Dynamical localization in a one-dimensional crystal with an impurity under the action of an electric field

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We have solved the problem of dynamical localization in a one-dimensional system with an impurity under the action of a dc field along the single-band tight-binding model. By fixing the impurity potential, we show that characteristic field values can make two on-site energies coincide, enhancing in this way the hopping of carriers between the two sites. The distance between the degenerate sites decreases with increasing field intensity. So for high-field values the sites can be nearest neighbors producing strong oscillations. On the other hand, for weak-field values the two degenerate sites are far apart from each other and, as a result, there is an almost complete localization at the impurity site. We propose a model which allows us to determine the impurity level in a superlattice.

INTRODUCTION

In this work we have solved the dynamical localization problem of diffusion of a carrier in a linear chain with a point impurity under the action of a dc electric field. The particle is initially in a well-localized state at the impurity site. We evaluate the time evolution of the probability propagator on each lattice site and the mean-square displacement.

The application of a dc electric field on a particle subject to a periodic potential would cause the appearance of an oscillatory movement of the particle, which can be well understood in a semiclassical picture that gives the time evolution of the quasimomentum. According to this simple approach, every time the zone boundary is reached there is an umklapp process that reverts the motion, i.e., we have Bloch oscillations of period $T=\hbar G/eE$, where G is a reciprocal-lattice vector.

Bloch oscillations[1] in the time domain are the counterpart of the Wannier-Stark ladder[2] in the energy (frequency) domain. But their detection in bulk samples is almost impossible, due to the fact that in bulk the time scattering of a wave packet is much shorter than the Bloch period of oscillation. This situation was overcome with the use of superlattices (SL's), which have long periods that make possible the application of not so strong fields, a prediction made by Esaki and Tsu.[3] These authors proposed the use of SL's to generate a source of electromagnetic radiation in the terahertz range. Mendez and Bastard[4] have recently written an interesting paper regarding this phenomenon of Bloch oscillations and Wannier-Stark ladders.

The superposition of the electric field (responsible for Bloch oscillations) and the presence of an impurity at a site in an otherwise perfect crystal gives place, as we shall show below, to different regimes depending on the magnitude of the characteristic quantities in the problem.

We will consider the treatment of this problem for the case of SL's that can be considered as one-dimensional (1D) systems. It is of great interest to investigate the way a particle diffuses in such a system when acted upon by an electric field E applied along its grown axis and injected at an impurity site. It is well known that in a perfect lattice and in the field-free case an initially localized state will diffuse through the lattice according to the following law for the propagator:[5]

$$P_n(t;E=0)=|j_n(2Vt/\hbar)|^2 , \tag{1}$$

and for the mean-square displacement one gets

$$\langle n^2;E=0\rangle=2(Vt/\hbar)^2 , \tag{2}$$

where n is the lattice site, J_n is the Bessel function of order n, and $2V$ is the half-bandwidth.

When a dc field is applied to the perfect crystal, the initially localized carrier will continue to be close to the starting point in the lattice.[6–11] In this case the relevant results are

$$P_n(t)=\{J_n[(4V/eEa)\sin(eEat/\hbar)]\}^2 , \tag{3}$$

$$\langle n^2\rangle=[8V^2/(eEa)^2]\sin^2(eEat/2\hbar) , \tag{4}$$

so that, in the perfect crystal, we recover the Bloch prediction, i.e., the particle performs an oscillatory motion with the characteristic frequency $\omega_c=eEa/\hbar$. Such oscillations should result in emission of electromagnetic radiation in the terahertz range for superlattices with periods of order $a=100$ Å and electric fields as high as 10^5 V/cm. Such radiation emission was detected in a series of experimental works recently done.[12–14]

THE MODEL AND THE MATHEMATICAL PROCEDURE

In this work we focus on the problem of the influence of an impurity of strength ε_0 at the origin in an otherwise perfect 1D crystal. We have solved the time-dependent Schrödinger equation along the tight-binding single-band

