Electron–LO-phonon scattering near a current-carrying core

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Abstract

A calculation is presented on the scattering rates of electrons via the *bulk* spectrum of longitudinal optical phonons near a current-carrying core of radius R employing the Fröhlich interaction Hamiltonian. The electrons are mainly confined near the core by an electric potential and are also under the influence of the current-induced spatially inhomogeneous static azimuthal magnetic field. The external magnetic field lifts the double degeneracy of the non-zero electron's axial wave number (k_z) states, while that of the non-zero azimuthal quantum number (m) states is preserved. In fact, the $k_z < 0$ electron's energy subbands are found to be characterized by minima in their variations with the field. The intrasubband scattering rates show a remarkable behavior in their variations with the field. *First,* for weak electric potential of the nanosystem, these exhibit a strong, nonetheless inharmonic, oscillatory behavior in their variations with the field. The oscillations are, however, smoothed out as the strength of the electrical potential is increased, commencing at lower values of the field, within the same range of values of the field used. *Second,* for the same strength of the electric potential, there arise phase variations of the scattering rates in their variations with the field, resulting from the variation in the electron's axial wave number.

Keywords: Electron–phonon interactions; Azimuthal magnetic field

1. Introduction

There is a great deal of renewed interest in the fundamental properties of electrons in low-dimensional structures, particularly under the influence of a spatially inhomogeneous magnetic field. This interest is in part due to potential device applications relying on the confinement of

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the charge carriers in nanosystems [1–3]. Rudimentary confinement of the charge carriers is due to the walls of electric potential in fabricated nanostructures [4,5], the broad character of which also depends to a large extent on the geometrical symmetry of the quantum system [6, 7]. Additional confinement of electrons in low-dimensional systems is also achievable through the vector potential of an applied magnetic field [8]. One basic fabrication technique that can be employed to tailor a spatially inhomogeneous magnetic field is simply to alter the geometrical shape of the end-face of the core of the electromagnet. A wide variety of confining potentials of spatially modulated magnetic fields have been generated through experimental design, for example, those relying on semiconductor–superconductor boundaries [10–12] or integrating semiconductors with ferromagnetics [13]. As noted by Sim et al. [9], new features of the quantum mechanical properties of the confined charge carriers emerge, these being the signature of the non-uniformity of the applied magnetic field.

The other important factor which also determines the broad character of the confined electrons in low-dimensional systems is the orientation of the applied magnetic field relative to the heterointerface(s) [14,15]. It is well known that even in nanosystems which possess the same geometrical symmetry, the orientation of the applied magnetic field leads to very different conclusions regarding, for example, the nature of the electron's energy spectrum. As is the case here, this has been the main motivating factor for the investigations of the influence of a spatially inhomogeneous azimuthally-directed magnetic field on the charge carriers [14,16].

Now, one of the most important processes in low-dimensional semiconductor materials is scattering of electrons by phonons, particularly LO-polar-optical modes [17]. The phonon spectrum in low-dimensional systems, in part, consists of interface modes, whose amplitudes decay away from the interface and bulk-like confined modes [17]. The total scattering rate, taken to be the sum of the rates due to these two types of phonon modes has, to a good approximation, been found to be equal to the rate calculated using the *bulk* phonon spectrum [18–20]. Clearly, in this simplistic formalism, the contributions of the specific phonon modes to the total scattering rate cannot be evaluated separately. This, however, is possible in the more realistic evaluations; for example, such as as those carried out within the framework of the memory-function formalism [21]. Several of the experimental techniques for probing electron–phonon interactions include spectroscopic measurements [22,23], femtosecond time-resolved differential transmission [24] and polaron cyclotron resonance measurements [25]. Indeed, the resonant magnetopolaron effect has proved to be a useful experimental tool as a means for determining the relative strengths of interactions of specific phonon modes [25].

The aim of the investigations undertaken here is to evaluate the scattering rates arising from the interactions between *bulk* longitudinal optical (LO) phonon modes and electrons confined near a current-carrying core. As stated earlier, the main motivation for these investigations rests on the novel features of the system studied. These include the spatial inhomogeneity of the external magnetic field as well as its orientation relative to the interface of the nanostructure. The layout of this paper is as follows. Section 2 is a brief description of the system studied as well as a resume of the electron's eigenstates and eigenvalues. The general formalism for the calculations of electron–LO-phonon scattering rates in systems with cylindrical symmetry is outlined in Section 3. Finally, the conclusions are contained in Section 4.

