Extended states and dynamical localization in the random-dimer model

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We study quantum diffusion of wavepackets in one-dimensional random binary subject to an applied electric field. We consider three different cases: Periodic, random, and random dimer (paired) lattices. We analyze the spatial extent of electronic wavepackets by means of the time-dependent inverse participatio ratio. We show that the delocalized states recently found in random dimer lattices become spatially localized under the action of the applied field (dynamical localization) but wavepackets are much less localized than in purely random lattices. We conclude that the resonant tunneling effects causing delocalization play an important role even in the presence of the electric field.

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I. INTRODUCTION

The existence of one-dimensional (1D) disordered lattices with a number of extended electronic states large enough to contribute to transport properties in a relevant fashion has been undoubtedly established during this decade. The interest on this problem arose from the pioneering works of Flores [1] and Dunlap, Wu and Philips [2], which stimulated a considerable effort devoted to understand these delocalization phenomena [3–9]. The common feature of the models studied so far is that they consist of a host (discrete or continuum) system where defects are placed randomly although their distribution exhibit spatial correlation. This spatial correlation is usually introduced by imposing that impurities appear always in pairs (dimers) or in more complicated grouping schemes. Specifically, results for 1D random models with paired disorder, i.e., with defects forming dimers, which exhibit delocalization have been put on solid theoretical grounds [10]. Interestingly, spatial correlations in 1D random systems lead to new and unexpected phenomena not only in electronic systems but also in the case of quantum ferromagnets [11], Frenkel excitons [12], classical vibrations [13] and excitations [14]. It thus becomes clear that the study of random systems with correlated disorder is of interest in a wide range of physical problems, and that, ultimately, such a line of research may lead to the development of a variety of new devices and applications.

In Ref. [11], it was shown that delocalized electronic states arise in spite of the inherent disorder due to resonant phenomena taking place at dimers which, in turn, lead to a transmission coefficient of different segments forming the lattice close to unity, no matter what the length of the segment is. The transmission coefficient is exactly unity for the resonant energy at a single dimer defect and, most important, is very close to unity for electron energies near the resonant one, as demonstrated by perturbative and numerical calculations. Once the existence of these bands of extended states is put forward and the reasons for its appearance are understood in the isolated, non-interacting model, an interesting question immediately arises, namely what is the effect of external perturbations on the delocalized states? In particular, since we are going to concern ourselves with electronic states, the first perturbation that has to be studied is an applied electric field; since applied electric fields lead to localization even in periodic lattices, one should expect that delocalized states in random correlated systems might also be spatially localized. But the key question is to elucidate whether the physical mechanisms giving rise to delocalization in unperturbed systems are of relevance in the presence of the electric field or, on the contrary, they are immaterial at all. The answer to this question is not trivial: Competition between quantum coherence due to correlated disorder and the loss of quantum coherence due to the misalignement of local electronic levels under the action of the field will be the main mechanism governing this system, and the prevailing factor among these two is difficult to foresee.

In this letter we present a first study in the above direction. We consider the problem of quantum diffusion of wavepackets initially localized in random-dimer models (RDMs), as introduced in Ref. [2], under the action of a uniform electric field. The way we carry out such an analysis is by comparing electronic amplitudes in three different binary systems, namely periodic, unpaired disordered lattices and paired disordered ones. The study of periodic systems will allow us to establish the main features of dynamical localization in periodic binary systems. This is required for a better understanding of wavepacket dynamics when an amount of randomness is introduced in the system. To get an estimation of the spreading of the wavepacket as a function of time we will
use the time-dependent inverse participation ratio (IPR). By means of this quantity, we will be able to show below that, although all states in random dimer models become localized under the action of the electric field, they acquire an spatial structure much more extended than their counterparts in the purely random lattice.

II. MODEL

The unperturbed random-dimer model is described by the following 1D tight-binding Hamiltonian [2]

$$\mathcal{H}_0 = \sum_n E_n c_n^\dagger c_n + V \sum_n (c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1}). \quad (1)$$

Here $c_n$ and $c_n^\dagger$ are electron annihilation and creation operators in the site representation. The hopping matrix element $V$ is assumed to be constant over the whole lattice, whereas on-site energies $E_n$ can only take on two values $E_A$ and $E_B$, with the additional constraint that $E_B$ are assigned at random to pairs of lattices sites. In Ref. [2], it was found that for $|E_A - E_B| < 2|V|$, an initially localized wavepacket becomes delocalized and its mean-square displacement grows in time as $t^{3/2}$ (super-diffusion). For $|E_A - E_B| = 2|V|$ the mean-square displacement behaves asymptotically as $t$ (diffusion). Otherwise the wavepacket remains localized.

