Propagation of carriers in a one-dimensional quasicrystal

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We have addressed the problem of dynamical localization in a one-dimensional system with a periodic potential incommensurate with the crystal lattice under the action of a dc electric field. For the chosen potential there exists a mobility edge, that is, a critical value of the ratio between the strength of potential to the half bandwidth, $\eta = \epsilon_0/2V$, which classifies the nature of the wave functions. We show that the effect of the field is to shift the mobility edge towards the delocalized region. We show that the field influence on localization is much stronger than that due to the disorder. It is also shown that when a resonance condition is reached the wave packet oscillates with a characteristic frequency in the terahertz range for superlattices; such an effect can be used to generate electromagnetic radiation of this frequency range.

I. INTRODUCTION

In a previous work[1] we have addressed the problem of the dynamical localization of carriers in a superlattice (SL) with an impurity under the action of a dc electric field. We have discussed the interplay between the impurity potential and the electric field intensity. For this particular case of disorder we have shown that under certain circumstances a resonance condition that results in strong oscillations of the wave packet can be reached. In fact when the field intensity E and impurity ϵ satisfy the relation $eEd = \epsilon$ the oscillation takes place between the impurity site and one of its nearest neighbors with a period $\tau = \hbar/2V$ where $2V$ is the half-bandwidth. This would indicate a very interesting application to SL's, since by varying the field intensity we can satisfy the resonance condition which would in turn give the value of the impurity potential.

In the present work we have undertaken the problem of a different case of disorder, namely, a quasiperiodic potential whose Hamiltonian along the single-band tight-binding model is

$$H_0 = \sum_n \epsilon_0 \cos(2\pi\sigma n) + V \sum_n c_n^\dagger c_{n+1}, \qquad (1)$$

where $\sigma = \frac{(\sqrt{5}+1)}{2}$ is the golden mean.

Since σ is irrational, the Hamiltonian H_0 is incommensurate with the underlying crystal lattice becoming quasiperiodic at large Fibonacci numbers.

We have taken the size of the lattice such as to make the potential as periodic as possible. The nature of the eigenfunctions of H_0 can be characterized by a single parameter $\eta = \epsilon_0/2V$. It is well know[2] that the Hamiltonian of Eq. (1) has a spectrum that develops many gaps which become wider and wider as ϵ_0 increases, showing a highly fragmented band structure. At the same time it presents a mobility edge; that is, for $\eta < 1$ all the eigenfunctions are extended (nondecaying), while for $\eta > 1$ the eigenfunctions are localized. This has to be contrasted to a random one-dimensional (1D) system for which almost all states are localized. As the mobility edge $\eta_c = 1$ is approached from below the eigenfunctions show strong fluctuations characterized by a length ξ, beyond which the eigenfunctions look uniform. In the localized regime, on the other hand, we can define an average decay length l_d. Both lengths blow up at the mobility edge.

II. FIELD-DRIVEN DIFFUSION

As was previously said our interest is the description of the diffusion of carriers via the time evolution of the propagators when an electric field is acting upon the system. In this case the total Hamiltonian is

$$H = H_0 + \sum_n eEdn\ c_n^\dagger c_n. \qquad (2)$$

The Wannier propagator amplitudes satisfy the following equation:

$$i\hbar \frac{d}{dt} f_n = V\,(f_{n-1} + f_{n+1}) + (\epsilon_n - eEd\ n)\, f_n, \qquad (3)$$

where the on-site energies ϵ_n are

$$\epsilon_n = \epsilon_0 \cos(2\pi\sigma n)\,. \qquad (4)$$

For the case of a finite lattice of size N, the Schrödinger equation (3) can be put in matricial form:

$$i\hbar \frac{d}{dt}\mathbf{f} = \mathbf{M}\mathbf{f}, \qquad (5)$$

where $\mathbf{M}$ is the $N \times N$ dynamical matrix and the vector $\mathbf{f}$ is formed from the on-site Wannier amplitudes. We have developed a scheme to solve Eq. (5) based on the stationary character of the Hamiltonian.[1] Starting with

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the initial condition $\mathbf{f}(t=0)$, we put the solution as

$$\mathbf{f}(t) = \mathbf{R}^t \exp(-i\mathbf{D}t/\hbar)\,\mathbf{R}\,\mathbf{f}(0)\,, \tag{6}$$

where $\mathbf{D}$ is the diagonal form of the dynamical matrix $\mathbf{M} = \mathbf{R}^t\mathbf{D}\mathbf{R}$. We have checked the normalization of the wave function after every time step. After obtaining the amplitude $\mathbf{f}(t)$, we can evaluate the mean-square displacement

$$\langle n^2 \rangle = \sum_n |f_n|^2 n^2, \tag{7}$$

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

We have studied the influence on the solutions of (i) the initial condition, (ii) the potential strength ϵ_0, and (iii) the field intensity $\mathbf{E}$. Energies were measured in units of the bandwidth $4V$. To be specific we have chosen a lattice parameter $d = 100$ Å and the total minibandwidth to be 50 meV. We have considered the way a carrier diffuses when injected in an otherwise empty band, and have followed along the lines presented in Anderson's classical work.[3] We say that if we start with a well-localized state 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. Since we are dealing with a finite lattice the amplitude for large times goes as $1/N$ (that is, the limit $N \to \infty$ goes to zero). The difference between unity and this finite value is a measure of the spreading of the wave packet to neighboring sites.

