1$, and $\alpha=1.8$.

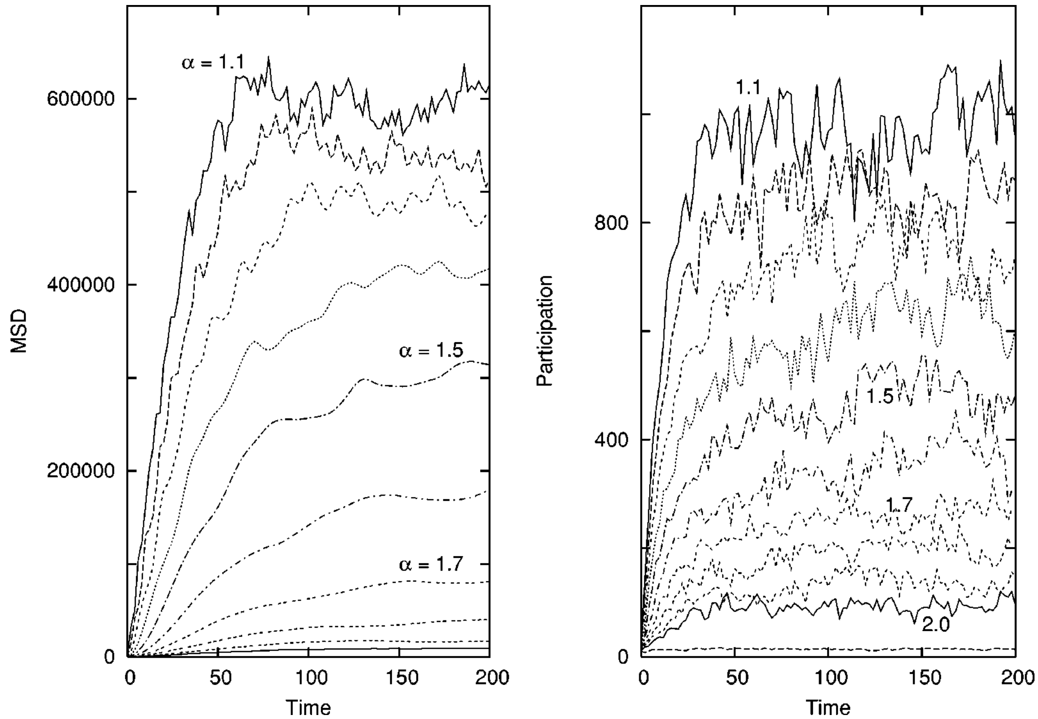

FIG. 2. Mean square displacement MSD (left panel) and participation function (right panel) for $\eta=2$ and the same values of α as in Fig. 1. The difference with the previous case is that already for $\alpha=1.5$ the localization is apparent.

V. EFFECT OF AN APPLIED dc ELECTRIC FIELD

We shall now consider the effect of an applied dc electric field on the propagating properties of wave packets. To include the field in the calculations we add to the Hamiltonian of Eq. (1) the following term: $\Sigma_n\, e\, E\, n\, d\, a_n^+ a_n$, where E is the field intensity and d is the lattice parameter. In terms of dimensionless units $\mathcal{E}=Eed/V$, we have to add to Eq. (2b) the term $\mathcal{E} n f_n$. We have considered various degrees of disor-

