Effects of a magnetic field on electron-phonon scattering in quantum wires

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We have rigorously calculated the bare electron-phonon scattering rates in semiconductor quantum wires in the presence of an external magnetic field. The magnetic field has several interesting effects on the scattering rates. It drastically reduces acoustic-phonon scattering (by orders of magnitude at easily achievable field strengths), but increases longitudinal-optical and surface optical-phonon scattering. It also enhances the difference between the acoustic-phonon scattering rates at energies just below and above a subband minimum. The latter effect may cause negative differential mobility to appear in quantum wires at electric fields far below the threshold for intervalley transfer.

I. INTRODUCTION

Recently, there has been a growing interest in the study of electron-phonon scattering in quasi-one-dimensional structures.[1-3] This was motivated by the belief that such structures can exhibit exceptionally high mobilities at reduced temperatures.[4] Field-effect transistors with quantum-wire channels have been fabricated and show very large transconductances as a result of this enhanced mobility. The increase in the mobility in these structures accrues primarily from a suppression of impurity scattering which is the dominant scattering mechanism at cryogenic temperatures and low electric fields. However, at room temperature and above, or at high electric fields, scattering in semiconductor quantum wires is mostly due to phonons. Phonon scattering not only determines the low-field mobility at room temperature, but it also determines the high-field saturation velocity of electrons, the homogeneous linewidth broadening of optical transitions, the relaxation rate for photoexcited carriers, and a host of other phenomena in quantum wires.

In this paper, we have rigorously calculated electron-phonon scattering rates in quantum wires using Fermi's golden rule. The application of this rule in quantum wires has been criticized in the past,[5] but the criticism is valid only for electron energies at a subband bottom. At these energies, the density of states in quasi-one-dimensional systems diverges, which makes the Fermi golden rule prescription (or more correctly, the Born approximation) invalid. Attempts at circumventing this problem by introducing arbitrary broadening of the density of states (presumably associated with surface roughness) have been reported in the literature.[6] We do not adopt this approach in our work since it is somewhat *ad hoc*; instead, we compute the scattering rates from the usual Fermi golden rule, but with the caveat that it is not valid for electron energies corresponding to subband minima.

Fermi's golden-rule-based calculations of electron-phonon scattering rates in quantum wires were reported by a number of researchers in the past. Arora[1] considered the scattering rates due to nonpolar acoustic phonons, while Basu and Nag[2] considered the scattering rates due to polar (piezoelectric) acoustic phonons as did Lee and Vassell.[2] Leburton and co-workers[7,8] and Constantinou and Ridley[9] have calculated electron-longitudinal polar-optical-phonon scattering rates in one-dimensional structures but without considering phonon confinement effects (the electrons are confined, but the phonon modes are assumed to be bulk modes). Recent experimental results have revealed that phonon confinement may be important in quantum wires. Signatures of *surface* modes in cylindrical wires[10] and *confined* optical modes[11] in rectangular wires have been observed. Calculations of optical-phonon scattering rates, in which phonon confinement effects were explicitly taken into account, were reported by some other researchers recently.[12-15] Based on these results, it appears that the scattering rates calculated by assuming bulk modes actually do not differ greatly from the sum total of scattering rates due to surface and confined optical modes. Presumably, this is because the confined optical modes have nulls at the wire surfaces, whereas the surface modes peak at the surfaces, so that the superposition of both modes looks approximately bulklike.[16] As a result, phonon confinement effects are generally not of paramount importance in electron–optical-phonon interaction in quantum wires.

While the above is true generally, there are two major exceptions. They correspond to the cases when either a transverse electric field or a transverse magnetic field is applied to the quantum wire. *In the presence of such fields, optical-phonon-confinement effects assume an added importance.* The fields skew in the electron wave functions towards an edge of the quantum wire thereby altering the overlap between the electron wave function and the confined longitudinal polar-optical-phonon modes or surface optical-phonon modes. This can modify the optical-phonon scattering rates significantly. Therefore, any experimental manifestation of a significant dependence of the optical-phonon scattering rates on transverse electric or magnetic fields may be viewed as a manifestation of optical-phonon confinement as well.

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In contrast to optical phonons, acoustic phonons, by their very nature, are almost always unconfined and bulk-like. Therefore, a transverse electric field does not have much of an effect on the acoustic-phonon scattering rate. However, a magnetic field still has a very significant effect and it is *not* linked to phonon confinement. The origin of this latter effect was elucidated by us in a recent publication[17] and will not be discussed in this paper. We only mention that the influence of a magnetic field on acoustic phonons is actually much stronger than the influence on optical phonons and may lead to rather intriguing effects, one of which is discussed later in this paper.

