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Optical absorption and delocalization in a quaternary tight-binding chain with correlated disorder

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ABSTRACT

We study electronic transport in a one-dimensional model with four kinds of atoms. The quaternary energy distribution is chosen in such a way that it contains long-range correlations. Localization properties and optical absorption are obtained by using numerical methods. Regarding the localization properties of the wave function, we show numerically that, for weak correlation on disorder, the participation number is finite, and the eigenstates are localized. For strong correlation, our results suggest that the model displays fully delocalized eigenstates. Weakly localized states are present in the regime of intermediate correlations. Our analysis of the optical absorption showed an interesting pattern of peaks and a strong dependence on the correlation degree. The structure of peaks is discussed in the light of the underlying density of states.

1. Introduction

According to Anderson localization theory, it is well known that extended eigenstates are absent in low-dimensional disordered systems for any level of uncorrelated disorder [1]. Exceptions to this statement are related to those cases with intrinsic correlation in the disorder distribution [2–21]. In general, it has been demonstrated that correlated disorder promotes the appearance of a metal–insulator transition, even in one-dimensional models. Moreover, the effect of correlated disorder on optical spectroscopy properties is also a key problem in the context of condensed matter physics [22–27]. It is well known that optical spectroscopy usually fails in detecting localization–delocalization transitions. However, a double-peak absorption spectrum profile has been numerically reported in a 1*d* lattice with long-range correlated diagonal disorder [24]. This phenomenon was also observed in a 1*d* lattice with long-range off-diagonal correlated disorder [25]. In [26], the optical properties in 1*d* models with heavy-tailed Levy disorder distribution were studied. These authors found a broadening of the optical line and a non-universal scaling of the distribution of exciton localization lengths. The optical absorption bandwidth and the non universality of the localization length within models with Levy disorder distribution were re-visited in [27].

Works on correlated disorder have considered systems in which the site energies are uniformly distributed in a finite range $[-W/2, W/2]$. Some years ago, models were considered in which the on-site energy could assume only discrete values (for example, binary and ternary models) [28–34]. The Anderson model with long-range correlated ternary disorder sequence was studied in [28]. These authors demonstrated that if the ternary sequence is generated in a fully random way, then the system is an insulator. Nevertheless, by creating a ternary diagonal disorder with long-range correlations, a localized–delocalized phase transition was observed [28]. The effect of long-range correlations in the sequence of

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capacitances of classical transmission lines (TL) was studied by Lazo and Diez [30,31]. To generate the ternary correlated distribution of capacitances, the Fourier filtering method was used [30] and also the Ornstein–Uhlenbeck (OU) process [31]. In both cases, a transition from non-conducting to conducting state of the TL induced by strong correlations was observed. More recently, a one-dimensional classical ternary harmonic chain with the mass distribution constructed from an OU process was studied [32]. The localization aspects of all vibrational eigenstates were obtained using the transfer matrix formalism. These authors concluded that only the zero frequency mode can propagate through the chain, thus contradicting previous works [28–31]. It has been latter clarified that the transition observed in Refs. [28–31] was actually a transition between disordered and ordered chains because the global disorder effectively vanished as the internal correlations were increased in their model systems. Forthcoming works unveiled the role played by local and global disorder in several models with discrete diagonal disorder [32–34], showing that a localization–delocalization transition can indeed occur when the global disorder is kept finite while the local disorder vanishes. In this case, delocalized states emerge when the two point correlation function develops a slow power-law decay. In the present work, we will focus in a model system with a finite global disorder and explore the signature of the localization–delocalization transition in the optical absorption spectrum.

We would like to stress that the study of models with discrete correlated disorder has received considerable interest from the experimental point of view. The possibility of generating real systems with a discrete correlated disorder can be a possible tool to compare theoretical and experimental procedures [35], also allowing for the design of new materials with adjustable properties.

Here, we will study the electronic transport in systems with correlated quaternary disorder distribution. In particular, we will examine localization properties and optical absorption using numerical methods. The term "quaternary disorder" represents a disorder distribution containing only four values $(\epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4)$. We will be particularly interested in identifying the distinct regimes of eigenstates localization and relate them with the typical regimes local disorder that emerge when the correlation degree is increased. Further, we will explore the optical absorption spectrum and relate its structure of peaks with the underlying characteristics of the energy band.

2. Model and formalism

We consider a standard one-electron Anderson Hamiltonian written as

$$H = \sum_n \epsilon_n |n\rangle\langle n| + \sum_n \tau_n (|n\rangle\langle n+1| + c.c) \tag{1}$$

where (ϵ_n) represents the quaternary correlated disorder distribution. We construct this sequence by mapping a continuous correlated series $\{V_n\}$ in a discrete group of four values $(\epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4)$. The continuous series $\{V_n\}$ is obtained through the trace of a fractional Brownian motion defined as [4–7]:

$$V_n = \sum_{k=1}^{N/2} \frac{1}{k^{\gamma/2}} \cos\left(\frac{2\pi nk}{N} + \phi_k\right). \tag{2}$$

Here, ϕ_k represent random phases distributed within the interval $[0, 2\pi]$.

The above series has no typical length scale, which is a characteristic of several stochastically generated natural series [36]. These sequences have a power-law spectral density of the form $S(k) \propto 1/k^{\gamma}$ derived from the Fourier transform of the two-point correlation function. k is related to the wavelength λ of the undulations on the random landscape. The widespread occurrence in nature of sequences with power-law noise is related to the general tendency of large driven dynamical systems to evolve for a self-organized critical state [37]. For $\gamma = 0$, the sequence is completely uncorrelated. The exponent γ is directly related to the Hurst exponent H of the rescaled range analysis ($\gamma = 2H + 1$) which describes the self-similar character of the series and the persistent character of its increments. In the case of $\gamma = 2$ the sequence resembles the trace of the usual Brownian motion. Long-range correlated sequences with persistent (anti-persistent) increments are obtained in the regime $\gamma > 2$ $(0 < \gamma < 2)$.

According to the approach used in [4], we also perform a normalization process such that : $\langle V_n \rangle = 0$ and $\sqrt{\langle V_n^2 \rangle - \langle V_n \rangle^2} = 1$. Once the correlated sequence $\{V_n\}$ was built, we proceed to the mapping in order to generate the quaternary correlated sequence $\{\epsilon_n\}$. The mapping is defined by the equation below:

$$\epsilon_n = \begin{cases} \epsilon_1 & \text{if } V_n < -b \\ \epsilon_2 & \text{if } -b < V_n < 0 \\ \epsilon_3 & \text{if } 0 < V_n < b \\ \epsilon_4 & \text{if } V_n > b. \end{cases} \tag{3}$$

The mapping parameter b introduced into this equation controls the type of mapping we use. In general, b controls the probability of each of the four values $(\epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4)$ appearing on the quaternary distribution. We choose $b \leq 2$, once 2 is approximately the largest value of the V_n sequence after the normalization process. Moreover, we set the following values for the on-site energies: $\epsilon_1 = -2, \epsilon_2 = -1, \epsilon_3 = 1$ and $\epsilon_4 = 2$.

In our calculations, hopping energy is $\tau_n = 1$. By exact diagonalization we compute all eigenstates $|\Phi(E)\rangle = \sum_n f_n(E)|n\rangle$, where $f_n(E)$ represents the Wannier amplitude on site n. From these eigenfunctions, we estimate participation average