We have considered lattices of different sizes in order to analyze the influence of the boundary. The effect of the electric field is to produce oscillations around the starting point so that for even moderate fields (10^3 V/cm) the carrier never gets a chance to reach the sample boundaries. The stronger the field is the more pronounced the localization becomes. In conclusion we have considered lattices of 111 sites for which the solutions of the Schrödinger equation are size independent.

III. RESULTS AND DISCUSSION

A. Zero field

As a test we have taken the field-free case imposing periodic boundary conditions $|\,1\rangle = |\,N+1\rangle$. In this case we have considered the time evolution of the propagators for two extreme initial conditions, namely, the perfectly localized state on site $\mathbf{M}$, $f_n(0) = \delta_{n,M}$, and the com-

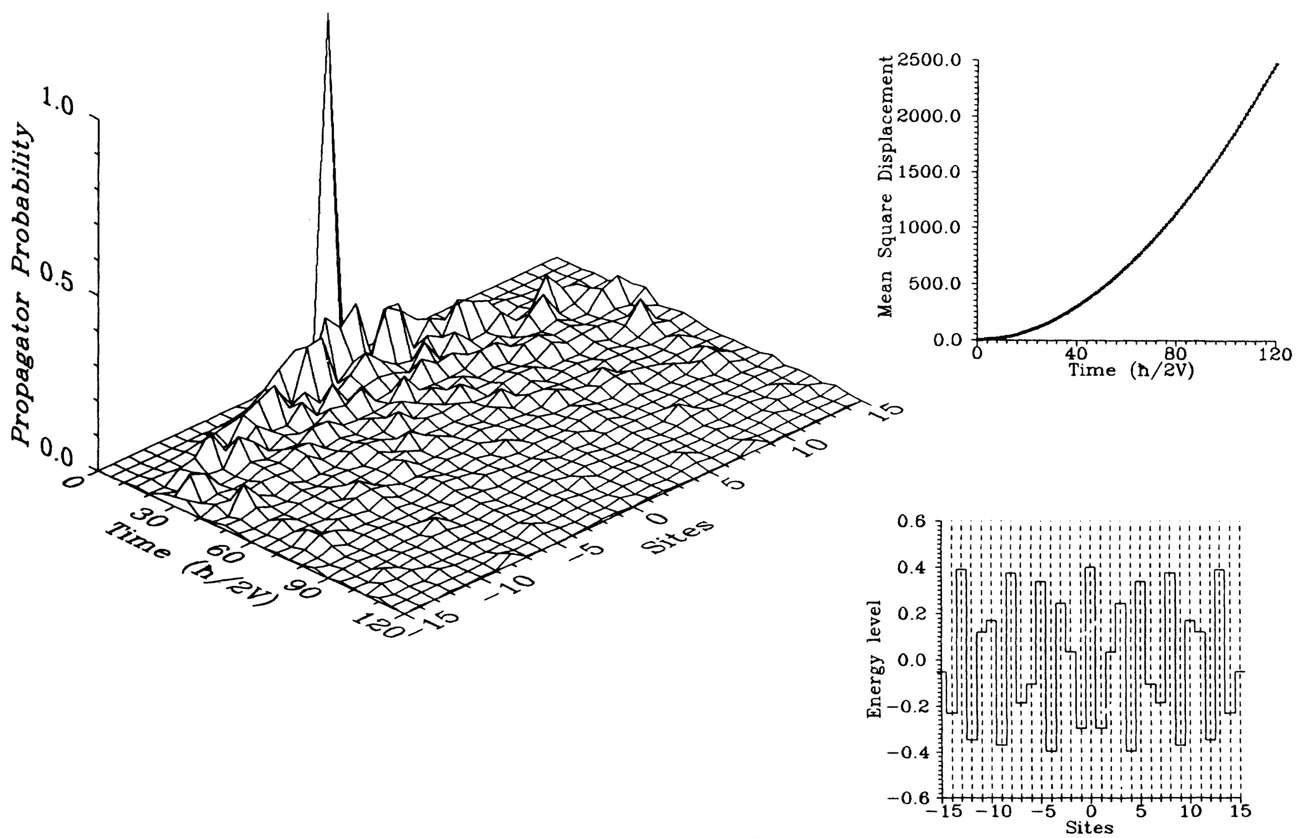

FIG. 1. We show the propagator probability as a function of time and lattice sites for the field-free case and potential strength $\epsilon_0 = 0.2\,|\,4V\,|$. The initial condition was $f_n(0) = \delta_{n,0}$. We show also the mean-square displacement and the on-site energy levels of Eq. (4). We notice the diffusion of the particle since we are below the mobility edge.