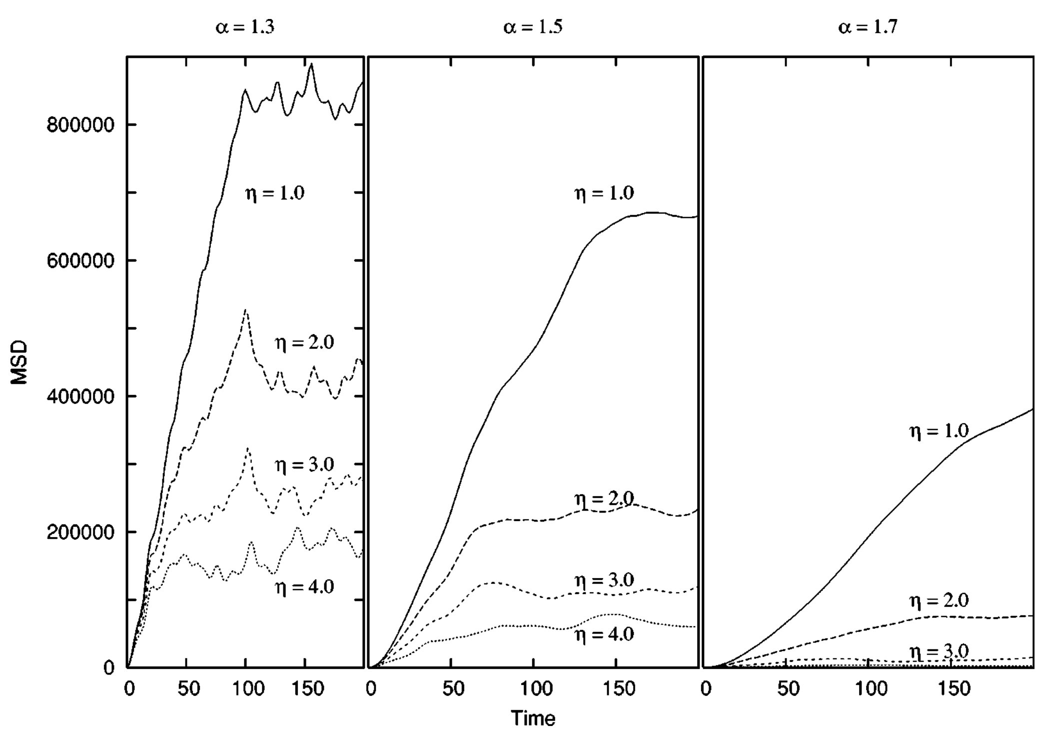

FIG. 3. MSD for η varying between 1 and 4 (small to moderate disorder), and three values of $\alpha=1.3$, 1.5, and 1.7. The figure shows the interplay between the degree of disorder and the hopping range while determining the propagation/localization of the wave packet.

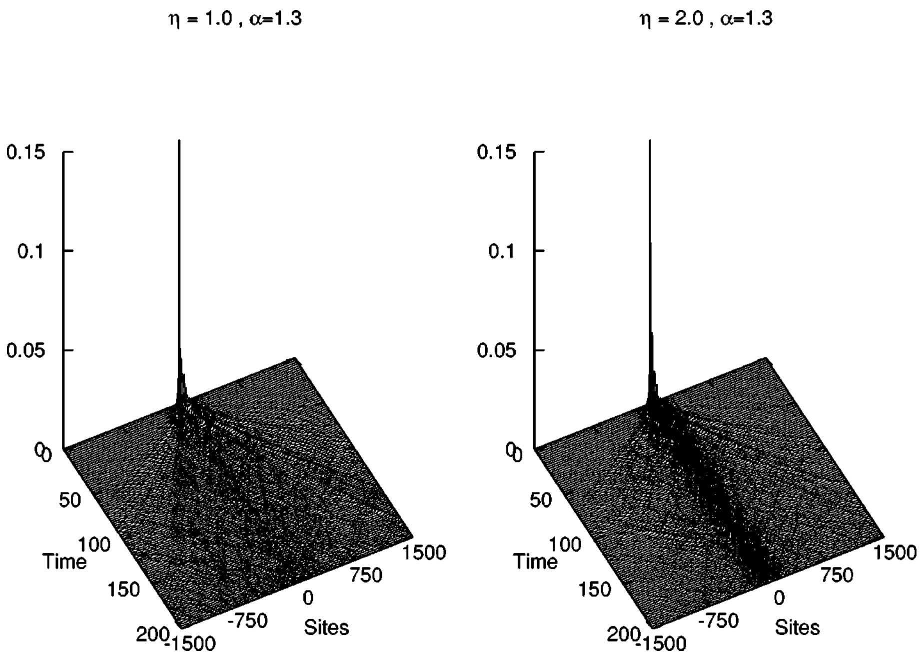

FIG. 4. Plots of the wave packet for $\sigma=3$, $\alpha=1.3$ and $\eta=1$ (left panel) and $\eta=2$ (right panel). Note the stronger localization of the wave packet around the starting sites for the latter case.

der as well as different hopping ranges together with several field intensities. Accordingly, we have to explore a 3D space parameters (η,α,E) at the same time that we analyze the time evolution of wave packets with two initial conditions associated with $\sigma=0$ and 3. To analyze the effect of the field on the displacement of the wave packet, we have included the time evolution of its centroid $\langle x(t)\rangle$. We shall present the results corresponding to the case in which the starting wave packet is more extended, namely when $\sigma=3$, since in the other cases of more localized initial conditions the effect of the field is more pronounced. First, we present the case for $\eta=2.0$, $\alpha=1.3$ and a weak field $\mathcal{E}=0.04$ ($E=1.0$ kV/cm). Note that for these parameters in the field-free case, the wave propagates rapidly, while in the presence of this field remains localized in a definite region of the lattice, is shown in Fig. 9.

