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Delocalization and ballistic dynamics in the two-dimensional Anderson model with long-range correlated disorder

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Abstract. – We study the nature of one-electron eigenstates in a two-dimensional ($2d$) Anderson model with long-range correlated disorder. Long-range correlations are introduced by using a $2d$ discrete Fourier method which generates an appropriated disorder distribution with spectral density $S(k) \propto 1/k^{\alpha_{2d}}$. Our numerical data suggest that the exponents governing the collapse of the participation function for low energies ($\xi \propto N^{D_2}$) and the long time decay of the autocorrelation function ($C(t) \propto t^{-\beta}$) satisfy the scaling relation $D_2 = \beta d$. They also imply that the system exhibits a crossover from a diffusive spread for weakly correlated disorder to a ballistic dynamics associated with the emergence of extended states in the strongly correlated disorder regime ($\alpha_{2d} > 2$).

Introduction. – The Anderson localization theory describes some relevant aspects concerning the properties of one-electron states and collective excitations in random media [1–3]. In one-dimensional ($1d$) and two-dimensional ($2d$) electronic systems, the scaling theory [2] predicts the absence of a disorder-driven metal-insulator transition (MIT) for any degree of uncorrelated disorder. For $1d$ systems, it is generally accepted that all eigenstates are exponentially localized for any amount of disorder and, therefore, an initially localized wave packet remains localized in a finite segment. In $2d$ systems, the overall picture is quite distinct. An extensive numerical analysis of the $2d$ Anderson model with dimerized disorder reported that distinct dynamical regimes can be observed according to the disorder strength [4]. The wave packet was shown to remain localized only in the regime of strong disorder. For weak disorder, a ballistic spread takes place. These regimes are separated by a phase with intermediate diffusive-like dynamics. This result points towards an anomalous scaling of the eigenfunctions momenta in the $2d$ Anderson model with intermediate disorder, since it has been demonstrated that the asymptotic scaling of a spreading wave packet is determined by multifractal dimensions characterizing the energy spectrum and eigenfunctions [5].

Recently, it has been reported that the presence of short- [6–12] or long-range correlations [13–15] is a possible mechanism to promote the appearance of truly delocalized states in the one-dimensional Anderson model. The absence of Anderson localization for some specific energy modes was put forward to account for transport properties of semiconductor superlattices with intentional short-range correlated disorder [16]. Further, much attention has been driven to the delocalization problem in $1d$ systems with long-range correlated disorder. It has been reported by several authors [13–15] that these systems display an Anderson transition with mobility edges separating localized and extended states in the limit of strong correlations. This theoretical prediction was confirmed by microwave transmission spectra of single-mode waveguides with inserted correlated scatters [17].

A first study of the effects of long-range correlations in the localization properties of $2d$ electronic systems was performed in ref. [18]. The authors considered a two-dimensional striped media in the x-y plane with on-site disorder. The on-site energies were generated by a superposition of an uncorrelated term and a long-range correlated one along the y-direction. It was predicted that this system displays a disorder-driven Kosterlitz-Thouless metal-insulator transition in the regime of strong correlations. More recently, the influence of long-range correlated disorder in the electron motion in a two-dimensional lattice was investigated [19] and relevant corrections to the conductivity were identified.

In this letter, we focus on the influence of isotropic scale-free long-range correlated disorder on the one-electron eigenstates of the Anderson model defined on a square lattice. In order to introduce long-range correlations in *both* x and y directions, the site energies of the Anderson Hamiltonian are distributed in such a way 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. In what follows, we use an exact diagonalization formalism to compute the participation function which can be used as a measure of the localized/delocalized nature of all eigenstates. In addition, the dynamics associated with the spread of an initially localized wave packet is investigated by numerically solving the $2d$ time-dependent Schrödinger equation. Our results suggest that this $2d$ Anderson model with isotropically long-range correlated disorder can support extended states in the strongly correlated regime.

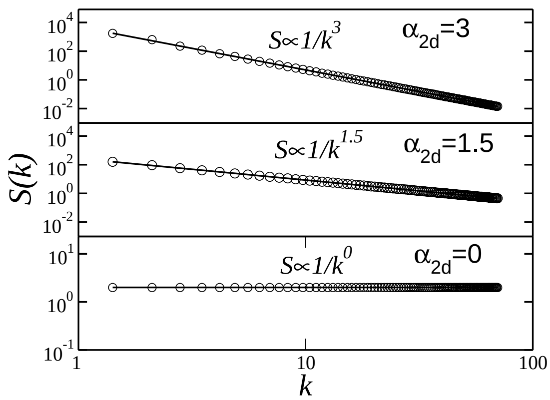

Fig. 1 – Spectrum $S(k)$ *vs.* k for $\alpha = 0$, 1.5, and 3 computed on a lattice with $N^2 = 100^2$. Notice that the power law scaling imposed by eq. (2) is fully satisfied.

