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Self-energy of a magnetopolaron at the interface of polar crystals

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Abstract. The self-energy of an interface electron interacting with bulk longitudinal-optical phonons as well as interface optical (IO) phonons in a magnetic field of arbitrary strength is studied using the Green function method. Our results show that the absolute value $|E^{(0)}_{e-ph}|$ of the ground-state self-energy of the electron is a rapidly increasing function of the magnetic field in the weak-magnetic-field region, but $|E^{(0)}_{e-ph}|$ is a slowly decreasing function of the magnetic field beyond a critical magnetic field B_c. For the excited states, $|E^{(n)}_{e-ph}|(n \geqslant 1)$ is an increasing function of the magnetic field in the pre-resonant region, while $E^{(n)}_{e-ph}$ is a positive and decreasing function of the magnetic field beyond the resonant region. Numerical results show that the electron–IO phonon interaction contributes only when the mean distance of the polaron from the interface is small and in the extremely-weak-magnetic-field region.

1. Introduction

An electron in a magnetic field possesses Landau levels. When the electron moves slowly in the conduction band of a polar crystal, it interacts with the polarization field of the crystal lattice to form a quasi-particle which is called a 'polaron'. The electron–phonon interaction produces a correction to the electron Landau levels and hence renormalizes the electron effective mass from its band value to a slightly larger polaron value. Recently, much attention has been centred around the polaron aspect in the quasi-two-dimensional (Q2D) electron systems (such as surface, interface, superlattice and quantum well structures). In the past, much work on Q2D magnetopolarons has been devoted to the calculation of the ground-state energy and the effective mass of polarons using the perturbation variational method or path integral approach [1–13]. Few investigations have studied the interface magnetopolaron by using the more powerful Green function method. To mention a few, using a Green function method, Das Sarma and co-workers [14, 15] made a formal calculation of the Landau-level correction and optical anomalies in the resonant region for pure two-dimensional (2D) systems. The issue of 'interface polarons' was discussed in [16].

It is generally accepted that in bulk semiconductors or polar crystals the effective mass of the electron is enhanced by the virtual coupling of a quasi-free electron with bulk longitudinal-optical (BO) phonons. However, for 2D or Q2D systems, one of the present authors and his collaborators [4–7] found that the interaction of electron with interface longitudinal-optical (IO) phonons must be considered as well as the interaction of electrons

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with BO phonons, especially when the distance between the electron and the interface is comparable with the radius of the polaron, a result which has been confirmed by experiments.

In this paper we study the self-energy of an interface polaron using the standard Green function method. We present a calculation of the self-energies of interface polarons for all the Landau levels for arbitrary magnetic field strengths. In our studies, both the BO phonon and the IO phonon are included in the interaction; the numerical results of the self-energies as well as the total energies of the interface magnetopolaron for the first three Landau levels will be given. The remainder of the paper is organized as follows: in section 2 we present the Hamiltonian of the system and outline the calculation of the Green function and the self-energies of the interface polaron. Section 3 contains our numerical results and discussion. A brief summary is presented in section 4.

2. Theory

Now we consider an interface polaron in polar–polar crystals. Suppose that 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 suppose that the barrier is infinitely high; therefore, the electron is restricted within crystal 1. The 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 [7]:

$$H = H_0 + H_\parallel + H_\perp \tag{1}$$

$$H_\parallel = H_{e\text{-BO}} + H_{e\text{-IO}} \tag{2}$$

$$H_0 = \frac{p_x^2}{2m_b} + \frac{1}{2m_b}\left(p_y + \frac{\beta^2}{2}x\right)^2 + \sum_k \hbar\omega_{BO} a_k^+ a_k + \sum_q \hbar\omega_{IO} b_q^+ b_q \tag{3}$$

$$H_{e\text{-BO}} = \sum_k [V_k^* \sin(zk_z)\exp(-i\boldsymbol{\rho}\cdot\boldsymbol{k}_\parallel)a_k^+ + \text{HC}] \tag{4}$$

$$H_{e\text{-IO}} = \sum_q [C_q^* \exp(-qz)\exp(-i\boldsymbol{\rho}\cdot\boldsymbol{q})b_q^+ + \text{HC}] \tag{5}$$

$$H_\perp = \frac{p_z^2}{2m_b} - \frac{e^2(\varepsilon_{\infty 1} - \varepsilon_{\infty 2})}{4z\varepsilon_{\infty 1}(\varepsilon_{\infty 1} + \varepsilon_{\infty 2})}. \tag{6}$$

