

Polaron effects on an anisotropic quantum dot in a magnetic field

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(Received 18 November 1998)

The polaronic effects for an electron confined in a parabolic quantum dot and a uniform magnetic field are calculated, taking into account the electron-bulk LO-phonon interaction. The variational wave function is constructed as a product form of an electronic part and a part of coherent phonons generated by the Lee-Low-Pines transformation from the vacuum. An analytical expression for the polaron energy is found by the minimization procedure, and from this expression the ground- and first-excited-state energies are obtained explicitly. It is shown that the results obtained for the ground-state energy reduce to the existing works in zero magnetic fields. In the presence of a magnetic field, the confinement of the electron is examined in three different limiting cases both for the ground and first excited states, depending on certain parameters, such as the magnetic-field strength, the electron-phonon coupling strength, the polaron radius, and the confinement length. [S0163-1829(99)03828-X]

I. INTRODUCTION

Recent technological advances in the fabrication of nanostructures have stimulated both experimental and theoretical interest in low-dimensional systems.¹ This interest arises for two major reasons: first, in these systems the length scales involved are typically of the order of a few nanometers, which paves the way for interesting fundamental physics; and second, they have potential use in designing devices. Of these structures, quantum wells, quantum wires, and quantum dots (QD's) are primarily important, since the electrons in quantum wells and wires are free to move in two directions and one direction, respectively, and in all the other directions confinement takes place, whereas the electrons in QD's are confined in all three spatial dimensions. The confinement feature brings in quantum effects when the electron wavelength is of the same order as the confinement length. It is therefore useful to consider quantized energy spectra of the confined electrons and their variations with the confinement lengths in order to assess electronic properties of these nanostructures. Furthermore, it is also of much interest to see the effects of electron-phonon interaction on these properties.

Electron-phonon interaction, which plays an important role in electronic and optical properties of polar crystalline materials in three dimensions, will have pronounced effects in low-dimensional systems as well. Apart from numerous works on polaronic effects in quantum wells and wires, recently there has been a considerable number of theoretical studies on the same effects including the confinement problem in the QD system. The main theme of the latter subject is the ground-state energies calculated in a spherical QD,²⁻⁵ and in a QD with parabolic potential,⁶⁻¹⁰ employing all types of interactions such as with bulk, interface, and surface LO phonons. Various other effects involving these phonons have been investigated theoretically in QD structures.¹¹⁻¹⁶ In particular, the authors of Refs. 2, 3, and 14 concluded that a bulk-type LO-phonon contribution into the polaron energies dominates.

Polaron effects in a QD become more interesting in a

magnetic field, whose existence now affects the confinement length in addition to the polaron properties. In the presence of a magnetic field, there are several theoretical studies. Zhu and Gu¹⁷ investigated the cyclotron resonance of a magnetopolarons in a QD with a strong magnetic field within the framework of the Rayleigh-Schrödinger perturbation theory. Zhu and Kobayashi¹⁸ used the Landau-Pekar variational treatment to calculate the binding energy of strong-coupling polarons in QD's. Recently, some theoretical works on cyclotron resonance in QD's have been done by several authors.^{19,20}

In this paper we shall consider a QD embedded in a three-dimensional (3D) material, where the dot electron is confined in a parabolic potential and in magnetic fields. Our attention will be focused on the electron bulk-phonon interaction effects in QD's. We develop a variational method, valid for an intermediate electron-phonon coupling strength.

The layout of the present paper as follows. In Sec. II, we construct a wave function as a product of the electronic and phonon parts, containing certain variational parameters, by which the polaron energy is calculated by a minimization procedure. In Sec. III, we obtain the ground- and first-excited-state energies, and compare with other works in certain limits. A conclusion is given in Sec. IV.

