Antiresonant hopping conductance and negative magnetoresistance in quantum-box superlattices

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Electric current in a one-dimensional chain of quantum boxes is characterized by a set of zero minima (antiresonances) due to the momentum selection rule for the interaction of acoustic phonons with Wannier-Stark localized electrons or due to the folded phonon gaps. Antiresonances manifest also in the conduction of superlattices in the presence of an external source of phonons. Negative magnetoresistance of superlattices in high electric fields is predicted. We also clarify general questions of boundary conditions in the hopping regime.

I. INTRODUCTION

Transport in quantum microstructures (QMS) manifests such fundamental phenomena as quantum interference and electron localization. QMS can be designed to achieve arbitrary spectra of electronic states and are flexible to geometrical confinement providing alternative windows for technological innovation. In particular, transport[1–4] and magnetotransport[5,7,6] in superlattices (SL) have been the subject of intense investigations. With magnetic field perpendicular to the layers SL realize a high degree of confinement of the electron gas and are well suited for simulating transport in quantum-box superlattice (QBSL) recently proposed to control phonon scattering.[8,9] In the present article, we investigate the conductance mechanisms in QBSL and predict a set of minima (antiresonances) in the current-voltage characteristics, due to the momentum selection rule for the interaction of acoustic phonons with the Wannier-Stark (WS) localized electrons. We also discuss the onset of antiresonances, due to the gaps in folded phonon spectrum and analyze resonant hopping of electrons between localized states, due to elastic and optical phonon scattering. We find that owing to the electron localization in high electric field the longitudinal magnetoresistance is negative over substantial range of magnetic field.

The effects we study are the manifestation of quantum confinement. We suggest that not only electron, but also phonon confinement can be observed in conductance experiments. In addition, we discuss critical issues on the importance of boundary conditions imposed on the electron chemical potential in the description of the nonequilibrium hopping conduction in QMS.

II. ELECTRONIC MODEL

In one-dimensional (1D) QBSL the electron motion is modulated by the periodic potential in the z direction of the chain and is strictly confined in the xy plane (Fig. 1). Consider the Wannier representation for the electron wave functions of QBSL,

$$\psi_{nmq\nu} = \Lambda_{nm}\left(x,y\right) u_q\left(z-\nu d\right), \tag{1}$$

where Λ_{nm} is the transverse wave function, m and n are the integer numbers, d is the period of QBSL, and $u_q\left(z-\nu d\right)$ is the wave function of an eigenstate E_q in a separate quantum well ν. The Hamiltonian in the presence of the uniform electric field $\mathbf{F} \parallel z$ is

$$\mathcal{H}_0 = \left(E_q + \epsilon_{nm} - eFd\nu\right)\delta_{\nu\nu'} + \Delta_q\left(\delta_{\nu,\nu'+1} + \delta_{\nu,\nu'-1}\right), \tag{2}$$

Δ_q is the tunneling matrix element (we consider only the tunneling between neighboring QB) and ϵ_{nm} is the transverse energy. Without essential loss of generality we discuss mostly the states corresponding to the lowest longitudinal mode. In this way, we set $E_1 = 0$ and omit the index q. In analogy with conventional crystals,[10] the Hamiltonian (2) in zero electric field results in a band spectrum with a width 4Δ. If the potential drop over the period of a structure, eFd, exceeds the collisional broadening of the electron levels $\hbar/\tau$, the electronic subband splits into WS ladder of localized states. The corresponding eigenvalues are

$$E_{nm\alpha} = \epsilon_{nm} - eFd\alpha, \tag{3}$$

and the wave functions are given by

$$\Psi_{nm\alpha} = \sum_{\nu} J_{\nu-\alpha}\psi_{nm\nu}, \tag{4}$$

where $J_k(2\Delta/eFd)$ are the Bessel functions of order k (Ref. 11) and α is the Stark diagonal representation index. Therefore, the band conduction breaks down and

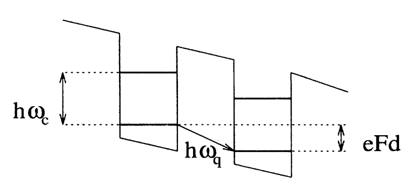

FIG. 1. Schematic QBSL with WS localization in the magnetic-field confinement.

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electrons move in the z direction only by hopping from one well to the other, due to scattering; direct tunneling between the WS states for $q = 1$ manifests in the electron spectrum and is taken into account in Eqs. (3,4). As for tunneling between states $q = 1$ and the WS states of higher minibands,[4] one can diagonalize the Hamiltonian for several minibands in electric field and, thus, include the effect of direct interband tunneling in the q component wave functions (see Ref. 12). Then only the scattering-assisted hopping results in a current.

