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Interband Tunneling and Wannier–Stark States in Superlattices with Complex Primitive Cell

Yu. Yu. Romanova, E. V. Demidov, and Yu. A. Romanov

Institute of the Physics of Microstructures, Russian Academy of Sciences, Nizhni Novgorod, 603950 Russia
e-mail: demidov@ipm.sci-nnov.ru

Abstract—Interband electron tunneling and Wannier-Stark states in superlattices with a complex primitive cell were investigated. The method developed in this study allows an arbitrary number of minibands to be considered.

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INTRODUCTION

Earlier [1–3], we showed that semiconductor superlattices (SLs) with a simple primitive cell and the sine dispersion law of electron minibands are not too promising for the creation of terahertz radiation sources on the Bloch oscillations (BO) of an electron. We believe that terahertz sources with a radiation frequency controlled by an electric field can be created on a SL with a complex primitive cell [4]. The band structure of such SLs can contain two or three low-lying close minibands (energy gap $\Delta_g \approx 1 - 10$ meV) considerably far apart (> 100 meV) from others. Such SLs are a new object of independent interest as well.

We investigated SL properties with three types of primitive cells: (a) simple symmetric, containing a single quantum well; (b) complex symmetric; and (c) and (d) complex asymmetrical, containing double quantum wells. Examples of their use are periodic $Al_xGa_{1-x}As/Al_yGa_{1-y}As$ heterostructures with two-layer (a) and four-layer (b, c, d) primitive cells. Their distinctive features are as follow: SL-A has a rather wide (260 meV) first forbidden miniband comparable to the others and two rather narrow allowed ones (27 and 100 meV). SL-B, C, and D are narrow-miniband with two close ($\Delta_g \approx$ 15, 7 and 18 meV) minibands considerably far apart from others. Symmetric SL-B and asymmetrical SL-D have similar miniband spectra. In asymmetrical SL-C, the widths of the first two allowed minibands ($\Delta_{1,2} \approx$ 40 and 70 meV) are considerably larger than the energy gap between them (7 meV). In SL-B and SL-D, the values of these three energies are on the same order of magnitude. SL asymmetry is manifested in the dependence of the tunneling probability on the field direction, the width of the forbidden miniband, and the character of the time evolution of the electron's interminiband transitions.

EXPERIMENTAL

The probabilities of interminiband tunneling and the energy levels of the electron in static electric field E were determined by the Schrödinger equation in the quasi-momentum representation (see, e.g., [5]):

$$\left[\varepsilon_n(k,E) - ieE\frac{\partial}{\partial k}\right]\Psi_n(k,t) - eE\sum_{n'\neq n} x_{nn'}(k)\Psi_{n'}(k,t) = i\hbar\frac{\partial}{\partial t}\Psi_n(k,t), \quad (1)$$

where $\varepsilon_n(k,E) = \varepsilon_n(k) - eEx_{nn}(k)$ is the dispersion law of the nth miniband renormalized by the electric field, $x_{nn'}(k)$ are the matrix elements of the coordinate, and $\Psi_n(k,t)$ is the component of wave function in the nth miniband. By substituting

$$\psi_n(k,t) = \exp\left\{-i\frac{d}{\hbar\Omega_c}\int_{k_i}^{k}\varepsilon_n(k,E)dk\right\}C_n(k)\delta\left(k - k_i - \frac{\Omega_c}{d}(t-t_0)\right),$$

(where $\Omega_c = eEd/\hbar$ is the Wannier–Stark frequency) in Eq. (1), we obtain the basic system of equations for $C_n(k)$:

$$\frac{dC_n(k)}{dk} - i\sum_{n'\neq n}\exp\left\{-i\frac{d}{\hbar\Omega_C}\int_{k_i}^{k}[\varepsilon_{n'}(k,E) - \varepsilon_n(k,E)]dk\right\} \times x_{nn'}(k)C_{n'}(k) = 0 \quad (2)$$

with initial condition $C_n(k_i) = C_n^{(0)}$. Let us introduce a unitary matrix $M_{nn'}(k_i,k_f,E)$ connecting the probabilities of finding the electron in the nth miniband at its passage the quasi-momentum interval (k_i,k_f):

