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DYNAMICS OF ONE-ELECTRON IN A ONE-DIMENSIONAL SYSTEMS WITH AN APERIODIC HOPPING DISTRIBUTION

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In this paper, we consider the effect of an aperiodic hopping distribution on a single electron. The aperiodic sequence of hopping energies was generated by using a sinusoidal function whose phase ϕ varies as a power-law, $\phi \propto n^{\nu}$, where n labels the positions along the chain. The exponent ν controls the degree of aperiodicity in the sequence hopping terms. Using the transfer matrix method, we compute the localization length within the band of allowed energies. Our numerical calculations indicate that, for an aperiodic sequence of hopping energies with $\nu < 1$, a new phase of extended states appears in this model. For a pseudorandom hopping distribution with $\nu > 1$, all eigenstates remain localized. In addition, we study the electronic dynamics subjected to an electric field. Our numerical calculations reveals perfect Bloch oscillations for $\nu < 1$. The typical frequency of these oscillations agree with the semiclassical predictions.

Keywords: One-electron; aperiodic hopping energy; Bloch oscillations.

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1. Introduction

In pure periodic systems, the one-electron eigenstates are Bloch waves delocalized in the thermodynamic limit. In the absence of scattering, the system behaves as a perfect conductor whenever the Fermi energy falls into the conduction band. Disorder, originating from lattice imperfections, modifies the nature of the one-electron eigenstates. For three-dimensional (3D) systems and a relatively weak disorder (of a magnitude smaller than the bandwidth), the states at the band center may remain extended.[1–4] In lower dimensions the effect of disorder is much more dramatic. In particular, uncorrelated disorder of any magnitude causes exponential localization of all one-particle eigenstates in one dimension (1D) and weak localization in two dimensions (2D).[2–4]

At the end of eighties it was realized, however, that extended states may survive in 1D systems when correlated disorder[5–13] or deterministic nonperiodic potentials[14–22] are involved. In fact, models with deterministic potential which is

incommensurate with the underlying lattice[14–22] depicts features that are in between those of the random Anderson model and the periodic Bloch model. The localized or extended nature of the eigenstates has been extensively investigated in the physics literature[14–18] and has been related to general characteristics of the aperiodic on-site distributions. The biased wave packet dynamics of a single electron moving in a lattice with an aperiodic potential was investigated in Ref. 20. It was numerically demonstrated that the electric field promotes sustained Bloch oscillations of an initial Gaussian wave packet whose amplitude reflects the bandwidth of extended states. The frequency of these oscillations exhibit unique features, such as a sensitivity to the initial wave packet position and a multimode structure for weak fields, originating from the characteristics of the underlying aperiodic potential.[20] In addition, the effect of aperiodicity in quantum Heisenberg ferromagnetic systems[20] and classical harmonic lattices[22] was numerically investigated. In general lines, the aperiodicity may induce the appearance of truly delocalized states.

In this work, we report further progress along this line. We consider a single electron moving in a lattice with an aperiodic slowly varying hopping term. The aperiodic sequence of hopping energies will be generated following the formalism used in Ref. 14. It consists in use a sinusoidal function whose phase ϕ varies as a power-law, $\phi \propto n^{\nu}$, where n labels the positions along the chain. The exponent ν controls the degree of aperiodicity in the sequence of exchange couplings. Using the transfer matrix method, we compute the localization length within the band of allowed energies. Our numerical calculations indicate that, for an aperiodic sequence of hopping energies ($\nu < 1$), a new phase of extended states appears in this model. For a pseudorandom hopping distribution $\nu > 1$, all eigenstates remain localized. In addition we study, by integration of the time-dependent Schrödinger equation, the electronic dynamics subjected to an electric field. The electric field promotes a bias which localizes the electron states. The resulting wave packet dynamics reveals perfect Bloch oscillations. The typical frequency of these oscillations agree with the semiclassical predictions.

2. Model and Formalism

We consider a tight-binding Hamiltonian on a 1D open lattice of spacing a with zero on-site energy, an aperiodic slowly varying hopping distribution and a uniform static electric field[20]

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

where $|n\rangle$ is a Wannier state localized at site n with energy $\tilde{\varepsilon}_n = 0$, $\mathcal{F}$ is the external uniform electric field and $-e$ is the charge of the particle. The hopping couplings $V_{n,n+1} = V_n$ will be considered to follow a deterministic rule given by

$$V_n = V_0 + [\cos(\alpha n^{\nu})]\,, \tag{2}$$

with α being an arbitrary rational number and ν being a tunable parameter.[14] From this sinusoidal form, one can control the degree of aperiodicity in the sequence of hopping couplings. In what follows, $V_0 = 2$ will be taken in order to avoid negative or null exchange interactions. In our calculations, we will use $\alpha = 0.5$. The main motivation for considering the specific model we study in this manuscript is that, from the sinusoidal form we can control the degree of aperiodicity in the hopping distribution. Within the context of on-site diagonal terms, the limit $\nu > 1$ was called "pseudorandom" at Ref. 16. It was shown that one-electron becomes localized at the presence of an aperiodic potential at this limit. For $\nu = 1$ this is just Harper's model, for which a rational α describes a crystalline solid, whereas an irrational α results in an incommensurate potential. It was demonstrated that an on-site energy distribution with $0 < \nu < 1$ induces a phase of extended states near the band center.

