Available online at www.sciencedirect.com
SCIENCE DIRECT
Solid State Communications 138 (2006) 585–589
solid state communications
www.elsevier.com/locate/ssc

Diffusive, super-diffusive and ballistic transport in the long-range correlated 1D Anderson model

B. Santos [a], L.P. Viana [b], M.L. Lyra [a], F.A.B.F. de Moura [a,*]

[a] *Instituto de Física, Universidade Federal de Alagoas, 57072-970 Maceió-AL, Brazil*
[b] *Laboratório de Métodos Numéricos e Simulação Computacional, Departamento de Tecnologia da Informação, Universidade Federal de Alagoas, 57072-970 Maceió-AL, Brazil*

Received 12 January 2006; received in revised form 3 April 2006; accepted 10 April 2006 by C. Lacroix
Available online 4 May 2006

Abstract

In this paper, we study the 1D Anderson model with long-range correlated on-site energies. This diagonal-correlated disorder is considered in such a way that the random sequence of site energies ε_n has a $1/k^{\alpha}$ power spectrum, where k is the wave-vector of the modulations on the random sequence landscape. Using the Runge–Kutta method to solve the time-dependent Schrödinger equation, we compute the participation number and the Shannon entropy for an initially localized wave packet. We observe that strong correlations can induce ballistic transport associated with the emergence of low-energy extended states, in agreement with previous works in this model. We further identify an intermediate regime with super-diffusive spreading of the wave-packet.

PACS: 63.50.+x; 63.22.+m; 62.30.+d

Keywords: D. Anderson model; D. Long-range correlated disorder; D. Delocalization; D. Electronic transport

1. Introduction

The time evolution of one-electron wave-packets in low-dimensional disordered systems is a well known problem with several connections with transport properties [1,2]. For low-dimensional systems with uncorrelated disorder, the Anderson localization theory predicts the absence of extended eigenstates [3]. This means that the width of the time-dependent wave-packet saturates in the long-time limit, i.e. the electron remains localized in a finite region around the initial position. The presence of short or long-range correlations is a key mechanism to induce extended states in the 1D Anderson model [4–9]. In fact, it has been established that short-range correlated on-site disorder may lead to the appearance of extended states at special resonance energies [4–6]. However, these states form a set of null measure of the density of states in the thermodynamic limit, which implies in the absence of mobility edges in such models.

On the other hand, long-range correlations can induce a metal–insulator transition in 1D systems [7–9]. A strategy to achieve this is to considered an 1D system with nearest-neighbor interactions and a long-range correlated on-site disorder distribution with a power-like spectrum behaving as $k^{-\alpha}$. Whenever, the standard deviation of the energy distribution is equal to the nearest-neighbor hopping, and $\alpha<2$, all states remain localized and the Lyapunov exponent is finite on the entire energy band. For $\alpha>2$, a phase of extended states appears at the center of the energy band, giving rise to two mobility edges. After this finding, models with long-range correlated on-site disorder distributions have attracted much attention. Scaling properties of the localization length [10] and local density of states [11] close to the critical point have been subjects of recent studies. Moreover, Bloch oscillations in an 1D disordered system with diagonal long-range correlated disorder was investigated. It was found that this type of correlated disorder does not destroy the coherence of such oscillations [12]. More recently, the metal–insulator transition in the 2D Anderson model with long-range correlations was characterized by measuring the participation number exponent from the long-time behavior of the wave-function spacial

* Corresponding author.
E-mail addresses: bsantos@df.ufal.br (B. Santos), lviana@tci.ufal.br (L.P. Viana), marcelo@df.ufal.br (M.L. Lyra), fidelis@df.ufal.br (F.A.B.F. de Moura).

0038-1098/$ - see front matter © 2006 Elsevier Ltd. All rights reserved.
doi:10.1016/j.ssc.2006.04.007

distribution [13]. The theoretical prediction of delocalization induced by correlated disorder has been confirmed by experimental works in semiconductor super-lattices [14] and microwave transmission spectra through a single-mode waveguide with correlated scatterers [15]. Several works suggest 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 [8].