2. The electron's eigenstates

The system studied here consists of a current I of uniform density passed along the axis of an infinitely long cylindrical core of arbitrary radius R ideally fashioned out of high-temperature superconducting material [14,16]. Note that high magnetic fields can be generated by passing a large current through a superconducting core while circumventing the Joule heating effect. The current-carrying core is then thought to be enveloped by a thick semiconductor which is also the host material for the electrons. However, the motion of the charge carriers is restricted to the region very much near the core by a confining electric potential of the host material, of the form

$$V(\rho) = \infty \quad \text{for } \rho < R$$
$$V(\rho) = \frac{1}{2}\mu\omega_o^2(\rho^2 - R^2) \quad \text{for } \rho \geq R, \tag{1}$$

where ω_o, a measure of the strength of the electric potential, is the angular frequency of a classical simple harmonic oscillator of mass μ, taken to be the same as the effective mass of an electron. This form of the electric potential, which can be tailored through the technique of doping, resembles somewhat the true potential of a heterojunction formed between AlGaAs and GaAs [26]. The vector potential of the current-induced spatially inhomogeneous external magnetic field, $\mathbf{B} = \mu_o I\hat{\phi}/(2\pi\rho)$, is taken in the gauge:

$$A_z = -\frac{1}{2}B_s R[1 + 2\ln(\rho/R)], \tag{2}$$

where $B_s = \mu_o I/(2\pi R)$ is the value of the magnetic field at the surface of the core. Clearly, a spatially inhomogeneous magnetic field cannot be uniquely described in terms of the cyclotron parameters of the radius and frequency, analogous to that of a static uniform magnetic field. This then raises the question of what scaling parameters should be used more so that the electron's orbits are not closed for a wide range of the relevant parameters [14] but are found to be predominantly snake-like in character [9,27,28]. Nevertheless, it is convenient to define a fictitious "cyclotron radius", $a_{cs} = (\hbar/eB_s)^{1/2}$, and a fictitious "cyclotron frequency", $\omega_{cs} = eB_s/\mu$, in terms of the value of the magnetic field at the surface of the core. In the usual notation, e is the electronic charge and $\hbar = h/2\pi$, in which h is Planck's constant. Now, in view of the symmetry of the problem posed here, the solution of the single-electron Schrödinger equation is sought in the general form:

$$\psi = C_{m\ell}\exp(\mathrm{i}k_z z)\exp(\mathrm{i}m\phi)\chi(\rho), \quad m = 0, \pm 1, \pm 2\ldots, \tag{3}$$

where $C_{m\ell}$ is a normalization constant, k_z is the axial component of the electron's wave vector, and ℓ and m are the radial and azimuthal quantum numbers, respectively. It is not possible, in particular, because of the logarithmic terms, to cast the full Schrödinger equation for the radial function $\chi(\rho)$ into a canonical form. However, solutions can be found in closed form if the logarithmic terms appearing in the full wave equation are replaced by their linear fitting forms [16]:

$$\ln x \approx c_1 + c_2 x \quad \text{and} \quad \ln^2 x \approx d_1 + d_2 x. \tag{4}$$

The constant factors c_i and $d_i (i = 1 \text{ or } 2)$, which depend on the range of the values of x used, are simply read off the computer using standard graphical software packages. With the logarithmic terms now replaced by their approximate linear graphical fittings, the substitution

$$\chi = \zeta^{|m|/2}\mathrm{e}^{-\zeta/2}\mathcal{F}, \tag{5}$$

where

$$\zeta = [d_2 + 4\omega_o^2/\omega_{cs}^2 + 2c_2(1 + k_z R/f_{cs})]^{1/2} \times \rho^2/2a_{cs}^2, \tag{6}$$

leads to

$$\zeta \frac{d^2\mathcal{F}}{d\zeta^2} + (b-\zeta)\frac{d\mathcal{F}}{d\zeta} - a\mathcal{F} = 0, \tag{7}$$

which is the canonical form of Kummer's equation for the confluent hypergeometric function. The solution of Eq. (7) which is well behaved within the region of interest; $1 \le \rho/R < \infty$ is $\mathcal{F} = U(a, b, \zeta)$, the specific relevant parameters a and b of which are given by

$$a = \frac{1}{2} + \frac{1}{2}|m| + \frac{1}{4}\beta \quad \text{and} \quad b + |m| + 1, \tag{8}$$

where

$$\beta = \frac{[k_z^2 R^2/f_{cs} - 4E_{m\ell}/\hbar\omega_{cs} + (1 - 4\omega_o^2/\omega_{cs}^2 + 2c_1 + d_1) f_{cs} + 2(1+c_1)k_z R]}{[d_2 + 4\omega_o^2/\omega_{cs}^2 + 2c_2(1 + k_z R/f_{cs})]^{1/2}}. \tag{9}$$

