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Coherent electronic dynamics and absorption spectra in an one-dimensional model with long-range correlated off-diagonal disorder

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ABSTRACT

In this work we study an one-dimensional Anderson model with long-range correlated off-diagonal disorder. We numerically demonstrate the presence of extended states and an anomalous optical absorption spectrum for high degrees of correlation. We also show that the electric field biased electronic wave packet dynamics shows Bloch-like oscillations.

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1. Introduction

Electronic transport in non-periodic lattices is a very relevant issue which has attracted the scientific interest during several decades. The scaling theory of Anderson localization predicts the absence of extended eigenstates in low-dimensional systems for any degree of uncorrelated disorder [1–3]. Therefore, electronic wave packets localize in a finite region around any given initial position. However, 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 [4–17]. The absence of Anderson localization in the presence of spatial short-range correlations in disorder was theoretically pointed out by Flores [4] and Dunlap et al. [5] at the end of eighties and the experimental confirmation was obtained by Bellani and co-workers [12] in a semiconductor superlattice with intentional correlated disorder. It has been reported [7,10,11,14] that systems with long-range correlated diagonal disorder display an Anderson metal–insulator transition with mobility edges separating localized and extended states for sufficiently strong correlations. Furthermore, the one-dimensional (1D) model with long-range off-diagonal disorder was investigated in Ref. [16]. It was demonstrated that a localization–delocalization transition occurs similar to that in 1D model with correlated diagonal disorder. The effect of long-range correlated scatters on the transport properties of microwave guides was ex-

perimentally studied and corroborated the predicted presence of mobility edges [15]. Furthermore, the theoretical prediction that is possible to see Anderson localization in a random multilayered filter [18] opened a wide field to investigate the effects of correlated disorder in optical systems. Random dielectric multilayers can be mapped on the problem of one electron in a random media with close connections with the random dimers and off-diagonal disorder versions of the Anderson model [19].

A key problem in condensed matter physics is to understand the electronic transport when disorder and electric field effects are simultaneously present. The interplay between disorder and dynamical localization due to an electric field was recently studied in Refs. [20,21]. It was numerically shown that coherent Bloch oscillations can appear whenever the disorder distribution displays appropriated long-range correlations in both one- [20] and two-dimensional [21] systems. This finding opens the possibility to perform experiments on coherent dc charge transport for measuring the bandwidth of the delocalized phase in disordered systems with long-range correlated randomness. Moreover, it is well known that optical spectroscopy usually fails in detecting localization–delocalization transitions. However, in Ref. [22] it was numerically reported an anomalous behavior of the absorption spectrum in an 1D lattice with long-range correlated diagonal disorder. The double-peak absorption spectrum found is the unique spectroscopic tool to monitor the Anderson transition.

In this Letter we will contribute to advance the understanding of electronic transport in low-dimensional systems with correlated disorder distribution. We will study a 1D Anderson model with long-range correlated off-diagonal disorder, generated by an 1D discrete Fourier method. The participation number and its scaling

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behavior will be obtained through direct diagonalization. The scaling analysis of the mean participation number around the band center will be used to identify the presence of extended states for high degrees of correlation and to explore the possible dependence of the transition point on the strength of disorder. We will also numerically investigate the signature of the delocalization–localization transition on the optical absorption spectrum. In addition we will consider the electric field biased dynamics of an initially localized wave packet by numerically solving the 1D time-dependent Schrödinger equation. Associated with extended states for high degrees of correlation, we will show that sustainable Bloch-like oscillations emerge with a dominant frequency given by the semi-classical prediction.

2. Model and formalism

We consider a tight-binding Hamiltonian with long-range correlated off-diagonal disorder under an external dc electric field on a regular 1D open lattice of spacing a [16]

$$H = \sum_{n=1}^N (-e\mathcal{F}an) |n\rangle \langle n| + \sum_{n=1}^{N-1} J_{n,n+1} |n\rangle \langle n+1|, \quad (1)$$

where $|n\rangle$ is a Wannier state localized at site n with zero site energy, \mathcal{F} is an external uniform electric field, and N is even. The intersite coupling is restricted to nearest-neighbors and assumed to be nonuniform over the entire lattice with $J_{n,n+1} = J_n$. The source of disorder is the stochastic fluctuations of intersite coupling J_n , which we are going to consider as being long-range correlated. One of the simplest ways to numerically generate a long-range correlated sequence of on-site potentials J_n is to write its Fourier decomposition as follows [24]

$$J_n = C_\alpha(N) \sum_{k=1}^{N/2} \frac{1}{k^{\alpha/2}} \cos\left(\frac{2\pi nk}{N} + \phi_k\right). \quad (2)$$