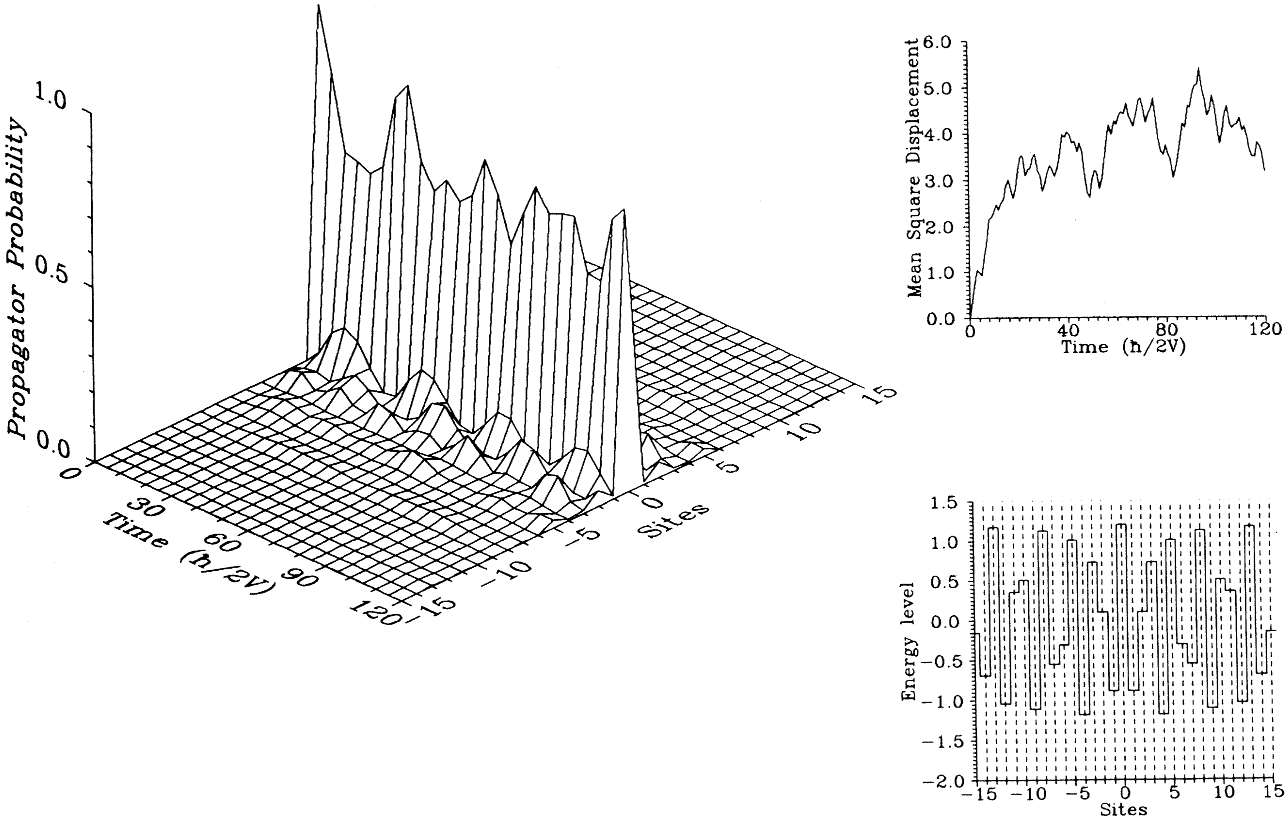

FIG. 2. The same as Fig. 1 but for $\epsilon_0 = 0.6 \mid 4V \mid$. In this case the particle localizes around the origin. Notice the small values of the MSD.

pletely delocalized case, $\mid f_n(0) \mid^2 = 1/N$, where N is the number of sites considered in our calculation.

It can be clearly seen in Fig. 1 that for values of the impurity potential less than the critical value $2V$, the particle that starts in a well-localized state propagates through the lattice, while for $\epsilon_0 = 0.2$, the mean square displacement shows a ballistic behavior: $\langle n^2 \rangle \propto t^2$. For the impurity potential $\epsilon_0 = 0.6$ (above the critical value 0.5) the particle localization is evident around the starting position (see Fig. 2).

A more complex pattern is obtained when the initial state considered was the completely delocalized one: $|f_n(0)|^2 = 1/N$. In this case we have taken $\epsilon_0 = 0.2$. As time goes we notice probability concentrations on the Fibonacci sites, i.e., sites for which $n = 3, 5, 8, \ldots$. The reason for that is that these sites are almost degenerate with the origin due to the form of the on-site energies [see Eq. (4)]. This produces depletion on the others sites, since hopping between degenerate sites is preferred.

B. Interacting case

We have considered different intensities of the dc field and looked at the time evolution of the wave packet. As is well known, the effect of the field on a carrier in a periodic potential is to produce oscillations [Block oscillations (BO)],[4–13] thus inhibiting diffusion in a lattice, an effect called dynamical localization. These oscillations are almost impossible to detect in bulk samples but, with the manufacturing of SL's, it was possible the detection of BO's through the emission of electromagnetic radiation in the terahertz range.[14] In the present case of a quasiperiodic potential, where we can define a mobility edge, the presence of the field should alter its position towards the delocalized states as we shall show. This situation was encountered in the case of electrons interacting with the lattice phonons. In fact, the work by Economou *et al.*[15] showed the formation of localized polarons in the vicinity of the mobility edge shifting it into the region of extended states. In this work, we have assumed sufficiently low temperatures as to neglect interaction of the carrier with the lattice phonons. The inclusion of this effect is currently under way.

To study the effect of the field on the assumed quasiperiodic potential we have taken values of the strength potential ϵ_0 well below the mobility edge and verified that small field intensities modify strongly the way a packet propagates in the lattice. In fact, starting with a well localized state at $t = 0$, we see that the wave packet remains partially localized, and at the same time it "appears" at other lattice sites with decreasing amplitudes as we go away from the origin.

