Interaction between longitudinal-optical-phonon modes of a rectangular quantum wire and charge carriers of a one-dimensional electron gas

Michael A. Stroscio
U.S. Army Research Office, P.O. Box 12211, Research Triangle Park, North Carolina 27709-2211
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The Fröhlich Hamiltonian describing the interaction of longitudinal-optical (LO) phonons and charge carriers in a three-dimensional polar semiconductor is generalized to the case where phonon modes are confined in two of the three spatial dimensions. The generalized Fröhlich Hamiltonian is used to calculate the total scattering rate for electron–LO-phonon scattering of electrons traversing a one-dimensional quantum wire with a rectangular cross section.

I. INTRODUCTION

Epitaxial techniques for the growth of new compound-semiconductor structures have advanced to a level where it is possible to grow wirelike regions of low-band-gap semiconductor material surrounded completely by regions of higher-band-gap semiconductor material. In particular, such wirelike structures have been grown with rectangular cross sections having dimensions small relative to the thermal deBroglie wavelength.[1] In these structures the electron–LO-phonon scattering rate is affected not only by changes in the electron wave function due to the confining rectangular potential but also by changes in the Fröhlich Hamiltonian caused by phonon confinement. Indeed, Fasol *et al.*[2] have recently presented striking evidence of phonon confinement. Size effects on the total scattering rates for polar-optical-phonon scattering of one-dimensional (1D) and two-dimensional (2D) electron gases in synthetic semiconductors have been evaluated previously by Leburton.[3] In this paper, Leburton's treatment of 1D electron–LO-phonon scattering is extended by incorporating effects of phonon confinement in the Fröhlich Hamiltonian.

II. FRÖHLICH HAMILTONIAN FOR LO PHONONS CONFINED IN TWO SPATIAL DIMENSIONS

Licari and Evrard[4] have calculated the operators describing the interaction between an electron and the phonon modes of an ionic crystal slab and have derived explicit expressions for two classes of phonon modes for such a slab: the bulklike sinusoidal modes and the localized surface modes. Furthermore, one of the operators derived by Licari and Evrard is equivalent to the Fröhlich operator for bulk LO phonons in the limit as the slab becomes very thick. The electron–surface-phonon interaction operator of Licari and Evrard leads to the classical image-charge theory result for the interaction energy of an electron external to a semi-infinite crystal and the polarization eigenmodes of the crystal.

To derive the Fröhlich Hamiltonian describing the interaction of LO phonons and electrons for a 1D electron gas, the three-dimensional Fröhlich operator for scattering in bulk semiconductor material, $H_{\rm Fr}^{(3D)}$, is subjected to boundary conditions requiring the LO-phonon potential to vanish in both the y and z directions. $H_{\rm Fr}^{(3D)}$ may be written as

$$H_{\rm Fr}^{(3D)}=\sum_K V_K e^{-i\mathbf{K}\cdot\mathbf{r}}(a_K+a_{-K}^{\dagger}) , \tag{2.1a}$$

where the phonon wave vector is $\mathbf{K}=(\mathbf{k},k_z)$ and

$$V_K=\left[\frac{2\pi e^2\hbar\omega}{VK^2}\left[\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right]\right]^{1/2} ; \tag{2.1b}$$

in Eq. (2.1b) $\hbar\omega$ is the phonon energy, V is the crystal volume, ϵ_∞ is the high-frequency dielectric constant, and ϵ_0 is the low-frequency dielectric constant. Writing the sum over K as a sum over $\mathbf{k}$ and as a sum over positive values of k_z;

$$H_{\rm Fr}^{(3D)}=\sum_{\mathbf{k},k_z>0} V_K e^{-\mathbf{k}\cdot\rho}[e^{-ik_z z}(a_{\mathbf{k},k_z}+a_{-\mathbf{k},-k_z}^{\dagger}) + e^{ik_z z}(a_{\mathbf{k},-k_z}+a_{-\mathbf{k},k_z}^{\dagger})] . \tag{2.2}$$

To derive the Fröhlich Hamiltonian for phonons confined in two dimensions, we first define

$$a_+(\mathbf{k})=\frac{1}{\sqrt{2}}(a_{\mathbf{k},k_z}+a_{\mathbf{k},-k_z}) , \tag{2.3a}$$

$$a_-(\mathbf{k})=\frac{-i}{\sqrt{2}}(a_{\mathbf{k},k_z}-a_{\mathbf{k},-k_z}) , \tag{2.3b}$$

and take $a_+^{\dagger}(-\mathbf{k})$ and $a_-^{\dagger}(-\mathbf{k})$ to be the adjoints of $a_+(-\mathbf{k})$ and $a_-(-\mathbf{k})$, respectively.

