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1994 J. Phys.: Condens. Matter 6 1893

(http://iopscience.iop.org/0953-8984/6/10/008)

J. Phys.: Condens. Matter 6 (1994) 1893–1902. Printed in the UK

Properties of an interface polaron in a magnetic field of arbitrary strength

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Received 6 September 1993, in final form 12 October 1993

Abstract. We study the induced potential of an interface electron interacting with bulk longitudinal-optical (BO) phonons as well as interface optical (IO) phonons using the Green-function method. The dependence of the induced potential on the magnetic field strength and on the distance of the electron from the interface is studied. The numerical results show that in weak magnetic fields both $|V_{e-BO}|$ and $|V_{e-IO}|$ are rapidly increasing functions of the magnetic field, but beyond a critical magnetic field B_c, $|V_{e-BO}|$ and $|V_{e-IO}|$ are slowly decreasing functions of the magnetic field. The numerical results also show that the electron–IO phonon interaction is dominant for weak magnetic fields and small electron departure from the interface. In the opposite limit, the electron–BO phonon interaction is dominant.

1. Introduction

With the advent of solid-state device science and technology, there has been increased interest in the properties of a surface or an interface polaron in crystals under the effect of a magnetic field of arbitrary strength. The importance of interface optical phonon modes in the polaron problem was discussed by Mori and Ando [1], and more recently Babiker *et al* [2]. In the past many works on interface magnetopolarons were devoted to the calculation of the ground-state energy and the effective mass of polarons by using the perturbation variational method or path integral approach [1–13]. Few works have studied the interface magnetopolaron by using the more powerful Green-function method. To mention a few, Das Sarma and co-workers [14–16], using the Green-function method, made a formal calculation of the Landau-level correction and optical anomalies in the resonant region for pure two-dimensional (2D) systems.

It is generally accepted that in bulk semiconductors or polar crystals the effective mass of an electron is enhanced by the virtual coupling of a quasi-free electron with bulk longitudinal-optical (BO) phonons. However, for 2D or quasi-two-dimensional (Q2D) systems, our studies [6–8] revealed that the interaction of an electron with interface LO phonons (IO phonons) must be considered in addition to that with BO phonons, especially when the distance between the electron and the interface is comparable to the radius of the polaron, as has been confirmed by experiments.

In this paper, we apply the standard Green-function method to study the effect of electron–phonon interactions on the induced potential of an electron at the interface of

0953-8984/94/101893+10$19.50

polar crystals. Both the BO phonons and IO phonons are included in the study. We present a calculation of the induced potential of the interface polaron for all the Landau levels at arbitrary magnetic field strengths. Our numerical results show that the induced potential of the interface polaron is strongly related to the magnetic field strength and the departure of the electron from the interface. The induced potential first increases with the magnetic field in weak magnetic fields, but beyond a critical field it slowly decreases with the magnetic field at different critical magnetic fields for V_{e-BO} and V_{e-IO} and for various electron departures z from the interface. It is also found that for weak magnetic fields and small departure of the electrons from the interface, the electron–IO phonon interaction is dominant, while in the opposite limit the electron–BO phonon interaction is dominant.

The paper is organized as follows. In section 2 we develop the Hamiltonian of the system and outline the calculation of the induced potential of an electron using the Green-function method. Section 3 contains our numerical results and discussion. A brief summary is presented in section 4.

2. Theory

In this section we limit ourselves to the weak-electron–phonon-coupling system and the zero-temperature case. The electron motion in the direction perpendicular to the interface is described by the lowest subband with the standard variational wave function.

