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Cyclotron resonance of a magnetopolaron in quantum well wires

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Abstract. The cyclotron resonance of magnetopolaron in quantum well wires (QWWs) has been studied with the use of variational solutions to the effective-mass equation. The results that we obtained show that both the absolute value of the electron–phonon interaction energy and the cyclotron resonance frequency decrease with increase in the sizes of the QWWs, and also that the cyclotron resonance frequency increases with increase in the external magnetic field.

1. Introduction

With the recent advances in the technique of molecular beam epitaxy, it has been possible to confine electrons in extremely thin semiconducting wires, namely quantum well wires (QWWs), with dimensions in the nanometre range. In these quasi-one-dimensional structures, the electron motion along the length of the wire is free but it is quantized in the two dimensions perpendicular to the wire. Much theoretical and experimental interest has been devoted to the study of the electronic properties of these one-dimensional semiconductor systems [1–3]. Recently, Degani and Hipolito [4] have calculated the binding energies of excitons in QWWs of GaAs surrounded by $Ga_{1-x}Al_xAs$ with the use of variational solutions to the effective-mass equation. They showed that the energies were dramatically dependent on the sizes of the wires, and also that their magnitudes were greater than those in comparable quasi-two-dimensional quantum-well structures. For quasi-two-dimensional quantum-well structures, the cyclotron resonance of magnetopolaron has been studied extensively [5–8]. Gu *et al* [9] have investigated the properties of a magnetopolaron at absolute zero temperature in a two-dimensional semiconductor quantum well. Wei *et al* [10] have discussed the properties of a magnetopolaron at a finite temperature in a two-dimensional semiconductor quantum well. By using the Green function approach, Sarma and Madhukar [11] made a formal calculation to investigate the Landau-level correction and the magneto-optical anomalies in the resonant region. They showed that the influence of the electron–phonon coupling in a two-dimensional system could lead to a splitting of the cyclotron resonance line when $\omega_c \rightarrow \omega_{LO}$. In their calculation, off-resonance terms in the perturbation theory were neglected. Vasilopoulos *et al* [12] have studied the magnetophonon resonances in a quasi-one-dimensional quantum wire. They were the first to find that the cyclotron resonance frequency decreases with increasing size of the quantum wire.

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In this paper, we have studied the cyclotron resonance of magnetopolaron in QWWs surrounded by a vacuum with the use of variational solutions to the effective-mass equations. Our results show that the cyclotron resonance frequency of the magnetopolaron is very sensitive to the length of the rectangular cross section of QWWs and decreases with increase in the length. Furthermore, the absolute value of the electron–phonon interaction energy decreases with increasing sizes of the QWWs. For the phonon system, we have used the bulk-phonon approximation instead of the combined-phonon modes as discussed by Babiker [13] and Babiker and Ridley [14] for the cases of quantum wells and superlattices. This approximation was recently nicely demonstrated by Hai *et al* [15] for the case of a quantum well. It is expected that similar conclusions hold for quantum wires.

2. Hamiltonian and energy

We consider an electron moving in QWWs with rectangular cross sections, which are made of polar crystals and are surrounded by a vacuum. On the assumption that an external magnetic field $B = (0, 0, B)$ (applied along with QWWs) exists, the motion of the electron, interacting with the bulk LO phonon, is described by the Hamiltonian under the effective-mass approximation:

$$H = H_e + H_{LO} + H_{e\text{-}LO} \tag{1a}$$

where

$$H_e = (P_x + eBy/2c)^2/2m_b + (P_y - eBx/2c)^2/2m_b + P_z^2/2m_b + V_{eff} \tag{1b}$$

$$H_{LO} = \sum_q \hbar\omega_{LO} a_q^+ a_q \tag{1c}$$

$$H_{e\text{-}LO} = \sum_q [\Gamma_q \exp(iq_z z + iQR)\, a_q + HC]. \tag{1d}$$

In the above expressions,

$$\Gamma_q = -i\hbar\omega_{LO}[(2\pi/V)(1/\varepsilon_\infty - 1/\varepsilon_0)e^2/\hbar\omega_{LO}]^{1/2}/q \tag{2a}$$

$$V_{eff} = \begin{cases} 0 & |x| \leqslant L_x/2 \quad \text{and} \quad |y| \leqslant L_y/2 \\ \infty & \text{otherwise.} \end{cases} \tag{2b}$$