Here, ϕ_k are $N/2$ independent random phases uniformly distributed within the interval $[0, 2\pi]$, and C_α is a normalization constant. We will displace the hopping sequence to have $\langle J_n \rangle = J_0 = 5$ and choose C_α to keep the variance size independent ($\sqrt{\langle J_n^2 \rangle} - \langle J_n \rangle^2 = \Delta$). The long-range nature of the potential correlations results from the power-law dependence of the amplitudes on the wave-vector characterizing each Fourier component. Several stochastic processes in nature are known to generate long-range correlated random sequences which have no characteristic scale as, for example, in the nucleotide sequence of DNA molecules [25]. The relevance of the underlying long-range correlations for the electronic transport in DNA has been recently discussed in Ref. [26]. Furthermore, interface roughness appearing during growth often displays height–height correlations with power-law spectra [27]; thus, the subsequent random potential arising from the rough interface would be long-range correlated. Recently, transport properties of systems with long-range correlated disorder was explored, both theoretically and experimentally, in the design of devices for filtering of electrical and optical signals [28].

2.1. Magnitudes of interest

Initially we will consider the model in the absence of an electric field ($\mathcal{F} = 0$). In order to study the localization properties we compute the static participation ratio defined by $P(E) = \sum_{n=1}^N \psi_n^2(E) / \sum_{n=1}^N \psi_n^A(E)$. Here $\psi_n(E)$ are the Wannier amplitude associated with an eigen-energy E , ($|\phi(E)\rangle = \sum_{n=1}^N \psi_n(E) |n\rangle$) in a chain of N sites. The eigenmodes are obtained by direct diagonalization of the Hamiltonian H . $P(E)$ diverges proportional to

the number of sites for extended states, but remains finite for exponentially localized ones. We average $P(E)$ in a small window around $E = 0$:

$$\langle \xi \rangle = \left[\sum_{E=-\Delta E/2}^{\Delta E/2} P(E) \right] / N_E. \quad (3)$$

We use $\Delta E \approx 1.0$ and a large number of samples such that the number of eigenmodes in each window (N_E) is close to 10^6 in order to obtain a good statistical accuracy. The sun avoids the band center ($-0.1 < E < 0.1$). Here, we will be particularly interested in computing the fluctuation of the participation number defined by

$$\Delta \xi = \sqrt{\langle \xi^2 \rangle - \langle \xi \rangle^2}, \quad (4)$$

where $\langle \xi^2 \rangle$ is the squared participation number averaged in the same energy window as in Eq. (3). The relative fluctuation of the participation number is given by

$$\eta = \Delta \xi / \langle \xi \rangle. \quad (5)$$

Within the framework of random and non-random long-range hopping models, it was demonstrated rigorously that the distribution function of the participation function is scale invariant at the Anderson transition [29]. Such scale invariance has been used to monitor the critical point of long-range hopping models [30] and shall also holds for general models exhibiting a localization–delocalization transition [31–33]. For extended states, the relative fluctuation $\eta(E)$ vanishes continuously with increasing system sizes since the participation function $\xi(E)$ diverges linearly while the fluctuation $\Delta \xi(E)$ has a weaker size dependence resulting from self-averaging. In the opposite regime of exponentially localized states, the relative fluctuation grows with increasing system size converging to a finite value. The relative fluctuation thus converges to a step function as $N \rightarrow \infty$, with a discontinuity at the mobility edge. Therefore, when plotting the relative fluctuation as a function of α , the curves obtained from different chain sizes shall cross roughly at a single point, identifying the localization–delocalization transition. In addition we will study the absorption spectrum defined as

$$A(E) = \frac{1}{N} \sum_{\beta} \delta(E - E_{\beta}) F_{\beta}, \quad (6)$$

where F_{β} is the oscillator strength associated with the eigenvalue β , namely $F_{\beta} = [\sum_n \psi_n(E_{\beta})]^2$. When $J_n > 0$ and disorder is uncorrelated, the eigenstates with higher oscillator strength are those at the top of the band.