Aiming to investigate how the emergence of delocalized states in 1D long-range correlated systems influences the electronic transport, we revisit the 1D Anderson Hamiltonian with long-range correlated on-site energies. We build an appropriate disordered long-range correlated on-site energy sequence using the formalism introduced in Refs. [7,9], which generates a random sequence with power spectrum proportional to $1/k^{\alpha}$, where k is the modulation wave-vector on the random sequence landscape. Solving numerically the 1D time-dependent Schrödinger equation, we present the dynamical evolution of an initially localized wave packet. We focus our studies on return probability $R(t)$, Shannon information entropy $S(t)$, and participation function $\xi(t)$ of an initially localized wave packet. We show in detail the time dependent form of these functions, characterizing their dependence with the degree of correlation in the disordered potential. Our results suggest ballistic transport for the electron wave-packet in the strong correlation regime ($\alpha>2$), a clean signature of extended states. A new super-diffusive regime will be reported to take place at intermediate correlations.

2. Model and formalism

The disordered 1D Anderson model is defined by the one-electron Hamiltonian

$$H=\sum_{n}\varepsilon_{n}|n\rangle\langle n|+t\sum_{n}[|n\rangle\langle n+1|+|n\rangle\langle n-1|], \tag{1}$$

where the random energies of the sites ε_n introduce diagonal disorder in the Hamiltonian, the hopping energy t is taken to be unitary, and the sum is taken over all N sites of an open chain. In order to introduce long-range correlations in the disorder distribution, the random sequence of site energies obeys the relation [7,9]

$$\varepsilon_{n}=\zeta(\alpha,N)\sum_{k=1}^{N/2}\left(\frac{1}{k}\right)^{\alpha/2}\cos\left(\frac{2\pi nk}{N}+\phi_{k}\right), \tag{2}$$

where $\{\phi_k\}$ are $N/2$ independent random phases uniformly distributed in the interval $[0,2\pi]$. This energy sequence is shifted in order to have $\langle\varepsilon_n=0\rangle$. $\zeta(\alpha,N)$ is used to set the energy sequence variance $\Delta\varepsilon_n=1$ for all system sizes. We shall consider time evolution of an initially localized wave packet at site n_0. The time-dependent Schrödinger equation for such a system can be written as [16]

$$i\dot{c}_{n}(t)=\varepsilon_{n}c_{n}(t)-c_{n+1}(t)-c_{n-1}(t), \tag{3}$$

where $c_n(t)$ is the wave amplitude on site n at time t, $\dot{c}_n(t)$ its time derivative, $\{c_n(t=0)=\delta_{n,n_0}\}$ stands for the initial wave-packet, and $\hbar=1$. To analyze the wave propagation, we solve Eq. (3) using the fourth-order Runge–Kutta method to obtain the temporal evolution of an initially localized wave-packet. We analyze the amplitude of the wave function at the initial site, calculating the so called return probability [1,16],

$$R(t)\equiv|c_{n_0}(t)|^{2}. \tag{4}$$

Usually, the electron escaping from its initial position occurs when the amplitude $c_{n_0}(t)$ vanishes as t evolves. Conversely, the amplitude remains finite for a localized wave-packet. However, the return probability does not completely characterize the dynamical wave-function evolution. In addition, we rely on two auxiliary measures to further analyze these properties: the Shannon information entropy,

$$S(t)=-\sum_{n}|c_{n}(t)|^{2}\ln|c_{n}(t)|^{2}; \tag{5}$$

and the participation function,

$$\xi(t)=\frac{1}{\sum_{n}|c_{n}(t)|^{4}}. \tag{6}$$

Note that $S(t)$ varies from 0, for a wave function confined to a single site, to $\ln N$, for a wave uniformly extended over the whole chain. The participation function $\xi(t)$ varies from 1 to N on these same limits [16]. These functions give information about the number of sites that are visited during the time evolution of the wave-packet over the underlying lattice.