Following this, we treated the case where $\eta=1$ (weak disorder) $\alpha=1.5$ and $\mathcal{E}=0.2$ ($E=5.0$ kV/cm), a field intensity that can be considered as moderate. The wave remains localized, but now in a smaller region since we have increased the field intensity, as it is shown in Fig. 10.

Now we present the wave packet evolution for the case of a strong electric field: $\mathcal{E}=0.4$ ($E=10.0$ kV/cm), $\eta=0.5$ (very weak disorder), and $\alpha=1.0$. It is a case of a strongly localized wave due to the electric field strength, as is evident in Fig. 11.

Note that the wave remains localized in *all* cases. The region of localization is reduced as the field intensity is increased. We would like to call attention to an interesting situation that arises when, by tuning the electric field, we can reach a situation in which the on-site energies of two neigh-

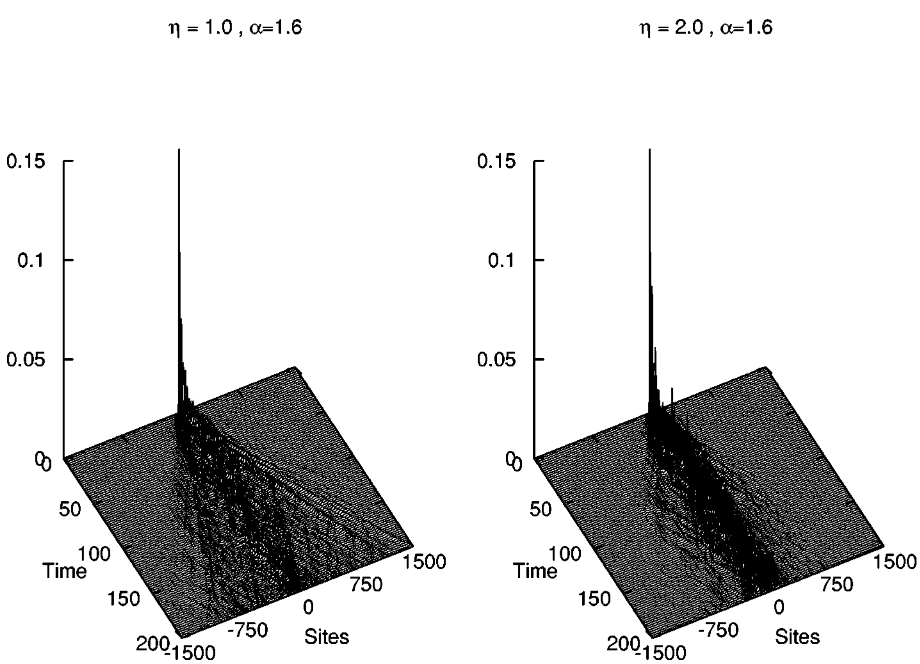

FIG. 5. Same as in Fig. 4, but for a shorter hopping range ($\alpha=1.6$).