2.2. Electric field effects

In terms of the Wannier amplitudes $\psi_n(t) = \langle n | \Psi(t) \rangle$, the Schrödinger equation reads [20]

$$i\dot{\psi}_n = -F n \psi_n + J_{n+1} \psi_{n+1} + J_n \psi_{n-1} \quad (7)$$

where we introduced the dimensionless parameter $F = e\mathcal{F}a/J_0$, and time is expressed in units of \hbar/J_0 . After the introduction of the disorder in the off-diagonal terms, we solve numerically Eq. (7) to study the time evolution of an initially Gaussian wave packet of width σ centered at site n_0

$$\psi_n(t=0) = Z(\sigma) \exp\left[-\frac{(n-n_0)^2}{4\sigma^2}\right] \quad (8)$$

where $Z(\sigma)$ is a normalization constant. Once Eq. (7) is solved for the initial condition (8), we compute the mean position of the wave packet (centroid)

$$x(t) = \sum_n (n - n_0) |\psi_n(t)|^2. \quad (9)$$

3. Results

3.1. Localization and absorption spectrum at zero bias

We start analyzing the results for the participation number and its fluctuations. We have considered $\Delta = 1$ in Fig. 1. In Fig. 1(a) we plot the mean participation number $\langle \xi \rangle$ versus N for $\alpha = 1.1$ up to 2. We observe clearly that $\langle \xi \rangle$ increases when α is increased. This feature agrees with the expected result concerning the emergence of extended states in long-range correlated disordered chains. For $\alpha > 2$ the participation number diverges linearly with the system size, indicating extended states. This result supports previous findings shown in Ref. [16]. However, it is interesting to note that for $1 < \alpha < 2$ the participation number also increase as the system size is increased. It was numerically proposed that this regime does not support true extended states [16]. However, the Lyapunov exponent derived from the transfer matrix formalism is vanishingly small in this intermediate regime [23]. The fluctuations of the participation number can be used as a precise tool to monitor the Anderson localization transitions [30–33]. In Fig. 1(c) we plot the relative fluctuation of the participation number $\Delta \xi$ versus the degree of correlation α for $N = 500$ up to 8000 sites. We observe that the curves obtained from different chain sizes cross roughly at a single point identifying the critical spectral exponent around $\alpha = 2$. A small dispersion at the crossing point is usually due to small corrections to scaling that are present in numerical calculations on finite systems. Before concluding the localization study, some words concerning the critical value $\alpha_c = 2$. In Ref. [14], it was numerically shown that in 1D electronic system with long-range correlated diagonal disorder, the critical spectral exponent α_c is rather independent on the magnitude of disorder Δ . In Fig. 2(a)–(b) we show the scaling behavior of the relative fluctuation on the participation number for $\Delta = 0.5$ and $\Delta = 0.75$. We can see that the critical spectral exponent is also universal, does not depending on the magnitude of the off-diagonal disorder.

Now we focus our attention to the absorption spectrum $A(E)$ for the present 1D model with off-diagonal correlated disorder. To solve numerically Eq. (6) we used $N = 1000$ sites, $\Delta = 1$ and 10^4 realizations of disorder for each value of α . Fig. 3 shows the output of these calculations. We observe that for $\alpha < 1$ the absorption spectrum displays a single and asymmetric peak slightly above the higher band edge $E = 10$ of the periodic lattice ($\sigma = 0$), i.e., only the highest states of the band contribute to the absorption spectrum. Therefore, we have the same trend observed in 1D systems with uncorrelated diagonal disorder. For $1 < \alpha < 2$ we observe an increase of the absorption bandwidth. Thus, models with weak long-range correlations in off-diagonal disorder have a stronger localization at the band edges as compared to the uncorrelated case, as it also occurs in the case of diagonal weakly correlated disorder [22]. However, for $\alpha > 2$ the absorption spectrum displays a well-defined doublet. One of the doublet components (at high energy) is located at the top of the band as usual, whereas the other one (at lower energy) lies deep inside the band. In contrast to the case of $\alpha < 2$, the broadening of the peaks drops down on increasing α and then saturates. To explain the origin of such double peak structure, we will follow Ref. [22] and present a simplified model that contains the basic ingredients needed to obtain the absorption spectrum. The heuristic calculation is started by considering the off-diagonal disorder given by Eq. (2). It is a sum of spatial harmonics. The amplitude of each term, $C_\alpha k^{-\alpha/2}$, decreases upon increasing the number k . For sufficient large α , the first term in the series (2) will be dominant. Therefore, the hopping distribution for a given realization represents a harmonic function of