3. Numerical Calculation

3.1. *Lyapunov exponent*

The localization length of each eigenstate in the absence of electric field ($\mathcal{F} = 0$) is taken as the inverse of the Lyapunov exponent γ defined by Ref. 14

$$\gamma = \lim_{N\to\infty} \frac{1}{N} \log \frac{|Q_N c(0)|}{|c(0)|}\,, \tag{3}$$

where $c(0) = \binom{u_1}{u_0}$ is a generic initial condition and Q_N is the product of all transfer matrices

$$Q_N = \prod_{n=1}^{N} \begin{pmatrix} \dfrac{E}{V_n} & -\dfrac{V_{n-1}}{V_n} \\ 1 & 0 \end{pmatrix}. \tag{4}$$

In our calculations we compute the average Lyapunov exponent $\langle\gamma\rangle$, defined by $\langle\gamma\rangle = (1/N_f)\sum_{E=-1}^{E=1} \gamma(E)$ where N_f is the number of eigenmodes within each interval $[-1, 1]$. Let me stress that the center of band ($E = 0$) was avoided in this sum because the localization length of this eigenstate is large even in the pseudo-random hopping energy distribution ($\nu > 1$). $\langle\gamma\rangle \approx 0$ for extended states and it is finite for exponentially localized ones.

3.2. *Biased dynamics*

In order to investigate the physical properties of the one-electron subjected to an external uniform electric field, we follow the time evolution of an initially localized wave packet. The Wannier amplitudes evolve in time according to the time-dependent Schrödinger equation as ($\hbar = 1$)[20]

$$i\dot{\psi}_n = (-Fn)\psi_n + V_n\psi_{n+1} + V_{n-1}\psi_{n-1}\,, \tag{5}$$

where we introduced the dimensionless magnitude $F = e\mathcal{F}a/V_0$. Time is expressed in units of $\hbar/V_0$. We consider a wave packet initially localized at site $n_0 = N/2$,

i.e. $|\Phi(t=0)\rangle = \sum_n \psi_n(t=0)|n\rangle$ where $\psi_n(t=0) = \delta_{n,n_0}$. The above set of equations were solved numerically by using a high-order method based on the Taylor expansion of the evolution operator $V(\Delta t)$:

$$V(\Delta t) = \exp(-iH\Delta t) = 1 + \sum_{l=1}^{l_o} \frac{(-iH\Delta t)^l}{l!} \tag{6}$$

where H is the Hamiltonian. The wave function at time Δt is given by $|\Phi(\Delta t)\rangle = V(\Delta t)|\Phi(t=0)\rangle$. The method can be used recursively to obtain the wave function at time t. To obtain $H^l|\Phi(t=0)\rangle$ we will use a recursive formula derived as follows. Let us define $H^l|\Phi(t=0)\rangle = \sum_n C_n^l|n\rangle$. Using the Hamiltonian formula [Eq. (1)] we can compute $H^1|\Phi(t=0)\rangle$ and obtain C_n^1 as

$$C_n^1 = (-Fn)\psi_n(t=0) + V_n\psi_{n+1}(t=0) + V_{n-1}\psi_{n-1}(t=0)\,. \tag{7}$$

Therefore, using that $H^l|\Phi(t=0)\rangle = H\sum_n C_n^{l-1}|n\rangle$, C_n^l can be obtained recursively as

$$C_n^l = (-Fn)C_n^{l-1}(t=0) + V_nC_{n+1}^{l-1}(t=0) + V_{n-1}C_{n-1}^{l-1}(t=0)\,. \tag{8}$$

The following results were taken by using $\Delta t = 0.01$ and the sum was truncated at $l_o = 15$. This cutoff was sufficient to keep the wave function norm conservation along the entire time interval considered ($t \leq 10^6$). This formalism is faster than high-order Runge–Kutta methods and it is easier to implement. The quantities that we will use to characterize the dynamics of the electron wave packet is its mean position (centroid)

$$x(t) = \sum_{n=1}^{N}(n - \langle n(t)\rangle)|\psi_n(t)|^2\,, \tag{9}$$

where $\langle n(t)\rangle = \sum_{n=1}^{N} n|\psi_n(t)|^2$. As the initial packet is assumed spatially narrow, one has contributions to the wave packet dynamics, coming from a wide spectrum of eigenstates of the Hamiltonian (1).