II. THEORY

We consider an electron, which is interacting with bulk LO phonons and subjected to a QD potential. In the presence of a uniform magnetic field along the z direction, the Fröhlich Hamiltonian of an electron-phonon interaction system confined in a 3D anisotropic harmonic potential is given by

$$H = H_E + \sum_{\mathbf{q}} \hbar \omega_0 b_{\mathbf{q}}^\dagger b_{\mathbf{q}} + \sum_{\mathbf{q}} (V_{\mathbf{q}} b_{\mathbf{q}} e^{i\mathbf{q} \cdot \mathbf{r}} + \text{H.c.}), \quad (1)$$

where

$$H_E = \frac{1}{2\mu} \left(\mathbf{p} + \frac{e}{c} \mathbf{A} \right)^2 + \frac{1}{2} \mu \omega_{\perp}^2 \mathbf{r}_{\perp}^2 + \frac{1}{2} \mu \omega_{\parallel}^2 z^2 \quad (2)$$

is the electronic part, and

$$|V_{\mathbf{q}}|^2 = (\hbar\omega_0)^2 \left(\frac{4\pi\alpha}{V} \right) \frac{r_0}{q_{\perp}^2 + q_z^2} \quad (3)$$

is the electron-phonon interaction amplitude. In Eq. (1), $b_{\mathbf{q}}^{\dagger}(b_{\mathbf{q}})$ is the creation (annihilation) operator of an optical phonon with a wave vector $\mathbf{q}=(\mathbf{q}_{\perp}, q_z)$ and an energy $\hbar\omega_0$, and \mathbf{p} and $\mathbf{r}=(\mathbf{r}_{\perp}, z)$ denote the electron momentum and position operators, respectively. α and r_0 are the electron-phonon coupling constant and polaron radius, respectively. By using the symmetrical Coulomb gauge $\mathbf{A} = B(-y, x, 0)/2$ for the vector potential, Eq. (2) can be written as a sum of two- and one-dimensional Hamiltonians in the form

$$H_E = H_{1D}(\omega_{\perp}, \mu) + H_{2D}(\omega, \mu), \quad (4)$$

where

$$H_{2D}(\omega, \mu) = -\frac{\hbar^2}{2\mu} \nabla_{\mathbf{r}_{\perp}}^2 + \frac{1}{2} \mu \omega^2 \mathbf{r}_{\perp}^2 + \frac{\omega_c}{2} L_z \quad (5)$$

is the well-known 2D isotropic oscillator Hamiltonian with frequency $\omega^2 = (\omega_c/2)^2 + \omega_{\perp}^2$ plus $(\omega_c/2)L_z$, and

$$H_{1D}(\omega_{\parallel}, \mu) = -\frac{\hbar^2}{2\mu} \nabla_z^2 + \frac{1}{2} \mu \omega_{\parallel}^2 z^2 \quad (6)$$

is the 1D oscillator Hamiltonian. Here ω_c is the cyclotron frequency, and ω_{\perp} and ω_{\parallel} are the measures of confinement strengths of the 3D anisotropic harmonic potential in the xy plane and the z direction, respectively.

The variational state vector for the Hamiltonian in Eq. (1) will be taken as

$$|\Psi_{nm}\rangle = |n, \mp m, l\rangle \otimes D(f)|0\rangle_{ph}, \quad (7)$$

where

$$D(f) = \exp \left[\sum_{\mathbf{q}} (b_{\mathbf{q}}^{\dagger} f_{\mathbf{q}} - b_{\mathbf{q}} f_{\mathbf{q}}^*) \right] \quad (8)$$

is the well-known Lee-Low-Pines transformation, by which coherent boson states are generated through the application on the zero-phonon state $|0\rangle_{ph}$.