$$C_n(k_f) = \sum_{n'} M_{nn'}(k_i,k_f,E)C_{n'}(k_i). \quad (3)$$

In the two-miniband approach, we have

$$\hat{M}(k_i,k_f,E)=\begin{pmatrix}\alpha(k_i,k_f,E) & \beta(k_i,k_f,E)\\ \gamma(k_i,k_f,E) & \delta(k_i,k_f,E)\end{pmatrix}, \qquad (4)$$

where $\alpha(k_i,k_f,E)\equiv D(k_i,k_f,E)\exp(i\varphi(k_i,k_f,E))$, and $\delta(k_i,k_f,E)$, $\beta(k_i,k_f,E)\equiv R(k_i,k_f,E)\exp(i\vartheta(k_i,k_f,E))$, and $\gamma(k_i, k_f, E)$ are the complex coefficients of the intraminiband passage and interminiband tunneling, respectively. Since $|\alpha(k_i,k_f,E)|^2 + |\beta(k_i,k_f,E)|^2 = 1$, $\alpha(k_i,k_f,E)=\delta^*(k_i,k_f,E)$, $\beta(k_i,k_f,E)=-\gamma^*(k_i,k_f,E)$, in the general case the $M(k_i,k_f,E)$ matrix contains three independent real functions. To find it, it is sufficient to solve equations (2) for a single K_0 period of the inverse SL (quasi-momentum interval $(k_i, k_i + K_0)$ with fixed $k_i$initial conditions $C_1(k_i) = 1$, $C_2(k_i) = 0$). In this case, we have $C_1(k_f)=\alpha(k_i,k_f,E)$, $C_2(k_f)=\gamma(k_i,k_f,E)$.

The M matrix determines the Wannier–Stark states of the electron as well [6]:

$$\varepsilon\to\varepsilon_n^{(1,2)}=\frac{\bar{\varepsilon}_1+\bar{\varepsilon}_2-eE(\bar{x}_1+\bar{x}_2)}{2}+\hbar\Omega_c\left(n\mp\frac{\phi(E)}{2\pi}\right), \qquad (5)$$
$$n=0,\pm1,\pm2,\ldots$$

$$\phi(E)=\arccos\left[D(k_i,k_i+K_0,E)\times\cos\left(\varphi(k_i,k_i+K_0,E)+\pi\frac{\bar{\Delta}_{21}(E)}{\hbar\Omega_c}\right)\right] \qquad (6)$$
$$0<\phi(E)<\pi,$$

where $\bar{\Delta}_{21}(E)\equiv\bar{\Delta}_{21}-eE(\bar{x}_2-\bar{x}_1)$, $\bar{\Delta}_{21}=\bar{\varepsilon}_2-\bar{\varepsilon}_1$, $\bar{\varepsilon}_n$ and $\bar{x}_n\equiv\bar{x}_{nn}$ are energies and diagonal matrix elements of the coordinate averaged on the Brillouin miniband. Relations (5) and (6) differ from those obtained in [6] by the presence of the average diagonal matrix elements of the coordinate and the φ phase, which is of fundamental importance even in weak electric fields (see below).

At $\alpha(k_i,k_i+K_0,E)=1$, the spectrum of the electron energies consists of two independent one-miniband Wannier–Stark ladders:

$$\varepsilon\to\varepsilon_\nu^{(1,2)}=\varepsilon_0^{(1,2)}+\nu\hbar\Omega_c,\quad \nu=0,\pm1,\pm2,\ldots,$$
$$\varepsilon_0^{(n)}=eE(x_o-\bar{x}_{nn})+\bar{\varepsilon}_n,\quad n=1,2, \qquad (7)$$

shifted with respect to each other by $\bar{\Delta}_{21}(E)$. From Eq. (7), one can see that the diagonal matrix elements of the $x_{nn}(k)$ coordinate usually not taken into account lead to an additional shift of the Wannier–Stark ladders, depending on the electric field. The sign of this shift changes with the change of the field direction, resulting in asymmetry of the electrical characteristics of the asymmetrical SLs.

In the E_n fields determined by the equidistant values

$$E_n^{-1}=\frac{e[nd+(\bar{x}_{22}-\bar{x}_{11})\mathrm{sign}(E_n)]}{\bar{\Delta}_{21}},\quad n=0,\pm1,\pm2,\ldots, \qquad (8)$$

the levels of different one-miniband Wannier–Stark ladders cross in pairs. The $[nd+(\bar{x}_{22}-\bar{x}_{11})\mathrm{sign}(E_n)]$ value is the distance between the centers of the one-miniband wave functions of the Wannier–Stark states that are in resonance with one another.

