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Coherent electron dynamics in a two-dimensional random system with mobility edges

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Abstract

We study numerically the dynamics of a one-electron wavepacket in a two-dimensional random lattice with long-range correlated diagonal disorder in the presence of a uniform electric field. The time-dependent Schrödinger equation is used for this purpose. We find that the wavepacket displays Bloch-like oscillations associated with the appearance of a phase of delocalized states in the strong correlation regime. The amplitude of oscillations directly reflects the bandwidth of the phase and allows us to measure it. The oscillations reveal two main frequencies whose values are determined by the structure of the underlying potential in the vicinity of the wavepacket maximum.

1. Introduction

Anderson localization theory describes many relevant aspects concerning the nature of one-electron states and collective excitations in random media [1–3]. In one-dimensional (1D) and two-dimensional (2D) electronic systems with time-reversal symmetry this theory predicts the absence of a disorder-driven metal–insulator transition for any degree of uncorrelated disorder. Recently, however, it has been reported that the presence of short-range [4–10] or long-range correlations [11–14] in disorder acts towards the appearance of truly delocalized states in 1D Anderson models. This theoretical prediction was put forward to account for the transport properties of semiconductor superlattices with intentional short-range correlated disorder [15] and microwave transmission spectra of single-mode waveguides with inserted long-range correlated scatters [16].

In 2D, the existence of extended states due to correlations in disorder has also been proved. Thus, in [17] the authors considered a two-dimensional striped medium in the (x, y) plane with on-site correlated disorder. The on-site energies were generated by a superposition of an

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uncorrelated term in the x-direction and a long-range correlated contribution along y-direction. It was predicted that this model displays a disorder-driven Kosterlitz–Thouless metal–insulator transition with strong correlations in disorder. More recently, the effect of an isotropic scale-free long-range correlated disorder on the one-electron eigenstates of the 2D Anderson model has been studied [18]. To introduce long-range correlations in *both* the x- and y-directions, the site energies were chosen to have a power-law spectral density $S(k) \propto 1/k^{\alpha_{2D}}$, where k is the magnitude of the typical wavevector characterizing the energy landscape roughness. The metal–insulator transition induced by strong correlations ($\alpha_{2D} > 2$) was monitored by measuring the participation number exponent from the long-time behaviour of the wavefunction spatial distribution [18].

It is well known that a uniform electric field applied to a periodic lattice causes the dynamic localization of electron wavepackets and gives rise to their oscillatory behaviour, the so-called Bloch oscillations [19]. Due to the advances in semiconductor technology, it has become possible to monitor the Bloch oscillations in uniform superlattices [20]. Remarkably, this phenomenon is not restricted to electronic systems. Recently, the authors of [21] reported the first experimental observation of photonic Bloch oscillations in two-dimensional periodic systems. In spite of the fact that the periodicity of the potential has been admitted to be the key ingredient for Bloch oscillations to exist, it has been demonstrated recently that a 1D Anderson model with diagonal long-range correlated disorder displays Bloch oscillations in the strong correlation limit [22]. It turned out that the period of oscillations agrees well with the one in an ideal Bloch band, while the amplitude of oscillations is proportional to the width of the delocalized phase, which has been predicted to appear in the strong correlation limit [11]. The spectral counterpart of Bloch oscillations—Wannier–Stark quantization of the energy spectrum—has also been found to be a remarkable feature of the model [23].

In this paper we focus on the interplay between the delocalization effect, arising from the long-range correlated disorder, and the dynamic localization, caused by an electric field acting on the system. By numerically solving the 2D time-dependent Schrödinger equation for the complete Hamiltonian, we compute the behaviour of an initial Gaussian wavepacket in the presence of a uniform electric field. We found clear signatures of Bloch-like oscillations [22] of the wavepacket between the two mobility edges of the phase of delocalized states. The amplitude of the oscillatory motion of the centroid allows us to determine the bandwidth of the delocalized phase.