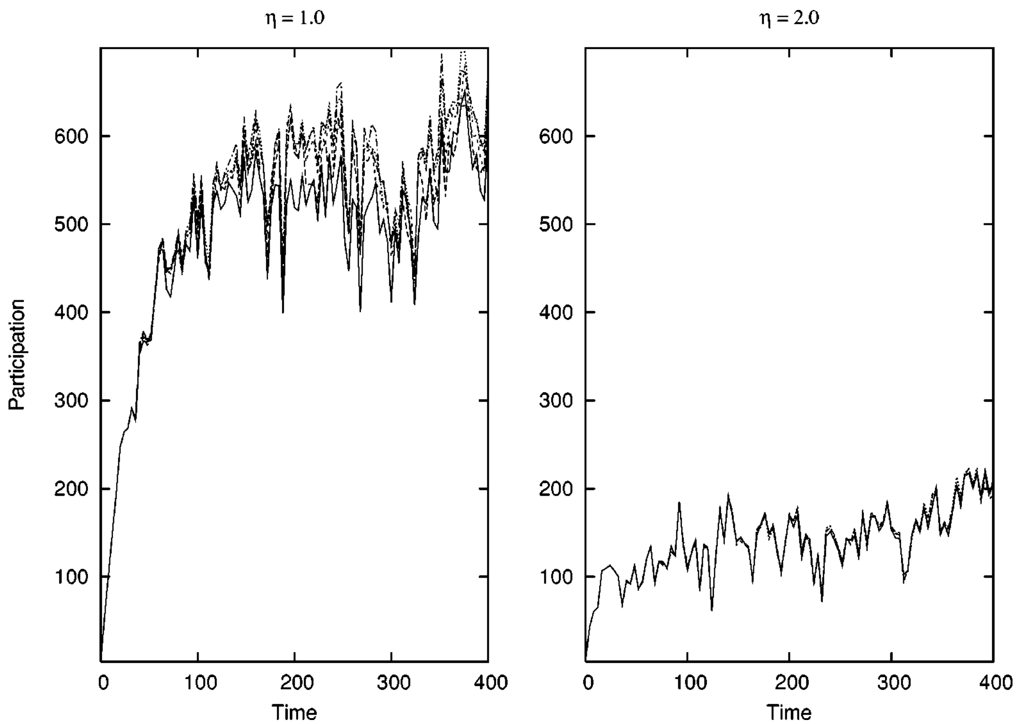

FIG. 6. Participation function for $\eta=1$ (left panel) and $\eta=2$ (right panel) with $\alpha=1.5$ and $\sigma=1$ in both cases. The calculations correspond to lattices from 2000 to 4000 sites (from bottom to top). Note that the dispersion of points obtained for different sizes in the case $\eta=1$ is greater than for the more localized wave corresponding to $\eta=2$.

boring atoms coincide. In this case the wave performs oscillations with precisely the Bloch frequency associated with this particular field value, as is shown in Fig. 12, where the field intensity $\mathcal{E}=4.0$ ($E=100$ kV/cm) was chosen such that the on-site energies at sites 0 and -1 are degenerate. Note that the centroid oscillates precisely between these sites. After we submitted the manuscript, we became aware of a work in which the existence of Bloch oscillations in 1D random

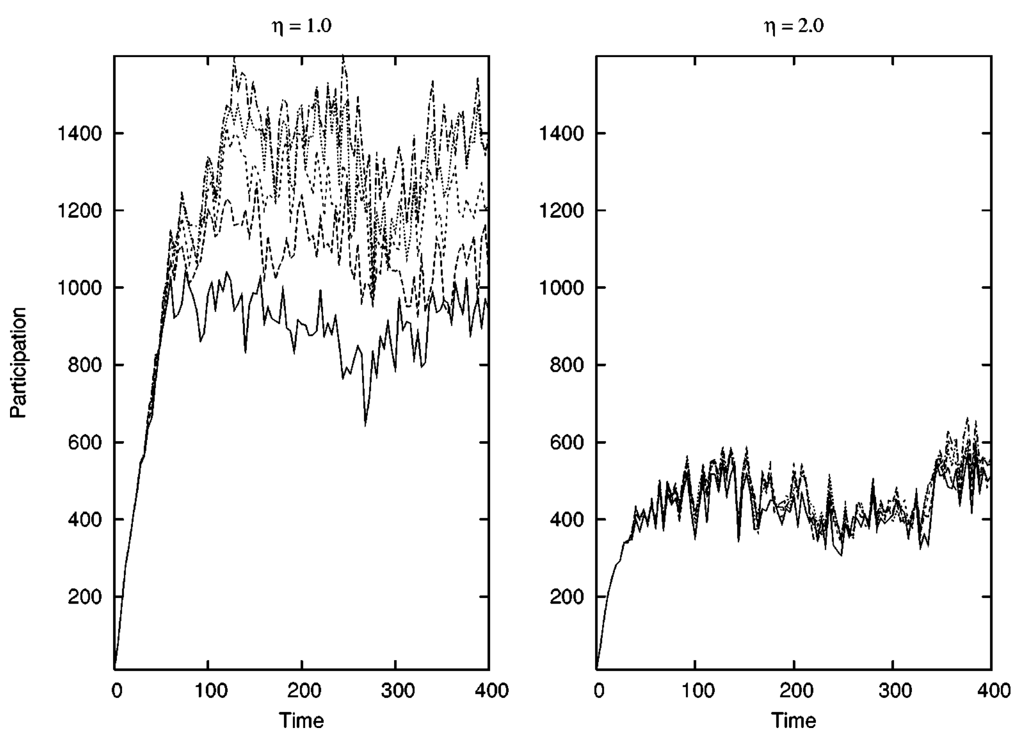

FIG. 7. Same as Fig. 6 but for a less localized initial wave packet ($\sigma=3$). The dispersion of points is greater than those shown in Fig. 6.