$|n, \mp m, l\rangle = |n, \mp m\rangle \otimes |l\rangle$ show the eigenfunctions of an electron in an anisotropic harmonic potential subjected to a uniform magnetic field in the z direction described by the Hamiltonian of Eq. (3), and its coordinate representation is given by

$$\begin{aligned} \langle \mathbf{r} | n, \mp m, l \rangle &= \psi_{n, \mp m}(\mathbf{r}_{\perp}) \psi_l(z) \\ &= N_{nm}(\gamma_{\mp}, \beta) e^{-\gamma_{\mp}^2 \mathbf{r}_{\perp}^2 / 2} \\ &\quad \times (x \mp iy)^m L_n^m(\gamma_{\mp}^2 \mathbf{r}_{\perp}^2) e^{-\beta^2 z^2 / 2} H_l(\beta z), \end{aligned} \quad (9)$$

where the functions L_n^m and H_l are associated Laguerre polynomials and Hermite polynomials, respectively. N_{nm} is the normalization constant, and is given by

$$N_{nm}(\gamma_{\mp}, \beta) = (-1)^n \frac{\gamma_{\mp}^{m+1}}{\sqrt{\pi}} \left[\frac{n!}{(n+m)!} \right]^{1/2} \frac{\beta^{1/2}}{[2^l l! \sqrt{\pi}]^{1/2}}. \quad (10)$$

In Eq. (9), n and m are the radial and the absolute value of the angular momentum quantum numbers, respectively, and l is the harmonic-oscillator quantum number confined in the z direction. Here γ_{\mp} , β , and $f_{\mathbf{q}}$ are used as variational parameters.

The part of H_{2D} of the Hamiltonian H_E was solved in a previous work,²¹ and the result is

$$\begin{aligned} \langle n, \mp m, l | H_{2D} | n, \mp m, l \rangle \\ = \frac{\hbar^2}{2\mu} \gamma_{\mp}^2 (2n+m+1) + \frac{1}{2} \mu \omega^2 \frac{1}{\gamma_{\mp}^2} (2n+m+1) \mp m \frac{\hbar\omega_c}{2}. \end{aligned} \quad (11)$$

It is also necessary to find the expectation value of H_{1D} , which is easily achieved by means of Hermite polynomials:

$$\begin{aligned} \langle n, \mp m, l | H_{1D} | n, \mp m, l \rangle &= \frac{\hbar^2}{2\mu} \beta^2 \left(l + \frac{1}{2} \right) + \frac{1}{2} \mu \omega_{\parallel}^2 \frac{1}{\beta^2} \\ &\quad \times \left(l + \frac{1}{2} \right). \end{aligned} \quad (12)$$

The expectation value of the total Hamiltonian in Eq. (1), including electron-phonon interaction term, is now $E_{n, \mp m, l} = E_{n, \mp m, l}^0 + E_{n, \mp m, l}^I$, where the first term is the sum of Eqs. (11) and (12) and the last term is the electron-phonon interaction energy, which is given by

$$\begin{aligned} E_{n, \mp m, l}^I &= \sum_{\mathbf{q}} [\hbar\omega_0 |f_{\mathbf{q}}|^2 + V_{\mathbf{q}} f_{\mathbf{q}} \sigma_{nm}(\mathbf{q}, \gamma_{\mp}, \beta) \\ &\quad + V_{\mathbf{q}}^* f_{\mathbf{q}}^* \sigma_{nm}^*(\mathbf{q}, \gamma_{\mp}, \beta)], \end{aligned} \quad (13)$$

where

$$\begin{aligned} \sigma_{nm}(\mathbf{q}, \gamma_{\mp}, \beta) &= \langle n, \mp m, l | e^{i\mathbf{q} \cdot \mathbf{r}} | n, \mp m, l \rangle \\ &= \rho_{nm}(\mathbf{q}_{\perp}, \gamma_{\mp}) \rho_l(q_z, \beta), \end{aligned} \quad (14)$$

with the matrix elements

$$\rho_{nm}(\mathbf{q}_{\perp}, \gamma_{\mp}) = \langle n, \mp m | e^{i\mathbf{q}_{\perp} \cdot \mathbf{r}_{\perp}} | n, \mp m \rangle \quad (15)$$

