Stationary, dynamical, and spectral electronic properties of a correlated random ladder model with coexisting extended and localized states

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We study some stationary, dynamical, and spectral properties of a tight-binding Hamiltonian model for noninteracting electrons in a random two-channels ladder with correlated disorder that presents superposed bands of localized and extended states. We compute the participation number, Kubo-Greenwood conductance, Lyapunov exponent, the spread of an initially localized wave packet, as well as the level-spacing statistics in the band of coexisting localized and extended states. All stationary quantities show a metallic character at the coexistence energy band, such as a finite conductance and vanishing Lyapunov exponent. The wave packet exhibits a ballistic spread due to the Bloch-type nature of the extended states. On the other hand, the level-spacing statistics is characterized by a new distribution function which accounts for the superposition of uniformly distributed Bloch-type states and Poissonian-distributed localized states.

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I. INTRODUCTION

The nature of electronic states in random systems is a central issue governing the electronic transport in condensed-matter physics. There are several quantities used to characterize electronic eigenstates in disordered systems, including stationary, dynamical, and spectral features. Among these, the level-spacing statistics has revealed itself as a very powerful tool.[1] It has been widely employed as an independent method based on the random matrix theory that is able to identify the presence of a disorder-induced metal-insulator transition.[5] It is well known that in the metallic regime of disordered systems with time-reversal symmetry and no spin dependence, the level-spacing distribution $P(s)$ is well described by the Gaussian orthogonal ensemble of random matrix theory, assuming the form $P(s)=(\pi/2)s\exp[-(\pi/4)s^2]$. Here, s denotes the energy-level spacing in units of the mean level spacing and $P(s)$ gives the distribution of normalized gaps in the spectrum in the limit of infinite system sizes. In the insulating regime, the level-spacing distribution follows a Poisson law $P(s)=\exp(-s)$. Usually, metallic (extended) and insulator (localized) eigenstates are not mixed within the energy band. Localized states have energies close to the band tails and are separated from the extended ones by mobility edges.[2] The disorder-induced metal-insulator transition takes place when the Fermi level crosses the mobility edge. At the metal-insulator transition, the level-spacing distribution has been shown to follow yet another behavior which is attributed to the existence of a critical ensemble.[3–7]

The scaling theory for the Anderson localization predicts that a metal-insulator transition can only take place above two dimensions.[8] According to general scaling arguments, all states shall be exponentially localized by any degree of disorder in one-dimensional (1D) systems, a scaling prediction widely supported numerically.[2] However, it has been reported along the last two decades that the presence of short-range[9–14] or long-range correlations[15–18] in the disorder distribution, as well as long-range couplings[19–22] can induce the appearance of truly delocalized states in low-dimensional Anderson models. In particular, such correlation-induced delocalization has been explored in several studies of the electronic transport along DNA-based chains motivated by recent claims of long-range correlations in the base-pairs sequence.[23–28] Based on a simple ladder model of a double-strand DNA, it has been shown that correlations and asymmetry on the sequence affect the electron localization.[24,28] Numerical calculation in double-strand DNA sequences have also identified a substantial increase in the one-electron localization length associated with the underlying correlations between the two nucleotide chains.[29,30] Two-channel random ladders have thus been considered as an interesting class of model systems on which correlations can strongly influence the electronic transport. Very recently, Sil *et al.*[31] showed that a quasiperiodic two-chain ladder presents metal/insulator transitions at multiple values of the Fermi energy. Further, the same group demonstrated analytically that a two-channel random ladder model can display a band of Bloch-type extended states when the on-site potentials and the hopping amplitudes display a particular correlation.[32] Remarkably, this band of extended states coexists with exponentially localized states, a new scenario that can lead to unusual transport properties.

Here, we explore in detail the effects of the coexistence of localized and extended states in the correlated random ladder model. We will show that stationary and dynamical properties are dominated by the extended states with the system presenting unusual features, such as a finite conductivity and a ballistic spread of the electronic wave packet. We further analyze the spectral statistics near the band center, where the superposition of localized and delocalized bands give rises to a new level-spacing distribution.