The interminiband tunneling of the electron blends the Wannier–Stark states of different minibands and removes the degeneracy in fields (8), and there is an anticrossing of levels. In the general case, the distance between the nearest steps of the double Wannier–Stark ladder is

$$\delta\varepsilon(E)=\frac{\hbar\Omega_c}{\pi}\min(\phi(E),\ \pi-\phi(E)). \qquad (9)$$

It is important to note that tunneling probability $R(k_i,k_i+K_0,E)$, just like that of passage $D(k_i,k_i+K_0,E)$, strongly depends on the initial value of quasi-momentum $\hbar k_i$. This was noted, in particular, in [7]. The $\hbar k_i$ phase strongly depends on $\varphi(k_i,k_i+K_0,E)$ as well. As a result, $\phi(E)$ phase (6), which determines Wannier–Stark levels (7) and their splitting (9), does not (as expected) depend on the initial quasi-momentum. Its choice is therefore dictated only by the convenience of the calculation. In the two-miniband model we consider, it is convenient to assume $k_i=0$, since in this case the functions $D(k_i,k_i+K_0,E)$ and $\varphi(k_i,k_i+K_0,E)$ are the smoothest functions of the electric field.

WEAK ELECTRIC FIELDS AND “WIDE” ALLOWED MINIBANDS

A situation like this arises in SL-C. In this case, tunneling occurs only in the vicinity of the extreme points of approach of minibands $k_0=\pm\pi/d$. The tunneling probability can therefore be easily found from the analytical properties of the dispersion law of the minibands close to k_0 [8]. Using the standard calculations, we obtain

$$R^2(0,K_0,E)=\exp\left(-\frac{\pi(\mu)^{1/2}\Delta_g^{3/2}}{2eE\hbar}\Phi(4\alpha\mu^2)\right),$$
$$\Phi(\xi)\approx1+\frac{3}{32}\xi+\frac{35}{1024}\xi^2, \qquad (10)$$

where $\mu^{-1}=|m_1^{-1}(k_0)|+|m_2^{-1}(k_0)|$, $\alpha=|m_{12}^{-1}(k_0)|^2+\frac{1}{4}(m_{22}^{-1}(k_0)-m_{11}^{-1}(k_0))^2$, $m_{1,2}(k_0)$ are the effective electron masses at the point of miniband approach, and $m_{nn'}^{-1}(k)$ are the matrix elements of inhomogeneous effective electron mass forming the SL material.

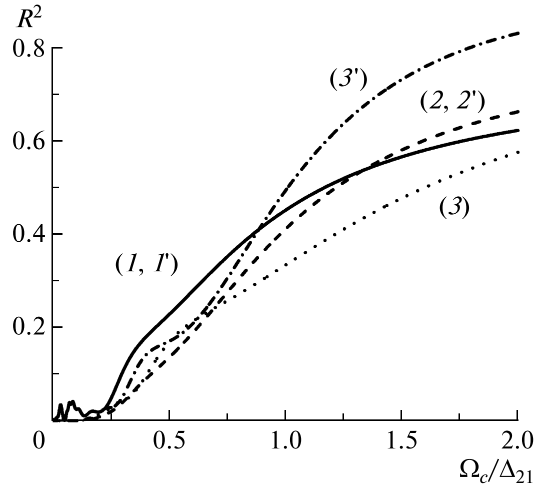

Fig. 1. Probability of tunneling $R^2(0, K_0, E)$ for three types of SL: (*1*) *1*', SL-A'; (*2*) *2*', SL-B; (*3*) *3*', SL-D. The apostrophe denotes negative field direction.

Equation (10) differs from the conventional equation for homogeneous semiconductors [8–10] by the presence of the $\Phi\left(4\alpha\mu^2\right)$ multiplier in the exponent index. Note that probability (10), determined only by the dispersion of minibands, does not take into account the symmetry of the SL's primitive cells.

Due to the weak tunneling, the Wannier–Stark states of the interacting and noninteracting minibands differ from each other only close to the crossing of the one-miniband Wannier–Stark levels. In particular, at the anticrossing we have $\delta\varepsilon(E) \approx \hbar\Omega_c R^2(0, K_0, E)/\pi$.

