

## The effect of electron-phonon interactions on the cyclotron mass and self-trapping energy of an interface polaron

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1992 J. Phys.: Condens. Matter 4 5087

(<http://iopscience.iop.org/0953-8984/4/22/008>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.159

The article was downloaded on 12/05/2010 at 12:03

Please note that [terms and conditions apply](#).

## The effect of electron–phonon interactions on the cyclotron mass and self-trapping energy of an interface polaron

Hu Zet, Wang You-Tang†, Shi-Wei Gu†‡, T C Au-Yeung§ and Y Y Yeung||

† Applied Physics Department and Institute of Condensed Matter Physics, Shanghai Jiao Tong University, Shanghai 200030, People's Republic of China

‡ CCAST (World Laboratory), Beijing 100080, and International Centre for Material Physics, Academia Sinica, Shenyang 110015, People's Republic of China

§ Applied Mathematics Department and || Applied Physics Department, Hong Kong Polytechnic, Hunghom, Hong Kong

Received 11 December 1991, in final form 5 February 1992

**Abstract.** Employing Haga's perturbation method, we derive an effective Hamiltonian for the interface magnetopolaron in polar crystals at zero temperature, in which the interactions of both bulk longitudinal optical (LO) phonons and interface (IF) phonons have been taken into account. Solving this effective Hamiltonian analytically, we obtain explicit formulae not only for the electron cyclotron mass associated with the Landau levels but also for the self-trapping energy of the magnetopolaron with respect to its first three quantum states in the direction normal to the interface of the system. Numerical results are calculated for some II–VI and III–V compounds, revealing that the effects of the bulk LO phonons and IF phonons on the electron in different quantum states do show different trends.

### 1. Introduction

As we know, an electron moving slowly in the conduction band of a polar crystal will interact with the phonon field produced by the polarization of the crystal lattice, forming a quasi-particle called a 'polaron'. However, fewer people recognize that such electron–phonon interactions will also cause a correction to the Landau levels, which are the harmonic oscillator levels formed in a magnetic field, and renormalize the band mass of the electron, the effects of which are observable in a cyclotron resonance experiment. Over the last few decades, many studies on three-dimensional (3D) polarons have been carried out [1, 2]. With the technological progress in materials science, various quasi-two-dimensional (Q2D) electronic systems have been fabricated (e.g. GaAs–Ga<sub>1-x</sub>Al<sub>x</sub>As and ZnAs–GaSb heterostructures and superlattices; InSb and Cd<sub>1-x</sub>Hg<sub>x</sub>Te metal–oxide–semiconductor structures). Most of the systems concerned are made up of crystals whose electron–phonon interactions are not strong, with the coupling constants being of the order of 0.1. Extensive experimental investigations have subsequently been done on these Q2D systems [3–7], in which the changes in the cyclotron resonance frequency of the electron, caused by the interactions between the phonons and the electron, have been discovered.

Since the electron in a Q2D system is generally confined to a thin layer of 10–100 Å, researchers usually neglect the finite extension of the electron wavefunctions in the direction normal to the surface and regard the system as an ideal 2D one. Moreover, they usually consider only the zero-temperature case. Based on the above-mentioned assumptions, several groups of researchers (see e.g. [8–13]) have employed various methods such as the Green function method, the Feynman path-integral technique and a novel perturbation method to calculate the shifts in the Landau levels and the magneto-optical anomalies due to the interactions between the electron in the resonant region of a 2D system and the bulk longitudinal optical (LO) phonons. Although systematic studies on surface and interface polarons have been performed in the past two decades (see e.g. [14–20]), as yet rather insufficient attention has been paid to surface and interface magnetopolarons in semi-infinite crystals. Recently, one of the authors (Gu Shi-Wei) and his collaborators [21] have made some detailed investigations on the properties of interface magnetopolarons with the generalized Larsen [13] method in the zero-temperature case, and subsequent extension to the finite-temperature case has also been made [22–24].