II. MODEL AND FORMALISM

Here, we study the two-channel ladder model within the first neighbors tight-binding approximation. Considering a single orbital per site, the Hamiltonian can be written as,

$$H=\sum_n \varepsilon_n \mathbf{c}_\mathbf{n}^\dagger \mathbf{c}_\mathbf{n} + t\sum_n \mathbf{c}_\mathbf{n}^\dagger \mathbf{c}_{\mathbf{n+1}} + t\sum_n \mathbf{c}_{\mathbf{n+1}}^\dagger \mathbf{c}_\mathbf{n}, \qquad (1)$$

where,

$$\mathbf{c_n} = \begin{pmatrix} \mathbf{c_{n,1}} \\ \mathbf{c_{n,2}} \end{pmatrix} \tag{2}$$

with $\mathbf{c_{n,i}}$ and $\mathbf{c^{\dagger}_{n,i}}$ being the usual fermionic creation and annihilation operators acting at site n of chain $i=1,2$. Also

$$\varepsilon_n = \begin{pmatrix} \varepsilon_{n,1} & \gamma_n \\ \gamma_n & \varepsilon_{n,2} \end{pmatrix}, \tag{3}$$

where $\varepsilon_{n,j}$ is the on-site energy at the nth site in chain j. γ_n corresponds to the interchain hopping parameter between the pair of sites at position n. Further, the coupling along each chain will be considered as site independent and can be put in the form

$$t = \begin{pmatrix} t & 0 \\ 0 & t \end{pmatrix} \tag{4}$$

with t being the intrachain hopping parameter between nearest neighbors.

In the above model, disorder is only present in the on-site potentials and in the interchain coupling. In Ref. 32 it was analytically demonstrated that when the ratios $\varepsilon_{n,2}/\varepsilon_{n,1}$ and $\gamma_n/\varepsilon_{n,1}$ follow constant proportions along the chain, i.e., $\varepsilon_{n,2}/\varepsilon_{n,1}=\varepsilon$ and $\gamma_n/\varepsilon_{n,1}=\gamma$, there is a similarity transformation that decouples the Hamiltonian eigenstates. The Hamiltonian can be written as the one of two uncoupled chains with effective on-site potentials being given by $\varepsilon^*_{n,i}=\lambda_i\varepsilon_{n,i}$, with

$$\lambda_1 = \frac{1+\varepsilon}{2} + \sqrt{\left(\frac{1-\varepsilon}{2}\right)^2 + \gamma^2}, \tag{5}$$

$$\lambda_2 = \frac{1+\varepsilon}{2} - \sqrt{\left(\frac{1-\varepsilon}{2}\right)^2 + \gamma^2}. \tag{6}$$

In general, both normal modes correspond to effective chains with random on-site potentials coupled through a nonrandom first neighbors hopping. Therefore, all eigenmodes are usually exponentially localized. However, for the particular case of $\gamma^2=\varepsilon$, one results with $\lambda_2=0$. Thus, one of the effective chains becomes disorder free with all on-site potentials being $\varepsilon^*_{n,2}=0$. Under this condition, all eigenmodes corresponding to this chain are Bloch type with energies ranging from $-2t<E<+2t$. On the other hand, all eigenmodes of the first set of normal modes remain exponentially localized. This situation represents a new scenario among the models of disordered electronic systems.[32] The mobility edges at the energies $E=\pm t$ actually separates exponentially localized states located near the band tails from the energy range around the band center on which Bloch type and exponentially localized states coexist.

III. STATIONARY, DYNAMICAL, AND SPECTRAL PROPERTIES

In what follows, we will analyze how such coexistence of localized and extended states influence the main physical quantities used to investigate disordered electron systems. We will consider all energies to be given in units of the intrachain hopping amplitude $t=1$. The on-site energies of the first chain will be taken from a uniform random distribution in the interval $[-0.5,0.5]$. Without any loss of generality, we will restrict the following study to the case of $\varepsilon=\gamma^2=1$. The main results we are going to discuss are quite independent of the actual value of ε. With the above setting $\varepsilon_{n,1}=\varepsilon_{n,2}=\gamma_n$ while being randomly distributed along the ladder. Initially, we numerically diagonalized the full Hamiltonian on a double-chain ladder up to $N=12\,000$ sites. In order to avoid spurious effects from a special disorder configuration, we averaged all quantities over distinct disorder configurations.