In this paper, we have examined the effect of a magnetic field on optical-phonon scattering rates. The analogous effect of a transverse electric field was studied by Ferreira and Bastard who assumed bulk phonon modes,[18] and by Tang, Zhu, and Huang,[19] as well as Weber,[20] who assumed confined optical and surface modes. We have also discussed one particular effect of the magnetic field on acoustic-phonon scattering rates which has rather intriguing consequences. A magnetic field dramatically enhances the difference between the acoustic-phonon scattering rates just above and just below a subband minimum. Riddoch and Ridley had pointed out that such a difference can trigger negative differential mobility if it is sufficiently large. Therefore, in quantum wires of nonpolar semiconductors (e.g., Ge), in which acoustic-phonon scattering is dominant over a wide range of temperatures, one can expect to observe negative differential mobility at electric fields far below the threshold for intervalley transfer (Ridley-Gunn-Hilsum effect) if the wire is subjected to a sufficiently strong magnetic field. The threshold electric field for the onset as well as the magnitude of the negative differential mobility can be tuned somewhat by the external magnetic field. Such an effect has many potential device applications.

This paper is organized as follows. In Sec. II we will discuss the theory for calculating phonon scattering rates in a quantum wire subjected to a magnetic field. The results of these calculations will be presented along with the appropriate interpretations in Sec. III. Finally, in Sec. IV, we will present the conclusions.

II. THEORY

We consider a quantum wire as shown in Fig. 1. Only one transverse subband is occupied along the z direction (for even the highest energy an electron can reach), but many are occupied in the y direction. The confining potentials along the y and z directions are assumed to be infinite. It was shown by Constantinou and Ridley[9] that finiteness of the potentials can reduce the scattering rates somewhat, but in this paper, we will neglect such effects. A magnetic field is applied along the z direction. In all calculations, we will assume that the phonons are unaffected by the magnetic field and are in thermodynamic equilibrium so that the phonon occupation probability is given by the Bose-Einstein factor at the lattice temperature. The electrons, however, are strongly affected by the magnetic field. The field imposes an additional degree of confinement on the electrons (in addition to the electrostatic quantum-wire confinement) so that the electron states become hybrid magnetoelectric states. This, of course, affects the electron-phonon scattering rates.

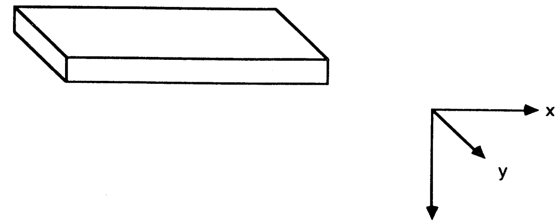

FIG. 1. A quasi-one-dimensional structure subjected to a magnetic field in the z direction. The thickness is small enough that only one subband is occupied in the z direction at all electron energies. Several subbands are occupied in the y direction.

The effect of the magnetic field on the scattering rate is completely accounted for (in every respect) by considering only three aspects: (a) the magnetic field changes the wave functions of the electron in various subbands, (b) it changes the energy and energy dispersion relation of the subbands (the subbands become hybrid magnetoelectric states), and (c) it changes the densities of states in various subbands. All these effects are rigorously taken into account in our calculations from first principles. We directly solve the Schrödinger equation in the quantum wire under a magnetic field to obtain the exact wave function in each magnetoelectric subband, the exact energies and energy dispersion relations for the magnetoelectric states, and the exact density of states in each magnetoelectric subband. These are then used in the calculation of the scattering rates. (The Schrödinger equation in a magnetic field is solved numerically using a finite difference method and the technique has been described in Ref. 21.)

In heavily doped quantum wires, screening of electron-phonon interactions and many-body effects may play an important role. Screening has been treated by Fishman,[22] Tanatar,[23] and by Campos, Das Sarma, and Stroscio.[24] Many-body effects have been treated by Ahn[25] and by Senna and Das Sarma.[26] Screening, especially dynamic screening, and also many-body effects are rather difficult to incorporate in the present approach and we will neglect them here. This limits the validity of the results to carrier concentrations where the screening length is large compared to phonon wavelengths. For our system, this means that the carrier concentration should be less than 10^6/cm. The effect of screening will be reported in a later publication.

Calculation of the acoustic-phonon scattering rates in a quantum wire subjected to a magnetic field has been discussed in Refs. 17 and 27. In this paper, we only present the calculation of the optical-phonon scattering rates in a magnetic field.

To calculate polar and nonpolar longitudinal-optical-(LO) as well as surface optical- (SO) phonon scattering rates, we have followed Stroscio[12] and Kim *et al.*[14] whose models assume confined (slab) phonon modes. A more accurate model would require calculation of the phonon modes from a microscopic model.[15,28,29] This is reserved for future work.