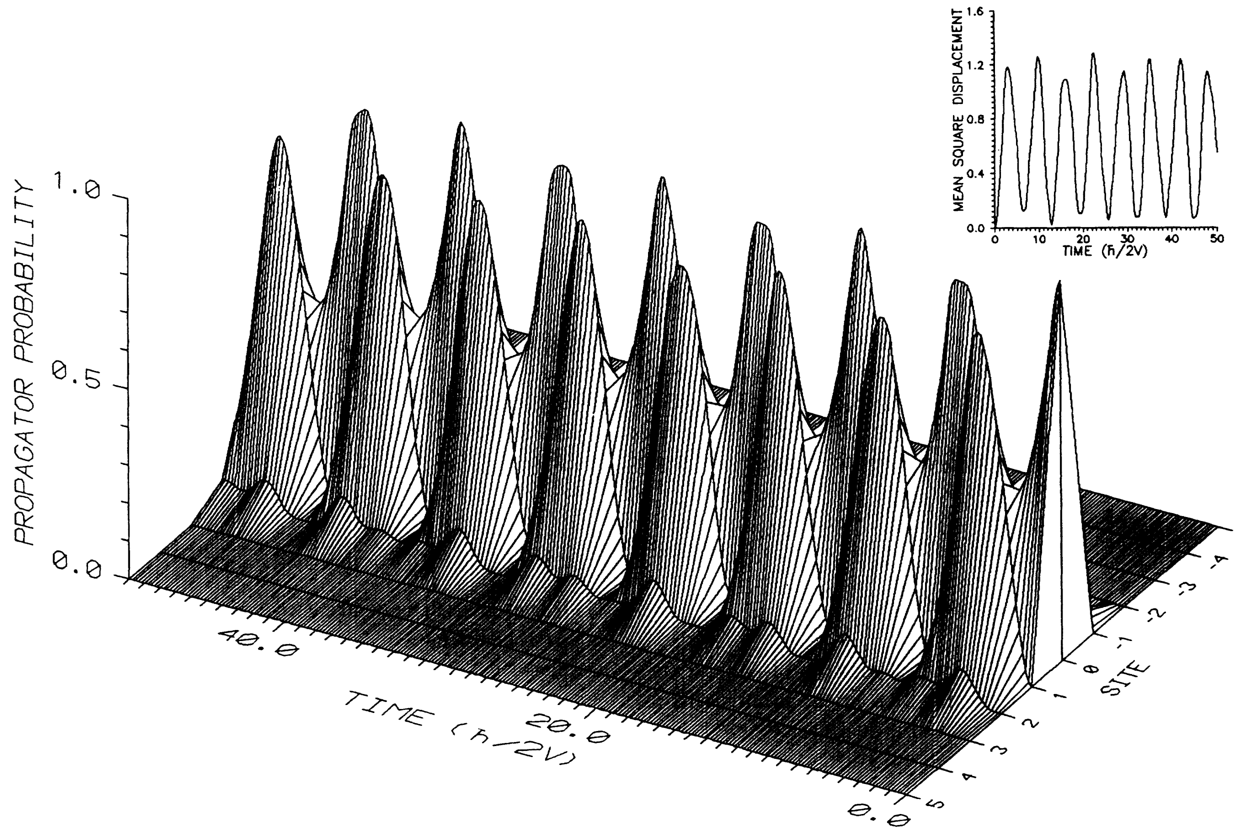

FIG. 1. We show the propagator probability as a function of time and lattice site for the following values: electric field intensity $E=5.0\times10^4$ V/cm and impurity energy $\varepsilon_0=-0.05$ eV. We also show the mean-square displacement as a function of time. We can see clearly a strong oscillation between impurity site and its first neighbor to the left [see Eq. (10)].

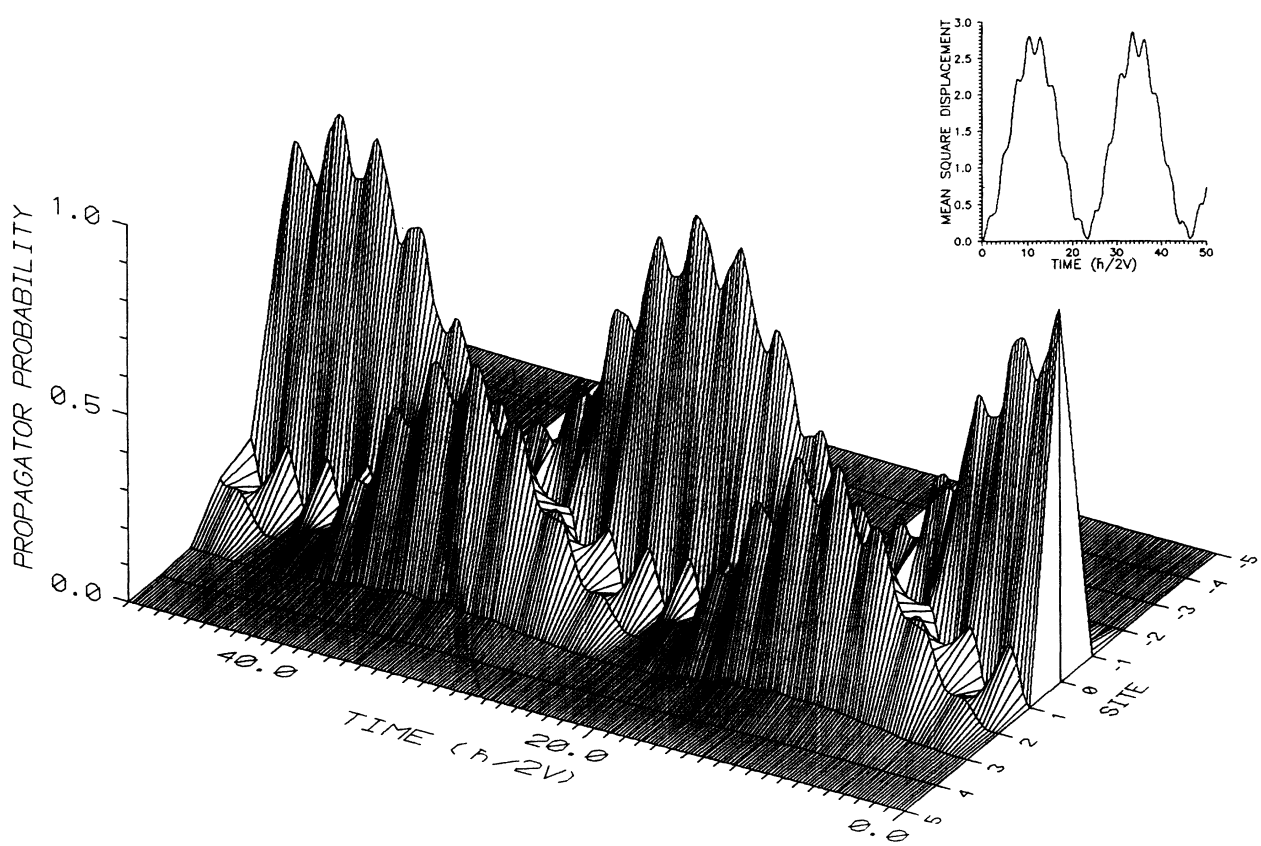

FIG. 2. The same as Fig. 1 for $E=5.0\times10^4$ V/cm and $\varepsilon_0=-0.10$ eV.

model, where we have the following set of differential equations for the Wannier propagator amplitudes:

$$i\hbar\frac{\partial}{\partial t}f_n = V(f_{n-1}+f_{n+1})-\varepsilon_0 f_n \delta_{n,0}-eEanf_n \ , \tag{5}$$

with the initial condition

$$f_n(0)=\delta_{n,0} \ . \tag{6}$$

For the case of a finite lattice of size N, the Schrödinger equation (5) written in matrix form is the following:

$$i\hbar\frac{\partial}{\partial t}\mathbf{f}=\mathbf{M}\mathbf{f} \ , \tag{7}$$

where $\mathbf{M}$ is the $N\times N$ dynamical matrix and the vector $\mathbf{f}$ is formed from the on-site amplitudes. The solution of the Schrödinger equation (7) can be written in the form

$$\mathbf{f}(t)=\exp(-i\mathbf{M}t/\hbar)\mathbf{f}(0) \ . \tag{8}$$

with the initial condition of Eq. (6).