2. Model and formalism

We consider a 2D electron moving in a random long-range correlated potential on a regular $N \times N$ lattice of unitary spacing and subjected to a uniform electric field $\boldsymbol{F}$. The corresponding tight-binding Hamiltonian reads [3]

$$\mathcal{H} = \sum_{\boldsymbol{m}} (\epsilon_{\boldsymbol{m}} + \boldsymbol{U} \cdot \boldsymbol{m}) \, |\boldsymbol{m}\rangle\langle\boldsymbol{m}| + J \sum_{\langle \boldsymbol{mn} \rangle} (|\boldsymbol{m}\rangle\langle\boldsymbol{n}| + |\boldsymbol{n}\rangle\langle\boldsymbol{m}|) \,, \tag{1}$$

where $|\boldsymbol{m}\rangle$ is a Wannier state localized at site $\boldsymbol{m} = m_x \boldsymbol{e}_x + m_y \boldsymbol{e}_y$, $\epsilon_{\boldsymbol{m}}$ is its energy and $\boldsymbol{U} = e\boldsymbol{F}$ is the energetic bias, e being the electron charge. Here $\boldsymbol{e}_x$ and $\boldsymbol{e}_y$ are the corresponding Cartesian unit vectors. We will assume that the electric field is applied along the diagonal of the square lattice. Then $\boldsymbol{U} = U(\boldsymbol{e}_x + \boldsymbol{e}_y)/\sqrt{2}$. Transfer integrals are restricted to nearest-neighbour sites and are given by J. Hereafter, we fix the energy scale by setting $J = 1$. The long-range correlated sequence of site energies $\epsilon_{\boldsymbol{m}}$ is generated by making use of a Fourier transform method as follows

$$\epsilon_{m} = \sum_{k_x=1}^{N/2}\sum_{k_y=1}^{N/2} \frac{\zeta(\alpha_{2D})}{k^{\alpha_{2D}/2}} \cos\left(\frac{2\pi m_x k_x}{N} + \phi^{(x)}_{k_x k_y}\right) \cos\left(\frac{2\pi m_y k_y}{N} + \phi^{(y)}_{k_x k_y}\right), \tag{2}$$

where $k^2 = k_x^2 + k_y^2$, and $\phi^{(x)}_{k_x k_y}$ and $\phi^{(y)}_{k_x k_y}$ are $N^2/2$ independent random phases uniformly distributed in the interval $[0, 2\pi]$ and $\zeta(\alpha_{2D})$ is a normalization constant, such that $\langle \varepsilon_{m}^2 \rangle = 1$. We also shift the on-site energies in order to have $\langle \varepsilon_{m} \rangle = 0$. The Wannier amplitudes evolve in time according to the time-dependent Schrödinger equation which can be written as [3]

$$\mathrm{i}\dot{\psi}_{m} = (\epsilon_{m} + \boldsymbol{U}\cdot\boldsymbol{m})\,\psi_{m} + \left(\psi_{m+e_x} + \psi_{m-e_x} + \psi_{m+e_y} + \psi_{m-e_y}\right), \tag{3}$$

with $\hbar = 1$. Having introduced the model of disorder, we numerically solve equation (3) to study the time evolution of an initially Gaussian wavepacket of width σ centred at site $\boldsymbol{m}_0$

$$\psi_{m}(t=0) = A(\sigma)\exp\left[-\frac{(\boldsymbol{m}-\boldsymbol{m}_0)^2}{4\sigma^2}\right]. \tag{4}$$

Once equation (3) is solved for the initial condition (4), we compute the projection of the mean position of the wavepacket (centroid) along the field direction

$$R(t) = \frac{1}{\sqrt{2}}(\boldsymbol{e}_x + \boldsymbol{e}_y)\cdot\sum_{m} \boldsymbol{m}|\psi_{m}(t)|^2. \tag{5}$$

3. Results and discussion

In the absence of disorder ($\epsilon_{m} = 0$), all the states are dynamically localized by the uniform electric field and the centroid oscillates in time, revealing Bloch oscillations [19]. The amplitude and the period of these oscillations are estimated from semiclassical arguments (see, e.g., [24]) as $L_U = W/U$ and $\tau_B = 2\pi/U$, respectively, where W is the width of the Bloch band in units of the transfer integral J ($W = 8$ in our case). The frequency of the Bloch oscillations is given by $\omega = 2\pi/\tau_B$ and, therefore, is equal to the bias magnitude U in the chosen units.

To study joint effects of the bias and correlated disorder, we performed numerical simulations of equation (3). In all simulations square lattices of size $N\times N = 250\times 250$ were used. The initial wavepacket was considered to be located in the centre of the lattice, $\boldsymbol{m}_0 = (N/2)(\boldsymbol{e}_x + \boldsymbol{e}_y)$, and its standard deviation was set to $\sigma = 1$.