In the above equations, $E_{m\ell}$ is the confinement energy of the electron and the dimensionless variable, $f_{cs} = R^2/2a_{cs}^2$ represents the applied magnetic field. The electron's total energy E_{Tot} is given by

$$E_{\text{Tot}} = E_{m\ell} + \frac{1}{2\mu}\hbar^2 k_z^2, \tag{10}$$

in which the second term, henceforth denoted as E_{k_z}, is the axial kinetic-like energy. The other convenient scaling parameter for later use, which nonetheless has no physical meaning, is the fictitious energy $E(R) = \hbar^2/(2\mu R^2)$. Now, the application of the standard boundary condition, that of continuity of the wave function at the surface of the core $\rho = R$, leads to the following eigenvalue equation for the determination of the electron's subband energies:

$$U(a, b, \zeta_R) = 0, \tag{11}$$

where ζ_R is given by Eq. (6) but with the replacement: $\rho = R$. Just like in the analysis of a two-dimensional system in a magnetic field [27], the quantity $k_z R$ may be regarded as the center of the electron's orbital motion which, for convenience here, is taken to be located in the plane exactly containing the axis of the core. Note that the external azimuthal magnetic field tends to project the electron's orbital motion onto a plane parallel to the core axis. This means that for a given value of the strength of the electric potential, the electron's wave functions and therefore the corresponding probability densities should be concentrated in a narrow channel near the surface of the core. There can hardly be any significant variations, therefore, of the expectation value of the radial distance for a wide range of the other relevant parameters of the system. The following result for the electron's energy subbands, obtained from employing the linear perturbation theory, should then be helpful in the interpretation of the numerical solutions of Eq. (11):

$$\langle E_{\text{Tot}}(B)\rangle = \langle E_{m\ell}(0)\rangle + E_{k_z} + \frac{1}{2}\hbar\omega_{cs}k_z R\langle[1 + 2\ln(\rho/R)]\rangle + \frac{1}{16}\frac{\hbar^2\omega_{cs}^2}{E(R)}\langle[1 + 2\ln(\rho/R)]^2\rangle, \tag{12}$$

where $\langle Q\rangle$ denotes a quantum mechanical expectation value of the quantity Q. In particular, $E_{m\ell}(0)$ is the zero-field electron's subband confinement energy. A more detailed discussion of

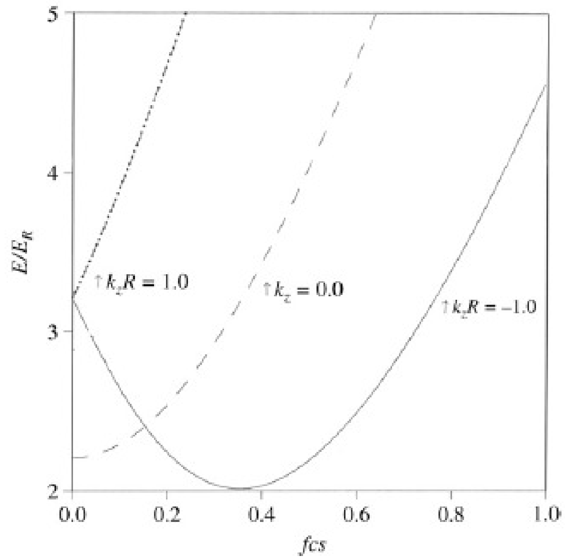

Fig. 1. The variations of the lowest-order ($\{m = 0, \ell = 1\}$) single-electron scaled energy subbands; $E_{01}/E(R)$, with the field $f_{cs} = R^2/2a_{cs}^2$. The key relevant parameters are: $\Omega = \hbar\omega_o/E(R) = 1.0, k_z = 0.0$ for the dashed curve and $k_zR = \pm 1.0$ for the thick broken curve and the smooth solid curve (with a minimum), respectively.

the electron's energy spectrum of this system is given in an earlier investigation [16] and is therefore not repeated here for brevity.