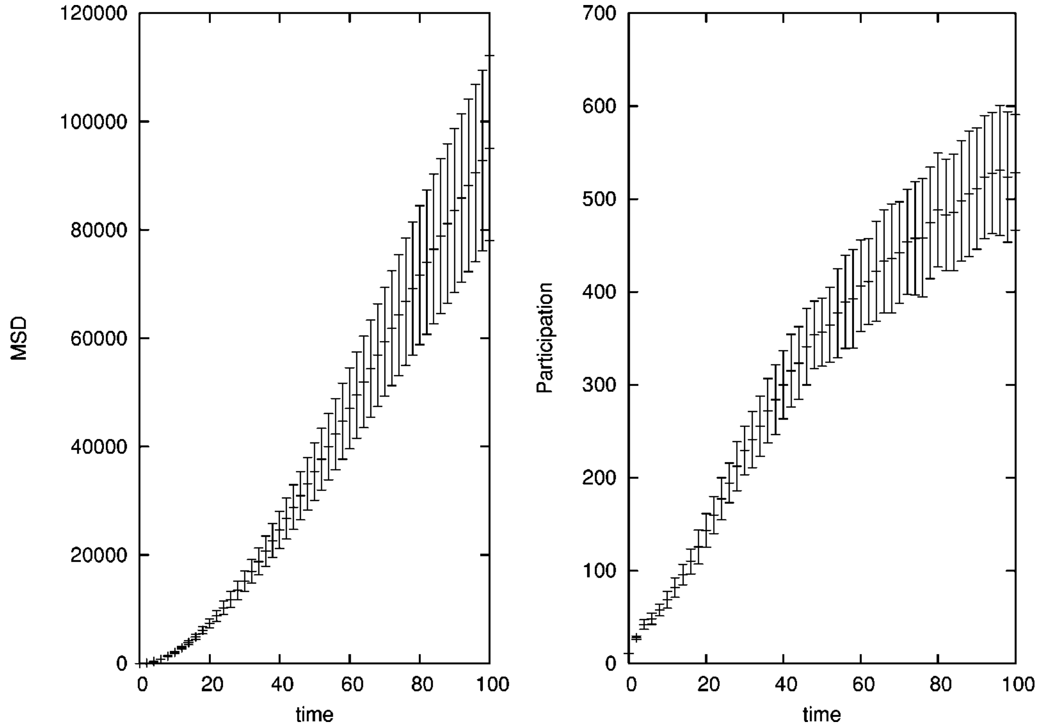

FIG. 8. Mean square displacement MSD (left panel) and participation function (right panel) for $\sigma=3$, $\eta=1$, and $\alpha=1.8$. The middle curve is the average, over 100 configurations. We also show the standard deviation.

systems is reported.[20] By using an experimental technique, Lyssenko *et al.*[21] were able to perform a direct measurement of the spatial displacement of Bloch oscillating electrons in ordered semiconductor superlattices.

We conclude in this section that the presence of an electric field introduces the effect of dynamical localization *even* when extended hopping range is considered, a similar situation as encountered in the perfect crystal case.[16]

VI. CONCLUSIONS

We have studied the effect of long-range hopping on the dynamics of wave packets in a random 1D Anderson system. We assumed nonrandom power-law decaying hopping with an exponent α, while the on-site energies were distributed randomly in the interval $[-\Delta/2,\Delta/2]$. We analyzed the influence of the spatial extent of the initial wave packet on the