3. Results and discussion

In this section, we show the results obtained for a wave-packet initially localized at site $n_0=N/2$, $\{c_n(t=0)=\delta_{n,n_0}\}$, as described in Section 2. The fourth-order Runge–Kutta method is used to solve the set of time-dependent Schrödinger coupled equations, written as Eq. (3) for the site n. Numerical convergence was ensured by conservation of the norm of the wave-packet at every time step, i.e. $\sum_n|c_n(t)|^2=1$. All calculations were averaged over 300 disorder configurations. In Fig. 1, we show the scaled asymptotic return probability, $R(t\to\infty)N$, as a function of the number of sites N for distinct correlation degrees. For $\alpha>2$ the return probability vanishes linearly, $R(t\to\infty)\propto 1/N$. This is a clean signature of extended behavior, in agreement with Ref. [7]. For weak correlations, $\alpha<1$, the return probability does not vanish in the thermodynamic limit ($N\to\infty$). This indicates that all eigenstates are localized in this regime. In the intermediate regime of $1<\alpha<2$, the asymptotic return probability vanishes slower than linearly. In this regime, the localization lengths are sensitive to the re-scaling of the local potential required to keep the potential variance scale invariant, but such scaling is not sufficient to promote an effective transport over the whole chain.

Furthermore, we analyze the time dependent Shannon entropy $S(t)$ and participation number $\xi(t)$. For the evaluation of these quantities, we numerically integrate the wave-

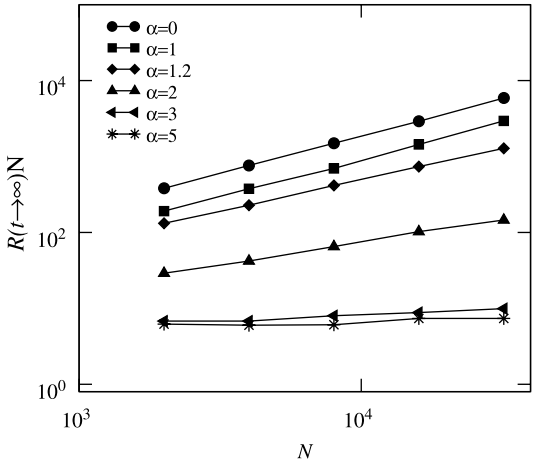

Fig. 1. The scaled return probability for long time, $R(t\to\infty)N$, versus number of sites N for distinct degrees of correlations (from top to bottom $\alpha=0$, 1, 1.2, 2, 3, 4, and 5). The return probability vanishes as $1/N$, $R(t\to\infty)N$ roughly a constant, for $\alpha>2$. This signs a metal–insulator transition induced by strong long-range correlations.

equation until a stationary state is reached even due to localization over a finite chain segment or after multiple reflections of the wave packet on the lattice boundaries. In Fig. 2(a), we show data for the Shannon entropy $S(t)$ versus

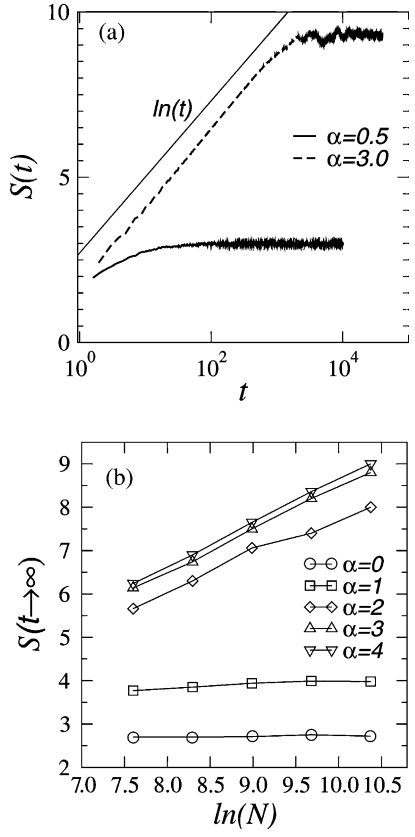

Fig. 2. (a) The Shannon information entropy $S(t)$ versus $\ln t$ for $\alpha=3$ (dashed line) and $\alpha=0.5$ (continuous line) and $N=8000$ sites. $S(t)$ evolves as $S(t)\propto\ln t$ in the strong correlated regime $\alpha=3$; (b) The asymptotic Shannon information entropy, $S(t\to\infty)$, versus $\ln N$. It scales with $\ln N$ in the strongly correlated regime, while it remains finite for weak correlations.