Model and formalism. – We consider the $2d$ Anderson Hamiltonian with disordered on-site energies ϵ_{im} on a regular $N \times N$ lattice [3, 18],

$$H = \sum_{i,m} \epsilon_{im} |i,m\rangle\langle i,m| + t \sum_{\langle im,jn\rangle} \big(|i,m\rangle\langle j,n| + |j,n\rangle\langle i,m|\big), \tag{1}$$

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 energy scale by setting the hopping energy $t = 1$. In order to generate a long-range correlated on-site energy landscape, we apply a $2d$ discrete Fourier transform method defined by

$$\epsilon_{i,m} = \sum_{k_x=1}^{N/2} \sum_{k_y=1}^{N/2} \frac{\zeta(\alpha_{2d})}{\left(k_x^2 + k_y^2\right)^{\alpha_{2d}/4}} \cos\left(\frac{2\pi i k_x}{N} + \frac{2\pi m k_y}{N} + \phi_{i,m}\right), \tag{2}$$

where $\phi_{i,m}$ are $N^2/4$ independent random phases uniformly distributed in the interval $[0, 2\pi]$ and $\zeta(\alpha_{2d})$ is a normalization constant which is chosen to have the energy variance $\langle \varepsilon_{i,m}^2 \rangle = 1$. We also shift the on-site energies in order to have $\langle \varepsilon_{i,m} \rangle = 0$. Typically, this sequence is the trace of a $2d$ fractional Brownian motion [20] with a well-defined power law spectrum $S(k) \propto 1/k^{\alpha_{2d}}$, where $k = \sqrt{k_x^2 + k_y^2}$. In fig. 1 we show the power law spectrum $S(k)$ for several values of α_{2d} computed from a sample energy landscape on a lattice with $N^2 = 100^2$ using the $2d$ Fourier transform of eq. (2). In order to investigate the physical properties associated with the nature of one-electron eigenstates ($|\Phi^{(E)}\rangle$), we numerically diagonalize the Hamiltonian and then calculate the participation function $\xi(E)$ defined by [3]

$$\xi(E) = \frac{\sum_{i,m} \left|c_{i,m}^{(E)}\right|^2}{\sum_{i,m} \left|c_{i,m}^{(E)}\right|^4}, \tag{3}$$

where $c_{i,m}^{(E)}$ are the amplitudes of the eigenstate $|\Phi^{(E)}\rangle$ in the Wannier representation ($|\Phi^{(E)}\rangle = \sum_{i,m} c_{i,m}^{(E)} \; |i,m\rangle$). In general, the participation number is a good estimate of the spatial extension of exponentially localized electronic states. For extended states, ξ is proportional to the total number of sites ($\xi \propto N^2$ for a square lattice). On the other hand, wave functions presenting power law decaying tails may display an anomalous scaling of the participation number $\xi \propto N^{D_2}$, with $D_2 < d$ [21].

We also study some dynamical aspects by examining the time evolution of an initially localized wave packet. The Wannier amplitudes evolve in time according to the time-dependent Schrödinger equation as ($\hbar = 1$) [3, 4]

$$i\frac{\mathrm{d}c_{i,m}(t)}{\mathrm{d}t} = \epsilon_{i,m} c_{i,m}(t) + t[c_{i,m-1}(t) + c_{i,m+1}(t) + c_{i-1,m}(t) + c_{i+1,m}(t)], \; i,m = 1,2,\ldots,N. \tag{4}$$

We consider a wave packet initially localized at site $i_0 = N/2$, $m_0 = N/2$, *i.e.* $c_{i,m}(t = 0) = \delta_{i,i_0}\delta_{m,m_0}$. A fourth-order Runge-Kutta method is used to solve the above set of coupled equations. We are particularly interested in calculating the wave packet mean-square displacement $\sigma^2(t)$ defined by [11, 21, 22]

$$\sigma^2(t) = \sum_{i=1}^{N} \sum_{m=1}^{N} \left[(i - i_0)^2 + (m - m_0)^2\right] |c_{i,m}(t)|^2, \tag{5}$$