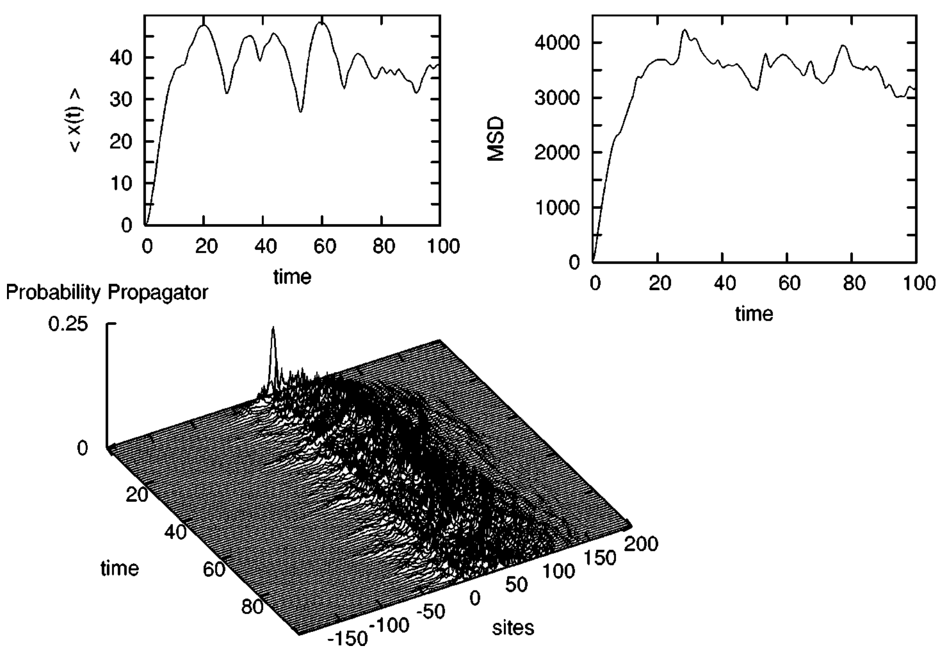

FIG. 9. Time evolution of the wave packet corresponding to the case: $\sigma=3$, $\eta=2.0$, $\alpha=1.3$, and $\mathcal{E}=0.04$. Also shown, the centroid and the MSD as functions of time.

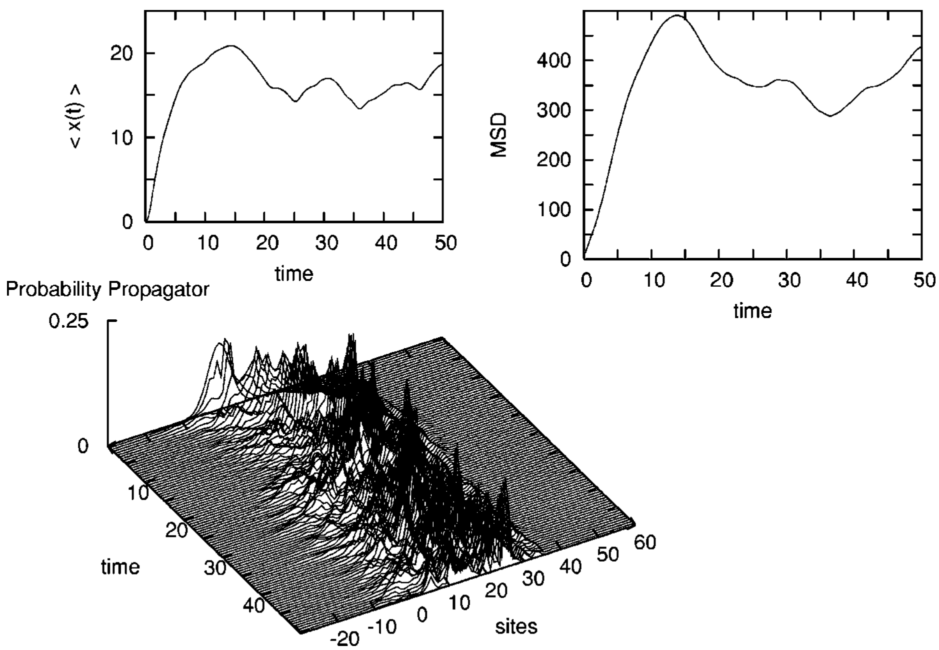

FIG. 10. The same as in Fig. 9, but for the case $\sigma=3$, $\eta=1.0$, $\alpha=1.5$, and $\mathcal{E}=0.2$.

dynamical properties, with and without the action of a dc electric field.

Fixing the degree of disorder η, and considering several values of α, we found that both the MSD and participation functions decrease when increasing α, i.e., the larger the hopping range, the more extended the wave packet as time evolves. When the disorder is increased, the wave packet tends to be more and more localized in a finite region of the lattice. The interplay between the degree of disorder and the hopping range determines the propagating properties. As an example of this, moderate degree of disorder while considering different extents of hopping range gives rise to different behaviors related to propagation or localization. This effect was evident in the plots of the time evolution of the wave packet.