1. Weak fields

We shall start the discussion considering first the case of very moderate fields intensities (10^3 V/cm) and different values of the disorder strength, going from the very delocalized region towards the mobility edge for H_0.

a. $E = 2.5 \times 10^3$ V/cm, $\epsilon_0 = 0.1 \mid 4V \mid$ (weak field and disorder). In this case $\eta = 0.2$ which means that we are far from the mobility edge. As it can be seen in Fig. 3, the particle starts to diffuse and due to the presence of the field it is more likely to be found on the left. We notice small hills as time goes on because at certain positions two on-site nearest neighbor energies are almost degenerate with the result that the packet is reinforced at such positions. The mean square displacement (MSD) shows a chaotic behavior at the same time that the particle is confined to a definite region of the lattice in spite of the fact that we are in the delocalized region of the spectrum of H_0.

b. $E = 2.5\times10^3$ V/cm, $\epsilon_0 = 0.4 \mid 4V \mid$. In this case, we notice in Fig. 4 the presence of three well-distinct hills, namely, around sites **0** (where the packet starts), **-3** and **-10**. If we consider the on-site energy levels shown in the figure, we can realize that site **-3** is almost degenerate with the origin so that hopping between these sites is enhanced. As for site **-10** it is almost degenerate with site **-11** so that when the packet reaches these sites it reinforces itself there. The MSD shows an oscillating pattern at the same time it presents smaller values than in the previous case (Sec. III B 1 a).

c. $E = 2.5 \times 10^3$ V/cm, $\epsilon_0 = 0.5 \mid 4V \mid$. By increasing the disorder strength up the critical value ($\eta = 1$) we see, in Fig. 5, two well-distinct hills, one at the origin and other at site **-3**. We can understand this since both on-site energies are degenerate as in the previous case but now the presence of large barriers around site **-3** strongly inhibits hopping. The MSD shows in this case a quasiperiodic movement of the wave packet but with much shorter quasiperiod than in the previous case. What we have is a clear oscillation between the origin and site **-3**.

2. Moderate fields

a. $E = 10^4$ V/cm, $\epsilon_0 = 0.115 \mid 4V \mid$. We notice in Fig. 6 that by increasing the field intensity but with a still weak disorder the packet localizes clearly around the starting position. If we compare the MSD for the present values with the corresponding to the case in Sec. III B 1 a (Fig. 3) we notice a drastic reduction which tells us that the field effect is predominant in determining the diffusion properties.

b. $E = 10^4$ V/cm, $\epsilon_0 = 0.438 \mid 4V \mid$. For this par-

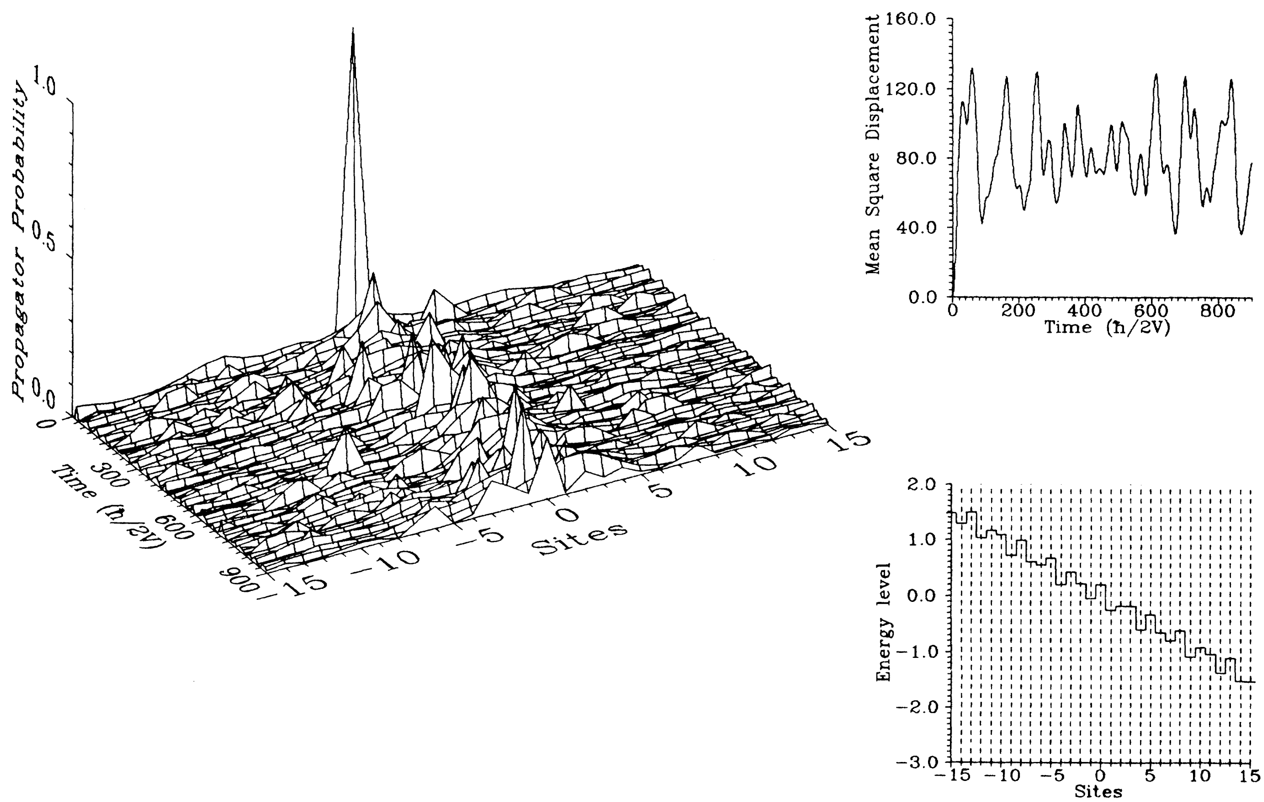

FIG. 3. The same as Fig. 1 but for the electric field intensity $E = 2.5$ kV/cm and $\epsilon_0 = 0.1 \mid 4\text{V} \mid$. Notice that in this case we are far from the mobility edge but, in spite of this, the MSD shows the confinement of the particle in a definite region.