The meaning of the terms in the above equations can be found in [7]; for conciseness, we do not rewrite them here.

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

$$E_0 = E_n + \sum_k \hbar\omega_{BO}\langle n_k\rangle + \sum_q \hbar\omega_{IO}\langle n_q\rangle \tag{7}$$

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

By using the standard Green function method [17], the electron proper self-energy parts corresponding to H_{e-BO} and H_{e-IO} are obtained as

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

$$= \frac{1}{\hbar}\sum_{s',k}|f_{s,s'}(z,k)|^2\left(\frac{\langle n_k\rangle + \langle n_{s'}\rangle}{i\omega_m - \omega_{s'} - \omega_{BO}} + \frac{\langle n_k\rangle + 1 - \langle n_{s'}\rangle}{i\omega_m - \omega_{s'} - \omega_{BO}}\right) \tag{8a}$$

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

$$= \frac{1}{\hbar}\sum_{s',q}|f_{s,s'}(z,q)|^2\left(\frac{\langle n_q\rangle + \langle n_{s'}\rangle}{i\omega_m - \omega_{s'} - \omega_{IO}} + \frac{\langle n_q\rangle + 1 - \langle n_{s'}\rangle}{i\omega_m - \omega_{s'} - \omega_{IO}}\right). \tag{8b}$$

In the above equations, $f_{s,s'}(z,k)$ and $f_{s,s'}(z,q)$ are defined in [7], $\mathcal{G}^{(0)}(s,i\omega_m)$ is the Matsubara Green function of a free electron, $\langle n_s\rangle$ is the mean number of electrons, and $\langle n_k\rangle$ and $\langle n_q\rangle$ are the mean numbers of the BO phonons and IO phonons, respectively.

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

$$\Sigma^*(s,z,i\omega_m) = \Sigma^*_{BO}(s,z,i\omega_m) + \Sigma^*_{IO}(s,z,i\omega_m). \tag{9}$$

We continue $i\omega_m$ analytically to the upper half of the complex ω plane and take the form $\omega = (E^*_n - \mu)/\hbar$. In the zero-temperature case the mean numbers of electron and phonons vanish, i.e. $\langle n_k\rangle = \langle n_q\rangle = \langle n_s\rangle = 0$; then equation (9) becomes

$$\Sigma^*(s,z,E^*_n) = \sum_{s',k}\frac{|f_{s,s'}(z,k)|^2}{E^*_n - E_{n'} - \hbar\omega_{BO}} + \sum_{s',q}\frac{|f_{s,s'}(z,q)|^2}{E^*_n - E_n - \hbar\omega_{IO}}. \tag{10}$$

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

$$\mathcal{G}^R(s,z,E^*_n) = \frac{1}{E^*_n - E_n - \Sigma^*(s,z,E^*_n)}. \tag{11}$$

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

$$\delta E_n(z) = \Sigma^*(s,z,E^*_n) = V^{(n)}_{e-BO}(z) + V^{(n)}_{e-IO}(z) \tag{12}$$

where $V^{(n)}_{e-BO}(z)$ and $V^{(n)}_{e-IO}(z)$ are the potentials of electrons induced from the electron–BO phonon interaction and electron–IO phonon interaction, respectively.