Despite all these previous works, we stress that the ideal 2D system is basically nothing more than an approximate one for real semi-infinite crystals. In a rigorous treatment, for an electron in systems composed of such crystals, the extension of its wavefunction in the direction perpendicular to the surface or interface cannot be disregarded. Therefore, it is very worth while to calculate the self-trapping energy as well as the cyclotron mass of a polaron with respect to its first three states in the direction normal to the interface of polar–polar crystals using Haga's perturbation method [25]. In our present approach, we consider the roles of both the half-space bulk longitudinal optical (LO) phonons and the interface (IF) phonons, and furthermore bring in an attractive image potential produced by the polarization of the electron clouds of the interface ions. Our work refers to weak and intermediate electron–phonon coupling conditions and an arbitrary magnetic field strength, but temporarily we restrict our discussion to the zero-temperature case. In section 2, we define the Hamiltonian of our system and apply two unitary transformations to it to separate out the perturbation term from the unperturbed term. Using a perturbation method up to second order, we then derive an effective Hamiltonian for the electron in section 3. After solving this effective Hamiltonian, explicit formulae for the electron cyclotron mass, the shift in Landau levels and the self-trapping energy are obtained in section 4. The numerical results for a few II–VI and III–V compounds are also given. The discussions and conclusion are presented in section 5.

## 2. The Hamiltonian

Suppose there are polar crystals 1 and 2 (see figure 1) in the  $z > 0$  and  $z < 0$  half-spaces, respectively, the  $xy$  plane is at their interface and a static uniform magnetic field  $B$  is applied along the  $z$  axis and described by a vector potential in the Landau gauge  $A = B(-y, 0, 0)$ . As the electron moves in crystal 1, i.e. the  $z > 0$  side, so there is a barrier from crystal 2 to it. For simplicity, we suppose that the barrier is infinitely high so that the electron is restricted within crystal 1. In this paper, we simultaneously take into account the interactions between the electron and both the bulk LO phonons in the  $z > 0$  half-space and the IF phonons. Besides, we also include an image potential produced by

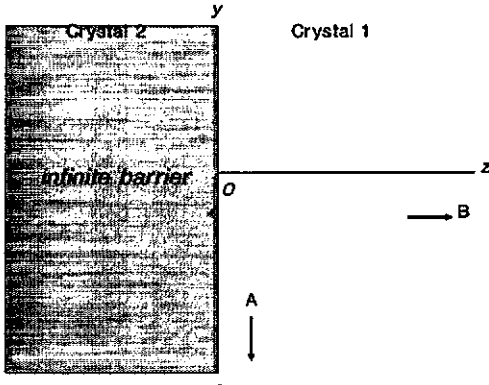


Figure 1. An infinite polar crystal 1 (at  $z > 0$ ) is interfaced with another crystal 2 at the  $xy$  plane. The applied magnetic field  $B$  and its associated vector potential  $A$  are pointing along the  $z$  and  $-y$  directions, respectively.

polarizing the electron cloud of the interface ions. Under the isotropic effective-mass approximation, the Hamiltonian of our system can be written as [21]:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{e-LO} + \mathcal{H}_{e-IF} \tag{1}$$

where

$$\begin{aligned} \mathcal{H}_0 = & \frac{1}{2m_b} \left( \hat{p}_x - \frac{eB}{c} y \right)^2 + \frac{1}{2m_b} \hat{p}_y^2 + \frac{1}{2m_b} \hat{p}_z^2 - \frac{\epsilon_{\infty 2} - \epsilon_{\infty 1}}{4\epsilon_{\infty 1}(\epsilon_{\infty 1} + \epsilon_{\infty 2})} \frac{e^2}{z} + \sum_K \hbar\omega_{LO} \hat{a}_K^\dagger \hat{a}_K \\ & + \sum_q \hbar\omega_{IF} \hat{b}_q^\dagger \hat{b}_q \quad (z \geq 0) \end{aligned} \tag{1a}$$

$$\mathcal{H}_{e-LO} = \sum_K [V_K^* \sin(zK_z) \exp(-i\boldsymbol{\rho} \cdot \mathbf{K}_\parallel) \hat{a}_K^\dagger + \text{HC}] \quad (z \geq 0) \tag{1b}$$

and

$$\mathcal{H}_{e-IF} = \sum_q [C_q^* \exp(-qz) \exp(-i\boldsymbol{\rho} \cdot \mathbf{q}) \hat{b}_q^\dagger + \text{HC}] \quad (z \geq 0) \tag{1c}$$

with

$$V_K^* = \frac{i}{|K|} \left( \frac{4\pi e^2 \hbar \omega_{LO}}{\epsilon V} \right)^{1/2} \tag{1d}$$

$$C_q^* = i \left( \frac{\pi e^2 \hbar \omega_{IF}}{\epsilon^* A |q|} \right)^{1/2} \tag{1e}$$

$$1/\epsilon = 1/\epsilon_{\infty 1} - 1/\epsilon_{01} \tag{1f}$$

$$1/\epsilon^* = 2/(\epsilon_{\infty 1} + \epsilon_{\infty 2}) - 2/(\epsilon_{01} + \epsilon_{02}). \tag{1g}$$

