

Absence of localization on the 2d model with long-range correlated off-diagonal disorder

F.A.B.F. de Moura^a

Instituto de Física, Universidade Federal de Alagoas, 57072-970 Maceió AL, Brazil

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Abstract. We study the one-electron eigenstates in a two-dimensional (2d) Anderson model with long-range correlated off-diagonal disorder, generated by a 2d discrete Fourier method. The dynamics of an initially localized wave packet is investigated by numerically solving the 2d time-dependent Schrödinger equation. In addition the participation number and its scaling behavior was obtained through direct diagonalization. Our numerical data suggest that the system exhibits a ballistic dynamics in the strongly correlated disorder regime. Moreover, the scaling analysis of mean participation number around the band center also indicates the presence of extended states for high degree of correlations.

1 Introduction

The Anderson localization theory predicts the absence of extended eigenstates on low-dimensional systems with uncorrelated disorder [1]. Therefore, at the long-time the width of the time-dependent wave-packet saturates in a finite region around the initial position. 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 [2–18]. The absence of Anderson localization in the presence of spatial short-range correlations in disorder was theoretically pointed out by Flores [2] and Dunlap [3,4] at the end of eighties and the experimental confirmation was obtained by Domínguez-Adame et al. [12] in a semiconductor superlattices with intentional correlated disorder. Since the end of the nineties the delocalization problem in one-dimensional (1d) systems with long-range correlated diagonal disorder have attracted attention. It has been reported [6,9–11,14] that these systems display an Anderson Metal-insulator transition (MIT) with mobility edges separating localized and extended states for sufficiently strong correlations. In particular, the 1d model with nearest-neighbor interactions and a on-site disorder distribution with a power-like spectrum behaving as $k^{-\alpha}$ has been studied in detail in references [6,11,14]. 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 [6,11,14]. Furthermore, the (1d) model with long-range purely off-diagonal disorder was investigated in reference [16,17]. It was proved that a localization-delocalization transition occurs similar to that in 1d model with correlated diagonal disorder [16,17]. Scaling properties of the localization length [14] and local density of states [18] close to the critical point have been the subject of recent studies. The effect of long-range correlated scatterers on the transport properties of microwave guides was experimentally studied and corroborated the predicted presence of mobility edges [15]. 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 [9,10]. Furthermore, the theoretical prediction that is possible to see Anderson localization in a random multilayered filter [19,20] opened a wide field of investigations of effects of correlated disorder in optical systems.

The existence of extended states due to correlations in two-dimensional (2d) disordered systems has been also proved. In reference [21] the authors considered a 2d striped medium in the (x, y) plane with on-site correlated disorder. The on-site energies were generated by a superposition of an uncorrelated term in the x -direction and a long-range correlated contribution along y -direction. It was predicted that this model displays a disorder-driven Kosterlitz-Thouless metal-insulator transition when strong correlations in disorder are provided. More recently, the existence of a Kosterlitz-Thouless transition in (2d) systems with hopping energies along the y -direction generated by a superposition of an

^a e-mail: fidelis@if.ufal.br

uncorrelated term and a long-range correlated one was numerically demonstrated [22]. Moreover, the effect of an isotropic scale-free long-range correlated disorder on the one-electron eigenstates of the 2d Anderson model has been studied [23,24]. To introduce long-range correlations in *both* x and y directions, the site energies were chosen to have a power-law spectral density $S(k) \propto 1/k^{\alpha_{2d}}$, where k is the magnitude of the typical wave-vector characterizing the energy landscape roughness. The metal-insulator transition induced by strong correlations ($\alpha_{2d} > 2$) was monitored by measuring the participation number exponent from the long-time behavior of the wave function spatial distribution [23,24]. Moreover, the interplay between the delocalization effect, arising from the long-range correlated disorder, and the dynamic localization, caused by an electric field was investigated [25,26]. It was predicted Bloch oscillations in both 1d [25] and 2d [26] geometries at the strong correlated limit. Moreover, the influence of correlated disorder on the conductivity of electron in a 2d lattice was investigated [27].