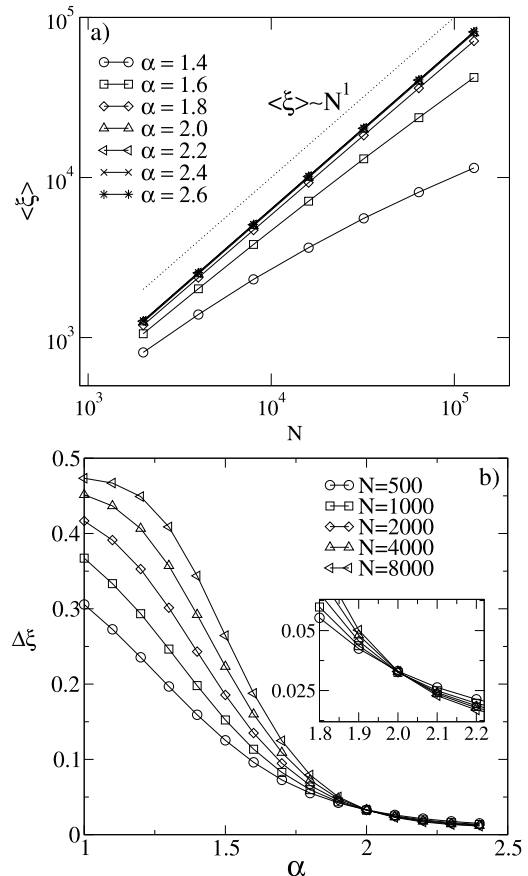


Fig. 1. (a) Mean participation number $\langle \xi \rangle$ versus N for $\alpha = 1.1$ up to 2. We clearly observe that for $\alpha > 2$ the participation number diverges linearly with the system size indicating extended states. (b) The relative fluctuation of the participation number $\Delta \xi$ versus the spectral exponent α for $N = 500$ up to 8000 sites. Curves obtained from different chain sizes cross roughly at a single point $\alpha = 2$. A small spread of the crossing point is usually due to small corrections to scaling that are present in numerical calculations on finite systems (see inset).

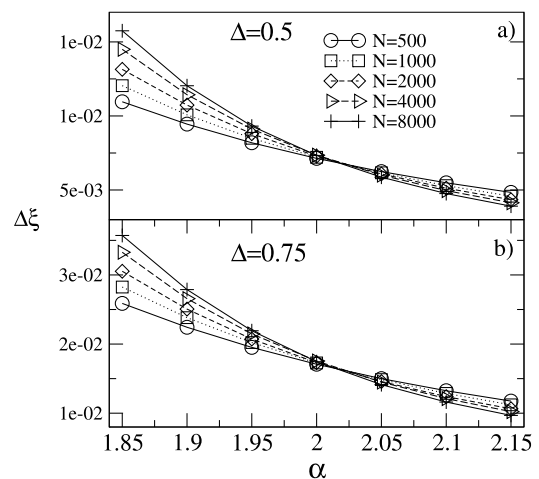


Fig. 2. Relative fluctuation of the participation number, averaged over an energy window $-1 < E < 1$, versus α for $\Delta = 0.5$ and 0.75 . Similarly to models with long-range correlated diagonal disorder [14], the model with off-diagonal correlated disorder also displays a critical point (α_c) that does not depend on the magnitude of disorder Δ .