A. Longitudinal polar-optical-phonon scattering rate in a magnetic field

The longitudinal polar-optical-phonon scattering rate of an electron with energy E_ν in the νth magnetoelectric subband is obtained from Fermi's golden rule as[12,14]

$$\frac{1}{\tau^{\pm}_{\mathrm{POP}}(E_\nu)}=\sum_{\nu'=1}^{\nu_{\max}}\frac{e^2}{4\pi\epsilon_0}\omega_{\mathrm{POP}}(N_{\omega_{\mathrm{POP}}}+\tfrac{1}{2}\pm\tfrac{1}{2})I_{\mathrm{POP}}D(E'_{\nu'}) , \tag{1}$$

where ω_{POP} is the longitudinal polar-optical-phonon frequency, $N_{\omega_{\mathrm{POP}}}$ is the phonon occupation probability (Bose-Einstein factor) for these phonons and $\nu_{\max}$ is the index of the highest phonon mode considered. The plus sign in the above expression refers to emission and the minus sign to absorption. The quantity $D(E'_{\nu'})$ is the density of states at the final energy $E'_{\nu'}$ in the magnetoelectric subband ν' and I_{POP} is given by

$$I_{\mathrm{POP}}=\left[\frac{1}{\epsilon_r(\infty)}-\frac{1}{\epsilon_r(0)}\right]\frac{(2\pi)^2}{L_yL_z}\sum_{m'=1,2,3,\ldots}\sum_{n'=1,2,3,\ldots}\left\{\frac{4P_{m'n'}}{\left[k_x^2+\left[\frac{m'\pi}{L_y}\right]^2+\left[\frac{n'\pi}{L_z}\right]^2\right]^{1/2}}\right\}^2 , \tag{2}$$

where $\epsilon_r(0)$ and $\epsilon_r(\infty)$ are the low- and high-frequency relative permittivities, k_x is the phonon wave vector along the length of the quantum wire, m' and n' are the transverse phonon mode indices along the y and z directions, L_y and L_z are the width and thickness of the quantum wire, and $P_{m'n'}$ is the overlap integral which can be written as

$$P_{m'n'}=\int_0^{L_y}\int_0^{L_z}\frac{dy}{L_y/2}\frac{dz}{L_z/2}\psi^*_{\mathrm{fin}}(y)\psi_{\mathrm{in}}(y)\phi^*_{\mathrm{fin}}(z)\phi_{\mathrm{in}}(z)\times\sin\left[\frac{m'\pi y}{L_y}\right]\sin\left[\frac{n'\pi z}{L_z}\right] . \tag{3}$$

In the above, $\psi_{\mathrm{in}}(y)$ $[\phi_{\mathrm{in}}(z)]$ and $\psi_{\mathrm{fin}}(y)$ $[\phi_{\mathrm{fin}}(z)]$ are the initial and final y (z) components of the wave functions of the electron in the presence of a magnetic field and the sine functions are the confined phonon (slab) modes.

To calculate the scattering rate, we need to know the eigenenergies E_ν, wave functions ψ_{E_ν}, and density of hybrid magnetoelectric states $D(E_\nu)$ in a magnetic field. As mentioned before, these are calculated exactly by solving the Schrödinger equation in a quantum wire subjected to a magnetic field.[21] Therefore, the magnetic-field effects are rigorously taken into account in the calculation of the scattering rates.

B. Longitudinal nonpolar-optical-phonon scattering rate in a magnetic field

The nonpolar longitudinal-optical-phonon scattering rate can be found likewise,

$$\frac{1}{\tau^{\pm}_{\mathrm{NPO}}(E_\nu)}=\sum_{\nu'=1}\frac{\pi D_0^2}{\rho\omega_{\mathrm{NPO}}L_yL_z}(N_{\omega_{\mathrm{NPO}}}+\tfrac{1}{2}\pm\tfrac{1}{2})\times I_{\mathrm{NPO}}D(E'_{\nu'}) , \tag{4}$$

where D_0 is the deformation potential for the optical phonon, ω_{NPO} is the frequency of the nonpolar longitudinal optical phonon, and I_{NPO} is the overlap integral given by

$$I_{\mathrm{NPO}}=\sum_{m'=1,2,3,\ldots}\sum_{n'=1,2,3\ldots}\left[\left[\int_0^{L_y}\int_0^{L_z}\frac{dy}{L_y/2}\frac{dz}{L_z/2}\psi^*_{\mathrm{fin}}(y)\psi_{\mathrm{in}}(y)\phi^*_{\mathrm{fin}}(z)\phi_{\mathrm{in}}(z)\right]\sin\left[\frac{m'\pi y}{L_y}\right]\sin\left[\frac{n'\pi z}{L_z}\right]\right]^2 . \tag{5}$$

C. Surface optical-phonon scattering rate in a magnetic field

The scattering rate due to surface optical (SO) phonons is given by[14]

$$\frac{1}{\tau^{\pm}_{\mathrm{SO}}(E_\nu)}=\sum_{\nu'=1}^{\nu_{\max}}\frac{e^2}{4\pi\epsilon_0}\omega_{\mathrm{SO}}(N_{\omega_{\mathrm{SO}}}+\tfrac{1}{2}\pm\tfrac{1}{2})I_{\mathrm{SO}}D(E'_{\nu'}) , \tag{6}$$

where ω_{SO} is the surface optical-phonon frequency and

$$I_{\mathrm{SO}}=\left[\frac{2\pi C'P_s}{\omega_{\mathrm{SO}}}\right]^2 , \tag{7}$$

with C' being the normalization constant[12] for phonon modes and P_s an overlap integral given by