In this paper we contribute to further understanding of the localization aspects in low-dimensional systems with correlated disorder distribution. To the best of our knowledge, the effect of correlated off-diagonal disorder was studied only in 1d models. Therefore, we study the nature of one-electron eigenstates in a two-dimensional (2d) Anderson model with long-range correlated off-diagonal disorder. The 2d correlated off-diagonal disorder distribution was generated by using a 2d discrete Fourier method. By solving the 2d time-dependent Schrödinger equation for the complete Hamiltonian, we compute the behavior of an initially localized wave packet. Our results suggest that the system exhibits a crossover from a diffusive spread for weakly correlated disorder to a quasi-ballistic dynamics associated with the emergence of extended states in the strongly correlated disorder regime.

2 Model and formalism

We consider the 2d Hamiltonian with disordered hopping energies $t_{im,jn}$ on a regular $N \times N$ lattice [1,21]

$$H = \sum_{i,m} \epsilon|i,m\rangle\langle i,m| + \sum_{\langle im,jn \rangle} (t_{im,jn}|i,m\rangle\langle j,n|), \quad (1)$$

where $|i,m\rangle$ is a Wannier state localized at site (i,m) and $\sum_{\langle im,jn \rangle}$ represents a sum over nearest-neighbor pairs. In our calculations, we fix the on-site energy $\epsilon = 0$. In order to generate a long-range correlated hopping energy landscape, we compute the following auxiliary long-range correlated sequence by applying a 2d discrete Fourier transform method [23,24,26] :

$$\eta_{i,m} = \sum_{k_i=1}^{N/2} \sum_{k_m=1}^{N/2} \frac{\zeta(\alpha)}{(k_i^2 + k_m^2)^{\alpha/4}} \times \cos\left(\frac{2\pi i k_i}{N} + \psi_{i,m}\right) \cos\left(\frac{2\pi m k_m}{N} + \phi_{i,m}\right), \quad (2)$$

where $\psi_{i,m}$ and $\phi_{i,m}$ are $N^2/2$ independent random phases uniformly distributed in the interval $[0, 2\pi]$ and the exponent α controls the degree of correlations. We shift the auxiliary sequence in order to have $\langle \eta_{i,m} \rangle = 0$ and chose $\zeta(\alpha)$ to have the variance $\langle \eta_{i,m}^2 \rangle = 1$. Typically, this sequence is the trace of a 2d fractional Brownian motion [23,24,26] with a well defined power-law spectrum $S(k) \propto 1/k^\alpha$, where $k = \sqrt{k_x^2 + k_y^2}$. The hopping energy $t_{im,jn}$ is given by $t_{im,jn} = \exp(-|\eta_{i,m} - \eta_{j,n}|)$. The exponential transformation of the difference $|\eta_{i,m} - \eta_{j,n}|$ brings the advantage of bounding the interval of the random variable without changing its asymptotic correlation function. Therefore, it is a numerical trick to impose long-range correlations in the off-diagonal disorder distribution. For $\alpha = 0$, we recover an 2d model with uncorrelated off-diagonal disorder. In order to investigate the physical properties of the one-electron eigenstates we follow the time evolution of an initially localized wave packet. The Wannier amplitudes evolve in time according to the time-dependent Schrödinger equation as ($\hbar = 1$) [23]

$$\begin{aligned} i \frac{dc_{i,m}(t)}{dt} &= t_{im,im-1}c_{i,m-1}(t) + t_{im,im+1}c_{i,m+1}(t) \\ &+ t_{im,i-1m}c_{i-1,m}(t) + t_{im,i+1m}c_{i+1,m}(t), \\ &i, m = 1, 2, \dots, N. \end{aligned} \quad (3)$$