Then we have the effective Hamiltonian

$$H_{n,\mathrm{eff}} = E^{(0)}_n + \frac{p_z^2}{2m_b} + V^{(n)}_{\mathrm{eff}}(z) \tag{13}$$

where the effective potential is

$$V^{(n)}_{\mathrm{eff}}(z) = V^{(n)}_{e-LO}(z) + V^{(n)}_{e-IO}(z) + V_{\mathrm{im}}(z). \tag{14}$$

$V_{\rm im}(z)$ is the image-potential energy of the electron, which is given in the second term of $H_\perp$.

For simplicity, we take into account only the lowest subband of $H_\perp$; so the relevant variational wavefunction with the variational parameter ξ_n can be written as [4]

$$\phi_n(z) = 2\xi_n^{3/2} z \exp(-\xi_n z) \tag{15}$$

and the polaron energy is given by

$$E_{\rm p}^{(n)} = \langle \phi_n(z)|H_{n,\rm eff}(z)|\phi_n(z)\rangle = (n+\tfrac{1}{2})\hbar\omega_{\rm c} + \frac{\hbar^2\xi_n^2}{2m_{\rm b}} - \frac{e^2(\varepsilon_{\infty 2}-\varepsilon_{\infty 1})\xi_n}{4\varepsilon_{\infty 1}(\varepsilon_{\infty 1}+\varepsilon_{\infty 2})} + E_{\rm e-BO}^{(n)} + E_{\rm e-IO}^{(n)} \tag{16}$$

where $E_{\rm e-BO}^{(n)}$ and $E_{\rm e-IO}^{(n)}$ are the self-energies induced by the electron–BO phonon interaction and electron–IO phonon interaction, respectively. The self-energy of the polaron corresponding to the Landau quantum number n is given by

$$E_{\rm e-ph}^{(n)} = E_{\rm e-BO}^{(n)} + E_{\rm e-IO}^{(n)} \tag{17}$$

and the variational parameter ξ_n can be decided by the equation $E_{\rm p}^{(n)} = \min[E_{\rm p}^{(n)}(\xi_n)]$, i.e.

$$\frac{\partial E_{\rm p}^{(n)}(\xi_n)}{\partial \xi_n} = 0. \tag{18}$$

Using equation (15), we can find the mean distance of the polaron from the interface:

$$\bar{z}_n = \int_0^\infty {\rm d}z\, \phi_n^*(z) z \phi_n(z) = \frac{3}{2\xi_n}. \tag{19}$$

Thus ξ_n is inversely proportional to the mean distance of the polaron from the interface.

Now we calculate the self-energies of the interface polaron; first we use [18]

$$\begin{aligned} |\langle n|\exp({\rm i}\boldsymbol{k}_\parallel\cdot\boldsymbol{\rho})|n'\rangle|^2 &= \frac{m!}{m'!}\zeta_\parallel^{(m'-m)}\exp(-\zeta_\parallel)[L_m^{m-m'}(\zeta_\parallel)]^2 \\ |\langle n|\exp({\rm i}\boldsymbol{q}\cdot\boldsymbol{\rho})|n'\rangle|^2 &= \frac{m!}{m'!}\zeta^{(m'-m)}\exp(-\zeta)[L_m^{m-m'}(\zeta)]^2 \end{aligned} \tag{20}$$

where $\zeta_\parallel = \hbar k_\parallel^2/2m_{\rm b}\omega_{\rm c}$ and $\zeta = \hbar q^2/2m_{\rm b}\omega_{\rm c}$. Then we change the sums over $\boldsymbol{k}$ and $\boldsymbol{q}$ in equation (12) into integrals. After a tedious but direct calculation, we can obtain the self-energies of the interface magnetopolaron with the Landau quantum number n as