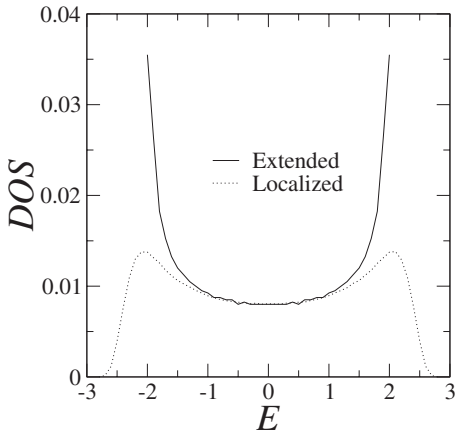

FIG. 1. DOS of the correlated ladder model evidencing the contribution of localized and extended states. At the band tails ($|E|>2$) only localized states are present. For $|E|<2$ continuous bands of localized and Bloch-type states coexist with a similar DOS at the band center. Data were obtained from 10^2 distinct disorder configurations on ladders with $N=10^4$ sites.

Figure 1 shows the density of states (DOS) for the localized and delocalized states separately. These have been classified by the spacial extension of each eigenmode. One can observe that the DOS corresponding to the extended state (continuous line) is indeed numerically identical to the DOS of a completely ordered chain. On the other hand, the DOS of the localized states (dotted line) corresponds to that of an uncorrelated disordered chain. This corroborates the previous discussion concerning the fact that this particular parameter setting leads to a decoupling of the ladder eigenmodes in Bloch-type and localized states, as well as to their coexistence in the energy range $-2<E<+2$. Notice that localized and extended states have a similar DOS at the center of the band.

In order to characterize the spacial extension of each eigenfunction, we measured their participation ratio. It is defined, within the tight-binding approximation, as[33]

$$\mathrm{P}_k/N = \frac{1}{N\sum_{n=1}^{N/2}\sum_{i=1}^{2}|a^k_{n,i}|^4}, \tag{7}$$

where $a^k_{i,j}$ is the amplitude of the kth wave function at the site (n,i). The participation ratio is roughly size independent for extended state, reaching a value of 2/3 for Bloch states. On

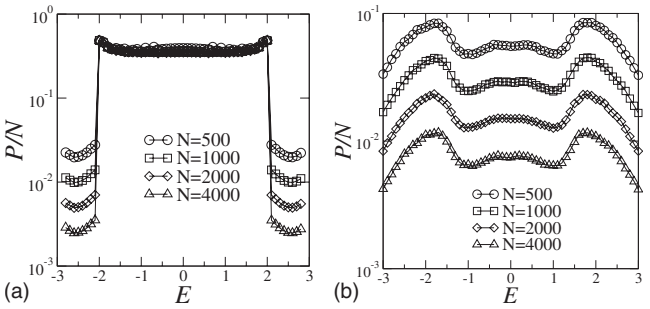

FIG. 2. (a) Averaged participation ratio P/N as a function of energy obtained from the exact diagonalization of the correlated ladder model for distinct ladder sizes N. In the coexistence region, the participation ratio is size independent showing the predominance of the extended states scaling behavior. (b) P/N for the counterpart ladder model with nonrandom interlayer hopping. As the ladder size increases, P/N decreases within the entire energy band, indicating that all sates are localized in this case. Distinct disorder configurations were considered up to a total of 1.5×10^6 states for each ladder size.

the other hand, it decays as $1/N$ for exponentially localized states. In what follows, we will report the averaged participation ratio, P/N, of the states with eigenenergies located within a small energy window around a given energy E. One expects it to decay as $1/N$ at the band tails where only localized states are present. In the coexistence region, the scaling behavior shall be asymptotically dominated by the extended states.