Then by defining

$$A_+(k_x)_\pm=\frac{1}{\sqrt{2}}[a_\pm(k_x,k_y)+a_\pm(k_x,-k_y)] , \tag{2.4a}$$

$$A_-(k_x)_\pm=-\frac{i}{\sqrt{2}}[a_\pm(k_x,k_y)-a_\pm(k_x,-k_y)] , \tag{2.4b}$$

expanding both $e^{\pm ik_y y}$ as well as $e^{\pm ik_z z}$, and taking $k_y=\pm m\pi/L_y$ and $k_z=\pm n\pi/L_z$ to ensure that the slab modes vanish[4] at $y=\pm L_y/2$ and $z=\pm L_z/2$ results in

$$H_{\mathrm{Fr}}^{(1\mathrm{D})}=2\alpha'\sum_{k_x}e^{-ik_x x}\left[\sum_{m=1,3,5,\ldots}\sum_{n=1,3,5,\ldots}\frac{\cos\left[\frac{m\pi}{L_y}y\right]\cos\left[\frac{n\pi}{L_z}z\right]}{\left[k_x^2+\left[\frac{m\pi}{L_y}\right]^2+\left[\frac{n\pi}{L_z}\right]^2\right]^{1/2}}[A_+(k_x)_+ + A_+^\dagger(-k_x)_+]\right.$$
$$+\sum_{m=1,3,5,\ldots}\sum_{n=2,4,6,\ldots}\frac{\cos\left[\frac{m\pi}{L_y}y\right]\sin\left[\frac{n\pi}{L_z}z\right]}{\left[k_x^2+\left[\frac{m\pi}{L_y}\right]^2+\left[\frac{n\pi}{L_z}\right]^2\right]^{1/2}}[A_+(k_x)_- + A_+^\dagger(-k_x)_-]$$
$$+\sum_{m=2,4,6,\ldots}\sum_{n=1,3,5,\ldots}\frac{\sin\left[\frac{m\pi}{L_y}y\right]\cos\left[\frac{n\pi}{L_z}z\right]}{\left[k_x^2+\left[\frac{m\pi}{L_y}\right]^2+\left[\frac{n\pi}{L_z}\right]^2\right]^{1/2}}[A_-(k_x)_+ + A_-^\dagger(-k_x)_+]$$
$$\left.+\sum_{m=2,4,6,\ldots}\sum_{n=2,4,6,\ldots}\frac{\sin\left[\frac{m\pi}{L_y}y\right]\sin\left[\frac{n\pi}{L_z}z\right]}{\left[k_x^2+\left[\frac{m\pi}{L_y}\right]^2+\left[\frac{n\pi}{L_z}\right]^2\right]^{1/2}}[A_-(k_x)_- + A_-^\dagger(-k_x)_-]\right], \tag{2.5a}$$

where $\alpha'=\left[\frac{2\pi e^2}{V}\hbar\omega\left[\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right]\right]^{1/2}$. (2.5b)

The one-dimensional Fröhlich Hamiltonian of Eq. (2.5a) describes the interaction of an electron and LO-phonon modes characterized by a traveling wave in the x direction and standing waves in the y direction and z direction. This result is approximate since the phonon modes in the y and z directions are not identically zero at $y=\pm L_y/2$ and $z=\pm L_z/2$. Physically, these modes should be small at heterojunctions since the dielectric constant changes at the heterojunction interface and since longitudinal modes propagate freely only at frequencies where the dielectric constant vanishes;[5] at other frequencies the modes are damped. Similar conclusions are reached on the basis of shell-model calculations.[6]

III. SCATTERING RATE FOR ELECTRON–LO-PHONON INTERACTIONS IN A QUANTUM WIRE

The 1D Fröhlich Hamiltonian of Eq. (2.5a) leads to especially simple scattering matrix elements when electron states are confined in infinitely deep potential wells in the y and z directions; in this case the electronic wave functions are given by eigenstates orthogonal to the phonon modes of Eq. (2.5a). While treatments with more realistic confining potentials are avaliable for LO phonons described by the 3D Fröhlich Hamiltonian,[7] they generally involve the extensive application of numerical techniques. Additionally, numerical treatments based on a 2D Fröhlich Hamiltonian have tended to emphasize superlattice structures; many such works are cited in Ref. 8.