period N , perturbed by a colored harmonic noise. To further simplify the model, we can divide the 1D lattice in two chains with $J_n \approx J_0 + J^*$ for $n < N/2$ and $J_n \approx J_0 - J^*$ for $n > N/2$ where $J^* = (2/\pi)C_\alpha$ is the average value of the effective harmonic hop-

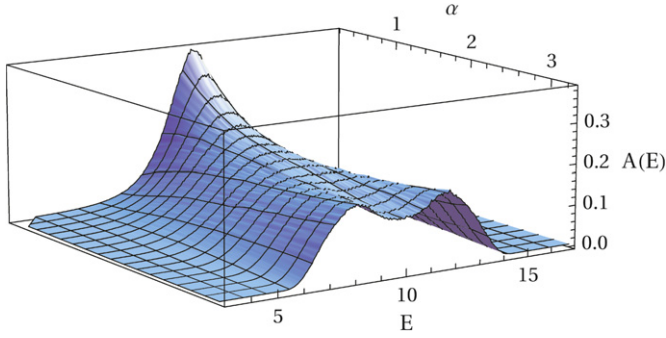


Fig. 3. Absorption spectrum $A(E)$ versus energy and α . Numerical calculations of Eq. (6) were done using $N = 1000$ sites, $\Delta = 1$ and 10^4 realizations of the disorder for each value of α . We observe that for $\alpha < 1$ the absorption spectrum displays a single and asymmetric peak slightly above the higher band edge $E = 10$ of the periodic lattice ($\sigma = 0$), i.e., only the highest states of the band contribute to the absorption spectrum. For $1 < \alpha < 2$ we observe an increase of the absorption bandwidth. For $\alpha > 2$ the absorption spectrum displays a well-defined doublet.

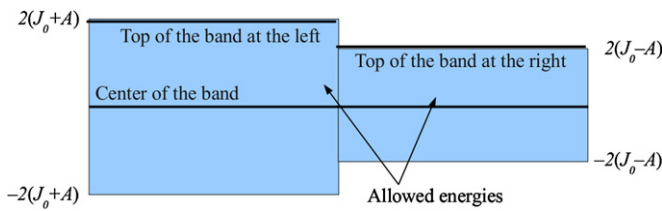


Fig. 4. The 1D model with strong long-range correlated off-diagonal disorder can be mapped into a chain with $J_n \approx J_0 + J^*$ for $n < N/2$ and $J_n \approx J_0 - J^*$ for $n > N/2$ where $J^* = (2/\pi)C_\alpha$ is the average value of the effective harmonic hopping distribution on the left half [Eq. (2)]. The band of allowed energies of each sublattice is showed, ranging from $-2(J_0 + J^*)$ to $+2(J_0 + J^*)$ and from $-2(J_0 - J^*)$ to $+2(J_0 - J^*)$ at the left and right sublattices, respectively. For this effective band distribution we expect an absorption spectrum with two peaks caused by the transitions from the ground state to the uppermost state of each subband. For $\Delta = 1$ their locations are $2(J_0 + J^*) \approx 12.0(1)$ and $2(J_0 - J^*) \approx 8.0(1)$, in good agreement with Fig. 3.

ping distribution on the left half. Therefore, we map the original lattice onto two uniform sublattices, coupled to each other through the hopping between sites $N/2$ and $N/2 + 1$. The allowed energies of each sublattice form a band, ranging from $-2(J_0 + J^*)$ to $+2(J_0 + J^*)$ and from $-2(J_0 - J^*)$ to $+2(J_0 - J^*)$ for the left and right sublattices, respectively (see Fig. 4). The absorption spectrum of such a system is expected to have two peaks caused by the transitions from the ground state to the top state of each subband. For $\Delta = 1$ their locations are $2(J_0 + J^*) \approx 12.0(1)$ and $+2(J_0 - J^*) \approx 8.0(1)$. We stress that these values are in good agreement with the numerical calculations presented in Fig. 3.