$\ln t$ using $\alpha=3$ (dashed line) and $\alpha=0.1$ (continuous line). Observe that $S(t)\propto\ln t$ for $\alpha=3$ and it saturates for $\alpha=0.5$. The logarithmic growth of $S(t)$ corroborates the existence of extended states for $\alpha>2$, while its saturation reflects the localization of the wave packet for weak correlations. In Fig. 2(b), one observes that $S(t\to\infty)\propto\ln N$ for $\alpha>2$; this indicates that the asymptotic wave-packet is uniformly distributed over the chain.

In Fig. 3, we show the numerical results for the scaled participation number $\xi(t)/N^{\gamma}$ versus scaled time computed from chains with distinct lengths and $\alpha=0.5$, 1.2, and 3. The scaling variables used to achieve the data collapse at $\alpha=3$ reveal that the participation number is a linearly increasing function of time $\xi(t)\propto t$, i.e. the wave-packet spreads ballistically until it reaches the lattice boundaries. Analyzing data for other values of α (not shown), we conclude that for any $\alpha>2$ the electron displays a ballistic dynamics associated with the emergence of extended eigenstates over the entire chain. In this regime, the wave-packet spreads uniformly over the chain. For weak correlations $\alpha<1$ all eigenfunctions remain localized in a finite segment and, therefore, the participation number in the thermodynamic limit quickly saturates as time evolves and it is size independent. Prior to the saturation the wave-packet spreads diffusively with $\xi(t)\propto t^{1/2}$.

A new regime is identified for intermediate values of the correlation exponent $1<\alpha<2$. The data collapse for the representative value of $\alpha=1.2$ is shown in Fig. 3(b). The non-trivial scaling exponents reveal that the wave-packet participation number exhibits a super-diffusive spread $\xi(t)\propto t^{2/3}$ before saturation. A similar scaling behavior of the participation number was shown to also take place at the critical point of the power-law bond-disordered Anderson model [17]. In that case, the super-diffusive spread was reflecting the power-law tail developed by the wave-packet in the super-diffusive regime, in agreement with the predicted behavior of quantum systems with fractal energy spectra and eigenfunctions [18]. In the present case, a different mechanism leads to super-diffusion and to the anomalous participation number scaling. In the regime of intermediate correlations, the electron eigenstates remain exponentially localized. Therefore, the wave-packet develops also exponential tails. To illustrate this feature, in Fig. 4 we display the average asymptotic wave-packet in this regime after a long spreading time. Its exponential tail is clearly seen in the inset. It is only at short distances that the wave-packet displays a power-law decay, as shown in the main picture. These two regimes may be represented by fitting the wave-packet to the form $|c_n(t\to\infty)|^2\propto e^{-n/\xi}/n^{2/3}$. The localization length ξ in this regime is sensitive to the normalization needed to keep the variance of the potential size independent. Such scaling is reflected in the slow divergence of the asymptotic participation number $\xi\propto N^{0.2}$. At short times, for which the wave-packet width is smaller than the localization length ξ, the pre-asymptotic power-law decay predominates, resulting in a super-diffusive spread.