We consider a wave packet initially localized at site $i_0 = N/2, m_0 = N/2$, i.e. $|\Phi(t=0)\rangle = \sum_{i,m} c_{i,m}(t=0)|i,m\rangle$ where $c_{i,m}(t=0) = \delta_{i,i_0}\delta_{m,m_0}$. The above set of equations were solved numerically by using a high-order method based on the Taylor expansion of the evolution operator $V(\Delta t)$:

$$V(\Delta t) = \exp(-iH\Delta t) = 1 + \sum_{l=1}^{n_o} \frac{(-iH\Delta t)^l}{l!} \quad (4)$$

where H is the Hamiltonian. The wave-function at time Δt is given by $|\Phi(\Delta t)\rangle = V(\Delta t)|\Phi(t=0)\rangle$. 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 $H^l|\Phi(t=0)\rangle = \sum_{i,m} C_{i,m}^l|i,m\rangle$. Using the Hamiltonian formula (Eq. (1)) we can compute $H^1|\Phi(t=0)\rangle$ and obtain $C_{i,m}^1$ as

$$\begin{aligned} C_{i,m}^1 &= t_{im,im-1}c_{i,m-1}(t=0) + t_{im,im+1}c_{i,m+1}(t=0) \\ &+ t_{im,i-1m}c_{i-1,m}(t=0) + t_{im,i+1m}c_{i+1,m}(t=0). \end{aligned} \quad (5)$$

Therefore, using that $H^l|\Phi(t=0)\rangle = H \sum_{i,m} C_{i,m}^{l-1}|i,m\rangle$, $C_{i,m}^l$ can be obtained recursively as

$$\begin{aligned} C_{i,m}^l &= t_{im,im-1}C_{i,m-1}^{l-1} + t_{im,im+1}C_{i,m+1}^{l-1} + t_{im,i-1m}C_{i-1,m}^{l-1} \\ &+ t_{im,i+1m}C_{i+1,m}^{l-1}. \end{aligned} \quad (6)$$

The following results were taken by using $\Delta t = 0.5$ and the sum was truncated at $n_o = 20$. This cutoff was sufficient to

keep the wave-function norm conservation along the entire time interval considered ($t \leq 10^6$). 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 [23]

$$\sigma(t) = \sqrt{\sum_{i=1}^N \sum_{m=1}^N [(i - i_0)^2 + (m - m_0)^2] |c_{i,m}(t)|^2}, \quad (7)$$

and the participation number $P(t)$ [23]

$$P(t) = \frac{1}{\sum_{i,m} |c_{i,m}(t)|^4}. \quad (8)$$

Note that $\sigma(t)$ varies from 0, for a wave function confined to a single site, to proportional to N , for a wave uniformly extended over the whole chain. The participation function $P(t)$ varies from 1 to N^2 on these same limits [23,26]. These functions give information about the number of sites that are visited during the time evolution of the wave-packet over the underlying lattice. In addition we compute the static participation ratio defined by $P(E) = \sum_{n,m=1}^N c_{n,m}^2(E) / \sum_{n,m=1}^N c_{n,m}^4(E)$. Here $c_{n,m}(E)$ are the wave-function component associated with an eigenmode $E(|\phi(E)\rangle = \sum_{n,m=1}^N c_{n,m}(E)|n,m\rangle)$ of a lattice of $N \times N$ sites. The eigenmodes are obtained by direct diagonalization of the Hamiltonian H defined by equation (1). $P(E)$ diverges proportional to number of sites (N^2) for extended states and it is finite for exponentially localized ones. In our calculations we compute the average participation number defined by $\langle \xi \rangle = \frac{1}{N_f} \sum_{E=0.5}^{E=1.0} P(E)$ where N_f is the number of eigenmodes within interval the $[0.5, 1.0]$. Let me stress that the center of band was avoided in this sum because the localization length of this eigenstate is large even in the absence of long-range correlations ($\alpha = 0$) [16,17]. A quantitative scaling analysis of the participation number can be derived by using the Θ function defined as

$$\Theta(N_1, N_2) = \left| \frac{N_2^2}{\langle \xi(N_2) \rangle} - \frac{N_1^2}{\langle \xi(N_1) \rangle} \right|. \quad (9)$$