In the present treatment, electron–LO-phonon scattering rates will be calculated in the extreme quantum limit (EQL) where only the lowest subband is occupied. For the infinite well potential, the ground-state 1D electron wave function has the well-known form

$$|q_{1\mathrm{D}}\rangle=\frac{e^{iq_x x}}{(L_x)^{1/2}}\left[\frac{2}{L_y}\right]^{1/2}\times\cos\left[\frac{\pi y}{L_y}\right]\left[\frac{2}{L_z}\right]^{1/2}\cos\left[\frac{\pi z}{L_z}\right], \tag{3.1}$$

where L_x is the length of the quantum wire, $-L_y/2\le y\le L_y/2$, and $-L_z/2\le z\le L_z/2$. The corresponding electron energy is

$$E_{1\mathrm{D}}=\frac{\hbar^2 q_x^2}{2m^*}+\frac{\hbar^2\pi^2}{2m^*}\left[\frac{1}{L_y^2}+\frac{1}{L_z^2}\right]. \tag{3.2}$$

Assuming that the Fermi-Golden rule gives an accurate value of the probability of making a transition from an initial state with electron wave vector $\mathbf{q}$ to a final state with electron wave vector $\mathbf{q}'$, the transition probability is

$$W^{\{e\}}_{\{a\}}(\mathbf{q},\mathbf{q}')=\left[\frac{2\pi}{\hbar}\right]|M^{\{e\}}_{\{a\}}|^2\,\delta(E(q')-E(q)\pm\hbar\omega), \tag{3.3}$$

where e stands for emission, a stands for absorption, $E(q')$ is the energy of the electron in the final state, $E(q)$ is the energy of the electron in the initial state, the upper

(lower) sign in the δ function corresponds to emission (absorption), and where

$$M^{\{e\}}_{a} = \langle \mathbf{q}', N_K + \tfrac{1}{2} \pm \tfrac{1}{2} | H^{(1D)}_{Fr} | \mathbf{q}, N_K + \tfrac{1}{2} \pm \tfrac{1}{2} \rangle \tag{3.4}$$

is the matrix element for electron–LO-phonon interaction; the phonon occupation number is taken as $N_K + 1$ or as N_K depending upon whether the process under consideration is emission or absorption and upon whether the state under consideration is the initial or final state. The y-dependent and z-dependent factors in Eq. (3.4) are given by

$$P_{mn} = \int_{-L_y/2}^{L_y/2} \frac{dy}{(L_y/2)} \int_{-L_z/2}^{L_z/2} \frac{dz}{(L_z/2)} \cos^2\left[\frac{\pi y}{L_y}\right] \cos^2\left[\frac{\pi z}{L_z}\right] \times \begin{cases} \cos\left[\frac{m\pi}{L_y} y\right] \cos\left[\frac{n\pi}{L_z} z\right] & \text{(3.5a)} \\ \cos\left[\frac{m\pi}{L_y} y\right] \sin\left[\frac{n\pi}{L_z} z\right] & \text{(3.5b)} \\ \sin\left[\frac{m\pi}{L_y} y\right] \cos\left[\frac{n\pi}{L_z} z\right] & \text{(3.5c)} \\ \sin\left[\frac{m\pi}{L_y} y\right] \sin\left[\frac{n\pi}{L_z} z\right] & \text{(3.5d)} \end{cases},$$