WEAK ELECTRIC FIELDS AND NARROW ALLOWED MINIBANDS

If the allowed minibands are narrow ($\Delta_1 + \Delta_2 \ll \bar{\Delta}_{21}$), even weak tunneling takes place in the wide region of the Brillouin miniband. A similar situation arises in SL-B and SL-D. In this case, it is more correct to use perturbation theory instead of (10). Assuming $C_1(k) = 1$ in (2) and, for simplicity, taking $x_{21}(k) = \bar{x}_{21} = \text{constt}$ and $\varepsilon_2(k, E) - \varepsilon_1(k, E) = \bar{\Delta}_{21}(E) = \text{constt}$, we obtain

$$R^2(0, K_0, E) \sim \left(\frac{\hbar\Omega_C}{\bar{\Delta}_{21}(E)}\right)^2 \frac{|\bar{x}_{21}|^2}{d^2} \sin^2\left(\pi\frac{\bar{\Delta}_{21}(E)}{\hbar\Omega_C}\right). \quad (11)$$

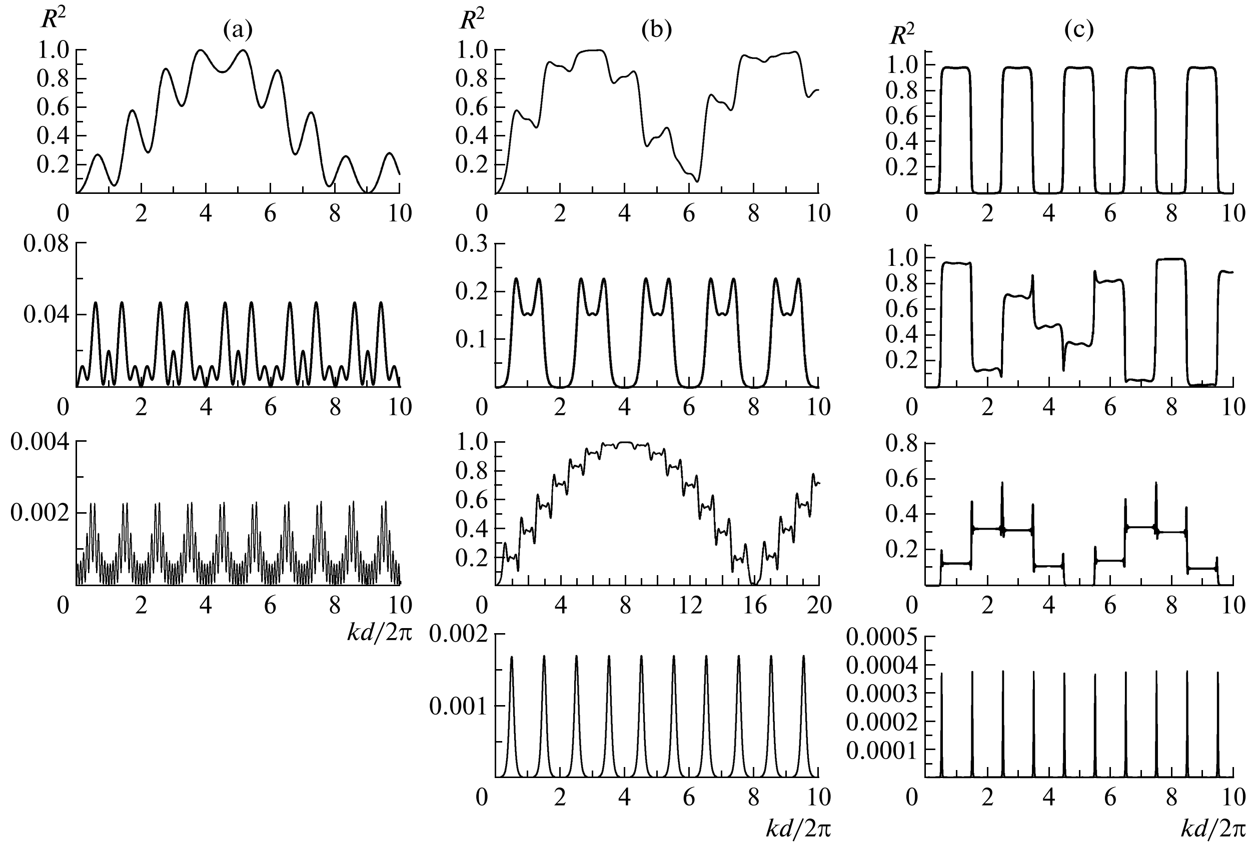

Fig. 2. Time evolutions of the probability of finding the electron in the second miniband upon its motion from initial state $k_i = 0$ of the first miniband in the field (from bottom to top): (a) $\hbar\Omega_c/\bar{\Delta}_{21} = 0.1, 0.4, 1.16$ in SL-A; (b) $\hbar\Omega_c/\bar{\Delta}_{21} = 0.05, 0.3, 0.5, 0.7$ in SL-B; and (c) $\hbar\Omega_c/\bar{\Delta}_{21} = 0.0005, 0.02, 0.6, 0.85$ in SL-C.