Now we consider an interface polaron in polar–polar crystals. Suppose there are polar crystals 1 and 2 in the $z > 0$ and $z < 0$ semispaces, respectively; the x–y plane is their interface. An electron moves in crystal 1, i.e., the $z > 0$ side, so there is a barrier from crystal 2 to it. Without loss of generality, we assume that the barrier is infinitely high and therefore the electron is restricted within crystal 1. A static uniform magnetic field $\boldsymbol{B} = (0, 0, B)$ is applied along the z direction and described by a vector potential in the Landau gauge $\boldsymbol{A} = B(0, x, 0)$. In this paper we simultaneously take the interactions of an electron with both BO and IO phonons into account. With the isotropic effective-mass approximation the Hamiltonian of the electron–phonon system can be written as follows [8]:

$$H = H_0 + H_\perp \qquad H_1 = H_{e-BO} + H_{e-IO} \tag{1a}$$

$$H_0 = \frac{p_x^2}{2m_b} + \frac{1}{2m_b}\left[p_y + \frac{\beta^2}{2}x\right]^2 + \sum_k \hbar\omega_{BO} a_k^+ a_k + \sum_q \hbar\omega_{IO} b_q^+ b_q \tag{1b}$$

$$H_{e-BO} = \sum_k [V_k^* \sin(zk_z)\exp(-i\rho\cdot k_\parallel) a_k^+ + HC] \tag{1c}$$

$$H_{e-IO} = \sum_q [C_q^* \exp(-qz)\exp(-i\rho\cdot q) b_q^+ + HC] \tag{1d}$$

$$H_\perp = p_z^2/2m_b + e^2(\epsilon_{\infty 1} - \epsilon_{\infty 2})/4z\epsilon_{\infty 1}(\epsilon_{\infty 1} + \epsilon_{\infty 2}) \tag{1e}$$

where

$$\beta^2 = 2eB/c \tag{2a}$$

$$V_k^* = (i/|k|)[(4\pi e^2/\epsilon V)\hbar\omega_{BO}]^{1/2} \qquad C_q^* = (i/|q|)[(\pi e^2/\epsilon^* S)\hbar\omega_{IO}]^{1/2} \tag{2b}$$

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

The coupling constants of the electron with the BO phonons and IO phonons are

$$\alpha_B = (e^2/2\hbar)(2m_b/\hbar\omega_{BO})^{1/2}/\epsilon \qquad \alpha_I = (e^2/2\hbar)(2m_b/\hbar\omega_{IO})^{1/2}/\epsilon^* \tag{3}$$

respectively. The cyclotron frequency of an electron with m_b as the bare band effective mass is

$$\omega_c = eB/m_b c. \tag{4a}$$

The first two terms in (1*b*) represent the kinetic energy of 2D motion of the electron in the x–y plane and the sum is denoted by $H_\parallel$; the third and fourth term are the BO and IO phonon energy, respectively. (1*c*) and (1*d*) are the interaction energy of the interface electron with the BO and IO phonons, respectively. The first term in (1*e*) is the kinetic energy of electron in the z direction and the second term is the attractive image potential. The notation is as follows: the electron position vector is denoted by $r = (\rho, z)$ and $\rho = (x, y)$ is a 2D vector in the x–y plane, $p = (p_x, p_y, p_z)$ is the momentum of the electron. The volume of crystal 1 is V and S is the area of the interface. We denote by $\epsilon_0(\epsilon_\infty)$ the static (optical) dielectric constant; $a_k^+(a_k)$ creates (annihilates) a BO phonon with wave vector $k = (k_\parallel, k_z)$ and $b_q^+(b_q)$ creates (annihilates) an IO phonon with 2D wave vector q. Moreover, ω_{BO} and ω_{IO} stand for the frequency of BO and IO phonons, respectively. We have [8]

$$\omega_{IO}^2 = \omega_{BO}^2\epsilon_{\infty 1}(\epsilon_{01} + \epsilon_{02})/\epsilon_{01}(\epsilon_{\infty 1} + \epsilon_{\infty 2}). \tag{4b}$$

In the weak-electron–phonon-coupling limit, H_I could be treated as a small perturbation. The unperturbed energy corresponding to H_0 is given by

$$E_0 = E_n + \sum_k \hbar\omega_{BO}\langle n_k\rangle + \sum_q \hbar\omega_{IO}\langle n_q\rangle \tag{5}$$

where $E_n = (n + \frac{1}{2})\hbar\omega_c$ is the electron Landau level energy with quantum number n, $\langle n_k\rangle$ and $\langle n_q\rangle$ being the mean number of BO and IO phonons respectively.