$$\begin{aligned} E_{\rm e-BO}^{(n)} &= -\alpha_{\rm B}\lambda_{\rm B}\hbar\omega_{\rm BO}\sum_{n'}\int_0^{X{\rm mB}}{\rm d}x\,\frac{V_{mm'}^2(x^2)}{(n'-n)\lambda_{\rm B}^2+1}\left(1-\frac{1}{(1+\sqrt{2}x/l_{\rm c}\xi_n)^3}\right) \\ E_{\rm e-IO}^{(n)} &= -\alpha_{\rm I}\lambda_{\rm I}\hbar\omega_{\rm IO}\sum_{n'}\int_0^{X{\rm mI}}{\rm d}x\frac{V_{mm'}^2(x^2)}{(n'-n)\lambda_{\rm I}^2+1}\frac{1}{(1+\sqrt{2}x/l_{\rm c}\xi_n)^3} \end{aligned} \tag{21}$$

where

$$\lambda_{\rm B}^2 = \omega_{\rm c}/\omega_{\rm BO} \qquad \lambda_{\rm I}^2 = \omega_{\rm c}/\omega_{\rm IO} \tag{22}$$

$$m = \min(n,n') \qquad m' = \max(n,n') \tag{23}$$

$$V_{mm'}(x) = \left(\frac{m'!}{m!}\right)^{1/2}\exp\left(-\frac{x}{2}\right)x^{(m-m')/2}L_{m'}^{m-m'}(x) \tag{24}$$

$L_n^{\alpha}(x)$ is the associated Laguerre polynomial and

$$l_c = \left(\frac{\hbar}{m_b \omega_c}\right)^{1/2} \tag{25}$$

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

$$X\mathrm{mB} = \frac{\hbar c k_m^2}{2eB} \qquad X\mathrm{mI} = \frac{\hbar c q_m^2}{2eB}. \tag{26}$$

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 a model system of an interface magnetopolaron to make the numerical computation. The parameters concerned are [4] $\varepsilon_{01} = 12.83$, $\varepsilon_{\infty 1} = 10.9$, $\hbar\omega_{\mathrm{BO}1} = 36.7$ meV, $m_{b1} = 0.0657m_0$, $\varepsilon_{02} = 14.44$ and $\varepsilon_{\infty 2} = 15.69$. The maxima of the two kinds of optical phonon wavevector are given by

$$k_m = \frac{\sqrt{3}\pi}{a} \qquad q_m = \frac{\sqrt{2}\pi}{a} \tag{27}$$

where $a = 5.654$ Å is the lattice constant of GaAs.

Figures 1 and 2 show the self-energy of the interface magnetopolaron as a function of the magnetic field B for the first three Landau levels ($n = 0, 1, 2$). From figure 1, we can see that in weak magnetic fields the absolute value of the ground-state self-energy $|E_{e-ph}^{(0)}|$ is a rapidly increasing function of B while, beyond a critical field B_c, $|E_{e-ph}^{(0)}|$ becomes a slowly decreasing function of B. From figure 1, we obtain $B_c \simeq 2.7$ T. The existence of a critical magnetic field can be understood as follows. It is well known that the self-energy of a polaron increases with increasing magnetic field for small fields [1, 2, 4–6, 14, 15]. As a result, the number of polar phonons (either BO phonons or IO phonons) increases. As the number of polar phonons in a crystal is not unlimited, when the magnetic field is increased beyond a critical field B_c, the number of polar phonons will reach a maximum. Beyond B_c, i.e. at relatively strong magnetic fields, a further increase in the magnetic field will convert some of the polar phonons into non-polar phonons, thus reducing the self-energy of the polaron. For the excited states, $|E_{e-ph}^{(n)}|(n \geqslant 1)$ is an increasing function of B in the pre-resonant region, but $E_{e-ph}^{(n)}$ becomes a positive and decreasing function of B beyond the resonant region. In that case, the excited polaron state becomes unbounded when the magnetic field is larger than the resonant magnetic field. From figure 2, one finds that the resonant magnetic field is roughly 21 T.