Since $\mathbf{M}$ is time independent, we can write the solution in the following form:

$$\mathbf{f}(t)=\mathbf{R}^t\exp(-i\mathbf{D}t/\hbar)\mathbf{R}\mathbf{f}(0) \ , \tag{9}$$

where $\mathbf{D}$ is diagonal form of the dynamical matrix

$$\mathbf{M}=\mathbf{R}^t\mathbf{D}\mathbf{R} \ . \tag{10}$$

We have diagonalized the dynamical matrix [Eq. (10)] through a numerical procedure.

Once we have solved for the amplitude $f_n(t)$, we can evaluate the mean-square displacement

$$\langle n^2\rangle=\sum_n |f_n|^2 n^2 \ , \tag{11}$$

which allows us to have a clear view of the localization problem.

This approach to the study of diffusion of an initially localized state follows along the lines presented by Anderson,[15] namely, we can conclude that diffusion has occurred if at $t\to\infty$ the Wannier amplitude on the given site goes to zero. If, on the contrary, the amplitude at the site remains finite while decreasing rapidly with distance, we say we have a localized state. The difference between unity and this finite value is a measure of the spreading of the wave packet to the neighboring sites.

DISCUSSION OF THE RESULTS

We have considered a lattice of different sizes in order to analyze the influence of the boundary. First, we would like to point out that even very weak fields can almost completely eliminate boundary effects. That is so because the effect of the field is to produce oscillations around the starting point, so that the carrier never gets a chance to

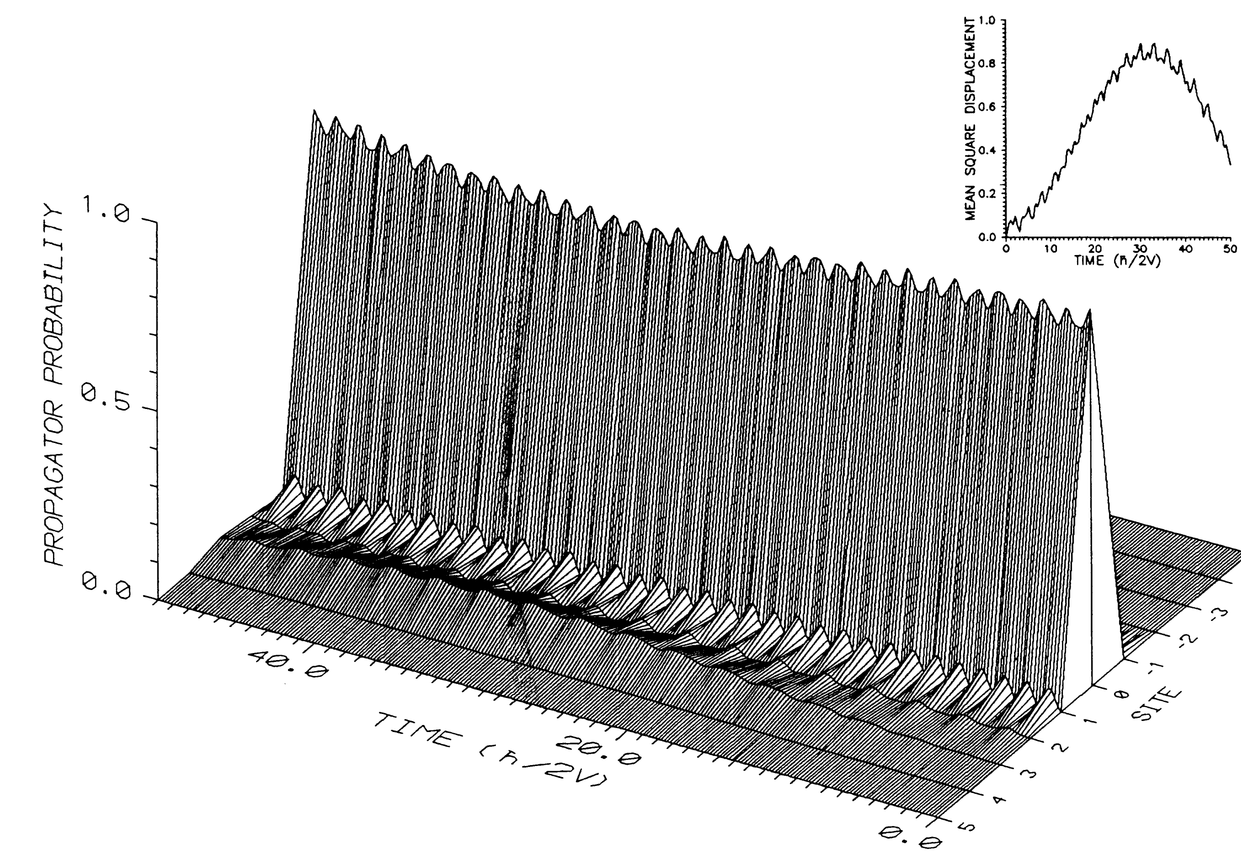

FIG. 3. The same as Fig. 1 for $E=5.0\times10^4$ V/cm and $\varepsilon_0-0.15$ eV. We notice the small amplitude for site 3, which becomes degenerate with the impurity and see that the maximum in $\langle n^2\rangle$ coincides with the maximum of $P_3(t)$.

reach the sample boundaries. The stronger the field is, the more pronounced the localization becomes.