In Fig. 2(a), we depict the averaged participation ratio as a function of energy for the present fully correlated random ladder model, as obtained from the exact diagonalization of ladders with distinct sizes. It clearly shows the mobility edges at $E=\pm2$. In the band tails, the participation ratio decays as $1/N$, as predicted due to the localized nature of the eigenstates in this energy range. In the coexistence region, the participation ratio is indeed size independent showing the predominance of the extended states scaling behavior. Near the band center, it assumes a value which is roughly equal to 1/3. This is consistent with the fact that localized and Bloch-type states have a similar DOS at the band center with the average P/N being given by the direct average between its value for Bloch-type $(P/N=2/3)$ and for localized $(P/N=0)$ states. At the mobility edges the averaged P/N reaches 2/3 due to the diverging DOS of the extended Bloch-type states. To explicitly show that both correlations (between the on-site couplings and between one of the on-site couplings and the intrachain hopping amplitude) are needed to obtain a band of extended states, we also considered a model with the same correlation between the on-site couplings, but with a nonrandom intrachain hopping $(\gamma_n=1)$. In Fig. 2(b), the P/N for this counterpart ladder model with nonrandom hoppings is shown. As the size of the system increases, P/N decreases within the entire energy band, indicating that all states are localized in this case.

In addition to the characterization of the spacial extension of the electronic states gotten from the exact diagonalization of the Hamiltonian, we also report the system's conductance. The conductance, for noninteracting electrons, and within the linear-response theory at zero temperature, is given by the Kubo-Greenwood formula,[34]

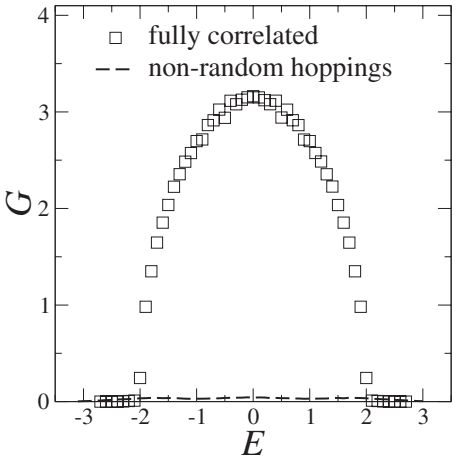

FIG. 3. Conductance for the fully correlated ladder model (symbols) and the counterpart ladder model with uncorrelated on-site potentials (dashed line). The finite conductance within the coexistence band of the fully correlated model reflects its metallic character. The small conductance of the ladder model with nonrandom hoppings is a finite-size effect that vanishes in the thermodynamic limit. Data were obtained from 5×10^2 distinct disorder configurations on ladders with 10^4 sites.

$$G(E)=\frac{2\pi}{\Omega}\sum_{a,b}|\langle a|\mathbf{n}H-H\mathbf{n}|b\rangle|^2\delta(E-E_a)\delta(E-E_b), \quad (8)$$

where $\mathbf{n}$ is the position operator along the ladder and $|a\rangle$ and $|b\rangle$ are stationary eigenstates. The above expression relates the nature of the one-electron eigenstates with the electrical conductance. If around the energy E there are delocalized states, the conductance has a finite value. However, if only localized states are present, the conductance goes to zero in the thermodynamic limit. In Fig. 3, we report the energy dependence of the conductance for the fully correlated random ladder model and its counterpart with nonrandom hoppings. The mobility edges separate the regime of vanishing conductance from the regime of finite conductance in the model with coexisting localized and delocalized states. The small conductance in the model with nonrandom hoppings is a finite-size effect. It continuously vanishes as the system size is increased.

Another standard quantity used to distinguish localized and extended states is the Lyapunov exponent Γ, which is the inverse of the localization length λ. The Lyapunov exponent is given by[2]

$$\Gamma\equiv\frac{1}{\lambda}=-\lim_{N\to\infty}\frac{2}{N}\ln|G^{\dagger}_{1,N/2}(E)|^2, \quad (9)$$

where $G^{\dagger}_{1,N/2}$ is the Green's-function operator between the first and the last pairs of sites. It can be numerically obtained through a decimation process. This aspect allows to compute the Lyapunov exponent for very long system sizes. Here, we used ladders with 12×10^6 sites. Further details about the computation of this parameter can be found in Refs. 35 and