As we mentioned above, we are interested in quantum diffusion of wavepackets under an applied electric field. In particular, we investigate the time behaviour for different sets of constituent parameter $E_A$, $E_B$, and $V$. The perturbed Hamiltonian is written as follows

$$\mathcal{H} = \mathcal{H}_0 - F \sum_n n c_n^\dagger c_n, \quad (2)$$

where $F$ is the electric field (we use units such that $\epsilon = \hbar = 1$ in the rest of the paper). In order to solve the corresponding Schrödinger equation we express the wave function in terms of localized Wannier states. In doing so, it can be seen that the time-dependent amplitudes $\psi_n(t)$ satisfy the following equation

$$i \frac{d}{dt} \psi_n(t) = (E_n - F n) \psi_n + V (\psi_{n-1} + \psi_{n+1}). \quad (3)$$

This equation is solved numerically with the initial condition $\psi_n(0) = \delta_{n,n_0}$, where $n_0$ denotes the initial site, using an implicit (Crank-Nicholson) integration scheme. Such a procedure preserves the normalization condition, which has been used at every time step to test the accuracy of results. Once the solution is found, the wavepacket dynamics can be characterized by means of the time-dependent IPR, defined as follows [15]

$$\text{IPR}(t) = \sum_n |\psi_n(t)|^4 \quad (4)$$

Usually the value of the IPR is a good estimation of the spatial extent of electronic states. Delocalized states are expected to present small IPR (in the ballistic limit, without applied field, it vanishes as $t^{-1}$), while localized states have larger IPR (in the limit of strong localization should be unity whenever the electron is localized at a single site).

III. RESULTS AND DISCUSSIONS

In the present work we study three different binary systems: periodic (ABABAB ...), unpaired and paired disordered lattices, with a given fraction $c$ of B-sites. For definiteness, we take $E_A = 0$ and $V = -1$, whereas $E_B = 1, 2, 3$ to include super-diffusive, diffusive and localized states of the unperturbed RDM. Although the local environment for different initial sites $n_0$ is different, we have checked that our main conclusions remain valid and only finer details of plots change upon setting several values of $n_0$ and different realizations of disorder.

We begin by studying the periodic lattice as a way to verify that we are carrying out our computations correctly. Figure 1 presents the results for $F = 0.02$ in a binary periodic lattice with $E_A = 0$, $E_B = 1$, and $V = -1$. Similar results are obtained for other values of the on-site energy $E_B$ and electric field $F$. The IPR displays marked peaks at times $t_k = k \pi (k = 0, 1 ...)$, where $\pi = 156.7$ for this value of the electric field. The value of maxima at $t_k$ is very close to unity, indicating that the wavepacket is strongly localized around the initial site $n_0$ (dynamical localization). This is consequence of the so called Bloch oscillations, where the wavepacket oscillates in time with period $\tau_B = 2\pi \hbar / FL$, $L$ being the lattice period (see, e.g., Ref. [16]). In our case $L = 2$ and, therefore, the corresponding period will be $\tau_B = 157.1$, in perfect agreement with that obtained from Fig. 1. We can therefore trust the results we are going to obtain for the random lattices.

FIG. 1. Inverse participation ratio as function of time in a binary periodic lattice with $E_A = 0$, $E_B = 1$, and $V = -1$, for $F = 0.02$. 

1.
Results corresponding to both kinds of disordered lattices are shown in Fig. 2, for $E_A = 0, V = -1, F = 0.02,$ and three different values of the on-site energy $E_B$. The concentration of B-sites is $c = 0.2$ in all cases. We can observe that Bloch oscillations are completely absent in random lattices. This fact can be explained by the absence of translational invariance and, consequently, by scattering of electrons with the lattice, which destroys the quantum coherence required to observe such phenomenon. In both kind of random lattices the IPR presents strong fluctuations at small time scales, but it can be observed that its average value over larger times is constant. Such small fluctuations depend on the particular realization of the disorder and on the initial position of the wavepacket. However, for a given concentration $c$, the mean value depends only on the electric field and on the hopping matrix element (the larger the electric field or the hopping matrix element, the closer to unity the IPR).