Some words concerning the comparison to static calculations are in order. As mentioned previously, the uppermost eigenstate of the Hamiltonian (1) is extended for a moderately high degree of disorder and undergoes a LDT on increasing the magnitude of the disorder, provided $1<\alpha<1.5$. The critical value of disorder in the thermodynamics limit ($N\to\infty$) depends on α and, for instance, it has been found that $\eta_c=10.9\pm0.2$. But this value diminishes on decreasing the system size due to the lowering of the uppermost band edge.[18] In addition, the static calculations (i.e., diagonalization of the Hamiltonian)[14,15,18] only refer to the uppermost state. It is also known that lower states are less extended[14] and, consequently, they are already localized when the uppermost state undergoes the LDT. Since the wave packet can be described as a superposition of all eigenstates, it is clear

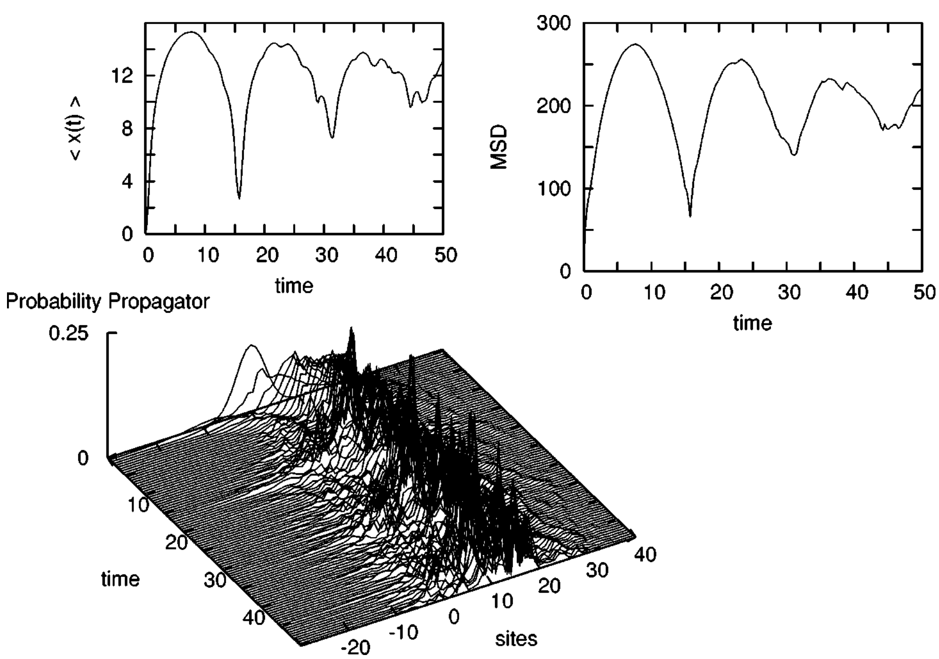

FIG. 11. The same as in Fig. 9, but for the case: $\sigma=3$, $\eta=0.5$, $\alpha=1.0$, and $\mathcal{E}=0.4$.

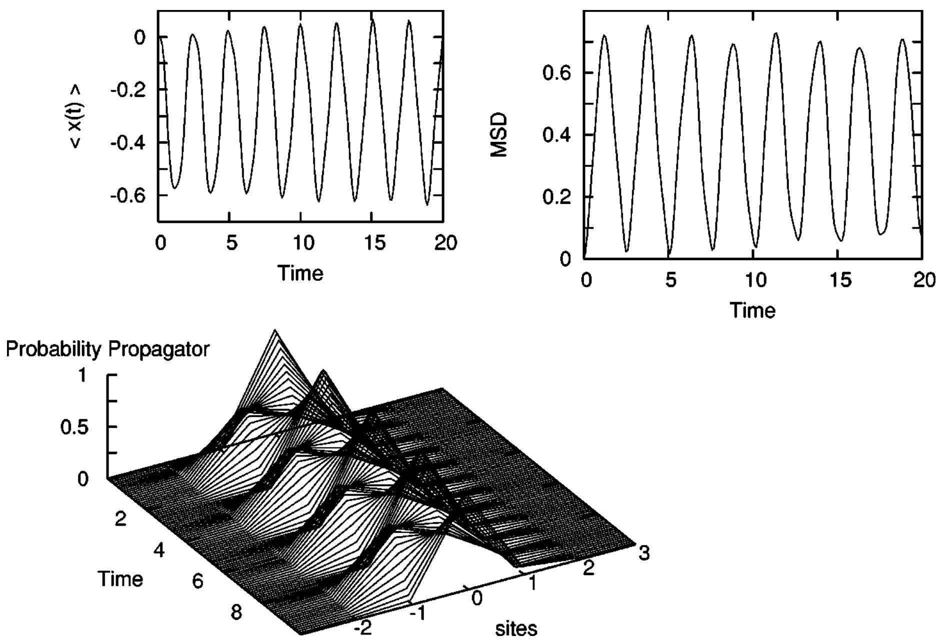

FIG. 12. The same as in Fig. 9, but for the case $\sigma=0$, $\eta=4.0$, $\alpha=4.0$, and $\mathcal{E}=4.0$. It clearly shows the oscillation of the centroid between sites 0 and -1.

that we cannot expect a perfect quantitative agreement between static and dynamics calculations. In particular, it is now rather clear the reason why the critical values for the wave packet obtained in this work, which involve all eigenstates, is lower than that corresponding to the uppermost state purported in Ref. 18.