4. Results

In Fig. 1 we show the average Lyapunov exponent $\langle\gamma\rangle$ as a function of ν obtained from the transfer matrix method. Calculations were done using $F = 0$, $N = 2.5\times10^6$ and 5×10^6 sites. One can see that this exponent vanishes in the $\nu < 1$ region. This feature is a clean signature of extended states. Now we will consider the biased case. In an ideal 1D system, a uniform field causes the electron wave packet to oscillate in space and time. The period of these oscillations are estimated semiclassically $\tau_B = 2\pi/F$. Subsequently, the frequency of the harmonic motion is $\omega = F$, for the chosen units. In what follows, we will restrict our analysis to field strengths producing oscillation amplitudes larger than the lattice spacing in order to be able to use the semiclassical formalism. In Fig. 2(left panel) we plotted the centroids of wave packets calculated for distinct field strengths for the initial position at the

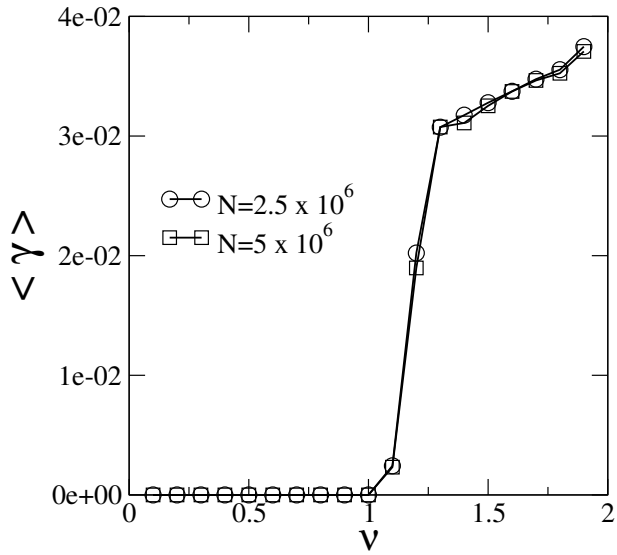

Fig. 1. Average Lyapunov exponent $\langle\gamma\rangle$ as a function of ν computed for $F = 0$, $N = 2.5 \times 10^6$ and 5×10^6 sites. The average Lyapunov exponent vanishes in the $\nu < 1$ region, thus indicating extended states.

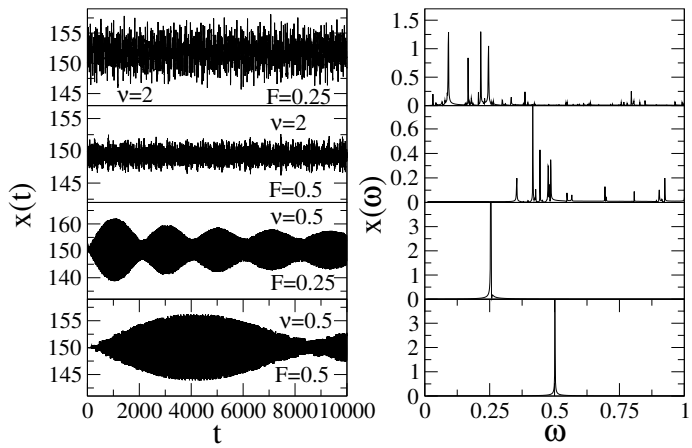

Fig. 2. (Left panel) Time-domain dynamics of the centroid of a biased wave packet ($n_0 = N/2$ at $t = 0$) for two values of the applied electric field $F = 0.25$ and 0.5. (Right panel) Fourier transform of the centroid.

chain center. It should be noticed that for $\nu < 1$ the Bloch oscillations remain sustained, i.e. no dephasing is taking place. Second, the oscillation amplitude is proportional to $1/F$ as predicted semiclassically.[20] To provide further confirmation of the semiclassical picture, we calculated numerically the Fourier transform of the centroid, $x(\omega)$, as shown in Fig. 2(right panel). Again, the estimated predominant frequency of the Bloch oscillations $\omega = F$ is corroborated for $\nu < 1$. In Fig. 2(left

panel) one can see that there are no signatures of Bloch oscillations for $\nu > 1$, at least for a moderate field amplitude. Oscillations, which are present at the very beginning, achieve in a short time a weakly fluctuating (stationary in average) value. For $\nu > 1$, the Fourier transform $x(\omega)$ is rather broad, confirming the absence of Bloch oscillations in this regime. The initial site n_0 was varied around the center of the chain and no qualitative change in the physical properties was found.

5. Summary and Conclusions

We studied a biased tight-binding model where the hopping energy are determined by a sinusoidal function whose phase ϕ varies as a power-law. By using a standard numerical transfer matrix method we compute the localization length within the band of allowed energies. Our numerical calculations indicate that, for aperiodic sequence of hopping energies ($\nu < 1$), a new phase of extended states appears in this model. Our main interest was the interplay between the delocalization effect, preserved by the aperiodicity, and the dynamic localization, caused by an electric field acting on the system. We computed the behavior of an initial localized wave packet in the presence of a uniform electric field solving numerically the 1D time-dependent Schrödinger equation for the complete Hamiltonian. The numerical solutions was done by using a high-order method based on the Taylor expansion of the evolution operator. We found clear signatures of Bloch-like oscillations for $\nu < 1$ and their absence for $\nu > 1$. The period of the oscillations agrees well with the period in an ideal Bloch band. However, contrary to what occurs in disordered systems, where scattering on site potential fluctuations gradually degrades the oscillations, these remain sustained with no signature of depletion. Our findings indicate that Bloch oscillations can indeed be observed in superlattices with slowly varying periodicity. We hope that the present work will stimulate experimental activities along this direction.

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