In order to study the influence of the size of the lattice on the solutions of Eq. (7), we have started with 121 sites and then we have reduced the size up to 41 sites. We could not notice any difference in the solutions as long as the field intensity was not less than 10^3 V/cm.

In the case of superposition of field plus impurity potential, we can distinguish different regimes. In order to be more specific, we have chosen a lattice parameter $a=100$ Å such that, for fields of the order 10^5 V/cm, the Bloch frequency comes to the terahertz regime. The total miniband width $4V$ was taken to be 50 meV, and we have normalized the characteristic energies in units of this bandwidth, which are of the order of those quoted in the work by Mendez, Agulló-Rueda, and Hong.[16]

Since the relevant quantities are the impurity potential and the field intensity we would like to discuss the nature of our solutions for (a) a given value of the field intensity while varying the impurity potential and (b) fixing the impurity potential and considering different values of the field.

Before presenting the results, we would like to anticipate them by stating that when the impurity potential ε_0 is such that it coincides with the on-site energy due to the field on a particular site n, i.e.,

$$eEan=\varepsilon_0 , \tag{12}$$

the packet oscillates resonantly between the impurity site and the particular site n. When n is close to the impurity, we have a strong oscillation between both sites in the lattice.

A. Fixed field intensity $E=5.0\times10^4$ V/cm

For this fixed value of the field intensity, we have considered different values of the impurity potential. By varying ε_0, different n values will satisfy Eq. (12). So, for $n=1$ ($eEa=\varepsilon_0$), we have strong oscillations taking place between the impurity site and the first neighbor to the left, as we can see clearly in Fig. 1. This is a quasiperiodic movement of short quasiperiod, as can also be inferred from the mean-square displacement, show in this figure. For an impurity potential such that $n=2$ in Eq. (12), we can see a similar trend for the particle oscillating between site 0 and 2, but with decreasing amplitude at this latter site (see Fig. 2). For a deeper impurity [$n=3$ in Eq. (12)], the amplitude at the impurity is much bigger than at site 3 (see Fig. 3).

For still deeper impurities, the resonance occurs between the origin and a very distant site, which results in a big probability of localization at the origin showing very small values for the propagator for this distant site.

On the other hand, when the impurity is such that we are far from resonance, the particle performs repeated