The meanings are as follows: $P = (P_x, P_y, P_z)$ is the electron momentum and m_b is the band mass of the electron. The volume of the polar crystal is V and the electron position vector is denoted by $r = (R, z)$. ε_0 and ε_∞ are the static and high-frequency dielectric constants, respectively. a_q^+ and a_q are the creation and destruction operators, respectively, for the optical phonons of wavevector $q = (Q, q_z)$ and frequency ω_{LO}. Γ_q is the Fourier coefficient of the electron–phonon interaction. The cyclotron frequency of an electron with m_b as the bare (band) effective mass is

$$\omega_c = eB/m_b c. \tag{3}$$

In order to eliminate the coordinate z of the electron, we make the transformation

$$H' = U_1^{-1} H U_1 \tag{4a}$$

where

$$U_1 = \exp\left(-i\sum_q q_z z a_q^+ a_q\right). \tag{4b}$$

2.1. The ground-state energy

Because the electron motion along the length of the wire (i.e. the z direction) is free but is quantized in the two dimensions perpendicular to the wire, the trial wavefunction in the ground state may be chosen as

$$\psi_0(x, y, z) = (4/L_x L_y L_z)^{1/2} \cos(\pi x/L_x) \cos(\pi y/L_y) \exp(iq_z z)\, U_2|0\rangle \tag{5a}$$

$$\int_{-L_x/2}^{L_x/2} \int_{-L_y/2}^{L_y/2} \int_{-L_z/2}^{L_z/2} \psi_0^*(x, y, z)\psi_0(x, y, z)\, dx\, dy\, dz = 1 \tag{5b}$$

where we assume that the length L_z of the wire is very large compared with L_x and L_y; so we simply assume L_z to be infinity. U_2 is a unitary transformation which displaces the phonon coordinates:

$$U_2 = \exp\left(\sum_q (f_q a_q^+ - f_q^* a_q)\right) \tag{5c}$$

and $|0\rangle$ is the phonon vacuum state. The functions f_q are to be determined by minimizing the expectation value of the Hamiltonian, i.e. $E_0 = \langle\psi_0|H'|\psi_0\rangle$. We then obtain the ground-state energy in the following form:

$$E_0 = E_{\text{kin}} + E_B + E_{\text{int}} \tag{6a}$$

where

$$E_{\text{kin}} = \hbar^2\pi^2/2m_b L_x^2 + \hbar^2\pi^2/2m_b L_y^2 \tag{6b}$$

$$E_B = e^2B^2(L_x^2 + L_y^2)(\tfrac{1}{6} - 1/\pi^2)/16m_b c^2 \tag{6c}$$

$$E_{\text{int}} = -\frac{e^2 q_{\text{LO}}}{\pi}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right) \int dQ \int dK \frac{|F(Q, K)|^2}{Q^2 + K^2 + q_{\text{LO}}(Q^2 + K^2)^{1/2}} \tag{6d}$$

In the above expressions,

$$F(Q, K) = (4/L_x L_y QK) \sin(L_x K/2) \sin(L_y Q/2) \times \{[1 - (L_x K/2\pi)^2][1 - (L_y Q/2\pi)^2]\}^{-1} \tag{7a}$$

$$q_{\text{LO}} = (2m_b\omega_{\text{LO}}/\hbar)^{1/2}. \tag{7b}$$

E_{kin} is the kinetic energy of the electron. E_B and E_{int} are the magnetic field and the electron–phonon interaction contributions, respectively, to the ground-state energy.