One can see that in fields (8), the probability of interminiband tunneling when the electron passes through the Brillouin miniband $(0, K_0)$ is zero. This does not, however, mean that tunneling and interaction between minibands are completely absent in such fields, since interminiband transitions upon the motion of the electron inside the Brillouin miniband occur with nonzero probability:

$$R^2(0,k_f,E) \sim \left(\frac{\hbar\Omega_C}{\bar{\Delta}_{21}(E)}\right)^2 \frac{|\bar{x}_{21}|^2}{d^2} \sin^2\left(\frac{\bar{\Delta}_{21}(E)}{2\hbar\Omega_C} k(t) d\right) \sim \sin^2\left(\frac{\bar{\Delta}_{21}(E)}{2\hbar} t\right). \quad (12)$$

The probability of finding the electron in the second miniband fluctuates with the interminiband frequency $\omega = \bar{\Delta}_{21}(E)/\hbar$, depending on the value and direction of the field. This corresponds to the oscillations between the Wannier–Stark states centered in the same primitive cell. According to (6) and (9), the splitting of the Wannier–Stark steps upon such anticrossing $D(0, K_0, E) = 1$, $R(0, K_0, E) = 0$:

$$\delta\varepsilon(E) = \frac{\hbar\Omega_c}{\pi} \min(\varphi(0, K_0, E),\ \ \pi - \varphi(0, K_0, E)). \quad (13)$$

The fluctuations in the probabilities of interminiband electron tunneling depending on the field have a general character (see below results of the numerical calculation). Fluctuations of a similar type were apparently found for the first time in [7], in a numerical study of the dynamics of ultracold atoms in optical lattices. They are not discussed there, however.

ARBITRARY ELECTRIC FIELDS

Our studies were performed by numerically solving equations (2). Figures 1 and 2 show the results. One can see that the classical formula of the (10) type for CP-A, -B, and -D does not hold even in weak fields, due to considerable tunneling of the electron in all of the Brillouin miniband and its value being finite. In SL-A, the fluctuations of the probability of tunneling in weak fields are qualitatively well described by formula (11). In other SLs, these oscillations are less expressed, since the widths of their allowed minibands are on the order of or larger than those of the forbidden miniband. In asymmetrical SL-C and -D, the probability of tunneling depends on the direction of the field. Such dependence should also exist in natural semiconductors without a center of symmetry.

The probabilities of electron tunneling depend strongly and in a fluctuating manner on the initial and final values of the electron's quasi-momentum. Similar fluctuations also exist in natural semiconductors, e.g., upon intersubband tunneling of holes in a complex valence band [11, 12]. Figure 2 shows the corresponding probabilities upon repeated passage of the Brillouin miniband by an electron. In the general case, there are three frequency fluctuations (and combination frequencies that accurately correspond to the transitions between steps of the double Wannier–Stark ladder): interminiband, $\sim\bar{\Delta}_{21}/\hbar$, Bloch Ω_c, and the lowest frequency (9). (In literature [13, 14], the fluctuations with the lowest frequency (9) are sometimes called Rabi fluctuations.) The narrow peaks on the curves (Fig. 2) are due to the partial return of the electron to the first miniband from the second upon its passage from the region of their maximum approach. An interesting feature is the character of tunneling in CP-C at field $\hbar\Omega_c/\bar{\Delta}_{21} = 0.85$. In this case, the probability of finding the electron in the second miniband oscillates with frequency $\Omega_R = \Omega_C/2$. This occurs due to the "fast" passage of the regions of effective tunneling (miniband approach) by the electron when it does not manage to return to the initial miniband due to the lag effect. In very strong fields, $\hbar\Omega_c/\bar{\Delta}_{21}(E) > 1$, the electron is strongly localized in space and thus undergoes interminiband transitions only within the limits of a single primitive cell.

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