There is an essential difference between conventional SL and QBSL. SL electrons are characterized by a continuous spectrum in the direction transverse to its axis and the energy conservation law can always be satisfied for any scattering process. For instance, in elastic scattering by impurities, the energy conservation is the result of an interchange betweeen longitudinal and transverse energies,[4,13] whereas phonon-assisted hopping is accompanied by a partial energy transfer to the lattice. On the other hand, in QBSL the transverse degree of freedom is characterized by a discrete spectrum ϵ_{mn} and electron hopping exists only when the transverse energy spacing is equal to the separation between the WS levels or differs from the latter by the phonon energy. It follows then that elastic and optical phonon scattering should manifest in a number of resonant peaks in the current. We note that elastic and optic phonon-assisted resonances are known to influence electron transport in double quantum well structures with transverse 2D continuous spectra.[14] However, the only background mechanism for conduction in SL is scattering by acoustic phonons. We are going to demonstrate that acoustic-phonon-assisted hopping in QBSL is characterized by a set of antiresonant minima. These minima are related to the quasi-one-dimensional character of the phonon propagation in QBSL, which dramatically affects both the phonon spectrum and the electron-phonon interaction.

III. TRANSPORT MODEL

In this section, we discuss the electric current in QBSL as a hopping current between the Wannier-Stark localized states, which is due to electron scattering of phonons, impurities, and various irregularities of superlattice structure. We describe the hopping conductance in QBSL, by the following transparent formula:

$$j_z = e \sum_{\alpha,\alpha',N,N'} \left(z_{\alpha,N} - z_{\alpha',N'}\right) W^{\alpha,\alpha'}_{N,N'}, \tag{5}$$

where $z_{\alpha,N} - z_{\alpha',N'}$ is the electron displacement (the hopping length) upon the scattering $(\alpha, N \rightarrow \alpha', N')$, N stands for the set of indices describing the transverse states, $W^{\alpha,\alpha'}_{N,N'}$ is the scattering probability. For elastic processes (due to impurities, surface or interface roughness), the scattering probability is

$$W^{\alpha,\alpha'}_{N,N'} = |V^{\alpha,\alpha'}_{N,N'}|^2 \delta(E_{\alpha N} - E_{\alpha' N'})(f_{\alpha N} - f_{\alpha' N'}), \tag{6}$$

where $V^{\alpha\alpha'}_{NN'}$ is the scattering matrix element ($|V|^2$ accounts for the number of defects and their correlation), $f_{\alpha N}$ is the nonequilibrium electron distribution function. For phonon-assisted hopping,

$$W^{\alpha\alpha'}_{NN'} = \sum_{\mathbf{q}_\perp q_z} |C^{\alpha,\alpha'}_{N,N'}|^2 \delta(E_{\alpha N} - E_{\alpha' N'} + \hbar\omega_q)\left[(f_{\alpha N} - f_{\alpha' N'})N_q - f_{\alpha' N'}(1 - f_{\alpha N})\right], \tag{7}$$

$C^{\alpha,\alpha'}_{N,N'}$ is the electron-phonon scattering amplitude, ω_q and N_q are the phonon frequency and the occupation number. The phonon occupation number, in a general case, is a nonequilibrium quantity and has to be determined by rate equation. Equation (7) accounts for spontaneous emission, emission, and absorption of phonons.

As far as we know, a formula similar to Eq. (5) was first derived by Luttinger,[15] and later on this approach was applied to conventional hopping in crystals[16] and conductance of SL.[3,17] However, it turns out that the derivation and applicability of Eq. (5) for hopping between localized states in QMS are nontrivial. In this paper, apart from the application of Eq. (5) to the QBSL, we would like to emphasize critical features regarding this formula and hopping regime in microdevices.