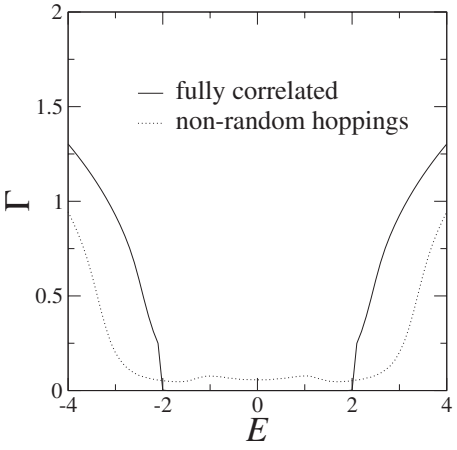

FIG. 4. Lyapunov exponent Γ for the fully correlated ladder model (continuous line) and the counterpart ladder model with nonrandom hoppings (dashed line). In the model with nonrandom hoppings, the Lyapunov exponent is finite within the entire energy band, reflecting the localized nature of all eigenstates. In the fully correlated model, the presence of extended states is signaled by the vanishing of Γ in the coexistence band.

36. If there are extended states in the vicinity of a given energy E, the Lyapunov exponent vanishes in the thermodynamic limit. It assumes a finite value when all states are localized in the vicinity of E, as well as outside the energy band. The Lyapunov exponent is shown in Fig. 4 for both fully correlated ladder model and the nonrandom hoppings ladder model. Once again the mobility edges are clearly depicted in the fully correlated model with the Lyapunov exponent being vanishingly small within the band of coexisting localized and delocalized states.

The localized/delocalized nature of one-electron eigenstates also influences the electronic transport. In order to study the one-electron wave-packet dynamics, we followed the time evolution of an initially localized wave packet. The time evolution of the wave function is obtained from the action of the unitary time-evolution operator,

$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle, \tag{10}$$

where $|\psi(t)\rangle$ is the electron state at time t and $|\psi(0)\rangle$ is the initial state. We solve Eq. (10) by expanding the time-evolution operator up to the 30th order. The wave-packet width $\sigma(t)$ is measured as the square root of the mean-square deviation of the electron from its initial position. In Fig. 5(a) we show the scaled wave-packet width $\sigma(t)/N$ as a function of the scaled time t/N for the fully correlated ladder model. Data from distinct chain sizes collapses into a single curve. The linear finite-size scaling of the asymptotic width indicates that the wave packet propagates until reaching the chain boundaries. The small oscillations during the convergence to the ultimate stationary state is due to the multiple reflections of the wave packet at the ladder boundaries and the coherent interference between the incident and reflected waves. Further, the initial linear behavior $\sigma(t) \propto t$ indicates a ballistic spread dominated by the unscattered Bloch-type states. For the ladder model with nonrandom hoppings, the data from distinct ladder sizes falls into a single curve without any rescaling. The size independence of the asymptotic wave-packet width indicates that the electron wave function spreads over a finite portion of the system.

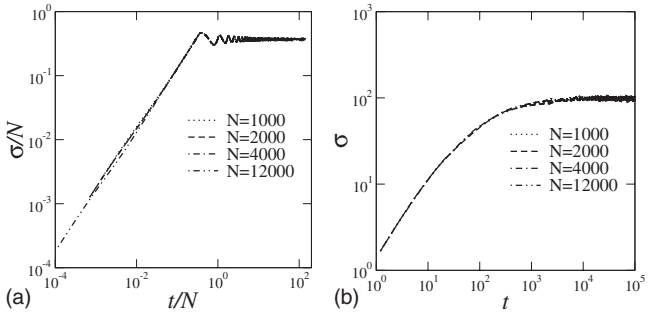

FIG. 5. (a) Time evolution of the wave-packet width of an initially localized electron in the fully correlated model for different ladder sizes. Data collapse into a single curve after a linear rescaling of the wave-packet width and time, indicating that the wave packet propagates ballistically until reaching the chain boundaries. (b) The corresponding time evolution in the counterpart ladder model with nonrandom hoppings. Data from distinct size falls into a single curve with no rescaling, showing that the electron wave packet spreads over a finite portion of the system.

Finally, we investigate how the coexistence of localized and extended states in the same energy range impacts the level-spacing statistics. Exponentially localized states are usually distributed in energy following a Poisson law $P(s) = \exp(-s)$, where s is the level spacing measured in units of the mean level spacing. Delocalized eigenfunctions repel each other. In the presence of disorder, the level spacing of extended states obeys the Wigner surmise, which takes the form $P(s) = (\pi/2)s \exp[-(\pi/4)s^2]$ in systems with time-reversal symmetry and no spin coupling. At the Anderson transition a new universal critical statistics intermediate between Wigner and Poisson has been suggested as a consequence of the multifractality of critical wave functions.[3–7] On the other hand, the level spacing of Bloch states is fully determined by the density of states at a given energy range.