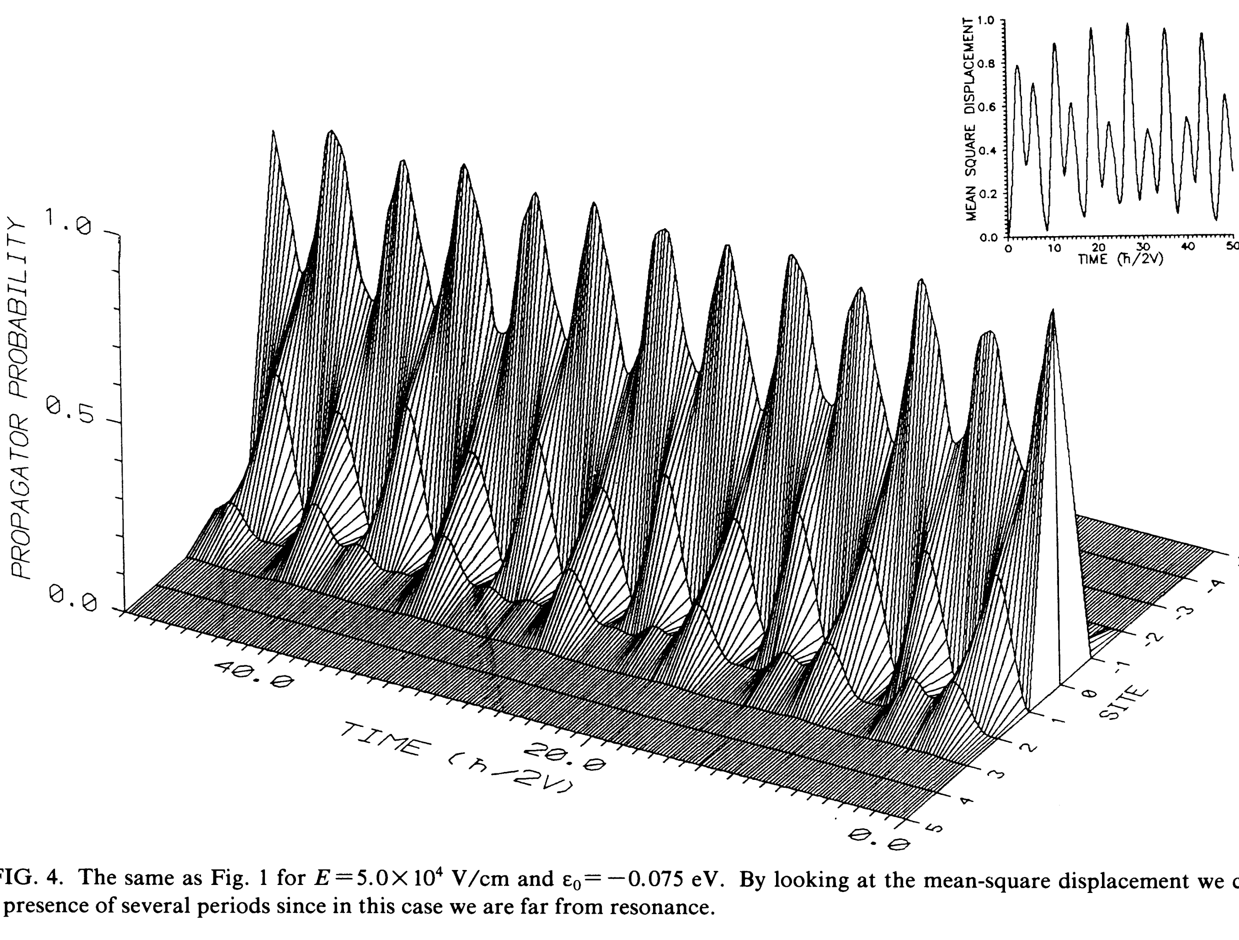

FIG. 4. The same as Fig. 1 for $E=5.0\times10^4$ V/cm and $\varepsilon_0=-0.075$ eV. By looking at the mean-square displacement we can see the presence of several periods since in this case we are far from resonance.

visits to the origin while making virtual transitions to neighboring sites (see Fig. 4).

B. Fixed impurity potential

Now, we analyze the effect of varying the field intensity for the following values of the impurity potential: $\varepsilon_0=-0.1$ and -0.5 eV. We can distinguish between three different regimes: (i) resonance between nearest-neighbor sites in the lattice which correspond to strong fields, (ii) resonance between distant sites in the lattice, which correspond to weak fields, and (iii) field and impurity are such that we are far from resonance.

In Figs. 5(a)–5(c) we show the propagators for

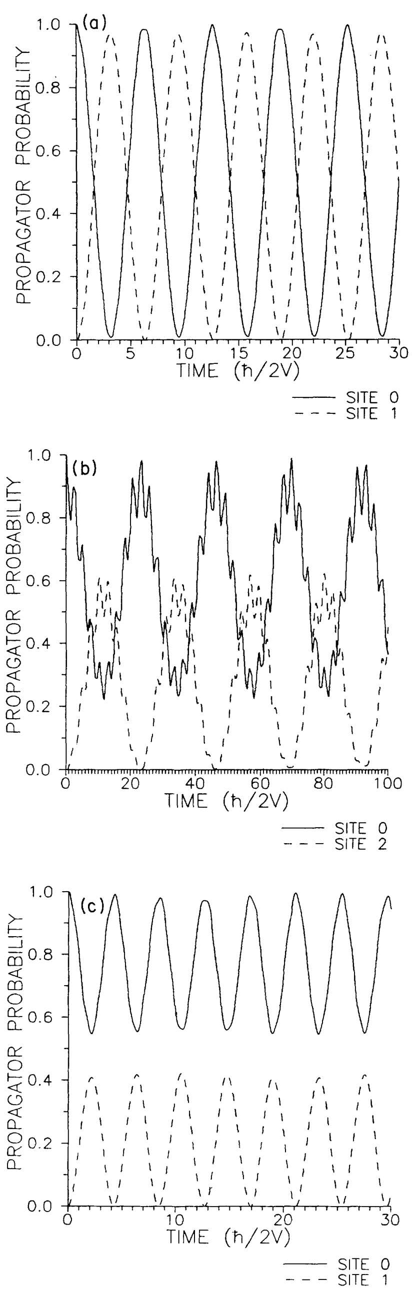

FIG. 5. (a) We show the propagators for sites 0 and 1 for the case $\varepsilon_0=-0.1$ eV and $E=1.0\times10^5$ V/cm. Notice that both sites are in resonance. (b) We show the propagators for sites 0 and 2 for the case $\varepsilon_0=-0.1$ eV and $E=5.0\times10^4$ V/cm. Notice that in this case the resonance occurs between impurity and site 2. (c) The same as (a) for $\varepsilon_0=-0.1$ eV and $E=7.5\times10^4$ V/cm. We notice that the hopping is inhibited since most of the time the particle is at the origin.

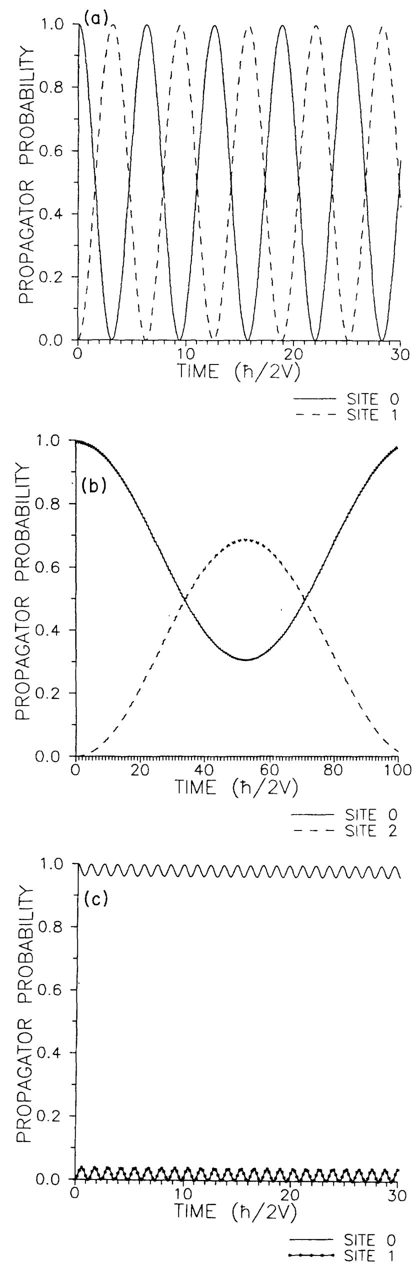

FIG. 6. (a) We show the propagators for sites 0 and 1 for a deeper impurity $\varepsilon_0=-0.5$ eV and $E=5.0\times10^5$ V/cm [$n=1$ in Eq. (10)]. A periodic oscillation between these two sites can be seen clearly with the period $T=2\pi\hbar/2V$. (b) We show the propagators for sites 0 and 2 for $\varepsilon_0=-0.5$ eV and $E=2.5\times10^5$ V/cm [$n=2$ in Eq. (10)]. We see an oscillation taking place between these two sites with a longer period than in (a). (c) The same as (a) for $\varepsilon_0=-0.5$ eV and $E=3.75\times10^5$ V/cm. In this case we are far from resonance. Again the hopping is inhibited and the particle remains almost completely localized at the impurity.