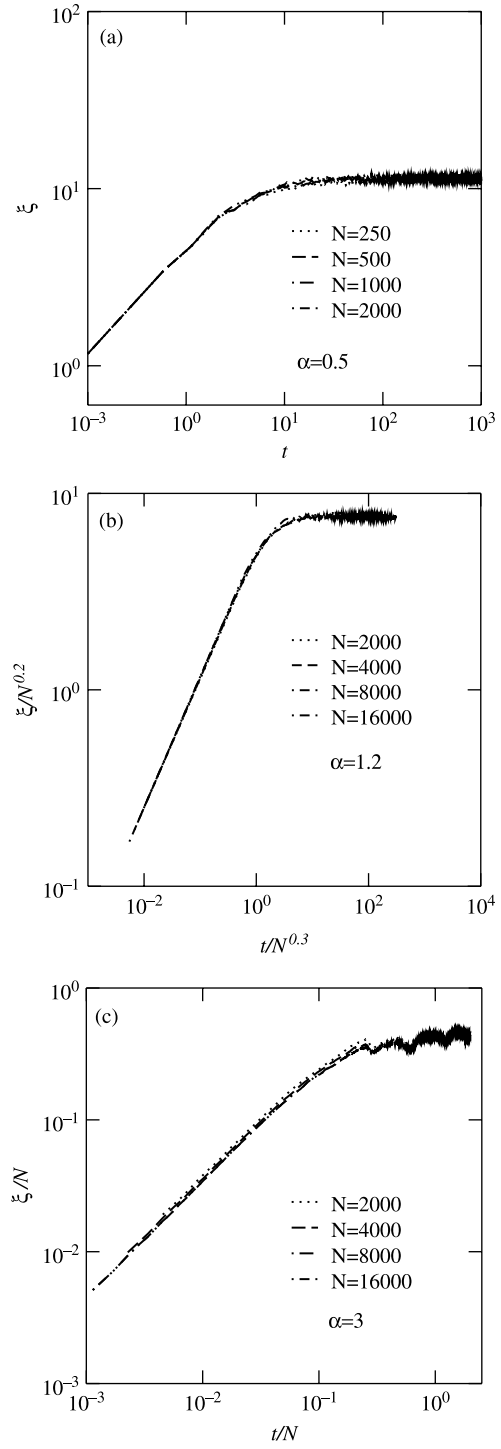

Fig. 3. (a) Participation number $\xi(t)$ as a function of time t for $\alpha=0.5$. The size independence reflects the localized nature of the wave-packet. Prior to the saturation, the participation number grows diffusively; (b) scaled participation number $\xi(t)/N^{0.2}$ as a function of scaled time $t/N^{0.3}$ for $\alpha=1.2$. Data collapse implies in a super-diffusive spread of the wave-packet; (c) scaled participation number $\xi(t)/N$ as a function of scaled time t/N for $\alpha=3$. Data collapse implies that the participation number grows ballistically prior to the reflection at the chain boundaries.

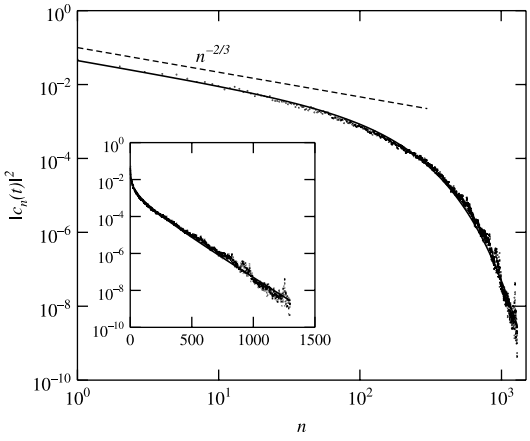

Fig. 4. Asymptotic wave-packet $|c_n(t\to\infty)|^2$ versus n ($n=0$ is the chain center at which the wave-function is initially localized). Here, we use $N=8000$ and $\alpha=1.2$. In this regime of intermediate correlations, the wave-packet develops exponential tails as shown in the inset. At short distances, it displays a power-law decay. The solid line is a fit to the form $|c_n(t\to\infty)|^2\propto e^{-n/\xi}/n^{2/3}$. The power-law regime predominates at short times giving rise to the super-diffusive spread of the wave-packet. The exponential tail promotes the saturation of the asymptotic participation number.

4. Conclusions

In this work, we studied the 1D Anderson model with long-range correlations. In order to introduce long-range correlations, we applied a Fourier method to construct an on-site energy sequence with spectral density $1/k^{\alpha}$. By solving the time-dependent Schrödinger equation for an initially localized wave-packet, we determined the return probability $R(t)$, the Shannon information entropy $S(t)$ and the participation function $\xi(t)$. We found three distinct dynamical regimes as a function of the correlation exponent. For $\alpha<1$, the wave-packet remains on a finite segment of the chain after an initial diffusive spread. In the strongly correlated regime $\alpha>2$, the asymptotic return probability vanishes linearly with $1/N$. The participation number grows ballistically prior to its reflection at the chain boundaries. The ballistic spreading indicates that the electron transport is weakly influenced by the underlying disorder in this strongly correlated regime. Such behavior is consistent with the recent demonstration of coherent Bloch oscillations of the wave-packet in the presence of external fields [12]. A new dynamical regime was reported for intermediate correlations with $1<\alpha<2$. In this case, the participation number grows super-diffusively and the asymptotic wave-packet remains non-uniformly distributed over the chain keeping exponential tails. At short distances, it displays a slow power-law decay. On the light of these findings, 1D chains with long-range correlated disorder can be used as a simple model that allows for a close investigation of the crossover from diffusive to ballistic transport in low-dimensional electron systems.