2.2. The first excited-state energy ($L_x \neq L_y$)

In this case, we assume further that $L_x > L_y$; then the trial wavefunction in the first excited state may be chosen as [16, 17]

$$\psi_1(x, y, z) = (4/L_x L_y L_z)^{1/2} \sin(2\pi x/L_x) \cos(\pi y/L_y) \exp(iq_z z)\, U_2|0\rangle \tag{8a}$$

$$\int \psi_1^* \psi_0\, dr = 0 \tag{8b}$$

$$\int \psi_1^* \psi_1\, dr = 1 \tag{8c}$$

where

$$U_2 = \exp\left(\sum_q (f_q a_q^+ - f_q^* a_q)\right). \tag{8d}$$

By minimizing the expectation value of the Hamiltonian, i.e. $E_1 = \langle\psi_1|H'|\psi_1\rangle$, we then obtain the first excited-state energy in the following form:

$$E_1 = E_{\text{kin}} + E_B + E_{\text{int}} \tag{9a}$$

where

$$E_{\text{kin}} = 4\hbar^2\pi^2/2m_b L_x^2 + \hbar^2\pi^2/2m_b L_y^2 \tag{9b}$$

$$E_B = e^2B^2[(L_x^2 + L_y^2)/6 - (L_x^2 + 4L_y^2)/4\pi^2]/16m_b c^2 \tag{9c}$$

$$E_{\text{int}} = -\frac{e^2 q_{\text{LO}}}{\pi}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right)\int \mathrm{d}Q \int \mathrm{d}K \frac{|F(Q,K)|^2}{Q^2 + K^2 + q_{\text{LO}}(Q^2+K^2)^{1/2}}. \tag{9d}$$

In the above expressions,

$$F(Q,K) = (4/L_x L_y QK)\sin(L_x K/2) \times \sin(L_y Q/2)/\{[1-(L_x K/4\pi)^2][1-(L_y Q/2\pi)^2]\}. \tag{10}$$

E_{kin} is the kinetic energy. E_B and E_{int} are the magnetic field and the electron–phonon interaction contributions, respectively, to the first excited-state energy.

2.3. *The first excited-state energy ($L_x = L_y = L$)*

In this case, the first excited state is degenerate; then the wavefunction may be chosen as

$$\psi_1(x,y,z) = (2/L^2 L_z)^{1/2}[\sin(2\pi x/L)\cos(\pi y/L) - \cos(\pi x/L)\sin(2\pi y/L)]\exp(\mathrm{i}q_z z)\, U_2|0\rangle \tag{11a}$$

$$\int \psi_1^* \psi_0 \,\mathrm{d}r = 0 \tag{11b}$$

$$\int \psi_1^* \psi_1 \,\mathrm{d}r = 1 \tag{11c}$$

where

$$U_2 = \exp\left(\sum_q (f_q a_q^+ - f_q^* a_q)\right). \tag{11d}$$

ψ_1 corresponds to the lower state of the first excited state, because the first excited-state energy will be split at this time. By minimizing the expectation value of the Hamiltonian, i.e. $E_1 = \langle\psi_1|H'|\psi_1\rangle$, we can obtain the lower first excited-state energy in the following form:

$$E_1 = E_{\text{kin}} + E_B + E_{\text{int}} \tag{12a}$$

where

$$E_{\text{kin}} = 5\hbar^2\pi^2/2m_b L^2 \tag{12b}$$

$$E_B = e^2 B^2 L^2(\tfrac{1}{3} - 5/4\pi^2)/16 m_b c^2 \tag{12c}$$

$$E_{\text{int}} = -\frac{e^2 q_{\text{LO}}}{\pi}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right)\int \mathrm{d}Q \int \mathrm{d}K \frac{|F(Q,K)|^2}{Q^2 + K^2 + q_{\text{LO}}(Q^2+K^2)^{1/2}}. \tag{12d}$$

In the above expressions,

$$F(Q,K) = (2/L^2 QK)(\sin(LK/2)\sin(LQ/2)[\{1/[1-(LK/4\pi)^2]\} \times \{1/[1-(LQ/2\pi)^2]\} + \{1/[1-(LK/2\pi)^2]\}\{1/[1-(LQ/4\pi)^2]\}] + 2\cos(LK/2)\cos(LQ/2)\{1/[1-(\pi/LK)^2] - 1/[1-(3\pi/LK)^2]\}\{1/[1-(\pi/LQ)^2] - 1/1 - (3\pi/LQ)^2\}). \tag{13}$$