By using the Green-function method [17], we calculate the electron-phonon interaction energy. In the Landau representation with a set of quantum number $s \equiv \{n, w_y\}$, we have

$$H_{e\text{–}BO} = \sum_{s,s',k} f_{s's}^*(z, k)C_{s'}^+C_s a_k^+ + \text{HC} \tag{6a}$$

$$H_{e\text{–}IO} = \sum_{s,s',q} f_{s's}^*(z, q)C_{s'}^+ b_q^+ + \text{HC} \tag{6b}$$

where

$$f_{s's}^*(z, k) = \sin(k_z z)V_k^*\langle s'|\exp(-ik_\parallel\cdot\rho|s\rangle \tag{7a}$$

$$f_{s's}^*(z, q) = \exp(-qz)C_q^*\langle s'|\exp(-iq\cdot\rho|s\rangle \tag{7b}$$

where w_y is the electron wave vector in the y direction, that is, $p_y = \hbar w_y$; $C_s^+(C_s)$ is the creation (annihilation) operator for an electron in the state s parametrized by z.

In the limit of weak electron–phonon couplings, it suffices to retain the contribution to the electron proper self-energy part by the lowest-order skeleton diagram. The Matsubara Green functions for a free BO phonon and a free IO are given by

$$\mathcal{D}_{BO}^{(0)}(k, iv_m) = 2\omega_{BO}/\hbar(v_m + \omega_{BO}^2) \qquad \mathcal{D}(0)_{IO}(q, iv_m) = 2\omega_{IO}/\hbar(v_m + \omega_{IO}^2) \tag{8}$$

with $v_m = 2m\pi/\hbar\beta$. The Matsubara Green function for a free electron is given by

$$\mathcal{G}^{(0)}(s, \mathrm{i}\omega_m) = 1/\hbar(\mathrm{i}\omega_m - \omega_s) \tag{9}$$

where $\omega_m = (2m+1)\pi/\hbar\beta$ and $\omega_s = (E_n - \mu)/\hbar\beta$ with chemical potential μ.

By using the standard frequency sum rules in [17], the electron proper self-energy parts corresponding to $H_{\mathrm{e-BO}}$ and $H_{\mathrm{e-IO}}$ are obtained as follows:

$$\sum_{\mathrm{BO}}^{*}(s, z, \mathrm{i}\omega_m) = -\frac{1}{\beta}\sum_{s',k,v_{m'}} \mathcal{G}^{(0)}[s', \mathrm{i}(\omega_m - v_{m'})]|f_{s,s'}(z, k)|^2 \mathcal{D}^{(0)}_{\mathrm{BO}}(k, \mathrm{i}v_{m'})$$

$$= \frac{1}{\hbar}\sum_{s',k}|f_{s,s'}(z, k)|^2\left[\frac{\langle n_k\rangle + \langle n_{s'}\rangle}{\mathrm{i}\omega_m - \omega_{s'} - \omega_{\mathrm{BO}}} + \frac{\langle n_k\rangle + 1 - \langle n_{s'}\rangle}{\mathrm{i}\omega_m - \omega_{s'} - \omega_{\mathrm{BO}}}\right]$$

$$\sum_{\mathrm{IO}}^{*}(s, z, \mathrm{i}\omega_m) = -\frac{1}{\beta}\sum_{s',q,v_{m'}} \mathcal{G}^{(0)}[s', \mathrm{i}(\omega_m - v_{m'})]|f_{s,s'}(z, q)|^2 \mathcal{D}^{(0)}_{\mathrm{BO}}(q, \mathrm{i}v_{m'})$$

$$= \frac{1}{\hbar}\sum_{s',q}|f_{s,s'}(z, q)|^2\left[\frac{\langle n_q\rangle + \langle n_{s'}\rangle}{\mathrm{i}\omega_m - \omega_{s'} - \omega_{\mathrm{IO}}} + \frac{\langle n_q\rangle + 1 - \langle n_{s'}\rangle}{\mathrm{i}\omega_m - \omega_{s'} - \omega_{\mathrm{IO}}}\right]$$