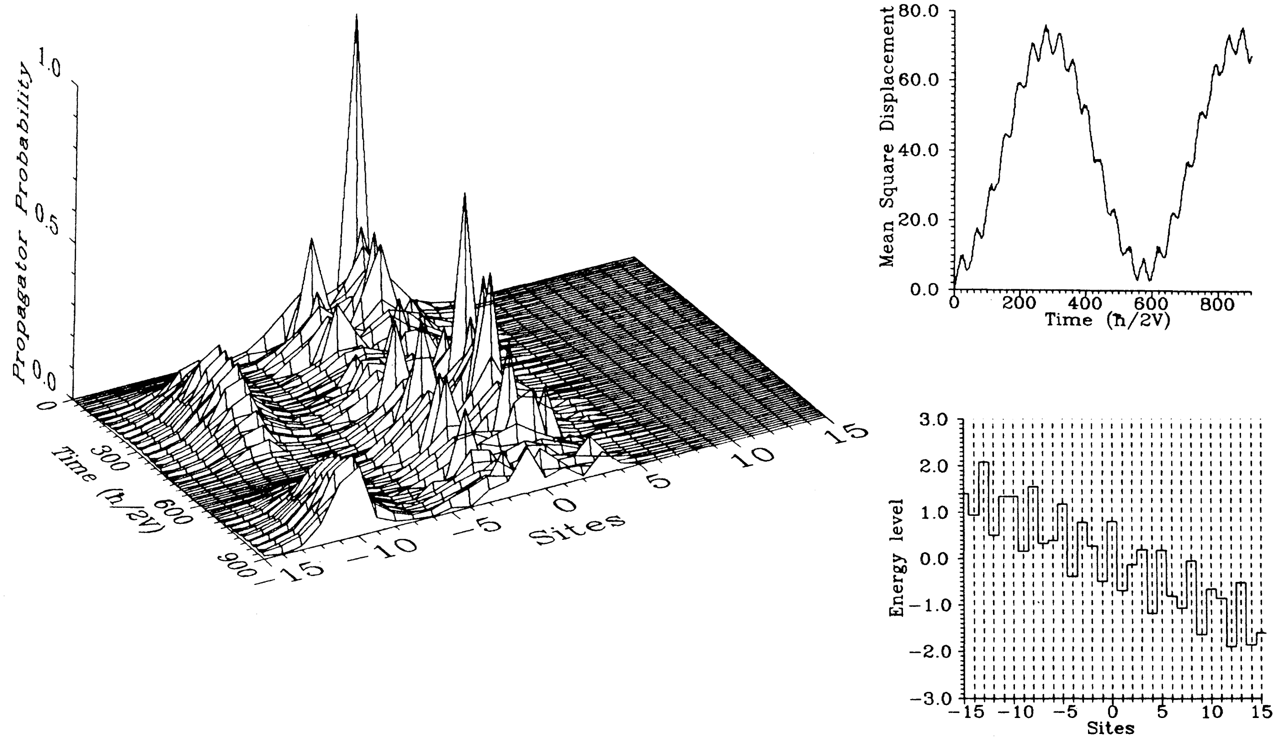

FIG. 4. The same as Fig. 3 for $E = 2.5$ kV/cm and $\epsilon_0 = 0.4 \mid 4\mathrm{V} \mid$. From the MSD we can notice an oscillation of the wave packet. From the on-site energy levels figure we realize that sites **0** and **-3** are degenerate and that the same happens between the sites **-10** and **-11** so that the packet gets reinforced in this neighborhood.