Θ is a measure of the difference between data from two consecutive lattices sizes investigated. For extended states $\Theta \approx 0$ for large lattices sizes. For localized states $\Theta \gg 0$ in the thermodynamic limite. Moreover it is well known that the relative fluctuation of the participation number defined by $\eta = \sqrt{\langle \xi^2 \rangle - \langle \xi \rangle^2} / \langle \xi \rangle$ where $[\langle \xi^2 \rangle = \frac{1}{N_f} \sum_{E=0.5}^{E=1.0} P(E)^2]$ is scale invariant at the Anderson transition [28,29]. This scaling can be used to monitor the critical point as it was suggested in reference [30]. Let me stress that the calculations based on exact diagonalization are quite limited to small sizes. The finite size effects are pronounced and becomes difficult a precise and complete description of the nature of eigenstates.

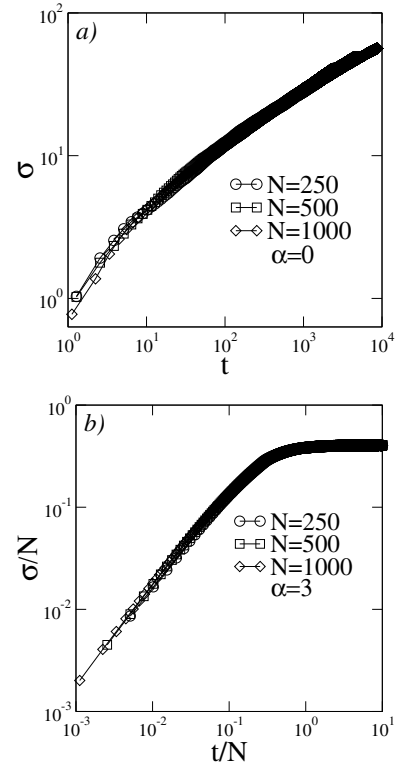


Fig. 1. (a) $\sigma(t)$ versus time t for $N \times N = 250 \times 250, 500 \times 500, 1000 \times 1000$ and $\alpha = 0$. The size independence reflects the localized nature of the wave-packet. (b) Scaled wave packet mean-square displacement $\sigma(t)/N$ versus scaled time t/N computed from lattices with $N \times N = 250 \times 250, 500 \times 500, 1000 \times 1000$ and $\alpha = 3.0$. The data collapse indicate a ballistic wave-packet spread.

3 Results

Our results were obtained following the time evolution of a wave-packet initially localized at site $(i_0, m_0) = (N/2, N/2)$, $\{c_{i,m}(t=0) = \delta_{i,i_0} \delta_{m,m_0}\}$, as described in the previous section. 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. (3)). Numerical convergence was ensured by conservation of the norm of the wave-packet at every time step, i.e., $|1 - \sum_{i,m} |c_{i,m}(t)|^2| < 10^{-10}$. All calculations were averaged over 100 disorder configurations. In Figure 1a we plot the wave packet mean-square displacement $\sigma(t)$ versus time t for $N \times N = 250 \times 250, 500 \times 500, 1000 \times 1000$ and $\alpha = 0$. Without correlations, $\alpha = 0$, all eigenfunctions remain localized in a finite segment and, therefore, the mean-square displacement is size independent. In Figure 1b, we show the numerical results for the scaled wave packet mean-square displacement $\sigma(t)/N$ versus scaled time t/N computed from lattices with distinct lengths and $\alpha = 3.0$. In this case, the wave-equation was integrated until a stationary state be reached after multiple reflections of the wave packet on the lattice boundaries. Therefore, the mean-square displacement saturates at a value $\propto N$ due to finite size