$$P_s^s=\frac{1}{\cosh(\alpha L_y/2)\cosh(\beta L_z/2)}\int_{-L_y/2}^{L_y/2}\int_{-L_z/2}^{L_z/2}\frac{dy}{L_y/2}\frac{dz}{L_z/2}\psi^*_{\mathrm{fin}}(y)\psi_{\mathrm{in}}(y)\phi^*_{\mathrm{fin}}(z)\phi_{\mathrm{in}}(z)\cosh(\alpha y)\cosh(\beta z) \tag{8}$$

for symmetric surface phonon modes, and

$$P_s^a = \frac{1}{\sinh(\alpha L_y/2)\sinh(\beta L_z/2)} \int_{-L_y/2}^{L_y/2} \int_{-L_z/2}^{L_z/2} \frac{dy}{L_y/2} \frac{dz}{L_z/2} \psi_{\rm fin}^*(y)\psi_{\rm in}(y)\phi_{\rm fin}^*(z)\phi_{\rm in}(z)\sinh(\alpha y)\sinh(\beta z) \qquad (9)$$

for antisymmetric surface phonon modes. The quantities α,β have been defined and the dispersion relation for SO phonons given in Ref. 14.

In our example, only one subband is occupied in the z direction. In that case, the SO phonon scattering is due to only the symmetric modes since the overlap integral in the z direction becomes zero for antisymmetric modes. This happens since the z component of the electron wave function (in the lowest subband) has even parity. Had multiple subbands been occupied in the z direction (some of whose wave function would have odd parity), the SO-phonon scattering would have had contributions from both the symmetric and antisymmetric phonon modes. This feature is not affected by a magnetic field as long as the field is directed along the z direction.

III. RESULTS AND DISCUSSION

We now present some results for a prototypical quasi-one-dimensional structure. The test structure is a GaAs quantum wire (surrounded by $Al_xGa_{1-x}As$) of width 500 Å (along the y direction) and thickness 40 Å (along the z direction). All phonon scattering rates are calculated for this system.