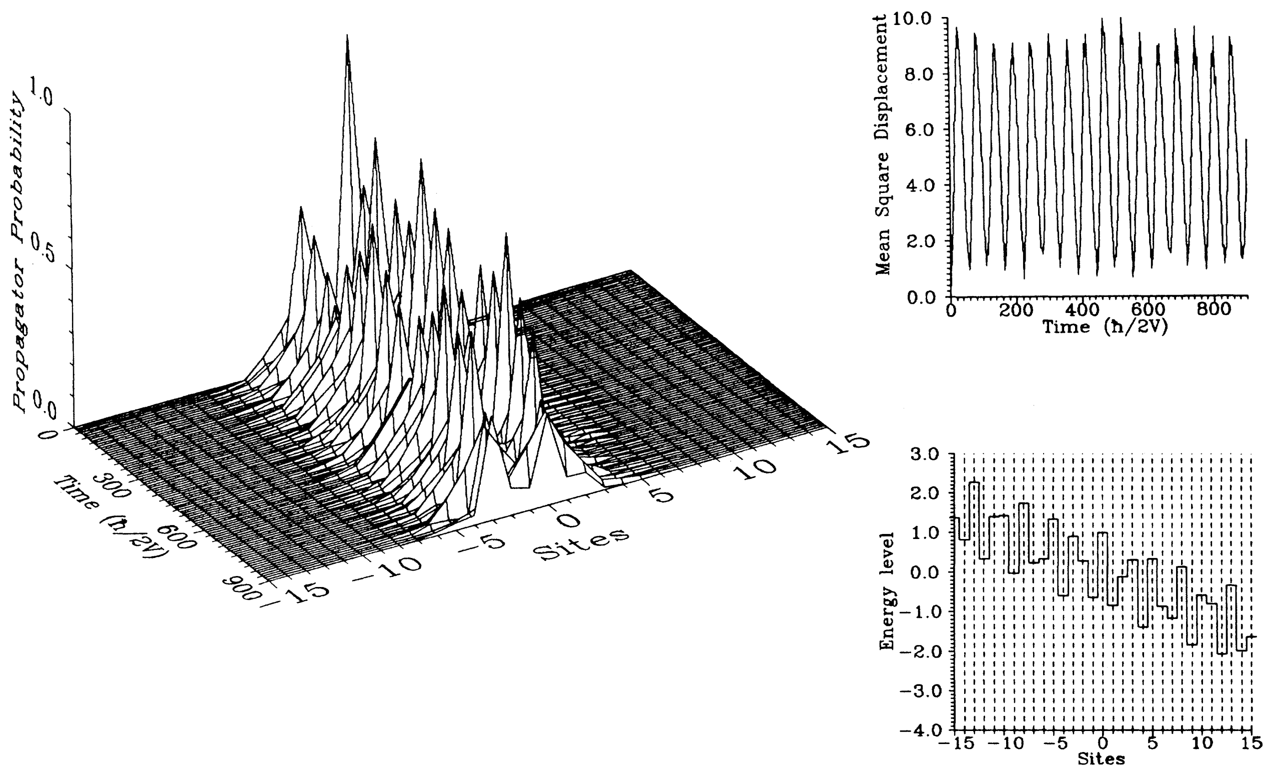

FIG. 5. The same as Fig. 4 for $E = 2.5$ kV/cm and $\epsilon_0 = 0.5 \mid 4V \mid$. This corresponds to the critical value $\eta = 1$. We see a clear oscillation between sites **0** and **-3**, with a period shorter than in Fig. 4 as well as smaller values of the MSD.

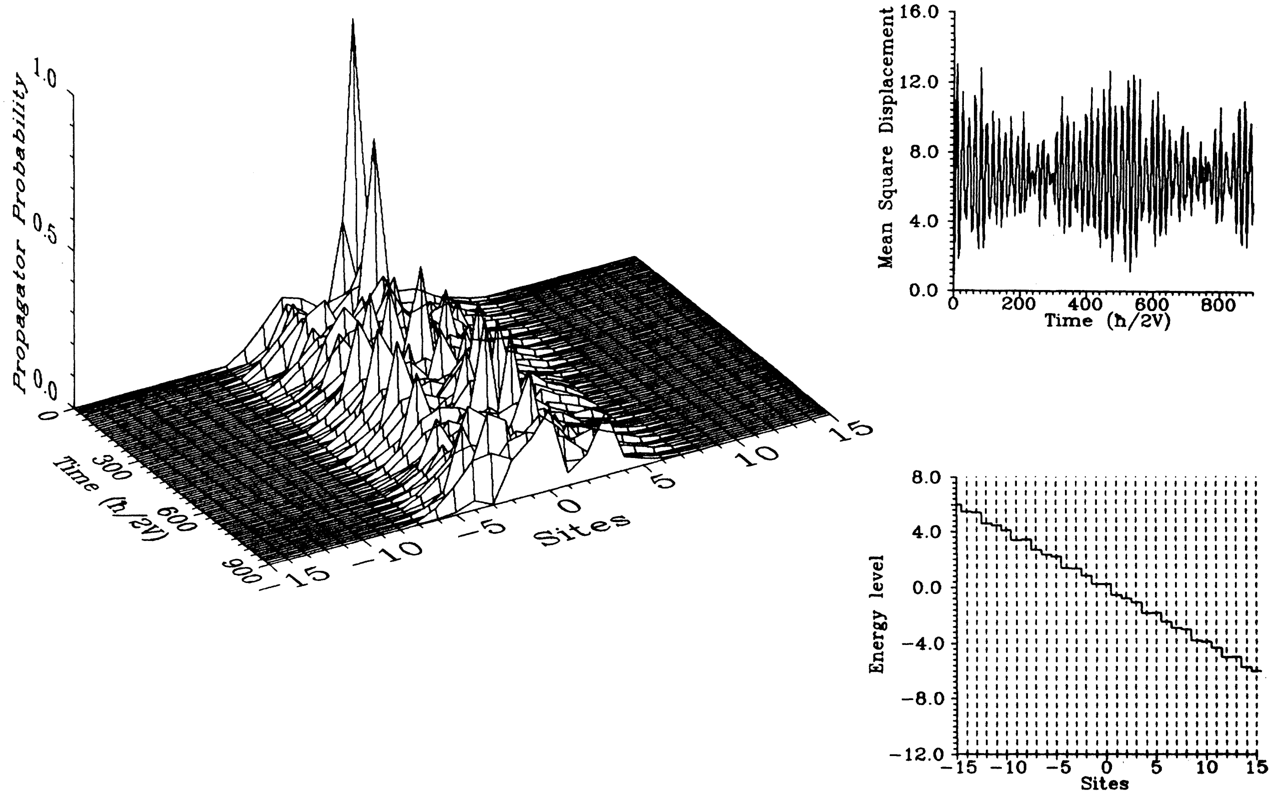

FIG. 6. The same as Fig. 4 for $E = 10$ kV/cm and $\epsilon_0 = 0.115 \mid 4V \mid$. We notice that even for this small potential strength the localization is severely enhanced with respect to the case shown in Fig. 3. The reason for that is the increasing of the field intensity.

ticular value, the on-site energies corresponding to the origin and site **-2** are almost degenerate which results in a strong localization, the particle is almost oscillating between sites **0** and **-2**.