In the limit of a large distance (i.e. $\xi_n \to 0$), which means that the electron is confined to the whole bulk of crystal 1, $E_{e-IO} \to 0$ and $E_{e-BO} \to$ three-dimensional self-energy E^{3D}, and in the opposite limit, i.e. $\xi_n \to \infty$, which means that the electron is confined on

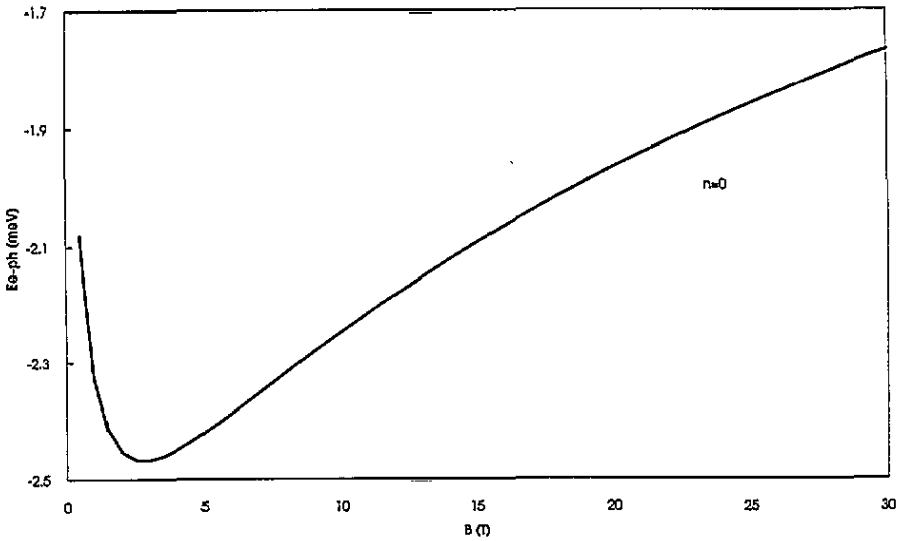

Figure 1. Self-energy of an interface polaron as a function of magnetic field B for the Landau ground state $n = 0$.

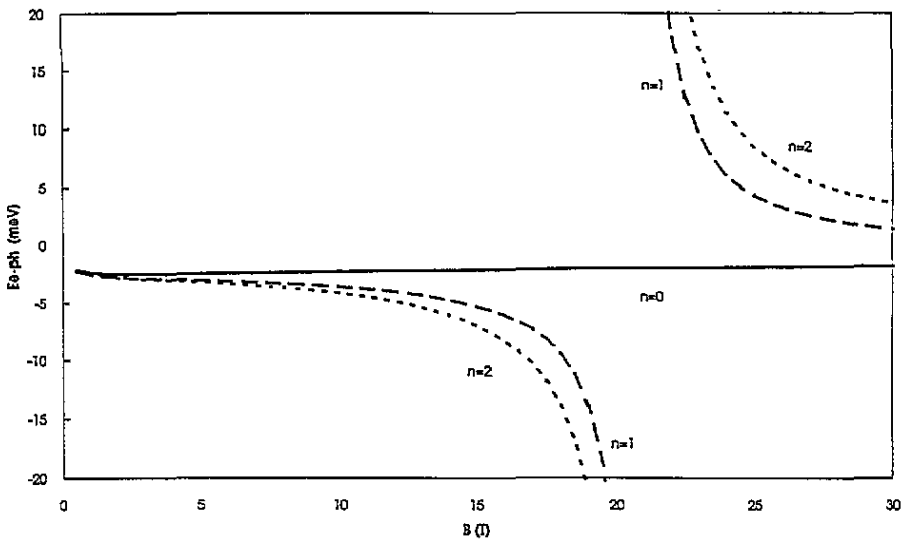

Figure 2. Same as figure 1 for different Landau levels $n = 0, 1, 2$.

the surface of crystal 1, $E_{e-BO} \to 0$ and $E_{e-IO} \to$ pure two-dimensional self-energy E^{2D}. For the value of $\bar{z}$ between the two limits our numerical results show that

$$E^{2D} > E^{Q2D}_{e-ph} > E^{3D}_{e-ph}. \tag{28}$$

That is to say, the self-energy of the Q2D system is larger than that of 3D system but smaller than that of pure 2D system, which has been confirmed by many other studies.