Here the electron has position vector  $(x, y, z)$  with  $\boldsymbol{\rho} = (x, y, 0)$  and momentum  $\mathbf{p} = (p_x, p_y, p_z)$ . The bulk LO phonon wavevector is  $\mathbf{K} = (K_x, K_y, K_z)$  with frequency  $\omega_{LO}$  and projection  $\mathbf{K}_\parallel = (K_x, K_y, 0)$ , whereas  $\mathbf{q}$  is the 2D IF phonon wavevector with frequency  $\omega_{IF}$ . The creation (annihilation) operators of the half-space bulk LO phonon and IF phonon are, respectively,  $\hat{a}_K^\dagger$  ( $\hat{a}_K$ ) and  $\hat{b}_q^\dagger$  ( $\hat{b}_q$ ). The  $V$  and  $A$  in (1d) and (1e) are the volume of crystal 1 and the interface area respectively; and  $\epsilon_{\infty 1}$  ( $\epsilon_{\infty 2}$ ) and  $\epsilon_{01}$  ( $\epsilon_{02}$ ) are the optical and static dielectric constants of crystal 1 (crystal 2), respectively. The chief

Hamiltonian term  $\mathcal{H}_0$  (1a) contains the electron kinetic energy under a magnetic field, the image potential and the energy of the bulk LO phonons and the IF phonons. The electron-bulk LO phonon and the electron-IF phonon interactions are given in (1b) and (1c) respectively.

The relation between the frequency of the bulk transverse optical (TO) phonon and those of the bulk LO phonon and the IF phonon (analogous with the surface optical phonon) have already been given in [21].

Contrary to Larsen's perturbational method used in [21], we presently employ Haga's [25] approach with two successive unitary transformations

$$U_1 = \exp \left[ -i \left( \sum_K \hat{a}_K^+ \hat{a}_K K_{\parallel} + \sum_q \hat{b}_q^+ \hat{b}_q q \right) \cdot \rho \right] \quad (2)$$

and

$$U_2 = \exp \left( \sum_K (\hat{a}_K^+ f_K - \hat{a}_K f_K^*) + \sum_q (\hat{b}_q^+ g_q - \hat{b}_q g_q^*) \right) \quad (3)$$

where the displacement amplitudes  $f_K$  and  $g_q$  are defined as

$$\begin{aligned} f_K &= (-2m_b/\hbar^2) V_K^*/(K_{\parallel}^2 + u_L^2) & u_L &= (2m_b \omega_{LO}/\hbar)^{1/2} \\ g_q &= (-2m_b/\hbar^2) C_q^*/(q^2 + u_I^2) & u_I &= (2m_b \omega_{IF}/\hbar)^{1/2} \end{aligned}$$

acting on equations (1a), (1b) and (1c). We can then eliminate the component  $\rho$  of the electron position coordinates (especially the phase factors  $\exp(-i\rho \cdot K_{\parallel})$  and  $\exp(-i\rho \cdot q)$ ) and obtain the transformed Hamiltonian

$$\mathcal{H}^* = U_2^{-1} U_1^{-1} \mathcal{H} U_1 U_2 = \mathcal{H}_0^* + \mathcal{H}_1^* \quad (4)$$

where

$$\begin{aligned} \mathcal{H}_0^* &= \frac{1}{2m_b} p_y^2 + \frac{1}{2} m_b \omega_c^2 y^2 + \frac{1}{2m_b} p_z^2 - \frac{\epsilon_{\infty 2} - \epsilon_{\infty 1}}{4\epsilon_{\infty 1}(\epsilon_{\infty 1} + \epsilon_{\infty 2})} \frac{e^2}{z} \\ &+ \frac{\hbar^2}{2m_b} \sum_K (K_{\parallel}^2 + u_L^2) (\hat{a}_K^+ \hat{a}_K + f_K^* f_K) \\ &+ \frac{\hbar^2}{2m_b} \sum_q (q^2 + u_I^2) (\hat{b}_q^+ \hat{b}_q + g_q^* g_q) \\ &+ \sum_K 2 \sin(zK_z) V_K^* f_K^* + \sum_q 2 e^{-qz} C_q^* g_q^* \quad (z \geq 0) \end{aligned} \quad (4a)$$