E_{kin} is the kinetic energy. E_B and E_{int} are the magnetic field and the electron–phonon

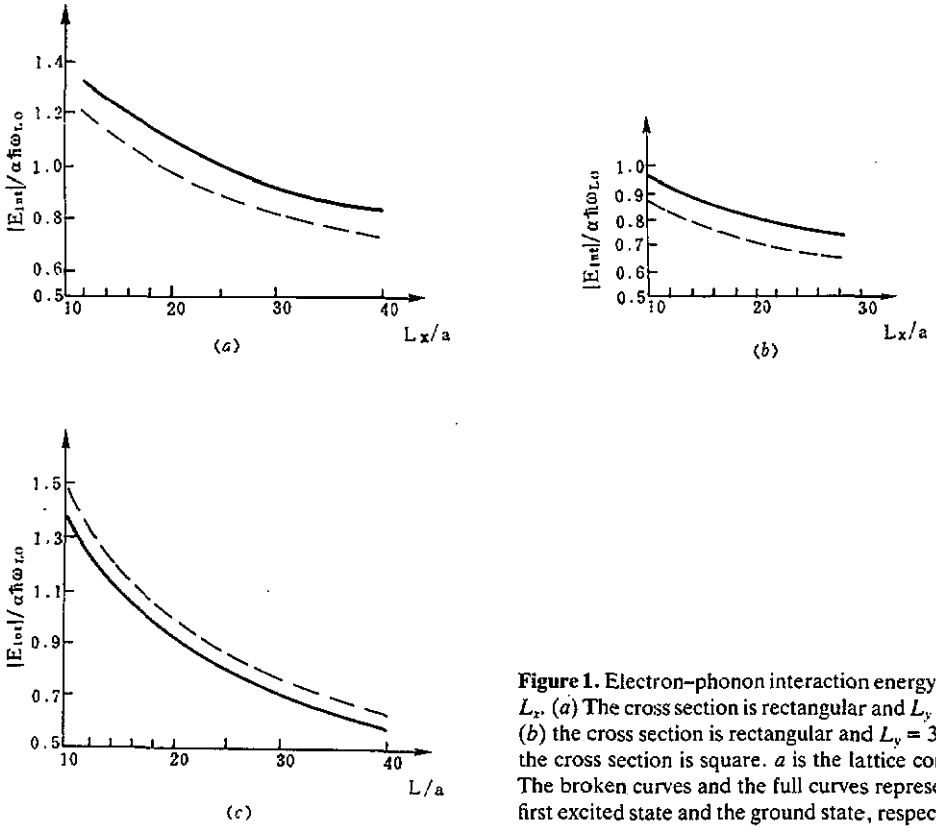

Figure 1. Electron–phonon interaction energy versus L_x. (*a*) The cross section is rectangular and $L_y = 10a$; (*b*) the cross section is rectangular and $L_y = 30a$; (*c*) the cross section is square. a is the lattice constant. The broken curves and the full curves represent the first excited state and the ground state, respectively.

interaction contributions, respectively, to the lower first excited-state energy. Then the cyclotron resonance condition is

$$\omega_c^* = (E_1 - E_0)/\hbar. \tag{14}$$

3. Numerical results and discussion

We choose GaAs as an example to present the numerical results. In the calculations we have used the following parameters: $\varepsilon_0 = 12.83$, $\varepsilon_\infty = 10.9$, $\hbar\omega_{LO} = 36.7$ meV, $a = 5.654$ Å, $m_b = 0.067\, m_e$ and the coupling constant α of the electron-phonon interaction given by $\alpha = 0.0681$. For simplification, the trial wavefunction (equation (5*a*)) has neglected the effect of the external magnetic field; so it is only valid for small magnitudes of the external magnetic field. From the condition that $\hbar\omega_c$ is much less than the size quantization energy, the magnetic field range of the present approach may be estimated to be $B < 0.64$ T).