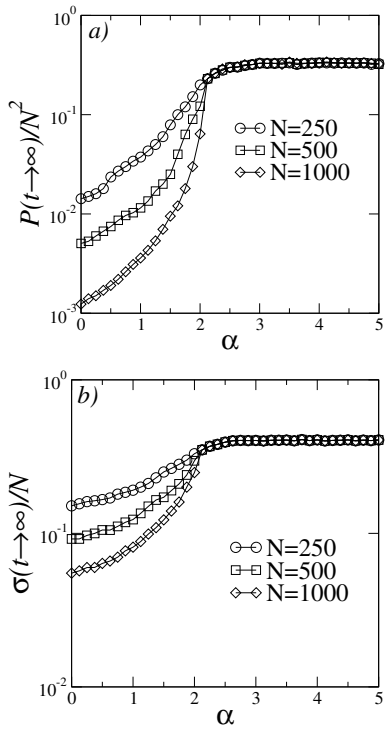


Fig. 2. (a) The long time participation number $P(t \rightarrow \infty)/N^2$ and (b) scaled mean-square displacement $\sigma(t \rightarrow \infty)/N$ versus α for $N \times N = 250 \times 250, 500 \times 500, 1000 \times 1000$. For $\alpha > 2$, both $\sigma(t \rightarrow \infty)/N$ and $P(t \rightarrow \infty)/N^2$ is roughly size independent indicating extended states.

effects. The scaling variables used to achieve the data collapse reveal that the wave-packet spread is a linearly increasing function of time $\sigma(t) \propto t$. The linear growth of the mean-square displacement saturates in the delocalized phase when the wave packet reaches the lattice boundaries. Therefore, our numerical calculations indicate a ballistic wave-packet spread. In Figure 2 we show the scaled asymptotic mean-square displacement $\sigma(t \rightarrow \infty)/N$ and participation number $P(t \rightarrow \infty)/N^2$ as a function of α for $N \times N = 250 \times 250, 500 \times 500, 1000 \times 1000$. Results were obtained by averaging over 100 realizations of the disorder. For $\alpha > 2$ the scaled mean-square displacement $\sigma(t \rightarrow \infty)/N$ and participation number $tP(t \rightarrow \infty)/N^2$ becomes size independent, i.e., the wave-packet spread is proportional to N . This feature is a clear signature of the existence of extended states for $\alpha > 2$. In Figure 3 we show our results about static participation number and its scaling behavior. Here we use exact partial diagonalization close to the band center ($0.5 < E < 1.0$). Let me stress that the center of the band was avoided due to the large localization length that exists in 2D systems with random hopping terms [16,17]. We are interested in the existence of extended states apart the band center. Our calculations were done using $N = 50$ up to 150 and over 1000 distinct disorder configurations to average. In Figure 3a we plot the logarithm of the mean participation number $\langle \xi \rangle$ versus logarithm of N for $\alpha = 0.5, 1.0, 1.5, 2.0, 2.5$ and