where $\langle n_s\rangle$ is the mean number of electrons. At zero temperature, the mean number of electrons and phonons vanish, that is, $\langle n_k\rangle = \langle n_q\rangle = \langle n_s\rangle = 0$; then the above self-energy part of the electrons reduces to

$$\sum_{\mathrm{BO}}^{*}(s, z, \mathrm{i}\omega_m) = \frac{1}{\hbar}\sum_{s',k}\frac{|f_{s,s'}(z, k)|^2}{\mathrm{i}\omega_m - \omega_{s'} - \omega_{\mathrm{BO}}} \tag{10a}$$

$$\sum_{\mathrm{IO}}^{*}(s, z, \mathrm{i}\omega_m) = \frac{1}{\hbar}\sum_{s',q}\frac{|f_{s,s'}(z, q)|^2}{\mathrm{i}\omega_m - \omega_{s'} - \omega_{\mathrm{IO}}} \tag{10b}$$

and the total proper self-energy part of the electron is given by

$$\sum^{*}(s, z, \mathrm{i}\omega_m) = \sum_{\mathrm{BO}}^{*}(s, z, \mathrm{i}\omega_m) + \sum_{\mathrm{IO}}^{*}(s, z, \mathrm{i}\omega_m). \tag{11}$$

We continue $\mathrm{i}\omega_m$ analytically to the upper half of the complex ω plane and take the form $\omega = (E_n^* - \mu)/\hbar$; then (11) becomes

$$\sum^{*}(s, z, E_n^*) = \sum_{s',k}\frac{|f_{s,s'}(z, k)|^2}{E_n^* - E_{n'} - \hbar\omega_{\mathrm{BO}}} + \sum_{s',q}\frac{|f_{s,s'}(z, q)|^2}{E_n^* - E_n - \hbar\omega_{\mathrm{IO}}}. \tag{12}$$

From Dyson's equation, the retarted Green function is obtained as

$$\mathcal{G}^{\mathrm{R}}(s, z, E_n^*) = \frac{1}{E_n^* - E_n - \Sigma^*(s, z, E_n^*)}. \tag{13}$$

As a result, the electron self-energy shift related to $H_{\|}$ is given approximately by

$$\delta E_n(z) = \Sigma^*(s, z, E_n^*) = V^{(n)}_{\mathrm{e-BO}}(z) + V^{(n)}_{\mathrm{e-IO}}(z) \tag{14}$$

where

$$V_{e-BO}^{(n)}(z) = -\frac{1}{\hbar}\sum_{s',k}\frac{|f_{s,s'}(z,k)|^2}{(n'-n)\omega_c + \omega_{BO}} \tag{15a}$$

$$V_{e-IO}^{(n)}(z) = -\frac{1}{\hbar}\sum_{s',q}\frac{|f_{s,s'}(z,q)|^2}{(n'-n)\omega_c + \omega_{IO}}. \tag{15b}$$

Then we have the effective Hamiltonian

$$H_{n,\text{eff}} = E_n^{(0)} + p_z^2/2m_b + V_{\text{eff}}^{(n)}(z) \tag{16}$$

where the effective potential is

$$V_{\text{eff}}^{(n)}(z) = V_{e-LO}^{(n)}(z) + V_{e-IO}^{(n)}(z) + V_{\text{im}}(z). \tag{17}$$

$V_{\text{im}}(z)$ is the image-potential energy of the electron, which is given in the second term of $H_\perp$. $V_{e-BO}^{(n)}(z)$ and $V_{e-IO}^{(n)}(z)$ are the energies induced by the electron-BO phonon interactions and electron–IO phonon interactions respectively, called the induced potential. It is generally accepted that self-trapping of the magnetopolaron depends entirely on the induced potential.