and

$$\begin{aligned} \mathcal{H}_1^* &= \frac{\hbar^2}{2m_b} \sum_K (K_{\parallel}^2 + u_L^2) (f_K^* \hat{a}_K + f_K \hat{a}_K^+) \\ &+ \frac{\hbar^2}{2m_b} \sum_q (q^2 + u_I^2) (g_q^* \hat{b}_q + g_q \hat{b}_q^+) \\ &+ \sum_K (f_K \hat{a}_K^+ + f_K^* \hat{a}_K) \left( \hbar \omega_c K_x y - \frac{\hbar}{m_b} K_y p \right) \end{aligned}$$

$$\begin{aligned}
 & + \sum_q (g_q \hat{b}_q^\dagger + g_q^* \hat{b}_q) \left( \hbar \omega_c q_x \varrho_y - \frac{\hbar}{m_b} q_y p_{\varrho_y} \right) \\
 & + \sum_K [V_K^* \sin(zK_z) \hat{a}_K^\dagger + \text{HC}] + \sum_q (C_q^* e^{-qz} \hat{b}^\dagger + \text{HC}) \\
 & + \text{higher-order terms in } \hat{a}_K^\dagger, \hat{a}_K, \hat{b}_q^\dagger \text{ and } \hat{b}_q \quad (z \geq 0). \tag{4b}
 \end{aligned}$$

We have introduced a new coordinate  $\varrho_y = y - cp_x/eB$  because  $p_x$  commutes with  $\mathcal{H}^*$  and so can be treated as a  $c$  number. The term  $\mathcal{H}_0^*$  is taken as the unperturbed Hamiltonian whereas  $\mathcal{H}_1^*$  can be regarded as a perturbation in the weak and intermediate electron-phonon coupling conditions [25].

### 3. Effective Hamiltonian at zero temperature

In the zero-temperature case, we need only consider the phonon vacuum state  $|0\rangle$  as our ground state and the energy levels of the electron are calculated from a perturbation approach on the average of the transformed Hamiltonian  $\mathcal{H}^*$  over the zero-phonon state  $|0\rangle$ . In other words, those electronic states are obtainable from an effective Hamiltonian defined as [26]

$$\mathcal{H}_{\text{eff}} \equiv \langle 0 | \mathcal{H}_0^* | 0 \rangle + \sum_n \frac{|\langle n | \mathcal{H}_1^* | 0 \rangle|^2}{E_0 - E_n} \tag{5}$$

where  $|n\rangle$  represents the general state occupied by  $n$  phonons.  $E_n$  and  $E_0$  are the energy of the unperturbed states that contain  $n$  phonons and no phonon, respectively. Note that the matrix element for the first-order correction is  $\langle 0 | \mathcal{H}_1^* | 0 \rangle = 0$  and the non-zero matrix elements for the second term of (5) are

$$\begin{aligned}
 \langle 1_K | \mathcal{H}_1^* | 0 \rangle & = (\hbar^2/2m_b) f_K \{ (K_\parallel^2 + u_\perp^2) [1 - \sin(zK_z)] \\
 & + (2m_b/\hbar^2) \omega_c K_x \varrho_y - (2/\hbar) K_y p_{\varrho_y} \} \quad (z \geq 0) \tag{6a}
 \end{aligned}$$

$$\begin{aligned}
 \langle 1_q | \mathcal{H}_1^* | 0 \rangle & = (\hbar^2/2m_b) g_q [(q^2 + u_\parallel^2)(1 - e^{-qz}) \\
 & + (2m_b/\hbar) \omega_c q_x \varrho_y - (2/\hbar) q_y p_{\varrho_y}] \quad (z \geq 0) \tag{6b}
 \end{aligned}$$

and their conjugates, where  $|1_K\rangle$  and  $|1_q\rangle$  stand for the states containing a bulk LO phonon of wavevector  $K$  and an IF phonon of wavevector  $q$ , respectively. Here we have ignored the contributions of the excitation of more than one phonon to the matrix elements. The energy differences between the states relevant to equations (6a) and (6b) are

$$E_{1K} - E_0 = (\hbar^2/2m_b)(K_\parallel^2 + u_\perp^2) \tag{7a}$$

and

$$E_{1q} - E_0 = (\hbar^2/2m_b)(q^2 + u_\parallel^2) \tag{7b}$$

respectively. Putting (6a), (6b), (7a) and (7b) into (5) and converting the summation over wavevectors into integration, it can be shown after some tedious manipulation that the effective Hamiltonian has the following explicit form:

$$\begin{aligned}
 \mathcal{H}_{\text{eff}} & = (1/2m_p^*) p_{\varrho_y}^2 + \frac{1}{2} m_p^* \omega_c^2 \varrho_y^2 + (1/2m_b) p_z^2 - [(\epsilon_{\infty 2} - \epsilon_{\infty 1})/4\epsilon_{\infty 1}(\epsilon_{\infty 1} + \epsilon_{\infty 2})] e^2/z \\
 & - \alpha_L \hbar \omega_{\text{LO}} (\pi/4 - F_L(z)) - \alpha_I \hbar \omega_{\text{IF}} F_I(z) \quad (z \geq 0) \tag{8}
 \end{aligned}$$

where the functions  $F_L$  and  $F_I$  have been defined explicitly in [26].

The first two terms of the expression (8) describe the cyclotron motion of the electron in the  $xy$  plane, which is represented concisely by a single coordinate  $\varpi y = y - cp_x/eB$  introduced earlier. The cyclotron mass  $m_p^*$  and cyclotron resonance frequency  $\omega_c^*$  are given in equation (4a) of [26] and they are dependent on the electron-phonon coupling strength  $\alpha_L$  (for bulk LO phonons) and  $\alpha_I$  (for IF phonons), which are also defined in [26]. However, they are independent of neither the states (see (9b) below) of the electron in the  $z$  direction nor the magnetic field strength, showing that  $m_p^*$  and  $\omega_c^*$  are determined completely by the optical and the static dielectric constants of both crystal 1 and crystal 2. Such a result is quite analogous to that of Liang's [27] studies on the magnetopolaron in a polar crystal slab. The rest of (8) expresses the motion of the electron in the  $z$  direction, and the last two terms, which are the induced potential originated from the interaction between the electron and the phonons, are those determining the self-trapping energy of the electron depending on its states in the  $z$  direction.

#### 4. The solutions and results

To solve the Schrödinger equation pertaining to the effective Hamiltonian  $\mathcal{H}_{\text{eff}}$  in (8), the wavefunction of the electron is written in product form

$$\Psi(\varpi y, z) = g(\varpi y)\varphi(z)$$

where  $g(\varpi y)$  and  $\varphi(z)$  satisfy

$$\left(\frac{1}{2m_p^*}\right)p_{\varpi y}^2 + \frac{1}{2}m_p^*\omega_c^{*2}\varpi y^2 g(\varpi y) = E_{\parallel}g(\varpi y) \quad (9a)$$

$$(\mathcal{H}_z + \mathcal{H}'_z)\varphi(z) = E_{\perp}\varphi(z). \quad (9b)$$

In (9b),

$$\mathcal{H}_z = \left(\frac{1}{2m_b}\right)p_z^2 - [(\epsilon_{\infty 2} - \epsilon_{\infty 1})/4\epsilon_{\infty 1}(\epsilon_{\infty 1} + \epsilon_{\infty 2})]e^2/z - (\pi/4)\alpha_L\hbar\omega_{\text{LO}}$$

and

$$\mathcal{H}'_z = \alpha_L\hbar\omega_{\text{LO}}F_L(z) - \alpha_I\hbar\omega_{\text{IF}}F_I(z).$$

The total energy is therefore  $E = E_{\parallel} + E_{\perp}$ . The Landau levels and the self-trapping energy of the interface magnetopolaron can be acquired by solving equations (9a) and (9b), respectively.

It is quite obvious that (9a) is the wave equation of a harmonic oscillator, whose eigenvalues (Landau levels) and eigenfunctions are

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega_c^* \quad n = 1, 2, \dots$$

and

$$g_n(\varpi y) = N_n \exp(-\lambda^2\varpi y^2/2)H_n(\lambda\varpi y)$$

where  $\lambda = (m_p^*\omega_c^*/\hbar)^{1/2}$ ,  $H_n$  are the  $n$ th-order Hermite polynomials and  $N_n$  are the normalization constants. Note that  $\omega_c^*m_p^* = \omega_c m_b$  and so the shift in the Landau levels is reflected as a renormalization of the band mass  $m_b$ .

As examples, we select some typical II-VI and III-V compounds (as crystal 1) interfaced with  $\text{TiO}_2$  (as crystal 2) for the numerical computation. Those compounds are very common semiconductor materials especially used for fabricating heterostructures and quantum-well devices. The parameters of the materials concerned and

**Table 1.** Parameters of selected materials and cyclotron masses. The interfaced crystal is  $\text{TiO}_2$  whose  $\epsilon_0 = 200$  and  $\epsilon_z = 78$ . Energies are in meV and  $m$  is the free electron mass.