This far, we have summarized the common features of states of both random lattices. It is now the moment to comment the main differences between paired and unpaired lattices. When $|E_A - E_B| < 2|V|$, i.e. whenever the defect energy lies within the allowed band [Fig. 2(a)], the mean value of the IPR is smaller for paired lattices, meaning that the wavepacket spreads over larger portions of the system. From this plot, it can be appreciated that the difference between both IPR values is about an order of magnitude, and hence the spatial extent of wavefunctions in paired and unpaired lattices will largely differ. Thus, when the unperturbed ($F = 0$) paired lattice supports extended states, the resulting dynamical localization under the action of the electric field is much less effective than in unpaired lattices. It is therefore reasonable to expect that the transport properties of the two systems will also exhibit specific features: For instance, the hopping conductivity has to be much larger in the dimer lattice than in the random lattice, due to the increased tunneling probability between neighboring localized states. A smaller degree of localization in the dimer lattice is also observed, although to a somewhat lesser extent, in the critical situation $|E_A - E_B| = 2|V|$ [Fig. 2(b)]. On the contrary, the dynamics in both lattices is almost identical whenever the unperturbed lattice only supports localized states [Fig. 2(c)].

A better understanding of this result is achieved if one considers that the (initially strongly localized) wavepacket is the combination of plane waves in a continuous band [7]. Since the energy spectrum of the paired disordered lattices presents a band of extended states, the lattice behaves as a selective electronic filter, and those components whose wavenumber belongs to this band can propagate over larger distances, producing a larger spreading of the resulting wavepacket. The observation of this behaviour, as we have reported, is therefore a clear consequence of the fact that the unperturbed lattice supports extended states. Finally, the absence of Bloch oscillations in paired disordered lattices indicates that their extended states are no longer Bloch states. Bloch states are characterized by a complete quantum coherence with a perfectly defined phase. This is not the case in the RDM, where electronic states increment its phase by a factor of $\pi$ whenever they pass over a dimer defect [2,4], and the position of each dimer defect is in any case a random variable.
IV. CONCLUSION

We have studied quantum diffusion of wavepackets driven by an applied external field in periodic and random (unpaired and paired) binary lattices. The spatial degree of localization of wavepackets initially localized at a single lattice site has been properly described by means of the time-dependent IPR. In binary periodic lattices we have confirmed the dynamical localization under electric fields as well as Bloch oscillations, for which the wavepacket oscillates in time with a well-defined period proportional to the inverse of the electric field. Quantum dynamics in disordered lattices also exhibits dynamical localization although it turns out to be much more intricate: In particular, no evidence of Bloch oscillations (regular behavior) is observed. What is most important for the purposes of the present work, we have determined that dynamical localization is less effective in paired disordered lattices than in unpaired ones, provided that the energy of defects lies within the band of extended states. Thus, it can be concluded that extended states can spread over larger segments of the lattice, giving rise to a smaller localization of the wavepacket in the presence of the electric field. Therefore, the resonant tunneling effects causing delocalization plays an important role, even in the presence of the applied field.

The results we have reported in this letter provide another piece of evidence supporting the true extended nature of states near the resonant energy in the random dimer model. From plots in Figs. 1 and 2(a), one can observe that the value of the IPR for the random dimer model is about the minimum. of the Bloch oscillations of the periodic lattice. This is to be compared with the random case, whose IPR is close to half of the IPR of the periodic lattice. It is then clear that electric-field-localized states in the random dimer model are much closer to those of the periodic lattice than to the purely random system. In view of this, we envisage that the transport properties of random dimer lattices under electric fields will also be close to those of periodic lattices, this being an experimentally verifiable, qualitative prediction. To conclude, we mention that another question stemming from this work is whether the same behavior will be found in more realistic models such as the continuum random dimer model [12] or the square well model [13]. These models have already given rise to quantitative predictions of effects that should be observed in real devices and therefore they are very appealing in order to find physically relevant consequences of dynamical localization in dimer models. Work in this direction is in progress.

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