3. High fields

Most interesting to discuss for its applications is the case of strong fields. Taking into account the on-site energies given by Eq. (4) the resonance condition between sites **0** and **n** can be written

$$[\epsilon_0/eEd]_n = n/\left[1 - \cos\left(2\pi\sigma n\right)\right], \quad (8)$$

which for the particular case of site **-1** can be written as

$$[\epsilon_0/eEd]_{-1} = 1/\left[\cos\left(2\pi\sigma\right) - 1\right]. \quad (9)$$

For strong fields we can satisfy the resonance condition [Eq. (9)]between the nearest neighbors (*NN*) in the lattice thus given place to strong oscillations with the shortest period: $\tau = 2\pi\,(\hbar/2V)$. This can be seen from Eq. (3) for the Wannier amplitudes. In fact, by neglecting the amplitudes other than f_0 and f_1 (approximation valid for strong fields) we obtain a pair of equations that couples both amplitudes with a perfectly periodic solution of precisely that period. Such oscillation between *NN* sites is clearly seen in Fig. 7(a) where we have plotted the propagators for sites **0** and **-1** for $\epsilon_0 = 1.15 \mid 4V \mid$. In Fig. 7(b) we notice the almost complete degeneracy between these sites. It is worth noticing that, for strong fields, the barriers between sites are big; consequently hopping to sites other than the degenerate ones is severely inhibited. In Fig. 7(c) we present the corresponding MSD which shows an almost perfect periodic motion of period $t = 2\pi\,(\hbar/2V)$.

We can compare this case with the one shown in Fig. 5 where we also have an oscillatory motion but with a larger period at the same time the MSD never vanishes. The importance of considering high field values is due to the fact that the oscillatory motion having the shortest period makes its detection simpler.

IV. CONCLUSIONS

A very interesting effect occurs when, by varying the field, we make a particular on-site energy become degenerate with the initial site energy. If the corresponding sites are close to each other (strong field case) we have a resonance effect which causes oscillations of the wave packet. The closer the sites corresponding to the degenerate level the stronger the oscillation and the shorter its quasiperiod, a picture that tells us that the response of the system to the external field is controlled by the short range configuration. In the case of *NN* resonance, the system behaves as a double quantum well as if ignoring