where the four expressions defined by Eqs. (3.5a)–(3.5d) correspond to the four terms of Eq. (2.5a) and the values of m and n correspond to those of Eq. (2.5a). The nonvanishing terms in Eq. (3.5a)–(3.5d) are those of Eq. (3.5a); using the identities $\cos 3x = 4\cos^3 x - 3\cos x$ and $\cos 5x = 16\cos^5 x - 20\cos^3 x + 5\cos x$, the integrals P_{mn} may be evaluated analytically. The lowest-order P_{mn} follow: $P_{11} = (8/3\pi)^2$, $P_{13} = P_{31} = \frac{1}{5}(8/3\pi)^2$, $P_{15} = P_{51} = -\frac{1}{35}(8/3\pi)^2$, $P_{33} = \frac{1}{25}(8/3\pi)^2$, $P_{35} = P_{53} = -\frac{1}{175}(8/3\pi)^2$, and $P_{55} = \frac{1}{1225}(8/3\pi)^2$. The phonon matrix elements are evaluated by use of Eqs. (2.3a), (2.3b), (2.4a), and (2.4b), as well as the amplitudes $\langle N_{\mathbf{K}} + 1 | -a_{\mathbf{K}} | N_{\mathbf{K}} \rangle = -(N_{\mathbf{K}} + 1)^{1/2}$ and $\langle N_{\mathbf{K}} - 1 | a_{\mathbf{K}} | N_{\mathbf{K}} \rangle = (N_{\mathbf{K}})^{1/2}$.

The matrix element of Eq. (3.4) is then a product of three factors: P_{mn} for the y- and z-dependent factors of the electron wave functions, $\mp(N_{\mathbf{K}} \pm 1)^{1/2}$ for the phonon amplitudes, and $\delta_{q_x - q_x' \mp k_x}$ from the orthonormality of the x-dependent factor of the electron wave function. The matrix element for a given phonon mode may then be written as

$$M^{\{e\}}_{m,n} = \mp 2\alpha' \frac{\delta_{q_x - q_x' \mp k_x}}{\left[k_x^2 + \left[\frac{m\pi}{L_y}\right]^2 + \left[\frac{n\pi}{L_z}\right]^2\right]^{1/2}} \times 2P_{mn}(N_{\mathbf{K}} + \tfrac{1}{2} \pm \tfrac{1}{2})^{1/2} . \tag{3.6}$$

The total transition rate $1/\tau^{\{e\}}_{1D}(q_x)$ for electron–LO-phonon scattering is obtained by first summing Eq. (3.6) over the continuous values of k_x and the discrete values of k_y and k_z, by then multiplying by the quantum-wire volume V, and finally by substituting the resulting expression in Eq. (3.3):

$$\frac{1}{\tau^{\{e\}}_{1D}(q_x)} = \frac{|\alpha'|^2 V}{4\pi^2 \hbar} (N_{\mathbf{K}} + \tfrac{1}{2} \pm \tfrac{1}{2}) \times \int_{-\infty}^{+\infty} dk_x I_{1D}(k_x, L_y, L_z) \times \delta(E(q_x \pm k_x) - E(q_x) \pm \hbar\omega) , \tag{3.7a}$$

where

$$I_{1D}(k_x, L_y, L_z) = \frac{(2\pi)^2}{L_y L_z} \left| \sum_{m=1,3,5,\ldots} \sum_{n=1,3,5,\ldots} \frac{4P_{mn}}{\left[k_x^2 + \left[\frac{m\pi}{L_y}\right]^2 + \left[\frac{n\pi}{L_z}\right]^2\right]^{1/2}} \right|^2 . \tag{3.7b}$$

The dominant contribution to the sum over phonon modes in Eq. (3.7b) is made by the mode with $m = n = 1$; this conclusion follows from the relations $P_{13} = \frac{1}{5}P_{11}$, $P_{33} = \frac{1}{25}P_{11}$, and for any remaining allowed combination of i and j, $P_{ij} \leq \frac{1}{35}P_{11}$.