In figure 1(a) we plotted the centroid time behaviour of a biased wavepacket ($U = 1$) in a weakly correlated random potential ($\alpha_{2D} = 1$). Recall that in the absence of bias all the states are localized for such a value of the correlation exponent α_{2D} [18]. As is seen, switching on the bias does not lead to coherent oscillations of the wavepacket. A more detailed inspection of these numerical data shows that Bloch oscillations in the weak correlation regime ($\alpha_{2D} < 2$) can be observed only for a short initial transient. They are strongly damped by disorder and rapidly transformed into an incoherent motion of the centroid, presented in figure 1(a). To provide a further confirmation of this claim, we calculated the Fourier spectrum $R(\omega)$ of the centroid $R(t)$. Figure 1(b) shows the results after averaging over 50 realizations of disorder. We observe that the Fourier spectrum $R(\omega)$ is rather broad, suggesting that $R(t)$ is similar to a short-range correlated noise signal with no typical frequency.

A rather different time-domain dynamics is found in the limit of strongly correlated disorder, $\alpha_{2D} > 2$, when a phase of extended states emerges in the centre of the band in the unbiased system [18]. We will show below that these states drastically affect the dynamics of the wavepacket, that now resembles the oscillatory motion of the electron in a biased disorder-free lattice. In figures 2 and 3 we plotted the centroid time behaviour of a biased wavepacket

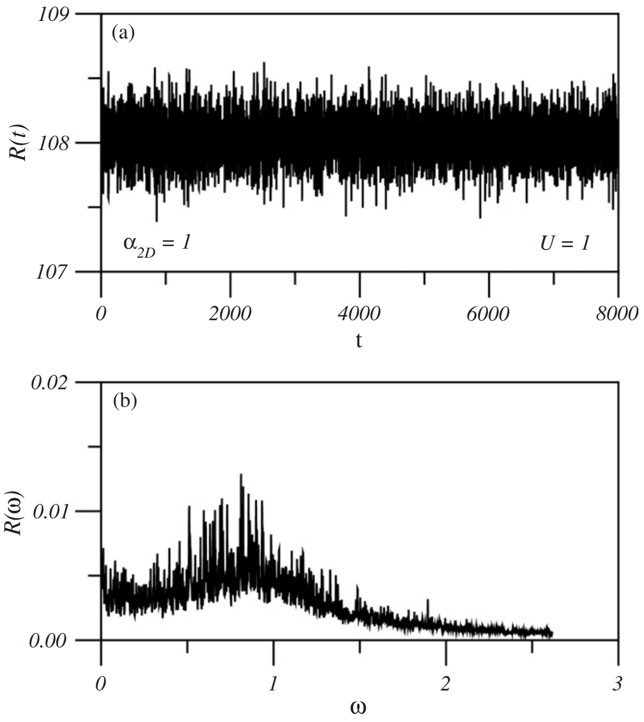

Figure 1. (a) Centroid dynamics of a biased wavepacket ($U = 1$) in a correlated random potential (2) with $\alpha_{2D} = 1$. (b) Fourier transform of the centroid, averaged over 50 realizations of disorder.

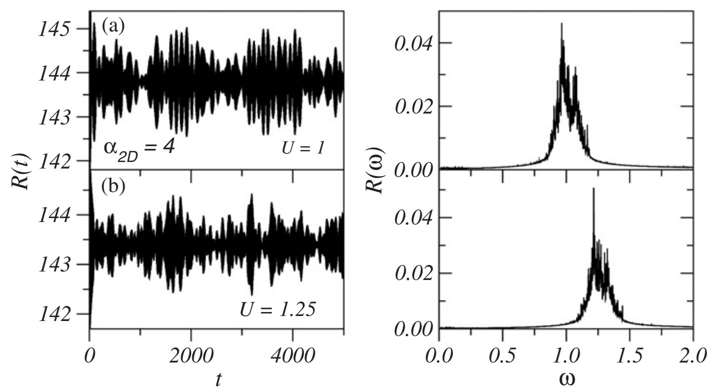

Figure 2. Centroid dynamics of a biased wavepacket in a correlated random potential (2) with $\alpha_{2D} = 4$ calculated for two bias magnitudes (a) $U = 1$ and (b) $U = 1.25$ (left panel). One can see a clear signature of sustainable Bloch-like oscillations. The corresponding Fourier spectra of the centroid, obtained by averaging over 50 realizations of disorder, are shown in the right panel.