Finally, we presented the results concerning the application of a dc electric field. It was clearly shown that the presence of the field causes the wave packet to remain in a definite region of the lattice; it is the phenomenon of dynamical localization, always noticeable irrespective of the degree of disorder and the extended range of the hopping. Clearly the stronger the field is, the more localized the wave, so as far as localization is concerned, the behavior of the wave packet is controlled mainly by the electric field. Furthermore, when the disorder is sufficiently small $(\eta<1)$ and for short-range hopping $(\alpha\geqslant 4)$, we recovered the Bloch oscillations by tuning the electric field intensity. Also we obtained the spatial displacement of the center of the wave packet as driven by the electric field.

ACKNOWLEDGMENT

The authors are thankful to Professor F. Dominguez-Adame for suggesting the problem and for very useful discussions.

[1] E. Abrahams, P. W. Anderson, D. C. Licciardello, and T. V. Ramakrishnan, Phys. Rev. Lett. **42**, 673 (1979).
[2] D. J. Thouless, Phys. Rep., Phys. Lett. **13**, 93 (1974).
[3] Elihu Abrahams, Sergey V. Kravchenko, and Myriam P. Sarachik, Rev. Mod. Phys. **73**, 251 (2001).
[4] X. G. Feng, Dragana Popovic, S. Washburn, and V. Dobrosavljevic, Phys. Rev. Lett. **86**, 2625 (2001).
[5] H. N. Nazareno, P. E. de Brito, and E. S. Rodrigues, Phys. Rev. B **66**, 012205 (2002).
[6] H. N. Nazareno, P. E. de Brito, and E. S. Rodrigues, Phys. Rev. B **68**, 054204 (2003).
[7] P. E. de Brito, C. A. A. da Silva, and H. N. Nazareno, Phys. Rev. B **51**, 6096 (1995).
[8] H. N. Nazareno, P. E. de Brito, and C. A. A. da Silva, Phys. Rev. B **51**, 864 (1995).
[9] P. E. de Brito, Jorge A. Gonzalez, and H. N. Nazareno, Phys. Rev. B **54**, 12820 (1996).
[10] D. H. Dunlap, H.-L. Wu, and P. Phillips, Phys. Rev. Lett. **65**, 88 (1990).
[11] J. C. Flores, J. Phys.: Condens. Matter **1**, 8471 (1989).
[12] V. Bellani, E. Diez, R. Hey, L. Toni, L. Tarricone, G. B. Parravicini, F. Domínguez-Adame, and R. Gómez-Alcalá, Phys. Rev. Lett. **82**, 2159 (1999).
[13] J. C. Cressoni and M. L. Lyra, Physica A **256**, 18 (1998).
[14] A. Rodriguez, V. A. Malyshev, and F. Domínguez-Adame, J. Phys. A **33**, L161 (2000).
[15] A. Rodriguez, V. A. Malyshev, G Sierra, M. A. Martín-Delgado, J. Rodríguez-Laguna, and F. Domínguez-Adame, Phys. Rev. Lett. **90**, 027404 (2003).
[16] H. N. Nazareno and P. E. de Brito, Phys. Rev. B **60**, 4629 (1999).
[17] P. W. Anderson, Phys. Rev. **109**, 1492 (1958).
[18] A. V. Malyshev, V. A. Malyshev, and F. Domínguez-Adame, cond-mat/0303092 (unpublished).
[19] F. Wegner, Z. Phys. B **36**, 209 (1980).
[20] F. Dominguez-Adame, V. A. Malyshev, F. A. B. F. de Moura, and M. L. Lyra, Phys. Rev. Lett. **91**, 197402 (2003).
[21] V. G. Lyssenko, G. Valusis, F. Loser, T. Hasche, K. Leo, M. M. Dignam, and K. Kohler, Phys. Rev. Lett. **79**, 301 (1997).