$\varepsilon_0 = -0.1$ eV and three values of the field, which correspond to the three regimes. We can clearly classify the regimes by the different periods. In fact, in the low-field case we have a large period [Fig. 5(b)], while for strong fields we have strong oscillations taking place with a short period [Fig. 5(a)]. On the other hand, far from resonance [Fig. 5(c)], we see strong oscillation and almost localized in site 0 with virtual transitions to the nearest neighbor.

In Figs. 6(a)–6(c), we show the propagators for $\varepsilon_0 = -0.5$ eV and three values of the field, which correspond to the three regimes. it is interesting to compare these results with the ones shown in Fig. 5(a)–5(c). In this case of a deeper impurity, we have to go to stronger fields in order to get the resonance between nearest-neighbor sites [Fig. 6(a)] and next-nearest-neighbor sites [Fig. 6(b)]. When far from resonance [Fig. 6(c)] the hopping is strongly inhibited even to the first neighbor.

We can see a very interesting behavior for the case of resonance between the impurity and first-site neighbor, namely, that independently of the particular values of the field and the impurity as long as they fulfill the relation $eEa = \varepsilon_0$, the quasiperiod is 2π (in units of $\hbar/2V$). This kind of universality can be understood from the equations of motion (5). In fact, by neglecting the amplitudes other than f_0 and f_1 (this is a good approximation for strong fields), we have a pair of equations that couples these amplitudes. In this case, the solution is strictly periodic with a period, which is always $2\pi\hbar/2V$.

This would indicate a very interesting application to SI's, since by varying the field we can satisfy the resonance condition of Eq. (12) for different lattice sites, which in turn give a different response from the sample. For strong fields, we can reach the situation of an oscillation between two neighboring sites in the lattice, which would indicate that the impurity potential should be precisely $\varepsilon_0 = eEa$.

CONCLUSIONS

We would like to conclude by stating that the effect of the field is to remove the degeneracy between the on-site levels, inhibiting the hopping effects. The presence of the impurity, on the other hand, brings the possibility that two on-site energies are nearly degenerate, thus enhancing hopping. However, if the sites are far from each other the tunneling through the lattice is damped severely (low-field case). When the two levels correspond to nearest neighbors in the lattice, the particle oscillates back and forth between the sites (strong-field case), resembling very closely the situation encountered in the case of a double-well potential, as was reported in the experiments done by Roskos *et al.*[17]

For a long time it was thought that Bloch oscillations, because of their large period, were almost impossible to detect, but Waschke *et al.*[14] showed conclusively that the particles perform a number of complete oscillations. Obviously the experiment should be done at low temperatures so that phonon-scattering processes do not mask the effect.

ACKNOWLEDGMENT

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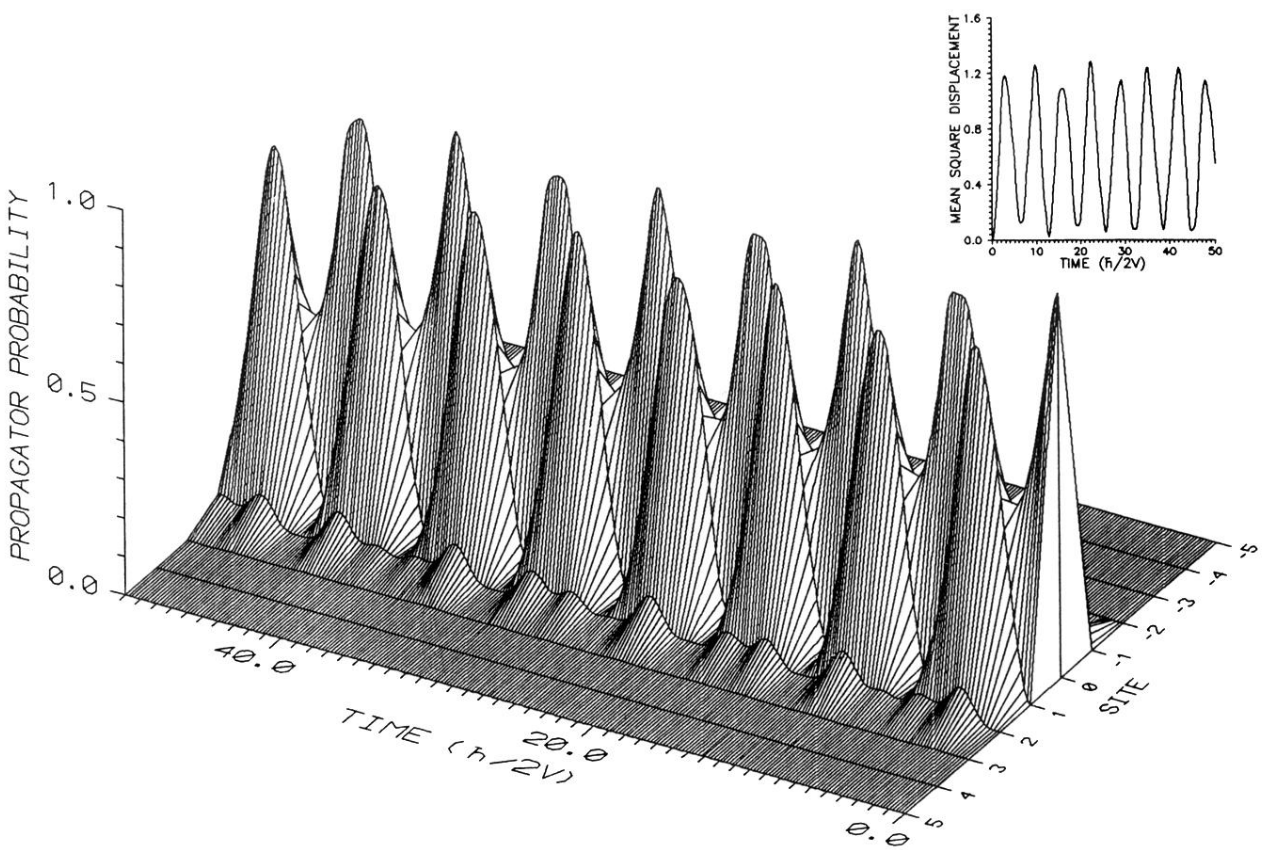