and

$$\rho_l(q_z, \beta) = \langle l | e^{iq_z z} | l \rangle. \quad (16)$$

The full calculation of $\rho_{nm}(\mathbf{q}_{\perp}, \gamma_{\mp})$ is derived in Ref.21; here we briefly summarize the results:

$$\begin{aligned}
\rho_{nm}(\mathbf{q}_\perp, \gamma_\mp) &= (-1)^{2n} \frac{\gamma_\mp^{2(m+1)}}{\pi} \frac{n!}{(n+m)!} \sum_{p=0}^{\infty} \frac{(i)^{2p}}{(2p)!} \\
&\times \int_0^{2\pi} (q_x \cos \varphi + q_y \sin \varphi)^{2p} d\varphi \int_0^\infty \rho d\rho \\
&\times \exp(-\gamma_\mp^2 \rho^2) \rho^{2(m+p)} [L_n^m(\gamma_\mp^2 \rho^2)]^2 \\
&= \frac{1}{n!m!} \sum_{p=0}^{\infty} \frac{(m+p)!}{[(p)!]^2} \left(-\frac{q_\perp^2}{4\gamma_\mp^2} \right)^p \Delta_{nm}(p),
\end{aligned} \tag{17}$$

with

$$\Delta_{nm}(p) = \frac{d^n}{dh^n} \left\{ \frac{F\left(\frac{1+m+p}{2}, 1 + \frac{m+p}{2}; 1+m; A^2/B^2\right)}{(1-h)^{1+m} B^{1+m+p}} \right\}_{h=0}, \tag{18}$$

in which only the even-order terms of p in the first integral are included, since the integration over the angle φ gives zero in odd-order terms and $\rho^2 = x^2 + y^2$, and the definition of the hypergeometric function ${}_2F_1$ with arguments $A = 4h/(1-h)^2$, $B = (1+h)/(1-h)$ is used. From Eq. (18) it is easy to verify that $\Delta_{00}(p) = \Delta_{0\mp 1}(p) = 1$ are independent of p and $\Delta_{10}(p) = 1 + p + p^2$, and thus, by use of these results in Eq. (17), we see that various values of $\rho_{nm}(\mathbf{q}_\perp, \gamma_\mp)$ take the forms

$$\begin{aligned}
\rho_{00} &= \exp(-x^2/2), \quad \rho_{0\mp 1} = \exp(-x^2/2)(1-x^2/2), \\
\rho_{10} &= \exp(-x^2/2)(1-x^2/2)^2,
\end{aligned} \tag{19}$$

where $x = q_\perp / \sqrt{2} \gamma_\mp$. The calculation of $\rho_l(q_z, \beta)$ can be straightforwardly carried out and the result is given in terms of Laguerre polynomials

$$\rho_l(q_z, \beta) = e^{-q_z^2/4\beta^2} L_l\left(\frac{q_z^2}{2\beta^2}\right). \tag{20}$$

Minimization of $E_{n,\mp m,l}$ with respect to $f_{\mathbf{q}}^*$ yields

$$f_{\mathbf{q}} = -\frac{V_{\mathbf{q}}^*}{\hbar\omega_0} \sigma_{nm}^*(\mathbf{q}, \gamma_\mp, \beta). \tag{21}$$

After substituting $f_{\mathbf{q}}$ into Eq. (13), $E_{n,\mp m,l}^I$ becomes

$$E_{n,\mp m,l}^I = -\frac{1}{\hbar\omega_0} \sum_{\mathbf{q}} |V_{\mathbf{q}}|^2 |\sigma_{nm}(\mathbf{q}, \gamma_\mp, \beta)|^2. \tag{22}$$

With the change of variables by $q_\perp / \sqrt{2} \gamma_\mp = x$ and $q_z / \sqrt{2} \beta = y$, Eq. (21) simplifies to the form

$$E_{n,\mp m,l}^I = -\alpha \hbar \omega_0 \frac{2\sqrt{2}}{\pi} \frac{\gamma_\mp^2}{\beta} I_{nm,l}(\Omega), \tag{23}$$

where $I_{nm,l}(\Omega)$ has the following form:

$$I_{nm,l}(\Omega) = \int_0^\infty x dx |\rho_{nm}(x^2/2)|^2 \int_0^\infty dy \frac{e^{-y^2}}{\Omega^2 x^2 + y^2} L_l^2(y^2). \tag{24}$$

Here $\Omega^2 = \gamma_\mp^2 / \beta^2$ is an important parameter, for which we will discuss three possible limiting cases.