One important observation is that the nonequilibrium character of the system in the hopping regime results only from the boundary conditions imposed on the electron distribution function. The nonequilibrium state of phonons in our case plays a minor role and in what follows, we use the Planck functions for phonon distribution. Now, if we interchange $(\alpha N) \Leftrightarrow (\alpha' N')$ in the second term between brackets of Eq. (5), we obtain

$$\begin{aligned} j_z &= e \sum_{\alpha N} z_{\alpha,N} \sum_{\alpha' N'} \left(W^{\alpha,\alpha'}_{N,N'} - W^{\alpha'\alpha}_{N'N}\right) \\ &= e \sum_{\alpha N} z_{\alpha,N} I_{\text{coll}}(f_{\alpha N}), \end{aligned} \tag{8}$$

where I_{coll} is the collisional integral, which determines the evolution of the electron distribution function in the rate equation,

$$\frac{\partial f_{\alpha N}}{\partial t} = I_{\text{coll}}(f_{\alpha N}). \tag{9}$$

At first glance, we have absolutely surprising results: In steady state, all the electron processes form a closed cycle, the collisional integral vanishes, and the current vanishes also. The solution of this puzzle is the following: The nonequilibrium factor in our system is the electric field. However, in Eq. (9), it determines only the equilibrium parameters, namely, the energies and wave functions of the localized states. In order to calculate the current, we are to take into account the difference of the chemical potentials between the left and right contact as the result of the applied voltage. Correspondingly, the electron distribution function in the contacts is determined by the boundary conditions, i.e., by the chemical potential, rather than by Eq. (9).

If we assume, that the distribution of electric field in SL or QBSL is uniform, the potential drop over any period is the same, and the boundary conditions may be imposed to one cell of the structure. Then, in the simplest case, there is no need to solve Eq. (9), since the electron distribution function, which determines the hopping current (8), is given by the boundary conditions for the nearest neighbor quantum wells. These electron distribution functions, in the mean energy gain approximation, are taken in equilibrium with the chemical potential varying from one cell to another and the electron concentration being kept constant. Actually this method was conventionally used for hopping conductance.[16,3,17] In general, distribution of the field may be nonuniform. Then a self-consistent calculation of the electron distribution functions with boundary conditions at contacts and current given by (8,9) is required. We notice that the self-consistent procedure may be important even for uniform electric field when heating is essential.

Evaluating the current as due to hopping processes, we explicitly take into account the perfect structure of a system, include direct tunneling between wells in a spectrum and wave functions of localized states and consider impurities, fluctuations, and inelastic scattering as a perturbation. This procedure in many cases may be more adequate for the description of microstructures than the calculation of the current due to direct tunneling. It is especially important when the electric field in a device cannot be considered as a perturbation, for instance, in the regime of the negative differential conductance.

IV. ANTIRESONANCES AND RESONANCES IN HOPPING TRANSPORT

We use now Eq. (5) for the hopping current in QBSL and demonstrate its peculiar features. The scattering matrix element in the basis of eigenfunctions (4) has the form

$$C^{\alpha,\alpha'}_{N,N'} = V_{\mathbf{q}} J_{\nu-\alpha} J_{\nu-\alpha'} \left\langle N | e^{iq_\perp r_\perp} | N' \right\rangle \left\langle \nu | e^{iq_z z} | \nu \right\rangle , \quad (10)$$

where $\mathbf{q}$ is the transferred momentum. The last multiplier in (11) is the matrix element, which is diagonal in Wannier index; within Wannier basis (1) only, the intrawell scattering[18] is taken into account. If we assume that the chain structure is invariant under the coordinate inversion transformation $z \leftrightarrow -z$, then the matrix element of the Fourier component is given by[19]

$$\left\langle \nu | e^{iq_z z} | \nu \right\rangle = e^{iq_z d\nu}, \quad (11)$$

and the summation over ν (Ref. 21) in (11) leads to

$$|C^{\alpha,\alpha'}_{N,N'}|^2 = |V_{\mathbf{q}}|^2 | \left\langle N | e^{iq_\perp r_\perp} | N' \right\rangle |^2 \times J^2_{\alpha-\alpha'} \left(\frac{4\Delta}{eFd} \sin \frac{q_z d}{2} \right) . \quad (12)$$

We see that phonons with $q_z = \frac{2\pi n}{d}$ result in vanishing electron transition between different wells α [$J_{\alpha-\alpha'}(0) = 0$ at $\alpha \neq \alpha'$]. Assume first that the dispersion of acoustical phonons is described by a constant speed of sound s and that phonons propagate in the z direction. Then the energy conservation law given by δ function in Eq. (7) determines q_z. At electric fields $F = nF_0$, n is the integer number, and