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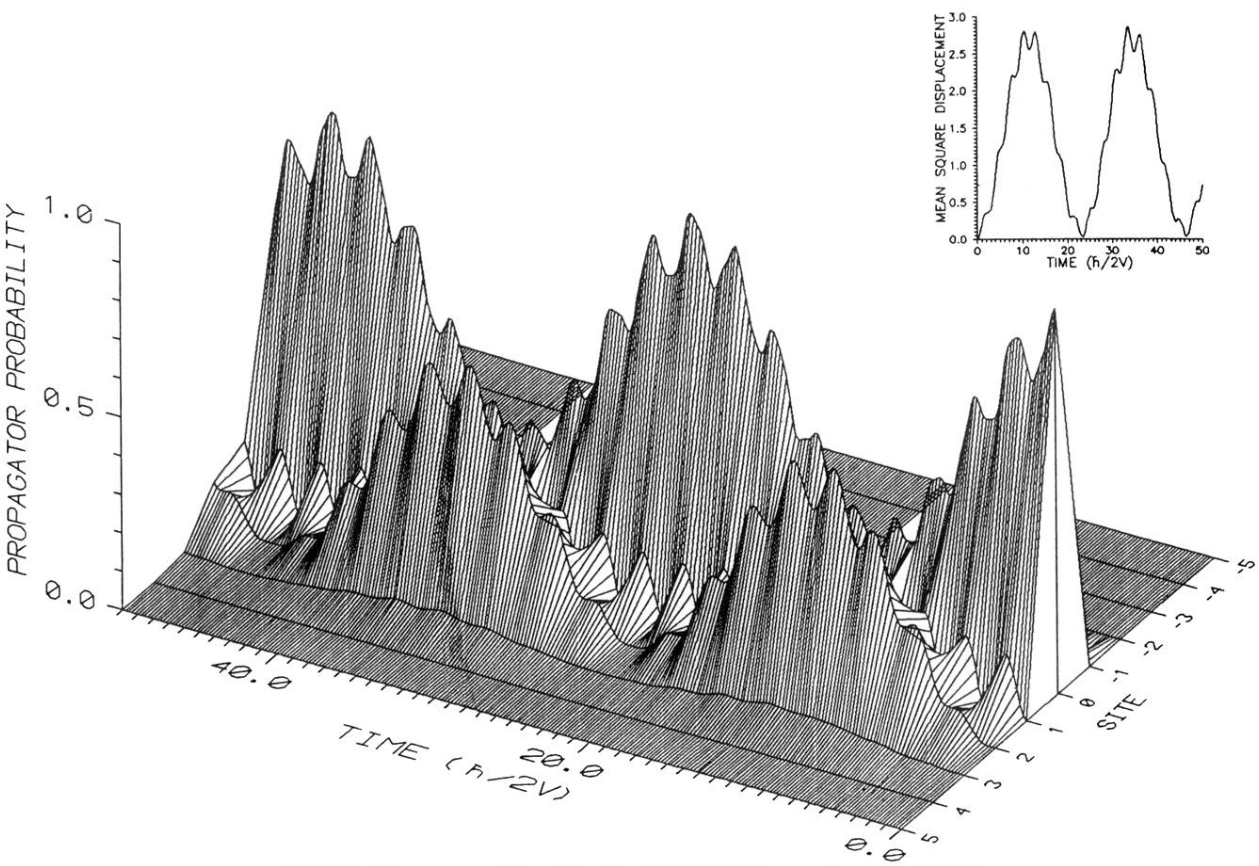