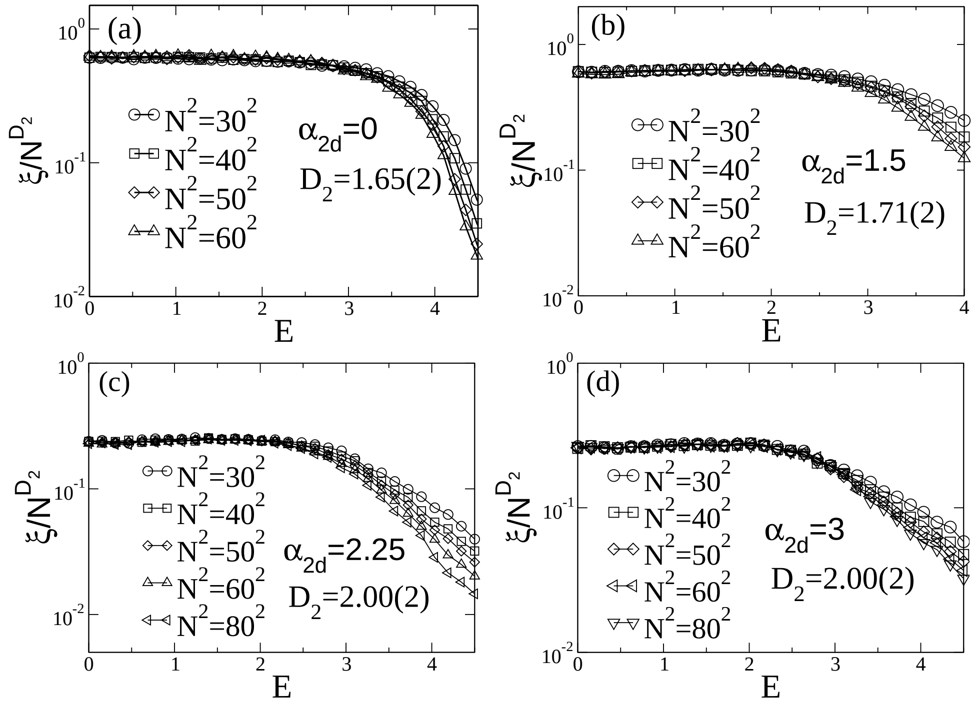

Fig. 2 – Scaled participation number, ξ/N^{D_2}, *vs.* energy E for (a) $\alpha_{2d} = 0$, (b) $\alpha_{2d} = 1.5$, (c) $\alpha_{2d} = 2.25$, and (d) $\alpha_{2d} = 3$. In (a) and (b), a low-energy phase with power law decaying wave functions is characterized the collapse of data with $D_2 < d$. In (c) and (d) $D_2 = d$, suggesting a phase of low-energy extended states.

as well as the temporal autocorrelation function $C(t)$ [21]:

$$C(t) = \frac{1}{t}\int_0^t R(t)\mathrm{d}t\,, \tag{6}$$

where $R(t) = |c_{i_0,m_0}(t)|^2$ denotes the return probability. In the asymptotic limit $t \to \infty$, the temporal autocorrelation function vanishes as $C(t) \propto 1/t^{\beta}$, with $\beta = D_2/d$. This scaling relation is a direct consequence of the fractal character of the eigenfunctions fluctuations [23, 24]. In the large-t limit, the return probability saturates at a finite value whenever the wave packet remains trapped in a finite region around the starting point. Otherwise, it vanishes as the wave packet continuously spread over the lattice [3]. Whenever the system presents a phase of truly extended states, the autocorrelation function vanishes linearly with $1/t$. A slower non-linear decay is usually a signature of an intermediate dynamical regime.