$$F_0 = 2\pi\hbar s/ed^2, \quad (13)$$

phonons are ineffective. The scattering probability (12) and the hopping current (5) vanish. This effect takes its origin in Bragg reflection: the transfer of phonon momentum equal to the momentum of reciprocal lattice does not change the longitudinal electron state. We have a specific momentum selection rule for the scattering of the WS localized electrons. The difference between SL with the continuous transverse spectrum and QBSL with the discrete one is very important here, and only the discrete spectrum results in a single value of q_z. If there are no other acoustic phonons in the structure, this means the absence of the background current and the appearance of zero minima in the conductance, i.e., antiresonant effect. (The accuracy of this zero is determined, as usual, by the width of levels and the accuracy of δ function approximation.) Let us notice, that there are also additional zero minima of the scattering probability [Eq. (12)] when the argument of the Bessel function $J_k(x)$, $k \neq 0$ coincides with one of its roots $x_i \neq 0$. However, in contrast to the momentum selection rule mentioned above, these minima are unlikely to be observed: if we consider the transitions between next-nearest neighbor wells,[3] the total current will be determined by Bessel functions of different orders. Correspondingly, the superposition of these transitions leads to nonzero current.

Let us consider the possibility for observation of the momentum selection rule. This effect is the result of the 1D propagation of phonons. It will be observable experimentally if either the density of states of 1D phonons is essential or the transverse scattering form factor given by

$$F(\mathbf{q}_\perp) = | \left\langle N | e^{iq_\perp r_\perp} | N' \right\rangle |^2 \quad (14)$$

has a sharp maximum at $\mathbf{q}_\perp = 0$. For instance, such a maximum is realized in SL in magnetic field, when the transverse modes are Landau levels. At the moment, this experimental geometry is the best way to simulate a quantum-box superlattice. In strong electric field, when the Wannier-Stark quantization is present, the 1D array of quantum boxes with magnetic- and electric-field-controlled discrete spectra are realized. If the energy difference between the initial and final WS levels satisfies the antiresonant condition, electron hopping occurs between partially filled Landau levels with the same quantum number and the form factor is

$$F(\mathbf{q}_\perp) \propto e^{-l_B^2 q_\perp^2}, \quad (15)$$

where l_B is the magnetic length. Consequently, the energy conservation law takes the form $eFd \simeq \hbar s q_z$, if the inequality

$$eFd/\hbar s \gg q_\perp \sim l_B^{-1} \quad (16)$$

or

$$(eFd)^2/ms^2 \gg \hbar\omega_c, \quad (17)$$

where ω_c is the cyclotron frequency, is satisfied. One sees that in high electric fields, only the q_z component of the phonon momentum is relevant and therefore hopping current reaches a minimum. We note that transitions to the next nearest QB states with the same number of Landau level are also in antiresonance. However, transitions between different Landau levels result in finite current. Its amplitude is much weaker than the one of the current, due to the transition to the nearest box, because phonon emission at low temperatures and $eFd < \hbar\omega_c$ requires a large hopping distance. Let us notice that one can also eliminate the transverse component of the phonon momentum by using an external source of phonons with a given direction of propagation. If the signal related to external phonons is extracted from the total current, the zero minima at the certain voltages can be found. In Fig. 2, we present the current calculated taking into account the transitions between nearest QB for the case of magnetically confined QBSL [Fig. 2(a)] and in the case of an external source of phonons[22] [Fig. 2(b)]. The two figures are remarkably similar.

The range of electric fields $eFd \gg \hbar/\tau$ turns out to be very interesting because of the negative magnetoresistance [Fig. 2(a)]. The physical origin of this effect in our case is that in the electric-field-induced localization regime, the current is proportional to the scattering probability, in contrast to Drude current at small electric fields, which is proportional to the scattering time and inverse proportional to scattering probability. The latter in the case of transition between zero Landau levels is proportional to the "density of states:"