for two values of the correlation exponent $\alpha_{2D} = 4$ (figure 2) and $\alpha_{2D} = 5$ (figure 3). Two magnitudes of the bias, $U = 1$ and $U = 1.25$, were considered for each value of α_{2D}. Figures 2 and 3 clearly demonstrate the occurrence of sustainable Bloch-like oscillations. Their amplitudes L_c are found to be $L_c \approx W_c/U$, where W_c is independent of the applied bias U.

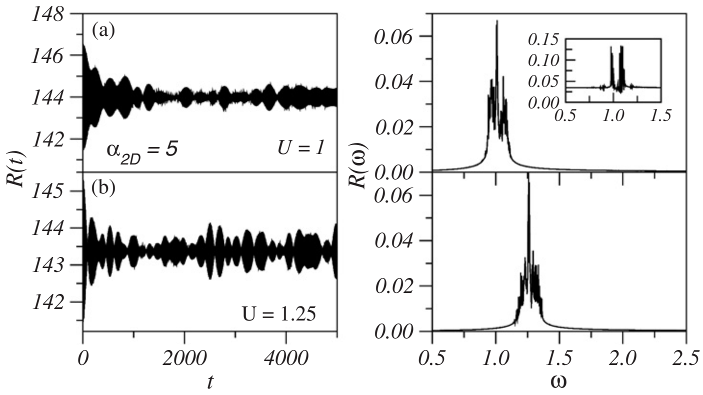

Figure 3. Same as in figure 2 but for $\alpha_{2D} = 5$. The inset shows the Fourier spectrum of the centroid for a single realization, clearly illustrating the fact that the oscillations reveal two dominant frequencies around $\omega = U$.

From the data in figure 2 we obtain $W_c \approx 2$. This value agrees remarkably well with the width of the band of extended states reported in [18].

The Fourier spectra $R(\omega)$ of the centroid, computed after averaging over 50 realization of disorder, show a single broad peak at about $\omega = U$. The peak frequency nicely agrees with the one in an ideal Bloch band. Looking, however, at the Fourier spectrum of a single realization (as shown in the inset in figure 3), one notices that $R(\omega)$ actually has two narrow peaks. The frequency of these peaks fluctuates from one realization to the other, which after averaging results in a broad single-peaked spectral density. This splitting is not found in 1D long-range correlated potentials.

With the aim of elucidating the anomalies found, we present a simplified model that sheds light on the origin of this doublet structure in the Fourier spectrum of the centroid oscillations. To this end, we recall that the random site potential $\epsilon_{\boldsymbol{m}}$ is given by the sum of harmonic terms (2). The amplitude of each term decreases upon increasing the harmonic number. For sufficiently high values of α_{2D}, the first term in the series will be dominant, while the others are considerably smaller. Consequently, the site potential for a given realization represents a harmonic function, perturbed by a coloured noise (see [25]). Based on this observation, we keep only the first term in (2) and neglect all others in our further arguments. Thus, the 'random' site potential now is $\epsilon_{\boldsymbol{m}} = \zeta \cos(2\pi m_x/N + \phi^{(x)}) \cos(2\pi m_y/N + \phi^{(y)})$, where phases $\phi^{(x)}$ and $\phi^{(y)}$ can be arbitrarily chosen.

The effective local bias is a superposition of the external one and the gradient of the local potential, $\boldsymbol{U}^{\text{eff}}_{\boldsymbol{m}} = \boldsymbol{U} - \nabla_{\boldsymbol{m}}\epsilon_{\boldsymbol{m}}$. At the initial position, $\boldsymbol{m}_0 = (N/2)(\boldsymbol{e}_x + \boldsymbol{e}_y)$, its components will be given by

$$U^{\text{eff}}_x = U + (2\pi\zeta/N) \sin\phi^{(x)} \cos\phi^{(y)},$$

$$U^{\text{eff}}_y = U + (2\pi\zeta/N) \sin\phi^{(y)} \cos\phi^{(x)}.$$

For $\phi^{(x)} = \phi^{(y)}$, the components of the effective bias are identical. As the frequency of the Bloch oscillations is proportional to the magnitude of the effective bias, only a single dominant frequency shall be present in this case. One just observes this in figure 4(a). Notice that for the particular case plotted ($\phi^{(x)} = \phi^{(y)} = 0$), the local bias at the central position does not acquire any contribution coming from the harmonic potential, which results in a null shift of the oscillation frequency. However, for the general case of $\phi^{(x)} \neq \phi^{(y)}$, the local bias