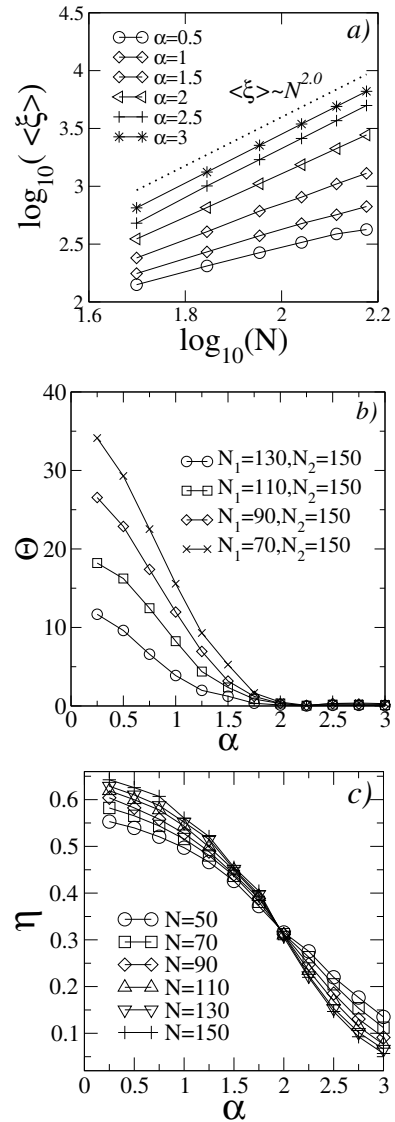


Fig. 3. (a) Log-log behavior of the mean participation number $\langle \xi \rangle$ versus N , computed using $N = 50$ up to 150 sites. For strong correlations ($\alpha > 2$), $\langle \xi \rangle \propto N^2$ indicating extended states. (b) Θ versus α data and (c) relative fluctuation of the participation number (η) versus α . Both results suggest, in good agreements with (a), that for $\alpha > 2$ there are a phase of extended modes close to center of band.

3.0. The dotted line indicates the power law behavior associated with delocalized states ($\langle \xi \rangle \propto N^2$). Therefore we can see that the data for $\alpha > 2$ display a clear signature of extended states. The best fit obtained for $\alpha > 2$ was $\langle \xi \rangle \propto N^{2.02(5)}$. Figure 3b shows data for Θ and Figure 3c relative fluctuations of the participation number η versus α . Both calculations also indicate the presence of extended states for $\alpha > 2$. In fact, analyzing in detail the Figures 3b, 3c we can see that the transition point happens about $\alpha \approx 1.95(5)$. The finite size effect that exists in this type of long-range correlated sequence is strongly related to the normalization used to keep fixed

the variance ($\langle \eta_{i,m}^2 \rangle = 1$) [6]. Therefore, the re-scale of the hopping distribution promotes finite size scaling corrections to the participation number as well as its fluctuations close to the critical point. This kind of finite size effect promotes some minor discrepancies in the critical point value obtained through the numerical formalisms used in this paper. However, within our numerical precision, the critical point value obtained through both formalisms are in perfect agreement.

4 Conclusions

In this paper we study the effect of long-range correlated off-diagonal disorder in 2d models. We consider one-electron in a lattice with long-range correlated off-diagonal disorder. The 2d correlated off-diagonal disorder distribution was generated by using a 2d discrete Fourier method. Our calculations were done solving the 2D time-dependent Schrödinger equation for the complete Hamiltonian by using a high-order method based on the Taylor expansion of the evolution operator. We followed the time evolution of an initial localized wave packet and computed the wave packet mean-square displacement and the time-dependent participation number. By analyzing the mean-square displacement and participation number for long-time we obtained strong evidences that the system exhibits a ballistic dynamics associated with the emergence of extended states in the strongly correlated disorder regime. In addition we provided a scaling analysis of the participation number close to the center of the band. In good agreement with time-dependent Schrödinger equation solution, we showed numerical evidences that indicate the existence of extended states around the band center. Therefore, correlations in the 2d models with off-diagonal disorder plays a similar role to those found in one-dimensional models with long-range correlated hopping terms. Therefore, we reported the existence of an Anderson transition in 2d models with off-diagonal correlated disorder. It is very instructive to stress the critical point value ($\alpha_c = 2$) is the same value obtained in 1d models with long-range correlated on-site energies [6], hopping terms [16,17] and 2d one-electron Hamiltonians with correlated on-site potentials [23,24]. It seems that this kind of self-affine long-range correlated distribution plays a universal role on the one-electron transport. We expect that the present work will stimulate further theoretical and experimental investigations along this line.

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