Extended states and dynamical localization in semiconductor superlattices

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We study the quantum dynamics of electronic wave packets in quantum-well based semiconductor superlattices subject to an applied electric field. Using a high-accuracy numerical method, we analyze the dynamical behavior of electronic wave packets in periodic, random and random dimer superlattices. The spatial extent of electronic states is characterized by means of the time-dependent inverse participation ratio. We show that the delocalized states recently found in random dimer superlattices become spatially localized under the action of the applied field (dynamical localization) but wavepackets are much less localized than in purely random superlattices at moderate field. We conclude that the resonant tunneling effects causing delocalization in dimer superlattices play an important role even in the presence of moderate electric field. © *1997 American Institute of Physics.* [S0021-8979(97)07801-8]

I. INTRODUCTION

There is at present much work devoted to dynamical properties of quantum-well based semiconductors superlattices (SLs). This interest is beyond the mere conceptual problem since time-dependent phenomena in semiconductor heterostructures are the basis for designing ultra-high speed electronic devices. Recently, GaAs–$Ga_{1-x}Al_xAs$ SLs operating as terahertz generators have been proposed.[1] The origin of the electromagnetic radiation is attributed to periodic and almost-periodic Bloch oscillations[2] (BOs) in perfect and imperfect systems, respectively. The idea of semiconductor SLs radiating at terahertz frequencies was proposed some time ago by Esaki and Tsu,[3] who argued that electrons should undergo BOs. A clear semiclassical picture of BOs may be attained by neglecting the coupling between different bands: Under an applied electric field F, electrons are accelerated until their crystal momentum satisfies the Bragg condition and then they are backward reflected. As a consequence, electrons oscillate back and forth with a characteristic period given by $\tau_B = 2\pi\hbar/(eFd)$, d being the spatial period of the SL.[4]

For sufficiently large electric fields, electron wave functions in periodic SLs are no longer extended but localized (Stark-Wannier localization). This localization is due to the loss of quantum coherence arising from the misalignment of levels of neighboring quantum-wells. Hence, an initially localized wavepacket, which consists of a linear combination of Stark-Wannier eigenstates,[5] will remain spatially localized during its time evolution (dynamical localization). Moreover, Bouchard and Luban found that BOs are not periodic but instead they become almost-periodic oscillations in SLs with GaAs contaminated by excess Al.[1] Thus, it seems that small fluctuations of local potentials cannot completely destroy BOs. This can be understood from the fact that the localization effects of disorder are not very strong and, consequently, signatures of BOs still occur in those SLs. From a fundamental point of view, an interesting task is to study intentionally disordered SLs, where electrons are localized within a few quantum-wells due to the higher degree of disorder,[6] in order to ascertain whether BOs are to be expected or not. Moreover, it is by now well-known that even intentionally disordered SLs may support a band of extended states when disorder presents some kind of spatial correlation.[7,8] In Ref. 9, it was shown that delocalized electronic states arise in spite of the inherent disorder due to resonant phenomena taking place at dimer quantum-wells of the same thickness. These resonances lead to a transmission coefficient of different segments forming the SL close to unity, no matter what the length of the segment is. In view of this, in random dimer SLs subject to an applied electric field, one expects that the competition between dynamical localization effects and resonant tunneling effects causing delocalization could lead to new kind of time-dependent phenomena.

In this work we present a first study of dynamical effects related to random and random dimer SLs subject to a dc electric field, and compare them with those obtained in periodic SLs. To be specific, we consider the problem of quantum evolution of electronic wavepackets initially localized in quantum-well based SLs, driven by an electric field. The study of periodic SLs will allow us to establish the main features of dynamical localization in the absence of disorder. This is required for a better understanding of wavepacket dynamics when an amount of intentional randomness is introduced in the SL. 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

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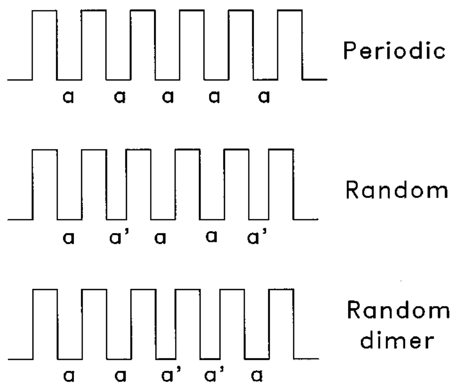

FIG. 1. Schematic diagram of the conduction-band edge of periodic, random (with unpaired quantum-wells of thickness a') and random dimer (with paired quantum-wells of thickness a') SLs. All barriers have the same thickness b.

quantity, we will be able to show below that, although all states in random dimer SLs become localized under the action of the electric field, they acquire an spatial structure much more extended than their counterparts in purely random SLs.