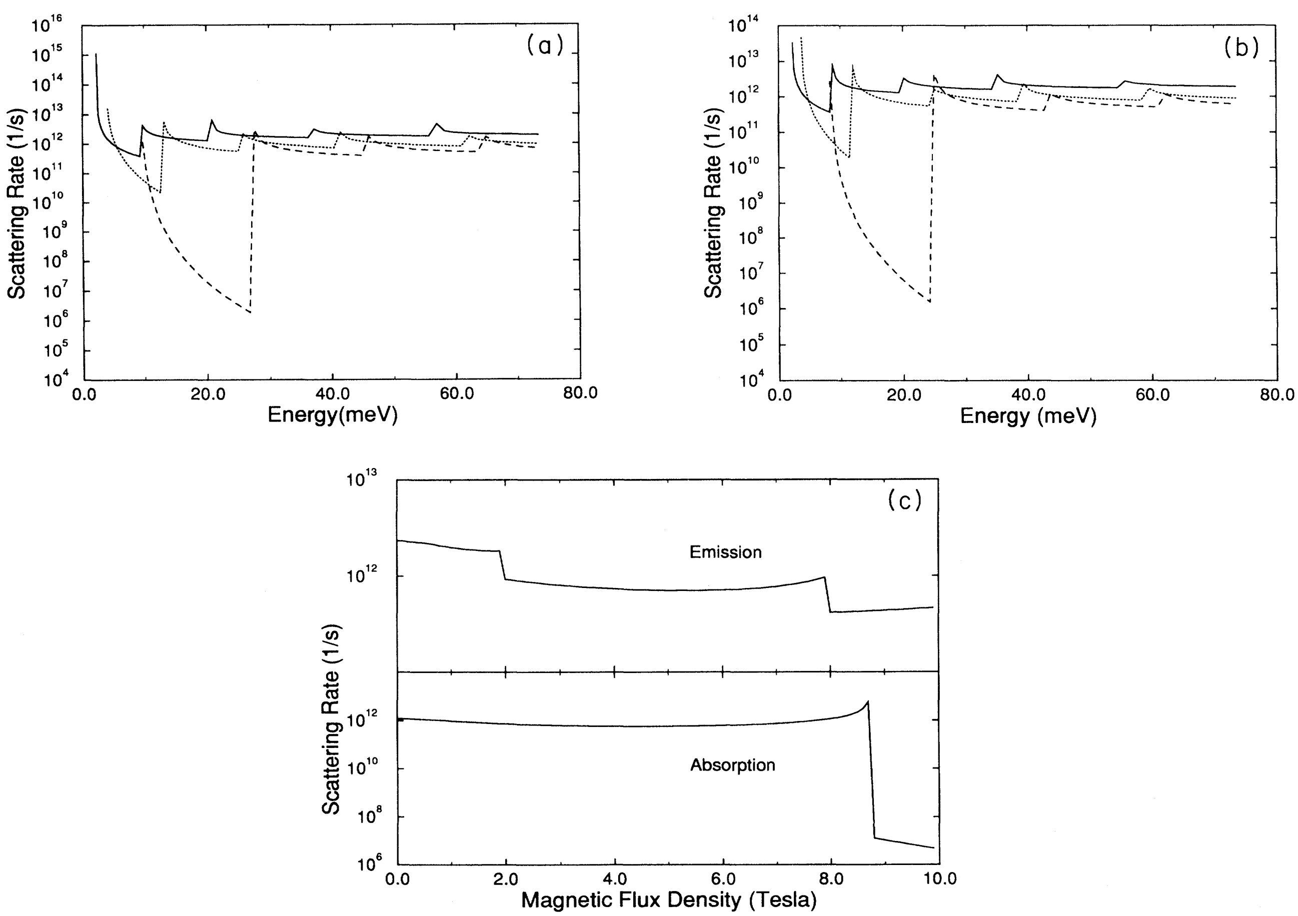

FIG. 2. (a) Electron nonpolar-acoustic-phonon scattering rate as a function of energy for electrons in the lowest magnetoelectric subband. (a) Emission rate and (b) the absorption rate. The lattice temperature is 300 K. The solid, short-dashed, and long-dashed lines represent magnetic flux densities of 0, 4, and 10 T. (c) The scattering rate as a function of magnetic flux density. The upper frame is for emission and the lower for absorption. In the upper frame, the electron energy is assumed to be 37 meV, and in the lower frame it is 25 meV.

A. Acoustic-phonon scattering rates

In Figs. 2(a) and 2(b), we show the nonpolar acoustic-phonon (deformation potential) emission and absorption rates at different magnetic-field strengths. The peaks in the scattering rates are associated with the divergence in the density of (final) states in a quasi-one-dimensional structure. These results are reproduced from Ref. 17.

The dramatic quenching of the acoustic-phonon scattering rate (by up to six orders of magnitude at a flux density of 10 T) was noted and its implications for the quantum Hall effect were discussed in Ref. 17. Here we discuss another interesting feature. A magnetic field significantly enhances the difference between the scattering rates just below and just above a subband minimum. The increase is several orders of magnitude. It was predicted that such a difference can cause negative differential mobility to appear in quantum confined systems at electric fields far below the threshold for intervalley transfer.[22] Later simulations failed to reveal such an effect in GaAs wires,[3] but we believe that a magnetic field may cause it to appear. The ideal materials for exhibiting this type of negative differential mobility are nonpolar semiconductors in which acoustic-phonon scattering predominates over a wide range of temperature. An example is germanium. Of course, only a complete Monte Carlo simulation of electron transport or some other solution of the Boltzmann transport equation can establish the existence of this effect. This is an important issue since (a) the threshold electric field for such negative differential mobility is presumably much lower than that associated with intervalley transfer (Ridley-Gunn-Hilsum effect). This may allow the realization of low power microwave oscillators (e.g., local oscillators in demodulation circuits), and (b) the threshold electric field can be engineered at will by altering the dimensions (width and thickness) of the wire. More importantly, both the threshold field and the magnitude of the negative differential mobility may be tuned somewhat by the magnetic field.