Acknowledgements

This work was partially supported by Brazilian research agencies CNPq and CAPES, and by Alagoas state research agency FAPEAL.

References

[1] B. Kramer, A. MacKinnon, Rep. Prog. Phys., 561469; For a review see, e.g., I.M. Lifshitz, S.A. Gredeskul, L.A. Pastur, Introduction to the Theory of Disordered Systems, Wiley, New York, 1988.

[2] R.A. Romer, H. Schulz-Baldes, Europhys. Lett. 68 (2004) 247.

[3] E. Abrahams, P.W. Anderson, D.C. Licciardello, T.V. Ramakrishnan, Phys. Rev. Lett. 42 (1979) 673.

[4] J.C. Flores, J. Phys.: Condens. Matter 1 (1989) 8471.

[5] D.H. Dunlap, H.L. Wu, P.W. Phillips, Phys. Rev. Lett. 65 (1990) 88; H.-L. Wu, P. Phillips, Phys. Rev. Lett. 66 (1991) 1366; P.W. Phillips, H.-L. Wu, Science 252 (1991) 1805.

[6] A. Sánchez, F. Domínguez-Adame, J. Phys. A: Math. Gen. 27 (1994) 3725; A. Sánchez, E. Maciá, F. Domínguez-Adame, Phys. Rev. B 49 (1994) 147.

[7] F.A.B.F. de Moura, M.L. Lyra, Phys. Rev. Lett. 81 (1998) 3735; F.A.B.F. de Moura, M.L. Lyra, Physica A 266 (1999) 465.

[8] F.M. Izrailev, A.A. Krokhin, Phys. Rev. Lett. 82 (1999) 4062; F.M. Izrailev, A.A. Krokhin, S.E. Ulloa, Phys. Rev. B 63 (2001) 41102.

[9] G.P. Zhang, S.-J. Xiong, Eur. Phys. J. B 29 (2002) 491.

[10] H. Shima, T. Nomura, T. Nakayama, Phys. Rev. B 70 (2005) 075116.

[11] G. Schubert, A. Weiße, H. Fehske, Physica B 359–361 (2005) 801.

[12] F. Domínguez-Adame, V.A. Malyshev, F.A.B.F. de Moura, M.L. Lyra, Phys. Rev. Lett. 91 (2003) 197402.

[13] F.A.B.F. de Moura, M.D. Coutinho-Filho, E.P. Raposo, M.L. Lyra, Europhys. Lett. 66 (2004) 585.

[14] V. Bellani, E. Diez, R. Hey, L. Toni, L. Tarricone, G.B. Parravicini, F. Domínguez-Adame, R. Gómez-Alcalá, Phys. Rev. Lett. 82 (1999) 2159; V. Bellani, E. Diez, A. Parisini, L. Tarricone, R. Hey, G.B. Parravicini, F. Domínguez-Adame, Physica E 7 (2000) 823.

[15] U. Kuhl, F.M. Izrailev, A. Krokhin, H.J. Stöckmann, Appl. Phys. Lett. 77 (2000) 633.

[16] H.N. Nazareno, P.E. de Brito, Phys. Rev. B 60 (1999) 4629.

[17] R.P.A. Lima, F.A.B.F. de Moura, M.L. Lyra, H.N. Nazareno, Phys. Rev. B 71 (2005) 235112.

[18] R. Ketzmerick, K. Kruse, S. Kraut, T. Geisel, Phys. Rev. Lett. 79 (1997) 1959.