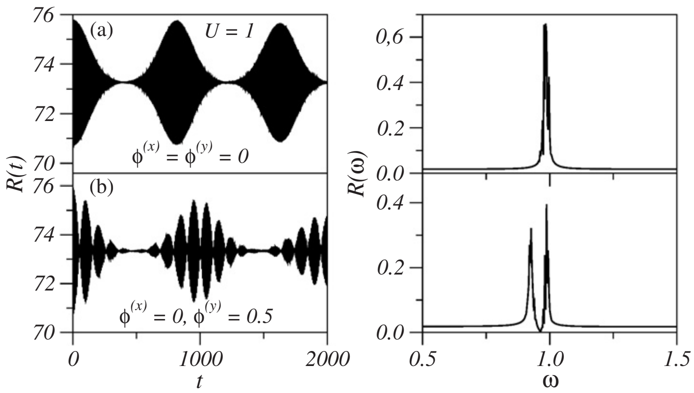

Figure 4. Left panels show the centroid time behaviour of a biased wavepacket moving in a potential $\epsilon_m = \zeta \cos(2\pi m_x/N+\phi^{(x)}) \cos(2\pi m_y/N+\phi^{(y)})$ for the two sets of phases $\phi^{(x)}$ and $\phi^{(y)}$ indicated in the plots. Right panels show the corresponding Fourier spectra.

components will differ by an amount of the order of $1/N$. Therefore, Bloch oscillations will have two dominant frequencies. This feature is exemplified in figure 4(b) where we used $\phi^{(x)} = 0$ and $\phi^{(y)} = 0.5$. For this case $U_x^{\rm eff}$ at $\boldsymbol{m}_0$ is not influenced by the local potential and the corresponding oscillation frequency is not shifted. On the other hand, the typical frequency associated with oscillations along the y-direction is shifted from the bare frequency $\omega = U = 1$. The two-peak structure depicted in the inset of figure 3(a) and the right-lower panel of figure 4(b) has, therefore, its origin in the distinct contributions given by the gradient of the local potential to the effective local bias. Averaging over random phases $\phi^{(x)}$ and $\phi^{(y)}$ results in a broader Fourier spectrum $R(\omega)$ around $\omega = U = 1$ with a mean width of the order of $1/N$.

4. Summary and concluding remarks

We studied the electron motion on a 2D square lattice with on-site long-range correlated disorder in the presence of an external uniform electric field. Long-range correlations were introduced by using a 2D discrete Fourier method which generates an appropriate disorder distribution with spectral density $S(k) \propto 1/k^{\alpha_{2D}}$. By numerically solving the Schrödinger equation, the time evolution of an initial Gaussian wavepacket was investigated, with the aim of finding coherent Bloch oscillations. Our results suggest that the oscillations are strongly damped in the weak correlation limit, $\alpha_{2D} < 2$, when all the states are localized because of disorder. The motion of the wavepacket on a large timescale is chaotic in this case. The sustained oscillations arise for $\alpha_{2D} > 2$, when a phase of the extended states emerges at the centre of the band. The amplitude of oscillations was found to be proportional to the energy difference between the two mobility edges of the delocalized phase [18], in good agreement with semiclassical arguments. Thus, we arrive at one of the principal conclusions of this work: (i) there exist clear signatures of the Bloch oscillations of a biased Gaussian wavepacket in the strong correlation regime ($\alpha_{2D} > 2$), originating from the presence of the two mobility edges, and (ii) the oscillations exhibit two dominant frequencies because the local bias has a contribution from the site energy potential. This is understood using semiclassical arguments.

The richness of the predicted dynamical behaviour can lead to new electro-optical devices, based on the coherent motion of confined electrons. We hope that the present work will stimulate experimental activities in this direction.

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