We now calculate the induced potentials; we use [18]

$$|\langle n|\exp(i\boldsymbol{k}_\parallel\cdot\boldsymbol{\rho})|n'\rangle|^2 = (m!/m'!)\xi_\parallel^{(m'-m)}\exp(-\xi_\parallel)[L_m^{m-m'}(\xi_\parallel)]^2 \tag{18a}$$

$$|\langle n|\exp(i\boldsymbol{q}\cdot\boldsymbol{\rho})|n'\rangle|^2 = (m!/m'!)\zeta^{(m'-m)}\exp(-\zeta)[L_m^{m-m'}(\zeta)]^2 \tag{18b}$$

where $\xi_\parallel = \hbar k_\parallel^2/(2m_b\omega_c)$, and $\zeta = \hbar q^2/(2m_b\omega_c)$. Then we change the sums over $\boldsymbol{k}$ and $\boldsymbol{q}$ in (15*a*) and (15*b*) into integrals. After a tedious but direct calculation, we can obtain the induced potential with the Landau quantum number n as

$$V_{e-BO}^{n} = -\alpha_B\lambda_B\hbar\omega_{BO}\sum_{n'}\int_0^{X_{mB}} dx\frac{V_{mm'}^2(x^2)[1-\exp(-\sqrt{8}zx/l_c)]}{(n'-n)\lambda_B^2+1} \tag{19a}$$

$$V_{e-IO}^{n} + -\alpha_I\lambda_I\hbar\omega_{IO}\sum_{n'}\int_0^{X_{mI}} dx\frac{V_{mm'}^2(x^2)\exp(-\sqrt{8}zx/l_c)}{(n'-n)\lambda_I^2+1} \tag{19b}$$

where

$$\lambda_B^2 = \omega_c/\omega_{BO} \qquad \lambda_I^2 = \omega_c/\omega_{IO} \tag{20}$$

$$m = \min(n,n') \qquad m' = \max(n,n') \tag{21a}$$

$$V_{mm'}(x) = [m'!/m!]^{1/2}e^{-x/2}x^{(m-m')/2}L_{m'}^{m-m'}(x) \tag{21b}$$

$L_n^\alpha(x)$ is the associated Lagurre polynomial, and

$$l_c = [\hbar/m_b\omega_c]^{1/2} \tag{22}$$

is the magnetic length characterizing the spread of the electron of the electron wave function in the x direction. The two upper integral limits in (19*a*) and (19*b*) can be written as

$$X_{mB} = \hbar ck_m^2/2eB \qquad X_{mI} = \hbar cq_m^2/2eB. \tag{23}$$

The maximum length of two kinds of optical phonon wavevector k_m and q_m are chosen on the boundaries of the first Brillouin zones.

3. Numerical results and discussion

A GaAs (crystal 1)/GaSb (crystal 2) structure is used for the model system of an interface magnetopolaron to perform the numerical computation. The parameters concerned are [8] $\epsilon_{01} = 12.83$, $\epsilon_{\infty 1} = 10.9$, $\hbar\omega_{BO1} = 36.7$ meV, $m_{b1} = 0.0657m_0$, $\epsilon_{02} = 14.44$, $\epsilon_{\infty 2} = 15.69$. The maximum of the two kinds of optical phonon wavevector is given by

$$k_m = \sqrt{3}\pi/a \qquad q_m = \sqrt{2}\pi/a \tag{24}$$

where $a = 5.654$ Å is the lattice constant of GaAs. In this paper we only give the ground-state-induced potential of the interface magnetopolaron.