The above scaling relation $\beta = D_2/d$ has been shown to hold for several models exhibiting multifractal eigenfunctions, in particular for models with power law decaying uncorrelated off-diagonal disorder [25, 26]. Although models with power law hopping and power law correlated on-site disorder present some similarities, delocalization is induced in these models by distinct mechanisms. In models with $1/r^{\mu}$ decaying random hopping amplitudes, delocalization is achieved by an increase of the effective dimensionality of the system as longer-ranged couplings are considered and extended states appears for $\mu < d$. For models with short-range couplings and disorder spectral density decaying as $1/k^{\alpha}$, delocalization is induced by the smoothing of the potential landscape and is achieved above a critical value of α. This feature makes the

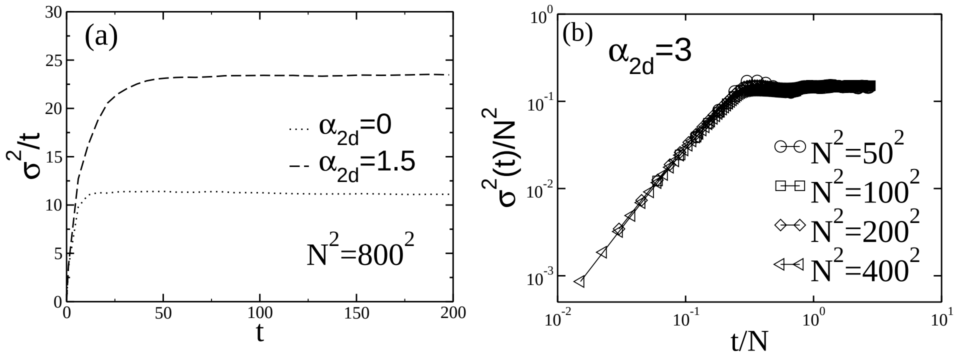

Fig. 3 – (a) Scaled mean-square displacement, $\sigma^2(t)/t$, *vs.* t for $\alpha_{2d} = 0$ (dotted line) and $\alpha_{2d} = 1.5$ (dashed line), with $N^2 = 800^2$ sites. After a short transient, a diffusive spread, $\sigma^2 \propto t$, is observed for $\alpha_{2d} < 2$. (b) Scaled mean-square displacement, $\sigma^2(t)/N^2$, *vs.* scaled time, t/N, for $\alpha = 3$ and $N^2 = 50^2$, 100^2, 200^2, 400^2 sites. The data collapse suggests a ballistic dynamics ($\sigma^2 \propto t^2$) for $\alpha_{2d} > 2$.

$d = 2$ case particularly interesting. Once this is the lower critical dimension for the Anderson transition, a regime of anomalous scaling behavior can emerge even for weak correlations (small α), as we are indeed going to report in the following section.

Results. – In figs. 2(a)-(b) we show the scaled participation number ξ/N^{D_2} *vs.* energy E for (a) $\alpha_{2d} = 0$ and (b) $\alpha_{2d} = 1.5$, with $N^2 = 30^2$, 40^2, 50^2, 60^2 sites, averaged over 100 samples. One can observe a well-defined data collapse for low energies: $D_2 = 1.65(2)$ and $1.71(2)$ for $\alpha_{2d} = 0$ and 1.5, respectively. Since $D_2 < d$, this phase is composed of wave functions with power law decaying tails. The participation number exponent remains smaller than the space dimension for any $\alpha_{2d} < 2$. Therefore, there are no truly delocalized states for this regime of weakly correlated disorder. Figures 2(c)-(d) display ξ/N^{D_2} *vs.* E for (c) $\alpha_{2d} = 2.25$ and (d) $\alpha_{2d} = 3.0$, with $N^2 = 30^2$, 40^2, 50^2, 60^2 sites, averaged over 100 samples, and $N^2 = 80^2$ sites averaged over 50 samples. We see that, in both cases, a well-defined data collapse in a wide region of low energies is obtained with $D_2 = 2.00(2)$. This result suggests the possibility of a phase of low-energy extended states for strongly correlated disorder, *i.e.*, $D_2 = d$. A direct study of the wave packet dynamics can be employed on much larger lattices and, therefore, allows for a finer control of finite-size effects. The long-time behavior of $\sigma^2(t)$ is obtained by numerical integration until the package arrives at one of the lattice boundary sites. In fig. 3(a), we show data for the scaled mean-square displacement, σ^2/t, for $\alpha_{2d} = 0$ and 1.5, with $N^2 = 800^2$ sites, displaying a diffusive behavior $[\sigma^2(t) \propto t]$. These results are compatible with a previous report on the dynamics of a two-dimensional binary alloy with dimerized uncorrelated diagonal disorder [4], where it was numerically shown that localization is only observed for strong disorder. For an intermediate disorder strength, as we simulated here, a diffusive-like dynamics was obtained. Therefore, our results for $\alpha_{2d} < 2$ suggest that a weak degree of correlations does not affect the time dependence of the wave packet mean-square displacement.