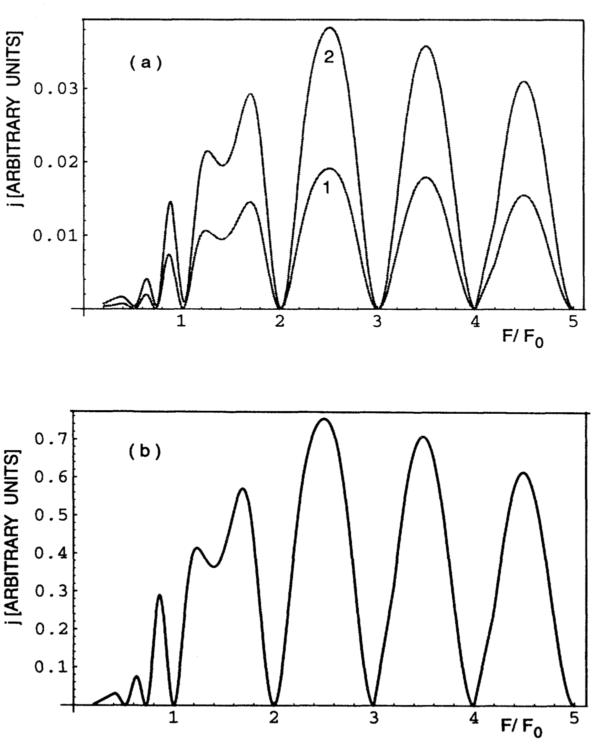

FIG. 2. (a) Hopping current in the conditions of the partial occupation of the zeroth Landau level. $F_0 = 2.17$ kV/cm. Curve 1: $B = 6$ T; Curve 2: $B = 12$ T. (b) Hopping current induced by an external source of phonons.

$$\int d\mathbf{q}_\perp e^{-l_B^2 q_\perp^2} = 2\pi/l_B^2, \tag{18}$$

and increases with magnetic field. Correspondingly, the current in the Wannier-Stark localization regime also increases and we see [Fig. 2(a)] that the bigger the magnetic field the bigger the hopping current. We predict that this negative magnetoresistance will be observed until the probability $1/\tau$ becomes the order of $eFd/\hbar$ with increasing magnetic field. Then the magnetic field destroys the Wannier-Stark localization, and the magnetoresistance becomes positive.

Consider now the effect of folded acoustical phonons[23] on conductance. The dispersion relation for folded phonons in the periodic potential is of the same form as the Kronig-Penney dispersion relation for electrons and spectrum can be considered as linear only at small q, while at the Bragg plane the wave velocity is zero and a gap arises. Obviously, if the energy conservation law Eq. (7) requires that $\hbar\omega_q$ falls into the gap, the current vanishes, and an antiresonant plateau is to be observed. Note that if the growth direction of a structure is (001), the gaps in the phonon spectrum are only at the Brillouin zone edge $q_z = \pm\pi/d$ and its center $q_z = 0$. Equations (7,11) determine the conditions for the current vanishing in the vicinity of the gaps. The current breakdown is not abrupt at $q_z = 0$, but at $q_z = \pm\pi$. This is another manifestation of the selection rule. Note that current peaks may arise due to the phonon "defects," which levels fall inside the folded phonon gap. These phonon modes come from the potential fluctuations.[24]

We would like to emphasize that the resonance and antiresonance features discussed in the present analysis are to be observed in hopping magnetoconductance experiments. For instance, the resonance, due to LO phonon scattering occur in the conductance, not in the resistance, and the absence of scattering will result in zero of the conductance, not in zero of the resistance. The claim on zero resistance in the absence of scattering in Ref. 25 is incorrect; the reason is that for $\hbar/\tau < eFd$ (and, naturally, in the absence of scattering) the electron states are localized, not delocalized, irrespective of an absolute value of electric field. Only for $\hbar/\tau > eFd$, in the conditions of the band conduction, the LO phonon resonance will result in a resistance maximum.

In order to observe antiresonances and resonances, it is necessary to study the SL magnetoconductance in the regime of WS localization. Evidence for the scattering-assisted resonant tunneling in SL in magnetic field was reported in Ref. 5. However, in these experiments, optical excitation plays an essential role and results in conductivity mechanisms varying from sample to sample. Different electron and hole subbands contribute to the conductivity and it appears difficult to extract the acoustic-phonon spectrum. In another experiment,[6] magnetoresistance in a quantizing magnetic field was studied in the band conduction regime, without WS localization. Finally, in Ref. 7, hopping conduction in magnetoresistance was investigated in the presence of strong disorder. The fact that no current oscillations were observed was due to the nature of localization, which was the result of disorder, but not of the electric field.

V. CONCLUSION

We have shown that the influence of quantum confinement on the electron and phonon states results in antiresonances in the hopping conductance of quantum-box superlattices. The momentum selection rule for the interaction of phonons with Wannier-Stark localized electrons as well as the folded phonon gaps are to be observed in the magnetoconductance. We predict negative magnetoresistance in high electric fields and point out the importance of boundary conditions imposed on the electron distribution in the description of the nonequilibrium character of the system.

Note added in proof. Recently, O. Raichev and F. Vasko [Phys. Rev. B **50**, 12 199 (1994)] considered the effect of an interference of matrix elements of transitions in a double-quantum-well system, which leads to minima of scattering probability. These minima are similar to minima in hopping current in superlattices due to one of the effects (Bragg reflection), which are considered in the present paper.

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