Materials	$\epsilon_0$	$\epsilon_z$	$\alpha_L$	$\alpha_I$	$\hbar\omega_{LO}$	$m_b/m$	$m_p^*/m_b$
ZnSe	8.33	5.90	1.37	0.108	30.5	0.171	2.38
ZnTe	9.86	7.28	1.15	0.111	25.5	0.160	1.98
CdTe	10.23	7.21	0.97	0.094	20.8	0.091	1.72
GaAs	12.83	10.9	0.39	0.054	36.7	0.0657	1.21
GaSb	15.69	14.44	0.261	0.047	29.8	0.047	1.14
InAs	14.61	11.8	0.232	0.035	30.2	0.0342	1.12

the cyclotron mass  $m_p^*$  obtainable from [26] are listed in table 1. The results reveal that the electron cyclotron mass  $m_p^*$  is apparently greater than its band mass  $m_b$ , owing to the interactions between the electron and the bulk LO phonons and the IF phonons. Furthermore, the polarity of the II-VI compounds is stronger than that of the III-V compounds, so the effect of the mass renormalization of the electron in II-V compounds is more obvious.

In equation (9b), the term  $\mathcal{H}_z$  has the wave equation isomorphic to the radial motion of an electron in a hydrogen atom, so we can readily obtain its solutions as follows:

$$E_l = -(m_b \gamma^2 / 2\hbar^2)(1/l^2) - (\pi/4)\alpha_L \hbar\omega_{LO}$$

$$\varphi_l(z) = z\psi_{100}(z) \quad l = 1, 2, 3, \dots$$

where

$$\gamma = [(\epsilon_{\infty 2} - \epsilon_{\infty 1}) / 4\epsilon_{\infty 1}(\epsilon_{\infty 1} + \epsilon_{\infty 2})]e^2$$

and  $\psi_{100}(z)$  is the wavefunction of the electron of the hydrogen atom in the (100) state.

The remaining term in (9b), namely  $\mathcal{H}'_z$ , can be regarded as a perturbation to  $\mathcal{H}_z$  and its first-order energy correction can be partitioned into the bulk LO phonon and the IF phonon parts as follows:

$$\Delta E_l = \langle \varphi_l | \mathcal{H}'_z | \varphi_l \rangle = \Delta E_l^{LO} + \Delta E_l^{IF} \tag{10}$$

where

$$\Delta E_l^{LO} = \frac{1}{2} u_L \alpha_L \hbar\omega_{LO} \iint \frac{\exp(-2K_{\parallel}z)}{K_{\parallel}^2 + u_L^2} |\varphi_l(z)|^2 dK_{\parallel} dz \tag{10a}$$

and

$$\Delta E_l^{IF} = -u_I \alpha_I \hbar\omega_{IF} \iint \frac{\exp(-2qz)}{q^2 + u_I^2} |\varphi_l(z)|^2 dq dz. \tag{10b}$$

Putting the explicit forms of  $\varphi_l(z)$  in (10a) and (10b), we have obtained the analytical expressions for those integrals in the first three principal quantum numbers  $l$  using the partial fraction method for integration, but they are too lengthy and cumbersome to be presented here.

Now, the self-trapping energy  $E_l^{IF}$  of the polaron (in the  $l$ th state of the  $z$  direction) is given by

$$E_l^{IF} = (\frac{1}{2}\pi\alpha_L \hbar\omega_{LO} - \Delta E_l^{LO}) - \Delta E_l^{IF} = E_l^{LO} + E_l^{IF}.$$

The position of the polaron in crystal 1 can be indicated by its mean distance from the



**Table 2.** Self-trapping energies  $E_l^F$  and mean distances  $\bar{z}_l$  from the interface of the polaron in selected materials interfaced with  $\text{TiO}_2$  as well as the first-order bulk LO phonon  $\Delta E_l^{LO}$  and the IF phonon  $\Delta E_l^F$  contributions to  $E_l^F$  for  $l = 1, 2$  and 3. Energies are in meV and distances in Å.