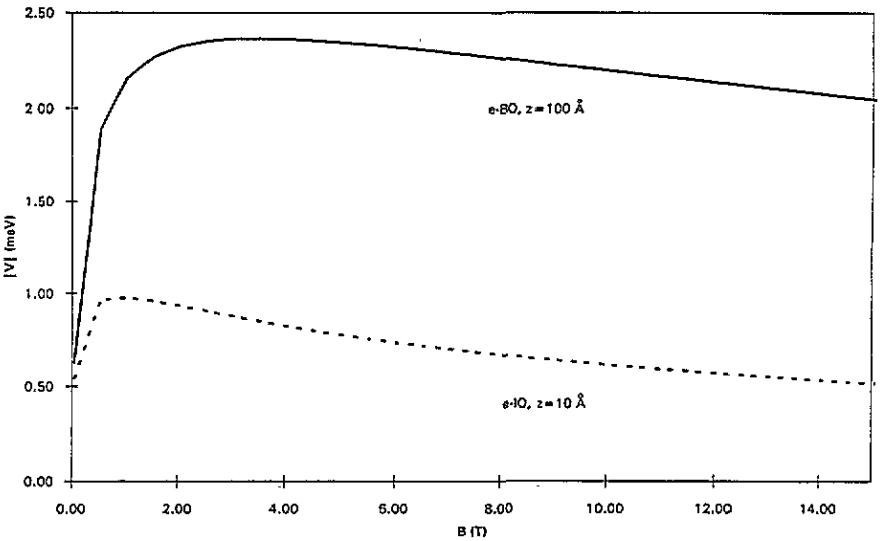

Figure 1. The induced potential as a function of the magnetic field B.

Figure 1 shows the induced potential as a function of the magnetic field. We can see that for a rather weak magnetic field and a small distance of the electron from the interface, the electron-IO phonon interaction is dominant, but for a large magnetic field and large distance of the electron from the interface the electron–BO phonon interaction is dominant. We can also see that in the low-magnetic-field region, the induced potential is a rapidly increasing function of the magnetic field, but beyond a critical magnetic field B_c the induced potential is a slowly decreasing function of the magnetic field. The critical point B_c is different for V_{e-BO} and V_{e-IO} and it also depends on the electron departure z. The above phenomena can be easily seen from (19*a*) and (19*b*), because the integrals included have a minimum point at some magnetic field B_c and departure z_c, which can be determined by the following equations:

$$\partial V_{e-BO}(B, z)/\partial B = 0 \qquad \partial V_{e-IO}(B, z)/\partial B = 0. \tag{25}$$

Many of previous works on the interface magnetopolaron were carried out in the low-field region and neglected the electron–IO phonon interaction so they could not find this

phenomenon. From figure 1 we can see that for the electron–BO phonon interaction, B_c is approximately 2.5 T when $z = 100$ Å, and for the electron–IO phonon interaction, B_c is approximately 0.5 T when $z = 10$ Å.

Let us give a physical discussion of this behaviour. The strength of the electron–phonon interaction is proportional to the number of *polarizable phonons* (either BO phonons or IO phonons). In weak magnetic fields, the number of polarizable phonons will increase with the magnetic field. When the magnetic field is increased beyond a critical field B_c, the number of polarizable phonons will reach a maximum. Beyond B_c, i.e. at relatively strong magnetic fields, a further increase in the magnetic field will decrease the number of polarizable phonons, thus reducing the strength of the electron–phonon interaction.

To our knowledge, we are not aware of any experiment that has detected directly the magnetic field dependence predicted for the induced potential. We suggest magneto-optical experiments be done to verify our results.

As a further illustration, figure 2 gives the z and B dependence of the induced potential; we can see these very clearly. To understand the induced potential magnitude, we also plot the image potential V_{im} as a function of z in figure 2.

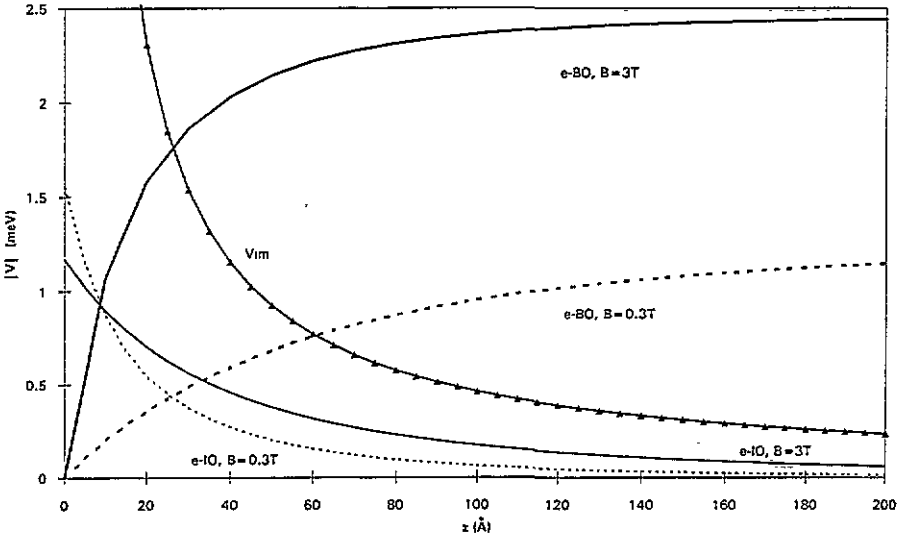

Figure 2. Induced potential and image potential of the electron as a function of the electron departure z from the interface for different magnetic fields.