We further collected in fig. 3(b) results for the wave packet mean-square displacement $\sigma^2(t)$, computed from lattices with $N^2 = 50^2$, 100^2, 200^2, 400^2 sites and $\alpha_{2d} = 3$, representing a strongly correlated energy landscape (similar results are also found for $\alpha_{2d} = 2.25$, 2.5 and 2.75). In this case, we numerically integrate the wave equation until a stationary state can be reached after multiple reflections of the wave packet on the lattice boundaries. Therefore,

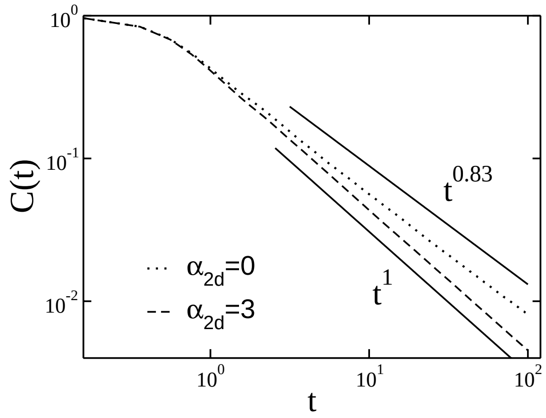

Fig. 4 – Temporal autocorrelation function $C(t)$ *vs.* t for $\alpha_{2d} = 0$ (dotted line) and 3 (dashed line) and $N^2 = 800^2$ sites. In the asymptotic limit $t \to \infty$, $C(t)$ vanishes as $C(t) \propto t^{-\beta}$ with $\beta \approx 0.83(1)$ and 1.0, respectively. These results agree with the reported scaling exponents for the participation number (see figs. 1(a) and (d)).

the mean-square displacement saturates at a value $\propto N^2$ due to finite-size effects. A fine data collapse is found by using the scaling variables $\sigma^2(t)/N^2$ and t/N, implying that, for $\alpha_{2d} > 2$, $\sigma^2 \propto t^2$, *i.e.*, the wave packet presents a ballistic spread before reaching the lattice boundaries.

Another signature of the occurrence of extended states in the strong correlated regime can be obtained by monitoring the temporal autocorrelation function $C(t)$. In fig. 4, we show data for $C(t)$ *vs.* t for $\alpha_{2d} = 0$ and 3, with $N^2 = 800^2$ sites averaged over 20 samples. $C(t)$ vanishes for long times as $C(t) \propto t^{-\beta}$, where $\beta \approx 0.83(1)$ and 1.0 (within our numerical accuracy), respectively. For $\alpha_{2d} = 1.5$, we find $\beta \simeq 0.86(2)$. Thus, the dynamic behavior of $\sigma^2(t)$ and $C(t)$ agrees remarkably well with the results of the participation number calculations, with $\beta = D_2/d$ [21,24]. Therefore, our results support the conclusion that this $2d$ Anderson model displays a phase of extended states induced by long-range on-site correlations.

Conclusions. – In this work we considered the $2d$ Anderson model with long-range correlations in both x and y directions. To introduce long-range correlations in this system we applied a $2d$ Fourier method to construct an on-site energy sequence with spectral density $S(k) \propto 1/k^{\alpha_{2d}}$. Using an exact diagonalization formalism, we investigated the participation function ξ of all energy eigenstates. For $\alpha_{2d} > 2$, we reported a data collapse indicating a phase of extended states in the low-energy regime, in agreement with a previous analytical prediction [19]. Further, by solving the time-dependent $2d$ Schrödinger equation for an initially localized wave packet, we determined the time-dependent mean-square displacement $\sigma^2(t)$ and the temporal autocorrelation function $C(t)$. Our data suggest that the exponents governing the collapse of the participation function for low energies ($\xi \propto N^{D_2}$) and the long time decay of the autocorrelation function ($C(t) \propto t^{-\beta}$) satisfy the scaling relation $D_2 = \beta d$. Also, in the weakly correlated regime ($\alpha_{2d} < 2$) a diffusive behavior ($\sigma^2 \propto t$) was found. In the strongly correlated case ($\alpha_{2d} > 2$) the system displays ballistic dynamics ($\sigma^2 \propto t^2$), with a linear vanishing of the autocorrelation function. This result further characterizes the extended nature of the low-energy states in the strongly correlated regime. We hope that the present work will stimulate further studies on semiconductors and superlattices with intentional long-range correlated disorder.

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