To investigate the effects of the electron–BO phonon interaction and electron–IO phonon interaction, the self-energy is plotted in figure 3 and figure 4 as a function of magnetic field for different mean polaron distances $\bar{z}$ from the interface (defined by equation (19)). From these figures we can see that the electron–IO phonon interaction should be considered only when the polaron is near the interface and in the weak-magnetic-field region. The critical magnetic field for the electron–IO phonon interaction is very small and, with the increase in the polaron mean distance $\bar{z}$ from the interface, the critical magnetic field will disappear. For the GaAs–GaSb interface structure, the mean distance of the polaron from the interface is very large; so the electron–BO phonon interaction plays a main role.

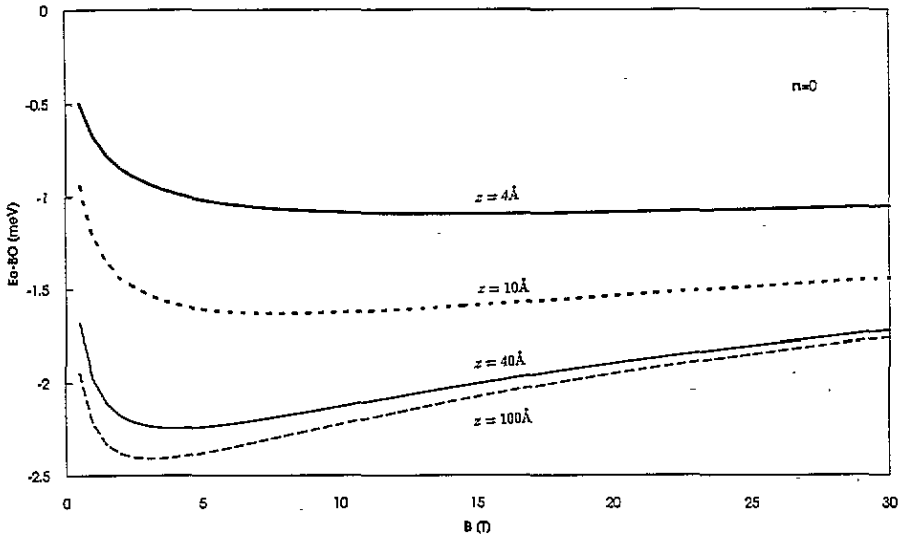

Figure 3. $E^{(0)}_{e-BO}$ as a function of magnetic field B for different polaron mean distances $\bar{z}$ from the interface equal to 4, 10, 40 and 100 Å.

Owing to the effect of the electron–optical phonon interaction, the electron Landau levels will be shifted. Figure 5 shows the total energy of the interface magnetopolaron as a function of the magnetic field, from which we can see that, before the resonant region, the Landau level will shift to a lower energy level and after the resonant region the Landau level will shift to a higher energy level, which is consistent with many previous studies [18, 19]. In the resonant magnetic field region the Landau levels will be split and this will be studied in our future papers.

4. Summary

In this paper, we have studied the self-energies of an electron at the interface of polar crystals interacting with both BO phonons and IO phonons in a magnetic field of arbitrary strength by using the Green function method. The self-energies as well as the total energies of the interface magnetopolaron for all the Landau levels have been studied. Our numerical results show that in the weak-magnetic-field region the Landau ground-state self-energy $|E^{(0)}_{e-ph}|$ is a rapidly increasing function of the magnetic field but, beyond a critical magnetic