In Fig. 6 we show results of the level-spacing distribution as obtained from the present two-channel model with correlated disorder and coexisting localized and Bloch-type states near the band center. To obtain the level-spacing distribution, we used an energy window near the band center $[-1,1]$. A spectral unfolding procedure was employed to keep the average level spacing equal to unity in each segment of the energy window.[4] Here, we have used $N = 12\,000$ sites and 5000 distinct disorder realizations. The emerging level-spacing distribution does not follow any of the standard forms. It displays an almost linear decrease with increasing level spacings, after which it develops a sharp increase as the level spacing approaches twice the average spacing. There is no level spacing larger than $s \simeq 2$. Actually, this distribution results from the fact that localized and Bloch-type states have roughly the same DOS in this energy range. After the spectral unfolding, the Bloch-type states become uniformly distributed in this energy range. On the other hand, the localized states are randomly distributed. Therefore, the spacing between Bloch states is equal to the average spacing between localized ones and twice the overall average level

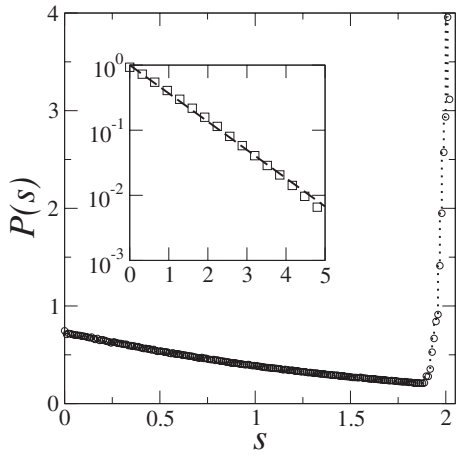

FIG. 6. The level-spacing distribution function for the states near the center of the coexistence band ($|E|<1$) of the fully correlated ladder model. Data were obtained from direct diagonalization of ladders with $N=12\,000$ sites and averaged over 5000 distinct disorder realizations. It displays an almost linear decrease followed by a sharp peak as the level spacing approaches twice the average spacing. This feature is related to the similar DOS of localized and Bloch-type states near the band center. The inset shows the Poissonian character of the level-spacing distribution for the counterpart ladder model with nonrandom hoppings.

spacing. Within this picture, the maximum level spacing is that between neighboring Bloch states and occurs when no localized state falls between them. The inset of Fig. 6 shows the level-spacing distribution of the counterpart ladder model with nonrandom hoppings that exhibits a pure Poissonian character.

IV. CONCLUSIONS

We investigated in detail some stationary, dynamical, and spectral aspects of a two-channels Anderson model with correlated disorder that depicts an energy band on which localized and Bloch-type states coexist. Following an exact-diagonalization procedure, we computed the participation ratio and the Kubo-Greenwood conductance. Moreover, the Lyapunov exponent was calculated using a Green's-function technique. All these stationary quantities clearly depict the mobility edges separating the energy range of purely localized states at the band tails from the energy range with coexisting localized and Bloch-type states. In the coexisting band, these quantities show signatures of the presence of delocalized states, namely, the size independence of the participation ratio, a finite conductance, and a vanishing Lyapunov exponent. We also followed the time evolution of an initially localized wave packet. The dynamics is also dominated by the presence of Bloch-type states with a ballistic spread until the saturation of the wave-packet width after the multiple reflections at the system's boundaries. Finally, we showed that the level-spacing statistics is described by a new distribution function due to the coexistence of localized and Bloch-type states. It results from the superposition of uniformly distributed Bloch state levels with the Poissonian-distributed levels of localized state. The resulting distribution exhibits a linear decay at small level spacings followed by a sharp increase when approaching a maximum level spacing which is roughly twice the average level spacing. It would be interesting to have its analytical form derived from general random matrix theory arguments. The present results gives further support to recent findings showing that quasi-1D random systems can display a true metallic behavior in the presence of specific short-range correlated disorder.[31,32]

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