Figures 3 and 4 show the induced potential as a function of the electron departure z for different magnetic fields. From the figures, we can see that the electron–IO phonon interaction is dominant in the low-magnetic-field region and for small electron departure from the interface, and the electron–BO phonon interaction is dominant in the strong magnetic field and for larger distance of the electron from the interface. We can also see that as the magnetic field increases, the induced potential increases rapidly in the low-magnetic-field region, but it decreases very slowly in the large-magnetic-field region; at the same time, with increasing electron departure z, V_{e-BO} (V_{e-IO}) rapidly increases (decreases) in the small-z region, and it increases (decreases) rather slowly in the larger-z region.

To further study the effect of the electron–IO phonon interaction, which was neglected in many previous studies, we plot the magnetic field and electron departure dependence of

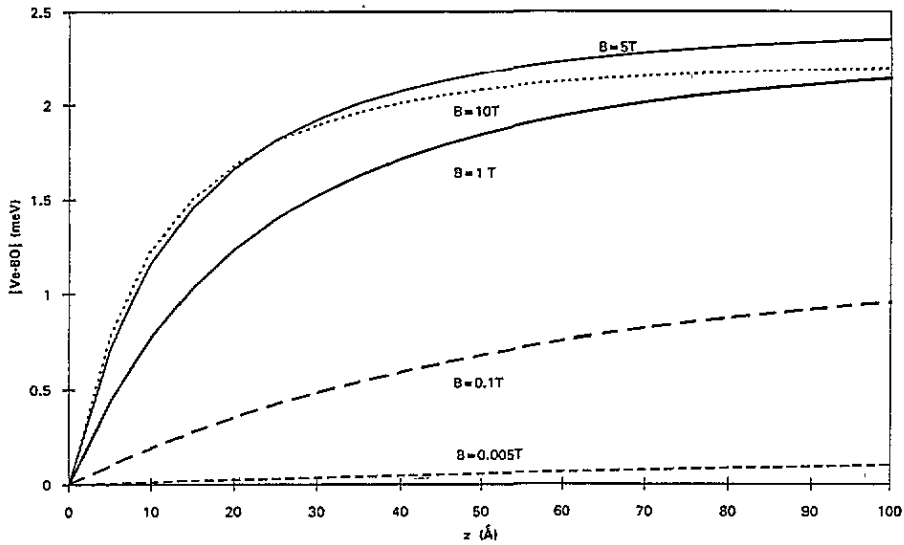

Figure 3. V_{e-BO} as a function of the electron departure from the interface for different magnetic fields.