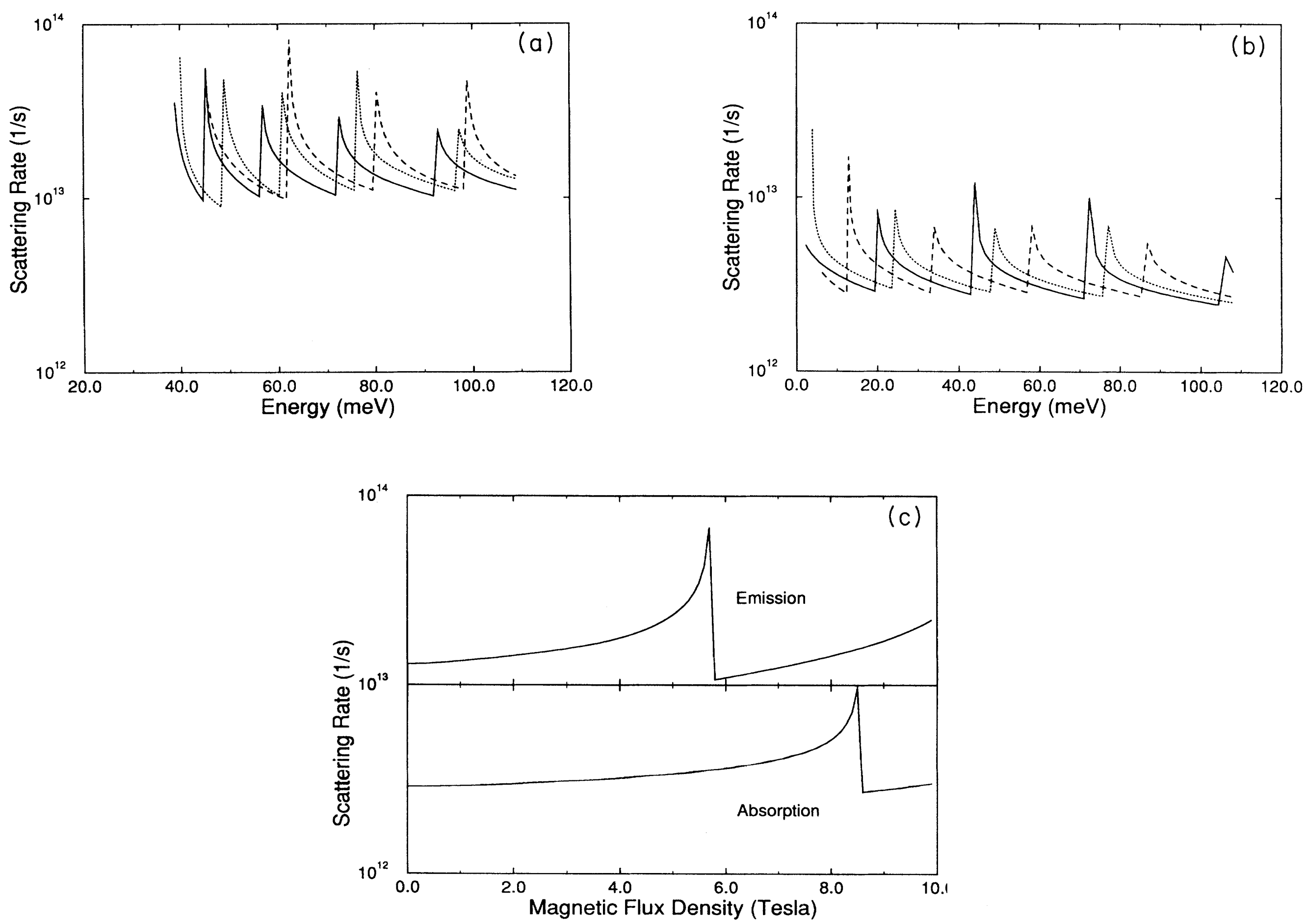

FIG. 3. Electron-longitudinal polar-optical-phonon scattering rates as a function of energy for electrons in the lowest magnetoelectric subband. The structure is the same as that in Fig. 2 and the lattice temperature is 300 K. (a) Emission rate and (b) absorption rate. Energy is measured from the bottom of the bulk conduction band edge. The solid, short-dashed, and long-dashed lines have the same interpretation as in Fig. 2. (c) The upper frame is the emission and the lower frame is the absorption rate as a function of magnetic flux density. In the upper frame, the electron energy is 60 meV and in the lower frame it is 40 meV.

B. Optical-phonon scattering rates

In Figs. 3(a) and 3(b), we have plotted the longitudinal polar-optical-phonon emission and absorption rates as a function of electron energy in the lowest magnetoelectric subband for various magnetic-field strengths. The nonpolar-optical-phonon scattering rates are shown in Figs. 4(a) and 4(b). The latter are for the L valley of GaAs since this scattering mechanism is forbidden in the Γ valley. Finally, the surface optical-phonon (SO) scattering rates are shown in Figs. 5(a) and 5(b).

Unlike in the case of acoustic-phonon scattering, all optical-phonon scattering rates tend to increase with magnetic flux density. This increase becomes more evident in the plots of the scattering rates versus magnetic field which are shown in Figs. 3(c), 4(c), and 5(c).

The increase for both polar and nonpolar longitudinal-optical-phonon scattering can be explained as follows. In the absence of a magnetic field, the electron wave function in the ith mode is orthogonal to the jth phonon mode if $i \neq j$. This makes the integrals I_{POP} and I_{NPO} (and the corresponding scattering rates $1/\tau_{\mathrm{POP}}^{\pm}$ and $1/\tau_{\mathrm{NPO}}^{\pm}$) vanish for $i \neq j$. This means that the jth phonon mode will not contribute to the scattering of an electron in the ith subband. However, when a magnetic field is present, it skews the electron wave functions towards one edge of the wire (owing to the Lorentz force) and this breaks the orthogonality between the electron wave function in the ith mode and the jth phonon mode ($i \neq j$). As a result, all phonon modes now contribute to the scattering of an electron. This opens up many new scattering channels which were previously forbidden. The result is an increase in the total scattering rate when a magnetic field is present.

In the case of the SO phonon, the increase in the scattering rate can be explained as follows. The magnetic field skews the electron wave functions towards one of the edges of the wire. This increases the overlap integral