Fig. 1 shows the variations of the lowest-order ($m = 0, \ell = 1$) scaled electron's total energies; $E_{\text{Tot}}/E(R)$, with the field, f_{cs}. The smooth dashed curve corresponds to $k_z = 0.0$ whereas the thick broken curve and the smooth solid curve (characterized by a minimum) correspond to $k_zR = \pm 1.0$, respectively. The other relevant parameters used are as follows: $c_1 = -0.11, c_2 = 0.37, d_1 = -0.85$ and $d_2 = 0.67$, corresponding to the range $1 \leq \rho/R \leq 15$ of the radial distance. The numerical value of the effective mass of the electron, relevant to the system of GaAs, is taken to be roughly 0.067 times that of the free electron and the strength of the electric potential is such that $\Omega = \hbar\omega_o/E(R) = 1.0$. Note that these are universal curves for the electron's energies, that is, for any radius of the core. In fact, both axes scale as R^2. As may easily be anticipated from the inspection of Eq. (12), the energy subbands corresponding to $k_z \geq 0$ increase monotonically with the increase of the field. The azimuthal applied magnetic field, however, lifts the double degeneracy of the $k_z \neq 0$ energy subbands. In particular, the $k_z < 0$ energy subbands initially decrease in energy and attain minima in their variations with the field. The condition for obtaining minima of the $k_z < 0$ energy subbands, based on the result obtained from the perturbation theory, that is, Eq. (12), may be cast as follows

$$\pi B_s < \rho^2 > \simeq \frac{\langle [1 + 2\ln(\rho/R)] \rangle}{\langle [1 + 2\ln(\rho/R)]^2 \rangle} \times \phi_o |k_z| R \sim \phi_o |k_z| R, \tag{13}$$

where $\phi_o = h/e$ is the elementary flux quantum. A paradoxical interpretation of Eq. (13) above is that minima of the $k_z < 0$ energy subbands occur whenever k_zR elementary fluxes are enclosed within the electron's fictitious cyclotron radius, a_{cs}. Physically, this corresponds to particular values of ω_o, B_s and k_z for which the corresponding electron's wave function is least perturbed by the walls of the constriction formed by the walls of the overall electric potential.

It is worth commenting that the electronic states of the system considered here are truly quasi-one-dimensional. This is because although the host material is a bulk sample, the motion of the electrons is restricted to within the constriction formed by the walls of the overall electric potential.

3. Electron–LO-phonon scattering rates

The two processes associated with the electron–phonon interaction considered here are annihilation or creation of a *bulk* phonon of wave vector $\mathbf{q}$, with axial (q_z) and off-axial (q_r) components such that $q^2 = q_r^2 + q_z^2$. Either of these processes is accompanied by a change of state of the electron, from the initial $|m, \ell, k_z>$ to the final $|m', \ell', k_z'>$. For these processes occurring in quasi-one-dimensional systems, overall conservation of the axial momentum is prescribed by $k_z' = k_z + q_z$ and $k_z' = k_z - q_z$ for absorption and for emission of a phonon, respectively. Here, it is assumed that the interaction of electrons with LO-phonon modes is described by the Fröhlich interaction Hamiltonian, given by [29]:

$$H_{\text{int}} = \sum_q C(q)[\mathbf{a}_q \exp(\mathrm{i}q.\mathcal{R}) + \mathbf{a}_q^{\dagger} \exp(-\mathrm{i}q.\mathcal{R})], \tag{14}$$

where $\mathbf{a}_q$ and $\mathbf{a}_q^{\dagger}$ are the phonon creation and annihilation operators, respectively, $\mathcal{R}$ is the position vector and $C(q)$ is a coupling factor, which for LO phonons, is given by

$$C(q) = \frac{\mathrm{i}}{q}[(\mathrm{e}^2\hbar\omega_L/2\varepsilon_o V_{\text{eff}})(\varepsilon_\infty^{-1} - \varepsilon_s^{-1})]^{1/2}, \tag{15}$$