For the cases of phonon emission (e) and absorption (a), Eq. (3.7a) may be expressed in a more convenient form by replacing the argument of the δ function by

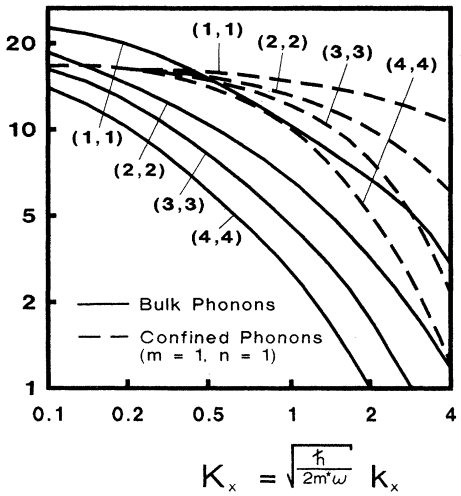

FIG. 1. $I_{1D}^{(0)}$ of Eq. (4.1) is displayed as a function of K_x for four pairs of $(L_y/L_0, L_z/L_0)$, where $L_0=[\hbar/(2m^*\omega)]^{1/2}$. $I_{1D}^{(0)}$ is displayed using dashed lines for four pairs: (1,1), (2,2), (3,3), and (4,4). The values of I_{1D} calculated in Ref. 3 are displayed for the same values of $(L_y/L_0, L_z/L_0)$; solid lines are used to display the results of Ref. 3.

$(k_x-k_+^{\{a\}})(k_x-k_-^{\{a\}})$, where

$$k_\pm^{\{a\}}=\epsilon q_x \pm \left[q_x^2-\epsilon\left[\frac{2m^*\omega}{\hbar}\right]\right]^{1/2}, \tag{3.8}$$

$\epsilon=+1$ for emission, and $\epsilon=-1$ for absorption. Integrating Eq. (3.7a) over k_x and using Eq. (2.5b) to eliminate α' yields

$$\frac{1}{\tau_{1D}^{\{a\}}(q_x)}=\frac{\alpha\omega}{2\pi}\left[N_K+\frac{1+\epsilon}{2}\right]\frac{I_{1D}(k_+^{\{a\}})+I_{1D}(k_-^{\{a\}})}{\sqrt{E/\hbar\omega-\epsilon}}, \tag{3.9a}$$

where

$$\alpha=\frac{1}{2}\frac{e^2}{(\hbar/2m^*\omega)^{1/2}}\left[\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right]\Big/\hbar\omega, \tag{3.9b}$$

$$E=\hbar^2 q_x^2/2m^*. \tag{3.9c}$$

IV. DISCUSSION

Equation (3.9a) gives the total scattering rate for emission (e) or absorption (a) of LO phonons. It is instructive to compare I_{1D} of Eq. (3.7b) with the results of Leburton.[3] In particular, for scattering to or from the lowest mode $(m=n=1)$,

$$I_{1D}^{(0)}=\frac{64(8/3\pi)^4}{(L_y/L_0)(L_z/L_0)[(K_x/\pi)^2+(L_0/L_y)^2+(L_0/L_z)^2]}, \tag{4.1}$$

where $K_x=k_xL_0$ and $L_0=(\hbar/2m^*\omega)^{1/2}$. In Fig. 1, dashed lines are used to display $I_{1D}^{(0)}$ as a function of K_x for several values of the pair $(L_y/L_0, L_z/L_0)$; namely, the pairs are (1,1), (2,2), (3,3), and (4,4). The results of Leburton are displayed on Fig. 1 as solid lines for the same pairs. Figure 1 illustrates that the magnitude of I_{1D} is at least one half of its value at $K_x=0$ unless $K_x \gtrsim \pi[(L_0/L_y)^2+(L_0/L_z)^2]^{1/2}$; for small K_x the discrete values of k_y and k_z control the magnitude of $I_{1D}^{(0)}$. For selected values of K_x, inclusion of the modes corresponding to P_{13} and P_{31} can lead to values of $I_{1D}^{(0)}$ nearly a factor of 2 larger than those of the corresponding $I_{1D}^{(0)}$. Equation (3.7b) illustrates clearly the extreme importance of the mode corresponding to P_{11}; by comparison, electron scattering with the mode corresponding to P_{13} or P_{31} is described by a value of $I_{1D}^{(1)}$ satisfying $I_{1D}^{(1)}<\frac{1}{25}I_{1D}^{(0)}$. While the mode corresponding to P_{11} dominates in the EQL, the higher-order phonon modes can be expected to make larger contributions when the electron wave functions from higher subbands are included.

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