3.2. Electric field effects

Finally, we study the time evolution of an initially localized wave packet subjected to a uniform electric field. It is well known that in disorder-free systems, a uniform electric field causes the dynamic localization of the electron and gives rise to an oscillatory motion of the wave packet, the so-called Bloch oscillations [20]. The size of the segment over which the electron oscillates and the period of the oscillations are estimated from semi-classical arguments to be $L_F = W/F$ and $\tau_B = 2\pi/F$, respectively, where W is the width of the Bloch band in units of the coupling integral J_0 . First, we compute the centroid $x(t)$ in a chain with weak long-range correlated off-diagonal disordered ($\alpha < 2$) of size $N = 1000$ with $F = 1.0$. As deduced from the upper panel of Fig. 5(a)–(b), there is no signature of Bloch oscillations in this case. Regular oscillations, which are present immediately after the initial wave packet is released, are quickly damped (not shown). The subse-

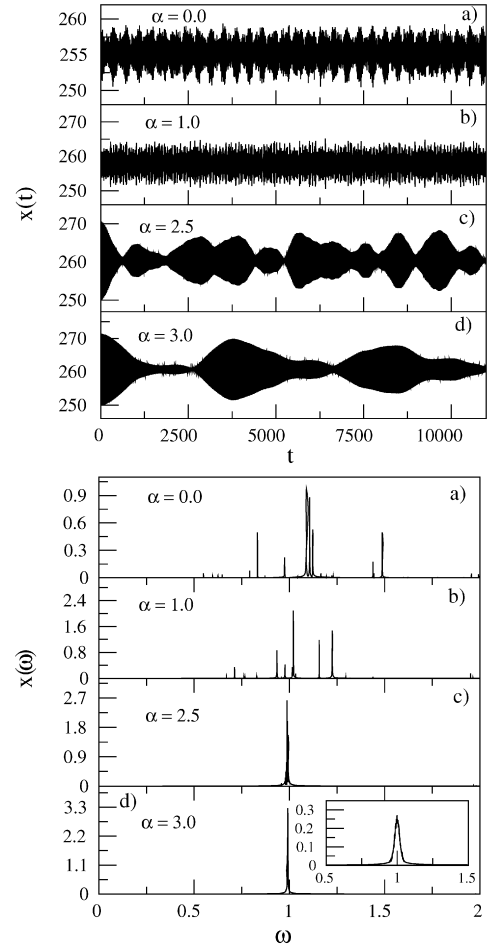


Fig. 5. Centroid $x(t)$ and its Fourier spectrum $x(\omega)$ and lower panels respectively) computed using a chain with $N = 1000$ sites, electric field $F = 1.0$ and several degrees of correlations $\alpha = 0, 1, 2.5$ and 3 . We observe that the oscillations have no predominant frequency for $\alpha < 2$. However, in the regime of $\alpha > 2$, a coherent oscillatory motion of the centroid sets up, with a well-defined peak at the Bloch frequency.

quent motion of the centroid resembles a stochastic motion around some mean position. The Fourier spectrum $x(\omega)$ of the centroid, plotted in the lower panel of Fig. 5(a)–(b), confirms this observation. The absence of a single peak in the Fourier spectrum $x(\omega)$ suggests that for $\alpha < 2$ the system shows a behavior similar to the standard Anderson model, with no signatures of Bloch oscillations. In the strong correlated case ($\alpha > 2$), the centroid reveals an oscillatory amplitude-modulated pattern, as shown in Fig. 5 (upper and lower panels c and d). Its Fourier transform $x(\omega)$ shows a well-defined narrow peak around $\omega = F$, as predicted by the semiclassical approximation [20].

4. Summary

In this Letter we study some aspects of localization, absorption spectrum and the biased electric field dynamics in a 1D Anderson model with long-range correlated off-diagonal disorder. The participation number and its scaling behavior were obtained through direct diagonalization. The scaling analysis of the relative fluctuations on the mean participation number around the band center indicates the presence of extended states for high degree of correlation and reveals that the critical spectral exponent does not depend of the disorder strength. We also numerically demonstrated that the delocalization–localization transition reveals itself in the optical absorption spectrum. The emergence of delocalized

states is signaled by the development of a well-defined doublet. One of the doublet components is located at the top of the band as usual, whereas the other one lies deep inside the band. By using a heuristic model we explain in detail the origin of the double peak absorption spectrum. In addition, the numerical calculations of the electric field biased dynamics of an initially localized wave packet have shown that, associated with extended states, sustainable Bloch-like oscillations sets up with the frequency obeying a semi-classical prediction.

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