The curves of E_{int} versus L_x are shown in figure 1. We can see that the absolute value of the electron–phonon interaction energy in the ground state (full curves) or in the first excited state (broken curves) decreases with increase in L_x. As we expect, owing to the decrease in the sizes of QWWs, the electron–phonon interaction becomes stronger; this result is consistent with the results on the quasi-two-dimensional quantum well discussed by Degani and Hipolito [18]. When the cross sections of QWWs are rectangular, the

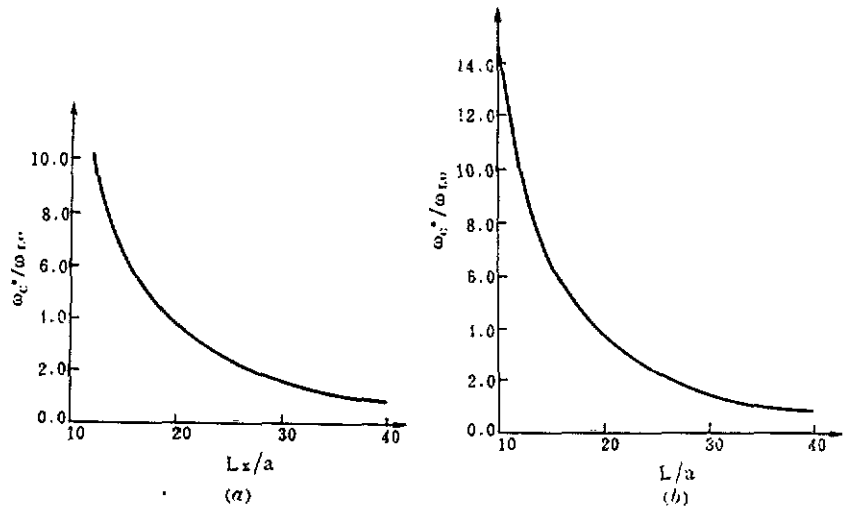

Figure 2. The cyclotron resonance frequency versus L_x, when $B = 0.5$ T. (*a*) The cross section is rectangular and $L_y = 10a$; (*b*) the cross section is square. *a* is the lattice constant.

absolute value of the electron–phonon interaction energy in the first excited state is smaller than that in the ground state, because the electron–phonon interaction energy is negative. Contrary to this, when the cross sections of QWWs are square, the absolute value of the electron–phonon interaction energy in the first excited state is larger than that in the ground state because of the degeneration of the first excited state, which means that the electron–phonon interaction in the first excited state is stronger than that in the ground state. Furthermore, from figure 1, we can see also that, on increase in L_x, the absolute value of the electron–phonon interaction energy decreases more rapidly in the case of a square cross section than in the case of a rectangular section.

The energy difference between the first excited state and the ground state (i.e. the cyclotron resonance energy) versus L_x is shown in figure 2. For the square cross section, the cyclotron resonance frequency decreases with increase in L_x while, for the rectangular cross section, two cases have to be discussed. The first case is that, an increase in the length L_x, the width L_y is constant and is always smaller than the length L_x. The second case is that, an increase in the width L_x, the length L_y is constant and is always larger than the width L_x. In the first case, the cyclotron frequency decreases rapidly with increase in the length L_x while, in the second case, the cyclotron resonance frequency is almost unchanged, because the total energy is decided mainly by the kinetic energy of the electron whose difference between the first excited state and the ground state is independent of the width of the rectangular cross section. These results are in agreement with the early work of Vasilopoulos *et al* [12].

Both the kinetic energy and the electron–phonon interaction energy are independent of the external magnetic field, but the total energy increase with increasing strength of the magnetic field and the curves of cyclotron resonance frequency versus the external magnetic field are parabolic.

From the above results, it is imaginable that the energy spectrum of a moving electron in QWWs can be changed by changing the sizes of QWWs or by changing the strength of the magnetic field. This could offer a theoretical guide to fabricating optical materials and devices.

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