in which ε_o is the permittivity of free space and V_{eff} is the effective volume of the crystal. Note that the volume of the core V_{core} is insignificantly small compared to that of the bulk host material: $V_C = V_{\text{eff}} + V_{\text{core}}$, hence to a very good approximation $V_{\text{eff}} = V_C$. The other parameters relevant to the system of GaAs are the high- and low-frequency dielectric constants $\varepsilon_\infty = 10.9$ and $\varepsilon_s = 13.1$, respectively. Finally, ω_L is the LO-phonon zone-center frequency, such that $\hbar\omega_L = 36.6$ meV [31]. As mentioned earlier, the system considered here is an addition to the configurations of interest for the evaluations of the interaction of electrons with LO phonons. The expressions for the scattering rates for this system are exactly the same as those of earlier similar investigations in systems with cylindrical symmetry [30–32] and are therefore not given here explicitly to avoid unnecessary repetition. In particular, the expressions for the emission intrasubband scattering rates possess a singularity when the electron's axial kinetic-type energy exactly matches the LO-phonon energy quantum. As anticipated, therefore, the scattering rates exhibit a divergent behavior whenever $E_{k_z} = \hbar\omega_L$; a feature attributable to the one-dimensional electron's density of states. Numerical results of these investigations are illustrated only for intrasubband scattering and for transitions within the lowest $\{m = 0, \ell = 1\}$ energy subband. The depth of the discussions of the results for the scattering rates is somewhat limited in view of the obvious gross assumptions made as well as the rather simplistic numerical analysis given here.

Fig. 2 shows the variations of the room temperature, $T \sim 300$ K, scaled intrasubband $(m = 0, \ell = 1)$ emission scattering rates; Γ^{em}/Γ_o, with the field and corresponding to $E_{k_z}/E(R) = k_z R = \pm 1.01$ for the thick broken curves and the smooth solid curves, respectively. The relative strengths of the electric potential are such that: (a) $\Omega = 2.0$, (b) $\Omega = 4.0$ and (c) $\Omega = 6.0$. It is seen from this series of graphs that for low values of Ω, the scattering rates