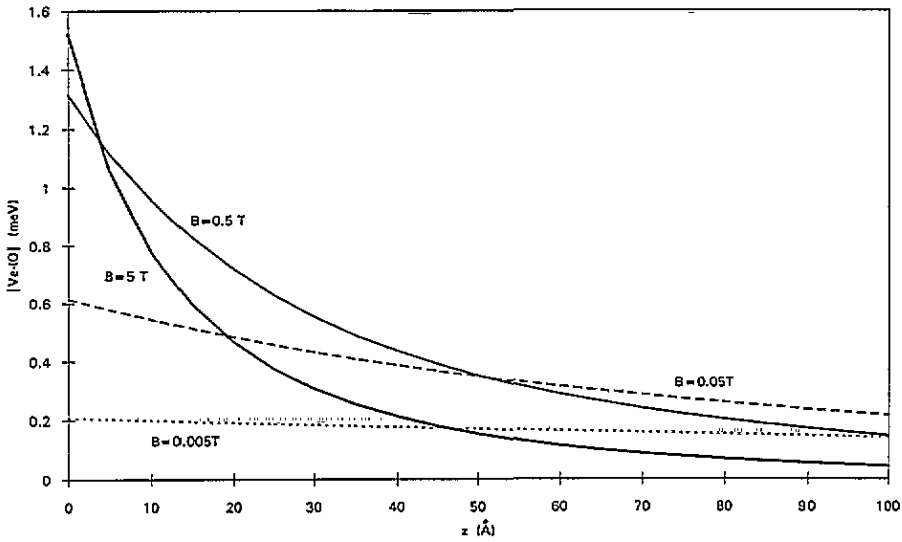

Figure 4. V_{e-IO} as a function of the electron departure from the interface for different magnetic fields.

V_{e-IO} in the weak-magnetic-field region in figure 5; we can see from this that the electron–IO phonon interaction is strongly affected by the motion of the electron in the weak magnetic field, especially when the electron is near the interface. We can neglect the effect of the electron–IO phonon interaction only in the strong magnetic field and when the electron is far from the interface.

Although the electron–electron interaction has been excluded from the present study, it

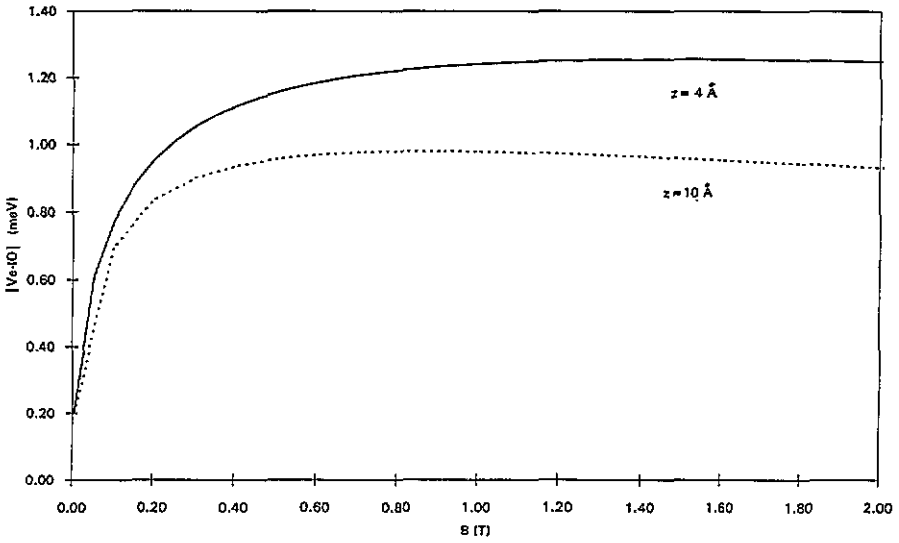

Figure 5. V_{e-IO} as a function of magnetic field in weak magnetic fields for different z.

would be interesting to see the implications of the results for the results for the problem of 2D electron-gas spectroscopic properties in the quantum limit [19]. We plan to treat the electron–electron interaction by the random-phase approximation and results will be reported elsewhere.

4. Summary

In this paper, we have studied the induced potential of an interface electron interacting with both the BO and IO phonons by using the standard Green-function theory method. The dependence of the induced potential on the magnetic field strength and electron departure from the interface is studied; the numerical results show that in a weak magnetic field both $|V_{e-BO}|$ and $|V_{e-IO}|$ are fast increasing functions of the magnetic field, but beyond a critical point B_c of the magnetic field, $|V_{e-BO}|$ and $|V_{e-IO}|$ are slowly decreasing functions of the magnetic field. The numerical results also show that the electron–IO phonon interaction is dominant in a rather weak magnetic field and small electron departure from the interface. In the opposite limit, the electron–BO phonon interaction is dominant. As the method suggested in this paper could only be applied for the weak-coupling limit and for arbitrary magnetic fields except near the resonant region, we shall study the self-energy and cyclotron resonance of the interface magnetopolaron in a future publication.

Acknowledgment

KWY acknowledges support from a UPGC grant under a project number 221-300-150.

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