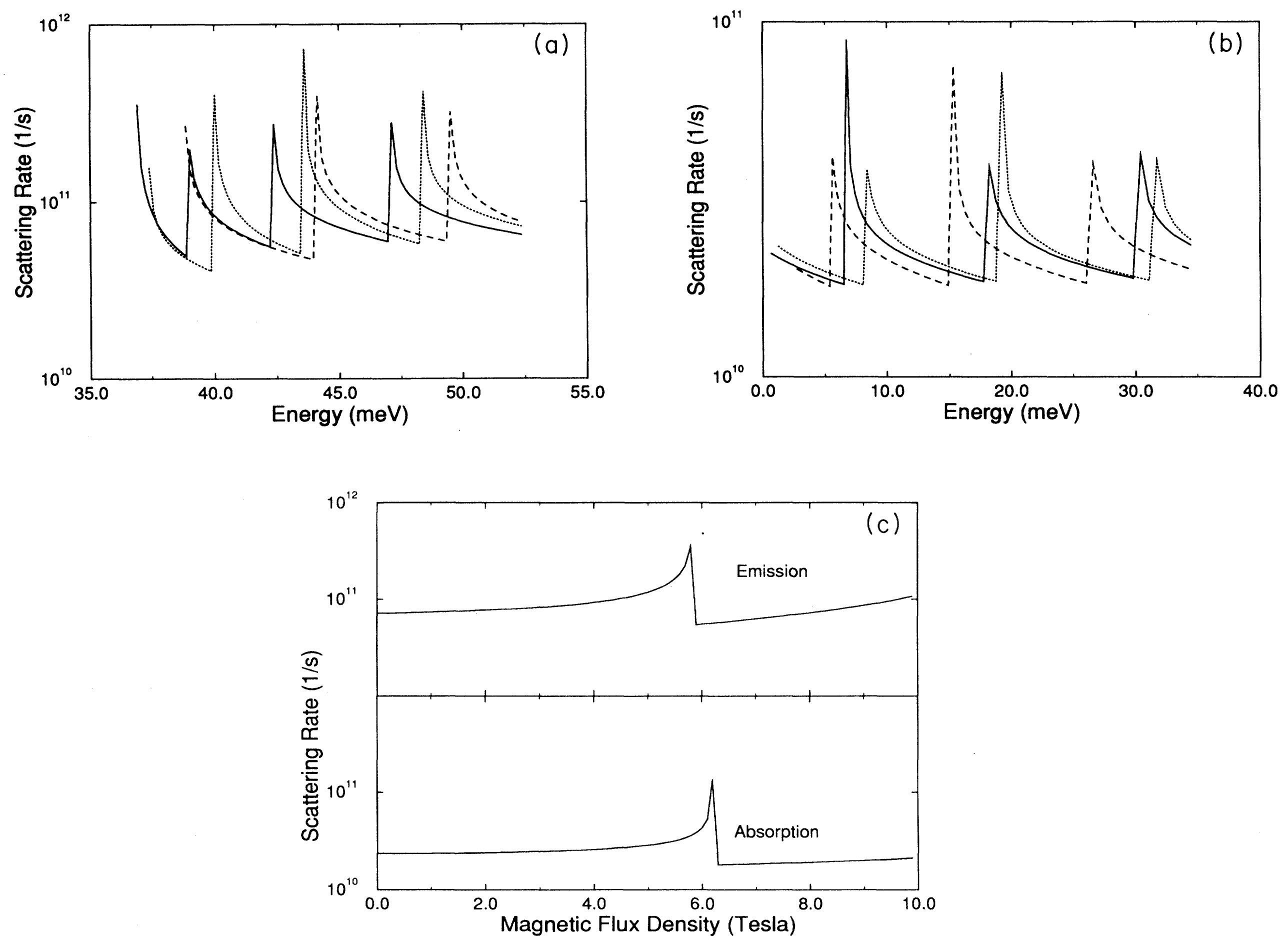

FIG. 4. Electron-longitudinal nonpolar-optical-phonon scattering rates as a function of energy for electrons in the lowest magnetoelectric subband. The structure is the same as that in Fig. 2 and the lattice temperature is 300 K. (a) Emission rate and (b) absorption rate. Again, energy is measured from the bottom of the bulk conduction-band edge. The solid, short-dashed, and long-dashed lines have the same interpretation as in Fig. 2. (c) The upper frame is the emission and the lower frame is the absorption rate as a function of magnetic flux density. In the upper frame, the electron energy is 45 meV and in the lower frame it is 10 meV.

P_s since the SO phonon modes are localized at the edges and decay away from the edges. Consequently, the scattering rate increases.

Another interesting feature in Fig. 5(b) is that, in the absence of any magnetic field, one cannot observe the peaks in the absorption rate associated with the divergence of the one-dimensional density of (final) states. This was also noted in Refs. 6 and 14. It was claimed in Ref. 6 that this happens because the peaks are due to intersubband scattering as opposed to intrasubband scattering. For SO phonon absorption, intrasubband scattering rate dominates over intersubband scattering rate and, therefore, the peaks in the intersubband rate are not discernible against the strong background of intrasubband scattering. However, when a magnetic field is turned on, the peaks appear (the two sets of peaks are associated with two phonon branches[14]). This indicates that a magnetic field *promotes intersubband SO phonon absorption over intrasubband SO phonon absorption.* We believe that this happens because the magnetic field breaks the orthogonality between the electron wave functions in two different subbands and increases the overlap integral P_s for intersubband transitions. This is true of SO phonon emission as well. Therefore, a magnetic field brings out the peaks in the scattering rate.

IV. CONCLUSION

In this paper, we have investigated rigorously the effect of a magnetic field on phonon scattering in a quantum wire. We have speculated on the possibility of a magnetic field causing negative differential mobility in a quantum wire at threshold electric fields far below that required for intervalley transfer. The magnitude of this negative differential mobility and the threshold electric field can be tuned somewhat by the magnetic field.