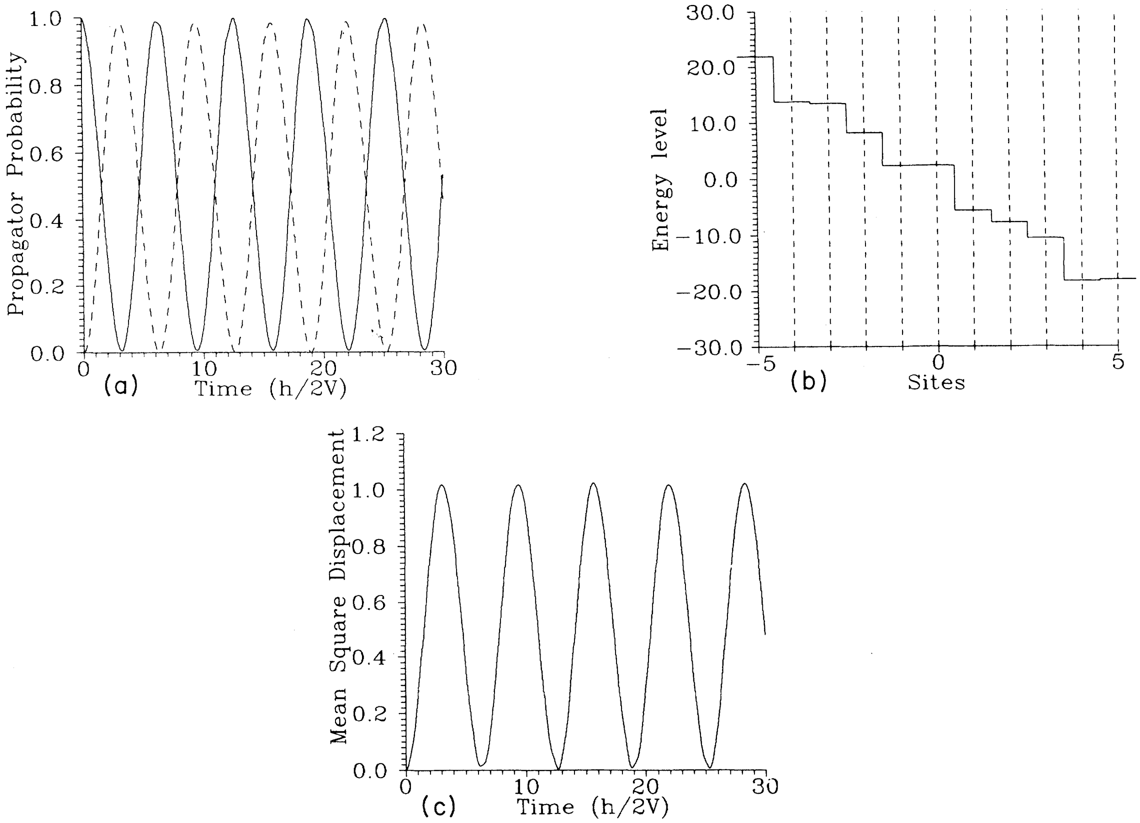

FIG. 7. (a) We show the propagator probabilities for sites **0** and **-1** for $E = 10^5$ V/cm and $\epsilon_0 = 1.15 \mid 4V \mid$. (b) We show the on-site energy levels and can see the degeneracy between the *NN* sites **0** and **-1**. (c) The mean-square displacement shows clearly a strong oscillation with the period $2\pi\,(\hbar/2V)$. Notice that the field and potential values were chosen in order to satisfy Eq. (9).

the rest of the lattice structure.

When far from resonance the pattern is very complex. As a matter of fact, there is always a pair of sites (quasi)degenerate but what we mean here by "far from resonance" is when these sites are far apart from each other. In this case, we see that the wave propagates in a very special way; namely, if the field and potential are not very strong, the particle is partially at the origin and meanwhile it prefers sites with close energies such that the wave packet gets reinforced in this neighborhood. For the particular case of disorder assumed in our work, the Fibonacci sites are the preferred ones in the field-free case. Clearly, when the strength of the disorder is large, the packet localizes itself and what the field does is to enhance localization. Beyond a definite neighborhood, a localized electron does not see the other sites in the crystal.

With regard to the limiting time taken is the calculation we went well beyond $800\hbar/2V$ shown in the figures. For such large times we got the same resulting patterns which allow us to keep our conclusions for the limit $t \to \infty$.

Our main conclusion is that, for the (1D) tight-binding model, the field influence on localization is much stronger than disorder is. While for disorder one needs to surpass a certain critical value to produce a delocalization-localization transition, any field intensity would produce the effect we call now dynamical localization which in the case of a pure crystal results in BO's.

Last but not the least, we would like to mention a possible application of the effect we have discussed in this work. Since the effect of the dc electric field is to produce oscillations of the wave packet, its application should result in the emission of electromagnetic radiation of a definite frequency [when field intensity and impurity potential satisfy the resonance condition of Eq. (9) between *NN* in the lattice]. By taking into account typical miniband widths for SL's, one should be able to generate radiation in the terahertz range provided the dephasing of the wave packet occurs for long times. Such results were already reported in Refs. 16, 17 for double quantum wells.

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[1] H.N. Nazareno, C.A.A. da Silva, and P.E. de Brito, Phys. Rev. B **50**, 4503 (1994).

[2] J.B. Sokoloff, Phys. Rep. **126**, 189 (1985); M.Ya. Azbel, Zh. Ekps. Teor. Fiz. **46**, 930 (1964) [Sov. Phys. JETP **19**, 634 (1964)]; S. Aubry and C. Andre, *Proceedings of the Israel Physical Society,* edited by C.G. Kuper (Adam Hilger, Bristol, 1979), Vol. 3, p. 133.

[3] P.W. Anderson, Phys. Rev. **109**, 1492 (1958).

[4] F. Block, Z. Phys. **52**, 555 (1928).

[5] G.H. Wannier, Phys. Rev. **181**, 1364 (1969).

[6] L. Esaki and R. Tsu, IBM J. Res. Dev. **14**, 61 (1970); R. Tsu and L. Esaki, Appl. Phys. Lett. **19**, 245 (1971).

[7] D.H. Dunlap and V.M. Kenkre, Phys. Rev. B **34**, 3625 (1986).

[8] J.B. Krieger and G.H. Iafrate, Phys. Rev. B **33**, 5495 (1986).

[9] H.N. Nazareno and J.C. Gallardo, Phys. Status Solidi B **153**, 179 (1989).

[10] N.H. Shon and H.N. Nazareno, J. Phys. Condens. Matter **4**, L611 (1992).

[11] M. Holthaus, Phys. Rev. Lett. **69**, 351 (1992).

[12] M. Dignam, J.E. Sipe, and J. Shan, Phys. Rev. B **49**, 10 512 (1994).

[13] For an interesting paper on BO's see E.E. Mendez and G. Bastard, Phys. Today **46** (6), 34 (1993).

[14] C. Waschke, H.G. Roskos, R. Schwedler, K. Leo, H. Kurz, and K. Köhler, Phys. Rev. Lett. **70**, 3319 (1993).

[15] E.N. Economou, O. Yanovitskii, and Th. Fraggis, Phys. Rev. B **47**, 740 (1993).

[16] H.G. Roskos, M.C. Nuss, J. Shah, K. Leo, D.A.B. Miller, A.M. Fox, S. Schmitt-Rink, and K. Köhler, Phys. Rev. Lett. **68,** 2216 (1992).

[17] M.C. Nuss, P.C.M. Planken, J. Brener, H.G. Roskos, M.S.C. Luo, and S.L. Chuang, Appl. Phys. B **58**, 249 (1994).