II. MODEL

In our model of disordered SL, the thickness of quantum-wells takes at random one of two values, a and a'. This will be referred to as random SL (RSL). The thickness of barriers separating neighboring quantum-wells is assumed to be the same in the whole SL, b. A random dimer SL (DSL) is constructed[8] by imposing the additional constraint that quantum-wells of thickness a' appear only in pairs, called hereafter a dimer quantum-well. Figure 1 presents a schematic diagram of the conduction-band edge of the SLs. As a typical SL we have studied a GaAs–$Ga_{0.65}Al_{0.35}As$ system with conduction-band offset 0.25 eV and effective mass $m^*=0.067m$ at the Γ valley, m being the electron mass. This is not a serious limitation of the model as our description can be easily generalized to include two different effective masses. In our computations we have taken $a=b=32$ Å and $a'=26$ Å. In RSLs as well as in DSLs the number of quantum-wells of thickness a' is 80 and the total number of quantum-wells is 200. It is worth mentioning that we have checked that our main results are independent of this fraction. We have already shown,[8] using the transfer-matrix method with standard boundary conditions, that this DSL presents a band of states whose transmission coefficient is close to unity, independently of the SL length (see Fig. 3 and Fig. 7 of Ref. 8). Finally, we also consider periodic SLs by taking $a=a'=b=32$ Å (see Fig. 1).

We focus on electron states close to the bottom of the conduction-band with $\mathbf{k}_{||}=0$. The envelope-functions for electron wavepackets satisfy the following quantum evolution equation

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \mathscr{H}(x)\Psi(x,t), \tag{1}$$

x being the growth direction. The time-independent Hamiltonian $\mathscr{H}(x)$ can be obtained within the one-band effective-mass framework as

$$\mathscr{H}(x) = -\frac{\hbar^2}{2m^*}\frac{d^2}{dx^2} + V_{SL}(x) - eFx, \tag{2}$$

where V_{SL} is the SL potential under zero bias condition, as shown in Fig. 1.

Before considering the quantum dynamics of electronic wave packets, it will be useful to provide a brief discussion of the main features of eigenstates of the Hamiltonian (2) with $F=0$ for the three kind of SLs we are considering, namely periodic, random a random dimer. Electron states in periodic SLs spread uniformly over the whole SL (Bloch states) and the energy spectrum is composed by minibands and minigaps. With our chosen parameters there exists only one miniband below the barrier, ranging from 102 up to 177 meV. On the contrary, electron states in RSLs are completely localized, according to the Anderson model, and the localization length depends on the electron energy and on the degree of disorder, as observed by several authors.[6] Finally, DSLs are intermediate between periodic SLS and RSLs in the sense that localized electronic states coexist with a band of delocalized states.[7,8] In the absence of electric field, these extended states are characterized by a transmission probability very close to unity. Specifically, in a previous work[7] we have shown analytically that there exists a particular energy E_r, whose value depends only upon the layer thicknesses and therefore can be easily controlled from the outset, for which the so build DSL is perfectly transparent. For the present values of the layer thicknesses a, a' and b, the resonant energy is found to be $E_r=155$ meV and, therefore, it lies within the allowed miniband. What is most important, electron states with energy close to E_r also display very good transmission properties. From the perspective of quantum evolution, those states could lead to oscillatory phenomena similar to BOs as they spread over the whole DLS. However this is not the case, as will be discussed in detail later.

III. RESULTS AND DISCUSSIONS

We study the quantum dynamics of an initial Gaussian wavepacket

$$\Psi(x,0) = [2\pi\sigma^2]^{-1/4} \exp\left[\frac{ik_0x - (x-x_0)^2}{4\sigma^2}\right], \tag{3}$$

where the mean kinetic energy is $\langle E\rangle = \hbar^2k_0^2/2m^*$ and σ measures the width of the electron wavepacket. The solution of Eq. (1) is given by

$$\Psi(x,t) = \exp\left(\frac{-i}{\hbar}\mathscr{H}(x)t\right)\Psi(x,0). \tag{4}$$

The finite difference representation of the exponential[10]

$$\exp\left(\frac{-i}{\hbar}\mathscr{H}(x)\,\delta t\right) = \frac{1 - \dfrac{i}{2\hbar}\mathscr{H}(x)\,\delta t}{1 + \dfrac{i}{2\hbar}\mathscr{H}(x)\,\delta t} + \mathscr{O}[(\delta t)^3],$$