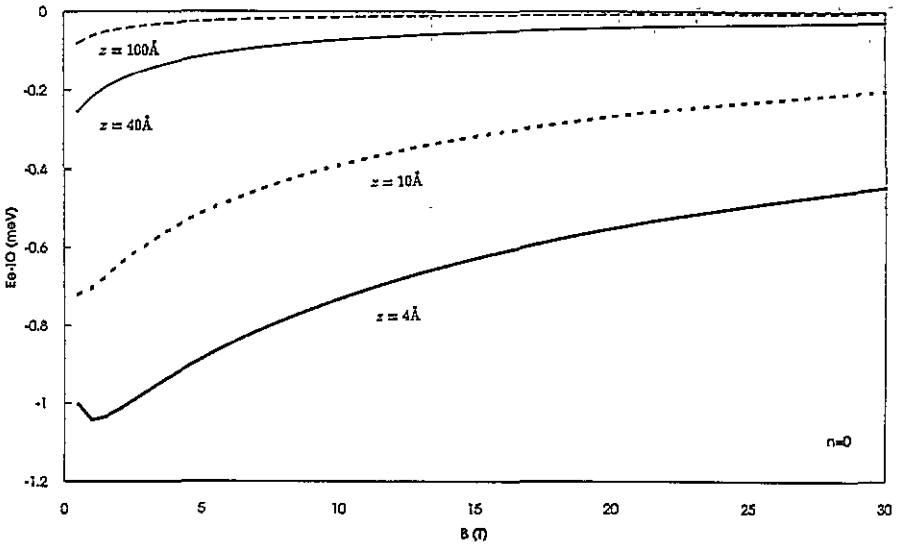

Figure 4. $E^{(0)}_{e-IO}$ as a function of magnetic field B for different polaron mean distances $\bar{z}$ from the interface equal to 4, 10, 40 and 100 Å.

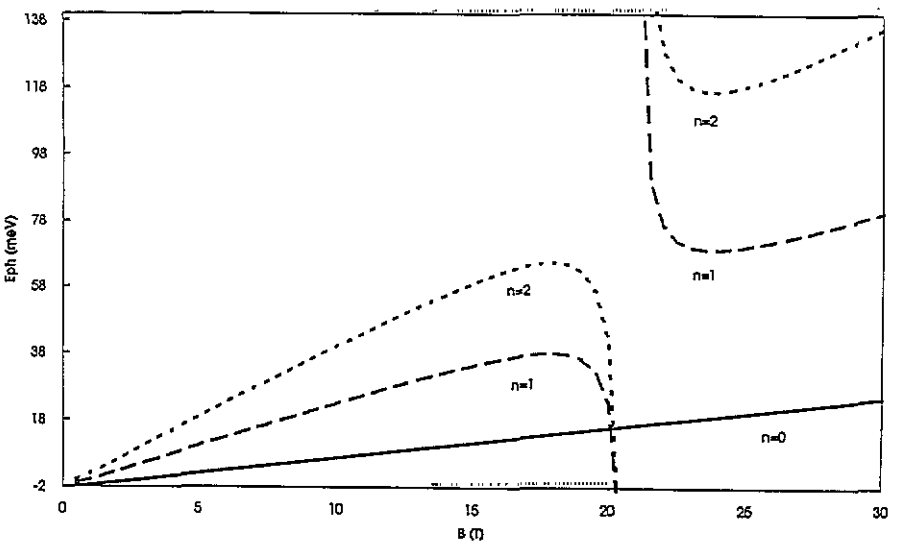

Figure 5. Energies of the interface polaron as a function of the magnetic field B for different Landau levels $n = 0, 1, 2$.

field B_c, $|E^{(0)}_{e-ph}|$ is a slowly decreasing function of the magnetic field. For the excited states, $|E^{(n)}_{e-ph}|(n \geqslant 1)$ is an increasing function of the magnetic field in the pre-resonant magnetic field region but, beyond the resonant magnetic field region, $E^{(n)}_{e-ph}$ become positive and a decreasing function of the magnetic field; thus the excited polaron state become unbounded. Our numerical results also show that, only in rather weak magnetic fields and for small mean

departures of the polaron from the interface, could the electron–IO phonon interaction make a contribution.

The method suggested in this paper could be applied to the weak electron–phonon-coupling limit and for arbitrary magnetic fields except in the resonant region; the cyclotron resonance of interface magnetopolarons in the resonant region will be studied in our future papers.

Acknowledgments

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