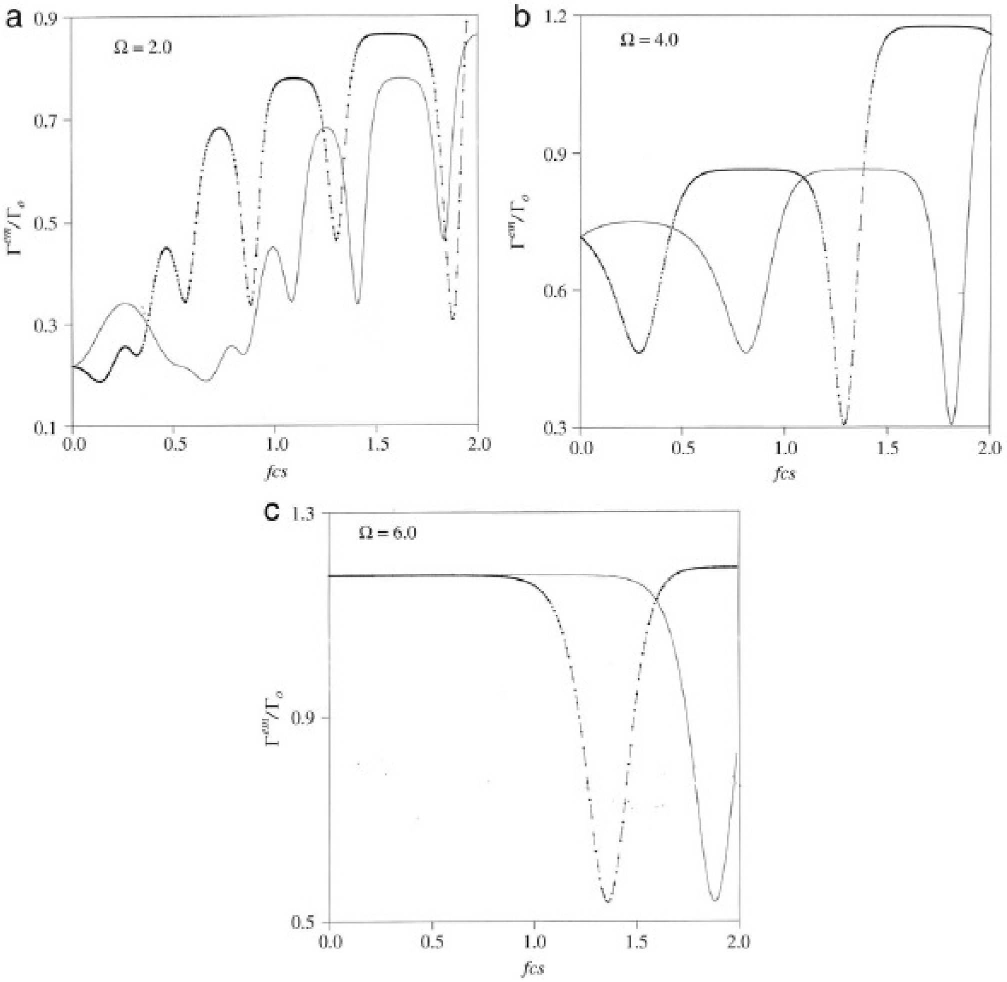

Fig. 2. The variations of the room temperature, $T \sim 300\ K$, intrasubband emission scattering rates ($m = 0$, $\ell = 1$) with the field corresponding to (a) $\Omega = 2.0$, (b) $\Omega = 4.0$ and (c) $\Omega = 6.0$. In each of this set of graphs; (a) to (c); the thick broken curves are for $k_z R = 1.0$ and the solid smooth curves are for $k_z R = -1.0$.

are characterized by very strong oscillations, nonetheless inharmonic, in their variations with the field. This behavior of the scattering rates is closely related to the general geometrical character of the corresponding scattering integrals; a characteristic believed to be an intrinsic property of the system considered [32]. As appreciated in earlier investigations [32], the intrasubband scattering integrals are oscillatory functions of the phonon radial wave number, nevertheless, enveloped by a rapid decay of their amplitudes. The onset of these oscillations occurs at smaller values of the phonon radial wave number, concurrent with the emergence of prominent amplitude modulation of the scattering integrals for a large radius of the core. It should also be noted that this behavior is in stark contrast to the corresponding results of a solid cylinder [31]. Again, as seen from a series of these figures, these oscillations are wiped out as the strength of the electric potential is increased. In fact, for large values of Ω, and within the same range of the field, these oscillations are completely wiped out. This means that in this regime of strong electric potential confinement, the functional form of the scattering rates becomes insensitive to variations of the field. It is also noted that for the same strength of the electric potential, different values of k_z used, both in magnitude and sign (positive or negative), lead to variations of phases of the scattering rates in their variations with the field. Note that for any value of the strength of the electric potential, the scattering rates remain finite in the limit of no hole, that is, as R tends to zero. Loosely speaking, this implies that overall the scattering rates increase as the radius of the core decreases. Again, this feature is believed to be an intrinsic property of the system studied here. Note, as may easily be anticipated, the double degeneracy of the scattering rates shown here, in the absence of the azimuthal applied magnetic field. The variations of the corresponding results for the absorption rates with the field are exactly the same as those for emission rates hence these (absorption rates) are not shown here for brevity. As a final worthy comment, in the experimental investigations corresponding to the theory presented here, specific values of k_z (and therefore E_{k_z}), can be selected by the "tuning" of an electric field applied in the axial direction [33].

4. Conclusions

A resume was given of the energy spectrum of an electron confined near a current-carrying core as functions of the azimuthal external magnetic field and the electric potential within the effective-mass approximation. A further analysis involved the evaluations of the interactions of electrons with the *bulk* LO-phonon spectrum based on the Fröhlich interaction Hamiltonian. The azimuthal external magnetic field was found to lift the double degeneracy of the $k_z \neq 0$ energy subbands while that of the $m \neq 0$ states is preserved. The situation is the other way around in the case of a parallel applied magnetic field. In fact, there is reciprocity correspondence between m and k_z in respect of the direction of the applied magnetic field. The Zeeman splitting is such that $k_z > 0$ energy subbands increase monotonically with the increase of the field. However, the $k_z < 0$ energy subbands initially decrease and attain minima in their variations with the field, at fields such that $\sim |k_z|R$ elementary flux quanta are enclosed within the electron's fictitious cyclotron radius. The $(m = 0, \ell = 1)$ intrasubband scattering rates were found to possess strong, although inharmonic, oscillations in their variations with the field, particularly for weak confinement of the electric potential of the system. Although based on a rather simplistic analysis, the results presented here are suggestive of considerable enhancement of the emission intrasubband scattering rates for a tiny radius of the core. This peculiar result points towards possibilities of attainment of high intrasubband scattering rates in three-dimensional systems which host well characterized cylindrical nanoheterojunctions. As a final comment, it is hopeful that the corresponding experimental investigations will be undertaken in the near future. This is in view of the relentless search for superconducting materials at increasingly higher temperatures and the advances in fabrication technologies to produce very fine wires, including carbon nanotubes.

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