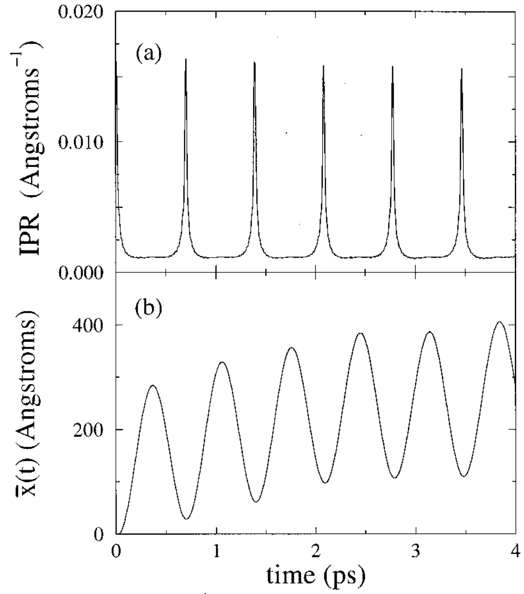

FIG. 2. Inverse participation ratio (a) and the position expectation value $\overline{x(t)}$ (b) as function of time for an initial Gaussian wave packet placed in a periodic SL, subject to an electric field $F=10$ kV/cm. The oscillation period is in excellent agreement with BOs period, $\tau_B=0.646$ ps.

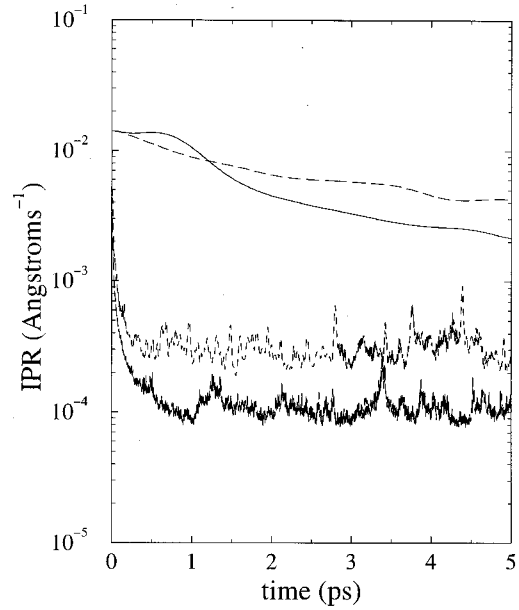

FIG. 3. Inverse participation ratio as function of time for an initial Gaussian wavepacket placed in a random SL (dashed line) and a random dimer SL with E_r lying within the miniband (solid line), subject to an electric field $F=10$ (lower lines) and $F=300$ kV/cm (upper lines). Note the absence of Bloch oscillations

where δt is the time step, brings a powerful and high-accurate numerical method. In addition, it ensures probability conservation,[5] which has been used at every time step as a first test of the accuracy of results. Boundary conditions read $\Psi(\infty,t)=\Psi(-\infty,t)=0$ and we have chosen the SL length sufficiently large to be sure than the wavepacket never comes close to the boundaries.

We use the position expectation value defined as

$$\overline{x}=\int_{-\infty}^{\infty}x|\Psi(x,t)|^2dx, \tag{5a}$$

and the time-dependent inverse participation ratio (IPR), defined as

$$\mathrm{IPR}(t)=\int_{-\infty}^{\infty}dx|\Psi(x,t)|^4, \tag{5b}$$

to get an estimation of the position and the degree of localization of electronic wavepackets. Much information can be extracted from the IPR, which can be viewed as a multifractal measure of the time-dependent probability density $|\Psi(x,t)|^2$. 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.

We study the influence of the electric field by using two values of the electric field, namely 10 and 300 kV/cm. Since the localization length of Stark-Wannier states is of the order of W/eF, W being the width of the allowed miniband, it is clear that the condition $W/eF\ll a+b$ ensures that the electric field is actually very large. On the contrary the condition $W/eF\gg a+b$ ensures that the electric field is very low. Upon taking $F=300$ kV/cm we obtain $W/eF=25$ Å, smaller than the period of the SL, and taking $F=10$ kV/cm we obtain $W/eF=750$ Å, much larger than the period of the SL. Then we can be sure that the fields selected represents the limits of high (300 kV/cm) and low voltages (10 kV/cm). We begin by studying the periodic SL as a way to verify that we are carrying out our computations correctly. Figure 2 presents the results for the position expectation value and for the IPR when the initial Gaussian wavepacket is located in the centermost quantum-well with $\sigma=20$ Å and mean kinetic energy $E=155$ meV with $F=10$ kV/cm. The IPR displays a periodic pattern with marked peaks at times $t_k=k\tau_B$, where k is any arbitrary, nonnegative integer and $\tau_B=0.646$ ps, whereas $\overline{x(t)}$ displays a clear oscillatory pattern. Notice that the value of the oscillation period is in excellent agreement with the theoretical prediction $\tau_B=2\pi\hbar/(eFd)$. It is also important to mention that the numerical value of the IPR at maxima is slightly larger than that obtained from (3) and (5), that is, $\mathrm{IPR}(0)=1/(2\sqrt{\pi}\sigma)=0.014$ Å^{-1}.