We have also presented the optical-phonon scattering

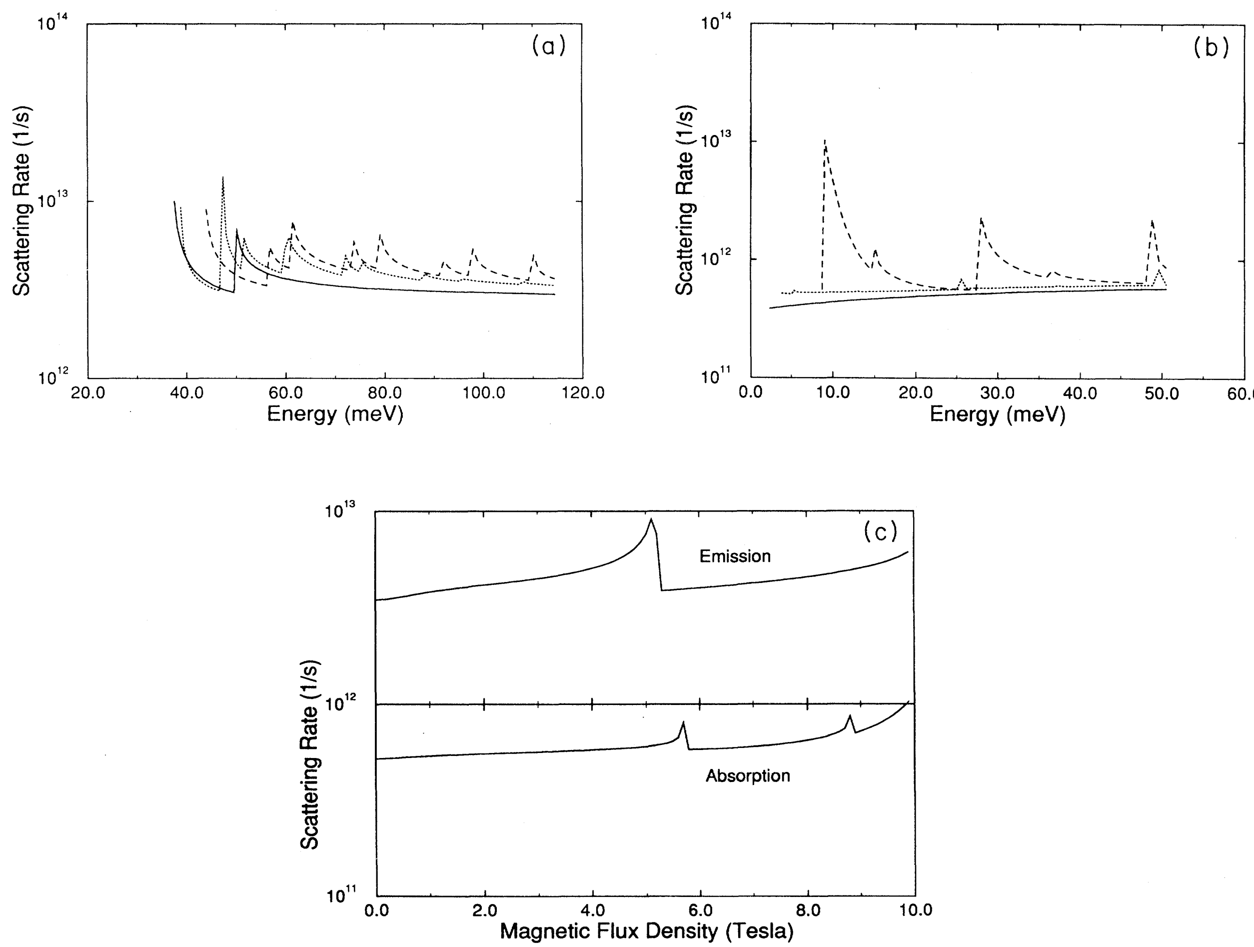

FIG. 5. Electron-surface optical-phonon scattering rates as a function of energy for electrons in the lowest magnetoelectric subband. The structure is the same as that in Fig. 2 and the lattice temperature is 300 K. (a) Emission rate and (b) absorption rate. Again, energy is measured from the bottom of the bulk conduction-band edge. The solid, short-dashed, and long-dashed lines have the same interpretation as in Fig. 2. (c) The upper frame is the emission and the lower frame is the absorption rate as a function of magnetic flux density. In the upper frame, the electron energy is 60 meV and in the lower frame it is 40 meV.

rates in a quantum wire subjected to a magnetic field. Optical-phonon scattering determines the saturation velocity in most materials at electric fields below the threshold for intervalley transfer. It also determines the relaxation rate for photoexcited carriers and the homogeneous linewidth broadening of the photoluminescence spectra. Therefore, it is important to understand the effect of a magnetic field on optical-phonon scattering rates. This work is an important step in that direction.

Recently, Masale and Constantinou have reported the effect of an axial magnetic field on electron-LO phonon scattering rates in a cylindrical quantum wire.[30] Their results are qualitatively similar to ours.

ACKNOWLEDGMENT

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