Materials	$l$	$E_l$	$\Delta E_l^{LO}$	$\Delta E_l^F$	$E_l^F$	$\bar{z}_l$
ZnSe	1	-35.86	3.05	-0.557	30.33	127.5
	2	-33.55	1.03	-0.195	31.98	509.9
	3	-33.12	0.82	-0.159	32.16	1147
ZnTe	1	-24.81	1.78	-0.409	21.66	174.2
	2	-23.49	0.63	-0.158	22.56	696.8
	3	-23.24	0.51	-0.136	22.65	1568
CdTe	1	-16.89	1.05	-0.241	15.04	302.8
	2	-16.12	0.40	-0.102	15.55	1211
	3	-15.98	0.34	-0.090	15.60	2725
GaAs	1	-11.5	0.37	-0.129	11.0	697.9
	2	-11.29	0.26	-0.098	11.07	2792
	3	-11.26	0.25	-0.096	11.08	6281
GaSb	1	-6.21	0.15	-0.079	6.039	1419
	2	-6.14	0.12	-0.070	6.055	5675
	3	-6.13	0.12	-0.069	6.057	12770
InAs	1	-5.57	0.15	-0.056	5.41	2210
	2	-5.51	0.13	-0.050	5.423	8839
	3	-5.50	0.13	-0.050	5.424	19890

interface, and in the  $l$ th state of the  $z$  direction, the mean distance is  $\bar{z}_l = \frac{2}{3}l^2a$ , where  $a = \hbar^2/(\gamma m_b)$ . We present in table 2 the numerical results of the self-trapping energy of the interface magnetopolaron in some materials. It is found that, with the increase of  $l$ , the self-trapping energy of the electron in both the II-VI compounds and III-V compounds increases and gradually converges to the limit  $\frac{1}{4}\pi\alpha_L\hbar\omega_{LO}$ . However, such changes in the energy of the electron in the former are much greater than that of the latter because II-VI compounds have stronger polarity than III-V compounds. In addition, it can be concluded that, with the increase of the mean distance of the polaron from the interface, the effects of the IF phonons weaken rapidly whereas the contributions of the bulk LO phonons are increasing. The magnetopolaron can then be treated as a three-dimensional one, disregarding the IF phonon contributions.

## 5. Discussions and conclusion

Using Haga's perturbation method, we have obtained an effective Hamiltonian for the interface magnetopolaron in polar crystals at zero temperature. Although we have assumed that the interface potential barrier is infinitely high, for any finite but high potential wall problem, it has been shown by Lee and Mei [28] that it can be solved approximately as an alternative problem with an infinite wall placed at a small (penetration) distance beyond the original wall. Hence our approach can similarly be adapted for a finite barrier. We have also solved that effective Hamiltonian analytically,

yielding explicit formulae for some interesting physical properties of the interface magnetopolaron, namely, cyclotron mass and self-trapping energy. Our formula for the self-trapping energy includes contributions from the interface phonons as well as the usual bulk LO phonons in a half-space. It is noted that the cyclotron mass of the interface magnetopolaron is mainly related to the optical and static dielectric constants of both crystals but independent of the magnetic field strength and the quantum states  $l$  of the electron in the direction normal to the interface.

For our numerical calculations, several typical II-VI and III-V semiconductor compounds are chosen to be interfaced with the  $\text{TiO}_2$  crystal, which has a very large dielectric constant so that the electron could be attracted much closer to the interface by the image potential and hence the interface phonon effect would be more conspicuous. Our results show that the stronger the polarity of the material, the more apparent the mass renormalization of the electron in the material. However, for the case of self-trapping energy, the stronger polarity  $\epsilon_{\infty 1}$  of crystal 1 will reduce the attractive image potential ( $= -\gamma/z$ ) and so the mean distance  $\bar{z}$  (which is inversely proportional to  $\gamma$ ) will increase, rapidly reducing the contributions of the IF phonons. On the contrary, the contributions from the bulk LO phonons will increase steadily. These two characteristics are in fact very similar to the previous work done by Gu *et al* [21] when they investigated the properties of a magnetopolaron at the interface of polar-polar crystals using Larsen's perturbational method. The same situation will also occur for increasing quantum number  $l$  as  $\bar{z}$  is directly proportional to  $l^2$ . Hence it is quite sufficient to consider the first three states only; thereafter the self-trapping energy will converge rapidly to the limit of  $\frac{1}{4}\pi\alpha_1\hbar\omega_{\text{LO}}$ . Besides, our calculations show that  $\Delta E_l^{\text{IF}}$  and  $\Delta E_l^{\text{LO}}$  in (10) are really small (less than 10%) compared with the first-order term  $E_l$  and this verifies the correctness of our perturbation approach in solving equation (9).