Results corresponding to both kinds of random SLs with the same initial condition as before are shown in Fig. 3. We have checked that our main results are independent of the particular disorder realization and of the initial position of the wave packet. First of all, we observe that BOs are completely absent in random SLs. This fact can be explained by the absence of translational invariance and, consequently, by scattering of electrons with the random potential, which destroys the quantum coherence required to observe such phenomenon. Except at very short times, when wave packets are so localized that electrons cannot see the long-range disorder, in both kind of random SLs the IPR presents strong fluctuations at small time scales, but it can be observed that its average value over larger times is roughly constant. Such small fluctuations depend on the particular realization of the disorder and on the initial position of the wavepacket. However, the mean value depends only on the electric field (the larger the electric field, the higher the IPR, see Fig. 3).

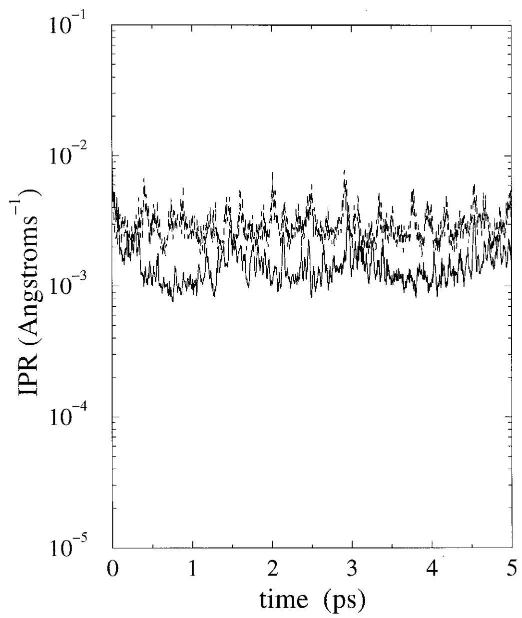

FIG. 4. Inverse participation ratio as function of time of an initial Gaussian wave packet placed in (a) a random SL (upper line) and (b) a random dimer SL with E_r out of the miniband (lower line), subject to an electric field $F=10$ kV/cm. Note the absence of Bloch oscillations.

So far, we have summarized the common features of states of both random SLs. It is now the moment to consider the main differences between RSLs and DSLs. The mean value of the IPR is smaller for DSLs, meaning that the wave-packet spreads over larger portions of the system. Thus, when the unperturbed $(F=0)$ SL supports extended states, the resulting dynamical localization under the action of the electric field is much *less* effective than in purely random SLs. It is therefore reasonable to expect that the transport properties of the two systems will also exhibit specific features: For instance, dc conductivity has to be much larger in the DSL than in the RSL, due to the increased tunneling probability between neighboring localized states. To get further support of our claim we have also studied DSLs without extended states at flat band. This we achieve by placing the resonant energy out of the allowed miniband. Thus, taking $a'=56$ Å and the same values of a and b as before, the resonant energy now is $E_r=78$ meV. Figure 4 shows that the difference of the IPR of both RSL and DSL is much smaller.

A better understanding of this result *at low field* is reached if one considers that the initially localized wave-packet is a combination of plane waves in a continuous band. Since the energy spectrum of the DSL presents a band of extended states, the SL 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 wave packet. The observation of this behavior, as we have reported, is therefore a clear consequence of the fact that the unperturbed SL supports extended states. Finally, the absence of Bloch oscillations in DSLs 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 DSL, where electronic states increment its phase by a factor of π whenever they pass over a dimer quantum-well,[7] and the position of each dimer quantum-well is in any case a random variable.

IV. CONCLUSION

We have studied quantum dynamics of wave packets driven by an applied external field in periodic, random, and random dimer SLs. The spatial degree of localization of wave packets initially localized has been properly described by means of the time-dependent IPR. In periodic SLs we have confirmed the existence of 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 random SLs 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 random dimer SLs than in purely random ones, if the unperturbed $(F=0)$ SL support extended states. Therefore, the resonant tunneling effects causing delocalization plays an important role, even in the presence of low applied field.

The results we have reported in this work provide another piece of evidence supporting the true extended nature of states near the resonant energy in the DSL. From plots in Figs. 2 and 3, one can observe that the value of the IPR for the DSL is about the minimum of the Bloch oscillations of the periodic lattice. This is to be compared with the purely random case, whose IPR is close to half of the IPR of the periodic lattice. It is then clear that dynamical localization effects in the DSL 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 DSL under electric fields will also be close to those of periodic SLs, this being an experimentally verifiable, qualitative prediction.

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