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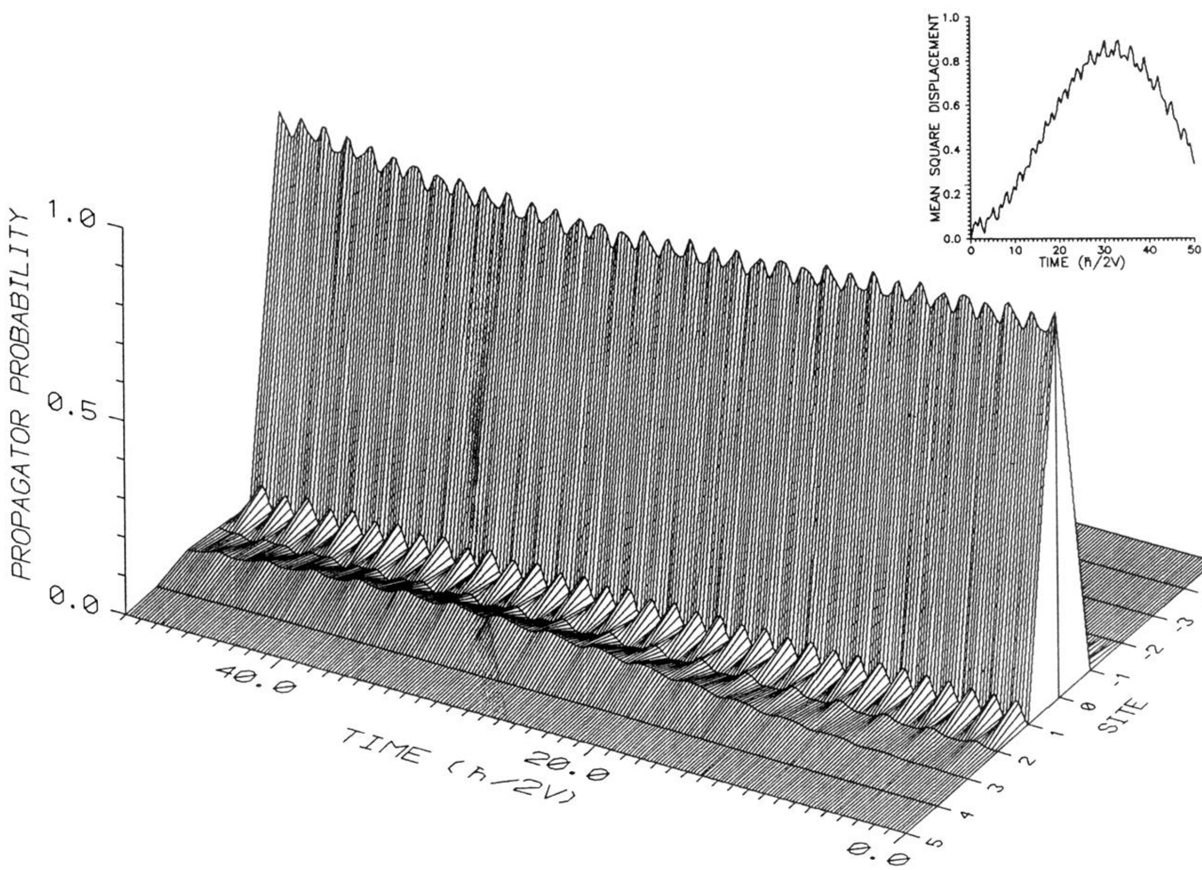

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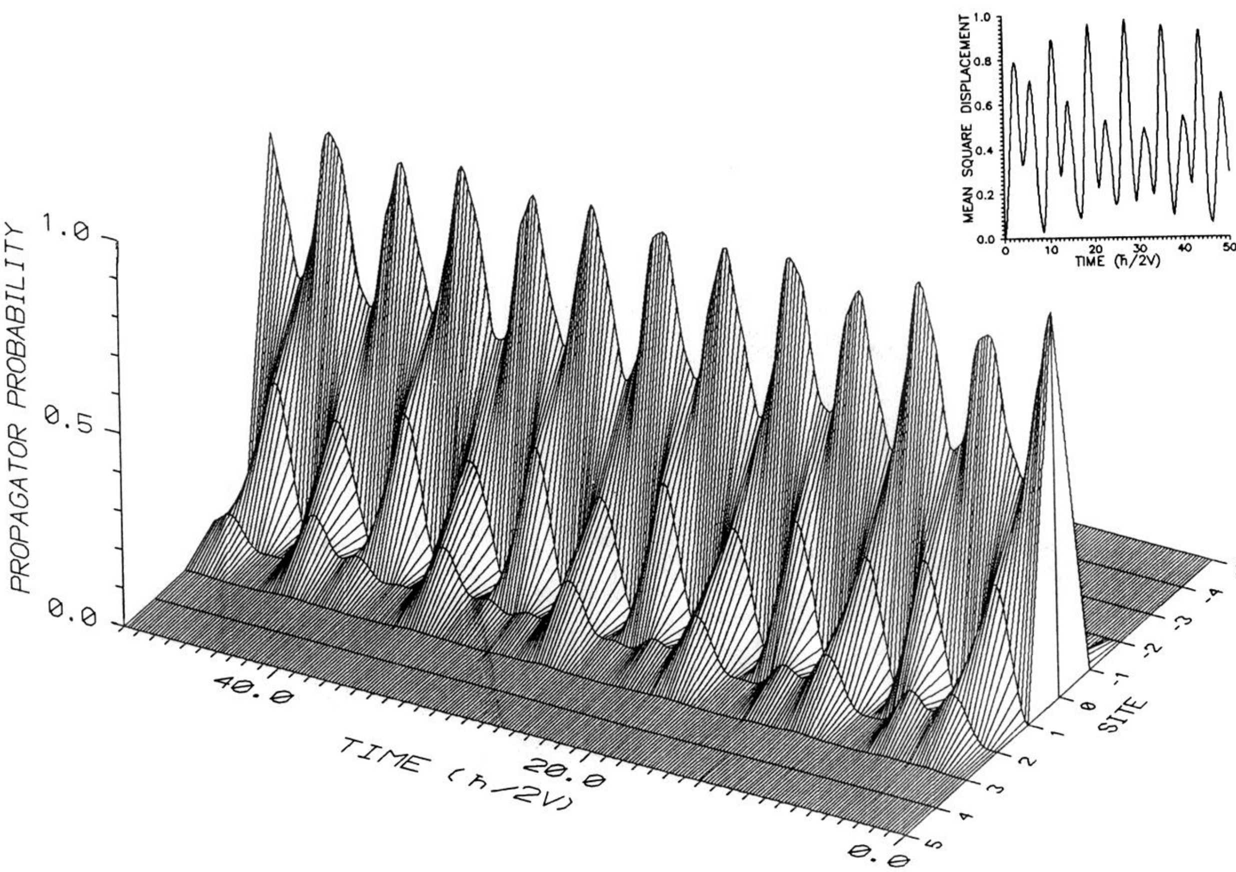

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