On the other hand, if we focus our interest on the energy level splittings ( $E_{l+1} - E_l$ ) of various quantum  $l$  states, we would find that the IF phonons will give significant contributions ( $\Delta E_l^{\text{IF}}$ ) that are opposite in sign to those of the bulk LO phonons. Furthermore, it is remarked that the calculated energy level splittings of our examples in table 2 are in the energy range of  $0.1$  to  $10 \text{ cm}^{-1}$ , which happen to be measurable by the conventional electron spin resonance technique. It is unfortunate that we could not find any experimental data from the literature to compare with our theoretical values.

## Acknowledgments

This work was partly supported by the Chinese National Natural Science Foundation Grant No. G9188006 and two of us (T C Au-Yeung and Y Y Yeung) would also like to thank the Hong Kong Polytechnic Research Sub-Committee for financial support. Besides this, we are very grateful to Dr W S Li for many valuable discussions.

## References

- [1] Devreese J T 1972 *Polarons in Ionic Crystals and Polar Semiconductors* (Amsterdam: North-Holland)
- [2] Kuper C and Whitfield G 1963 *Polarons and Excitons* (Edinburgh: Oliver and Boyd)  
Devreese J T and Peeters F M 1984 *Polarons and Excitons in Polar Semiconductors and Ionic Crystals* (New York: Plenum)
- [3] Tsui D C, Englert Th, Cho A Y and Gossard A C 1980 *Phys. Rev. Lett.* **44** 341  
Kido G, Miura N, Ohno H and Sakaki H 1982 *J. Phys. Soc. Japan* **51** 2168

- [4] Horst M, Merkt U and Kotthaus J P 1983 *Phys. Rev. Lett.* **50** 754
- [5] Seidenbusch W, Lindemann G, Lassnig R, Edlinger J and Gornik G 1984 *Surf. Sci.* **142** 375
- [6] Horst M, Merkt U, Zawadzki W, Maan J C and Ploog K 1985 *Solid State Commun.* **53** 403
- [7] Sigg H, Wyder P and Perenboom J A A 1985 *Phys. Rev. B* **31** 5253
- [8] Das Sarma S and Madhukar A 1980 *Phys. Rev. B* **22** 2823
- [9] Das Sarma S 1984 *Phys. Rev. Lett.* **52** 859, 1570
- [10] Larsen D M 1984 *Phys. Rev. B* **30** 4595
- [11] Peeters F M and Devreese J T 1985 *Phys. Rev. B* **31** 3689
- [12] Wu X G, Peeters F M and Devreese J T 1985 *Phys. Rev. B* **31** 3420
- [13] Larsen D M 1986 *Phys. Rev. B* **33** 799
- [14] Ibach H 1970 *Phys. Rev. Lett.* **24** 1416; 1971 *Phys. Rev. Lett.* **26** 1543
- [15] Evans E and Mills D L 1972 *Phys. Rev. B* **5** 4126; 1973 *Phys. Rev. B* **8** 4004
- [16] Sak J 1972 *Phys. Rev. B* **6** 3981
- [17] Hipolito O 1979 *Solid State Commun.* **32** 515
- [18] Ueba H 1980 *Phys. Status Solidi b* **100** 705
- [19] Gu S-W and Zhang J 1984 *Phys. Status Solidi b* **121** K165
- [20] Liang X X and Gu S-W 1984 *Solid State Commun.* **50** 505  
Zheng R S, Gu S-W and Lin D L 1986 *Solid State Commun.* **59** 331
- [21] Gu S-W, Kong X J and Wei C W 1987 *Phys. Rev. B* **36** 7977
- [22] Wei B H, Zhou G Z and Gu S-W 1989 *Phys. Rev. B* **40** 7866
- [23] Wei B H, Zhou X J and Gu S-W 1990 *Phys. Rev. B* **41** 1386
- [24] Wei B H and Gu S-W 1991 *Phys. Status Solidi b* **163** 161
- [25] Haga E 1954 *Prog. Theor. Phys.* **11** 449
- [26] Hu Ze, Wang Y-T, Gu S-W, Au-Yeung T C and Yeung Y Y 1992 *Solid State Commun.* **81** 325
- [27] Liang X X 1988 *Phys. Rev. B* **38** 3459
- [28] Lee Y C and Mei W N 1982 *J. Phys. C: Solid State Phys.* **15** L545