Hence the expectation value of the Hamiltonian of Eq. (1) is now

$$\begin{aligned}
E_{n,\mp m,l}(\gamma_\mp, \beta) &= \left(\frac{\hbar^2}{2\mu} \gamma_\mp^2 + \frac{1}{2} \mu \omega^2 \frac{1}{\gamma_\mp^2} \right) (2n+m+1) \\
&\mp m \frac{\hbar \omega_c}{2} + \left(\frac{\hbar^2}{2\mu} \beta^2 + \frac{1}{2} \mu \omega_\parallel^2 \frac{1}{\beta^2} \right) \left(l + \frac{1}{2} \right) \\
&- \alpha \hbar \omega_0 \frac{2\sqrt{2}}{\pi} r_0 \frac{\gamma_\mp^2}{\beta} I_{nm,l}(\Omega).
\end{aligned} \tag{25}$$

In the absence of the electron-phonon interaction, that is, when $\alpha = 0$, if we minimize $E_{n,\mp m,l}^0$ with respect to γ_\mp and β , then we obtain $\gamma_\mp^4 = (\mu\omega/\hbar)^2$ and $\beta^4 = (\mu\omega_\parallel/\hbar)^2$. If we now substitute these results into Eq. (24), we obtain the familiar result

$$E_{n,\mp m,l}^0 = \hbar \omega (2n+m+1) + \hbar \omega_\parallel \left(l + \frac{1}{2} \right) \mp m \frac{\hbar \omega_c}{2}, \tag{26}$$

where the first term represents 2D isotropic oscillator eigenvalues with $\omega^2 = (\omega_c/2)^2 + \omega_\perp^2$, and the second term is 1D oscillator eigenvalues with ω_\parallel . For convenience we introduce dimensionless parameters as follows:

$$\left(\frac{\hbar}{\mu\omega} \right)^{1/2} \gamma_\mp = \frac{1}{\bar{\gamma}_\mp} \quad \text{and} \quad \left(\frac{\hbar}{\mu\omega} \right)^{1/2} \beta = \frac{1}{\bar{\beta}}. \tag{27}$$

It should be noted that after this change Ω becomes $\bar{\Omega}^2 = \bar{\beta}^2 / \bar{\gamma}_\mp^2$. Finally it is also convenient to make $E_{n,\mp m,l}$ dimensionless dividing by $\hbar \omega_0$. Hence the total energy takes the form

$$\begin{aligned}
\bar{E}_{n,\mp m,l}(\bar{\gamma}_\mp, \bar{\beta}) &= \left(\frac{1}{2\bar{\gamma}_\mp^2} + \frac{1}{2} \bar{\omega}^2 \bar{\gamma}_\mp^2 \right) (2n+m+1) \mp m \frac{\bar{\omega}_c}{2} \\
&+ \left(\frac{1}{2\bar{\beta}^2} + \frac{1}{2} \bar{\omega}_\parallel^2 \bar{\beta}^2 \right) \left(l + \frac{1}{2} \right) \\
&- \alpha \frac{\bar{\beta}}{\pi \bar{\gamma}_\mp^2} I_{n\mp m,l}(\bar{\Omega}).
\end{aligned} \tag{28}$$

This is our fundamental result, from which we obtain the ground- and excited-state energies according to the values of $\bar{\Omega}$ in three different cases.

III. RESULTS AND DISCUSSION

We now consider Eq. (28) in three different cases of $\bar{\Omega}$, each of which corresponds to a physical case and reduces, on

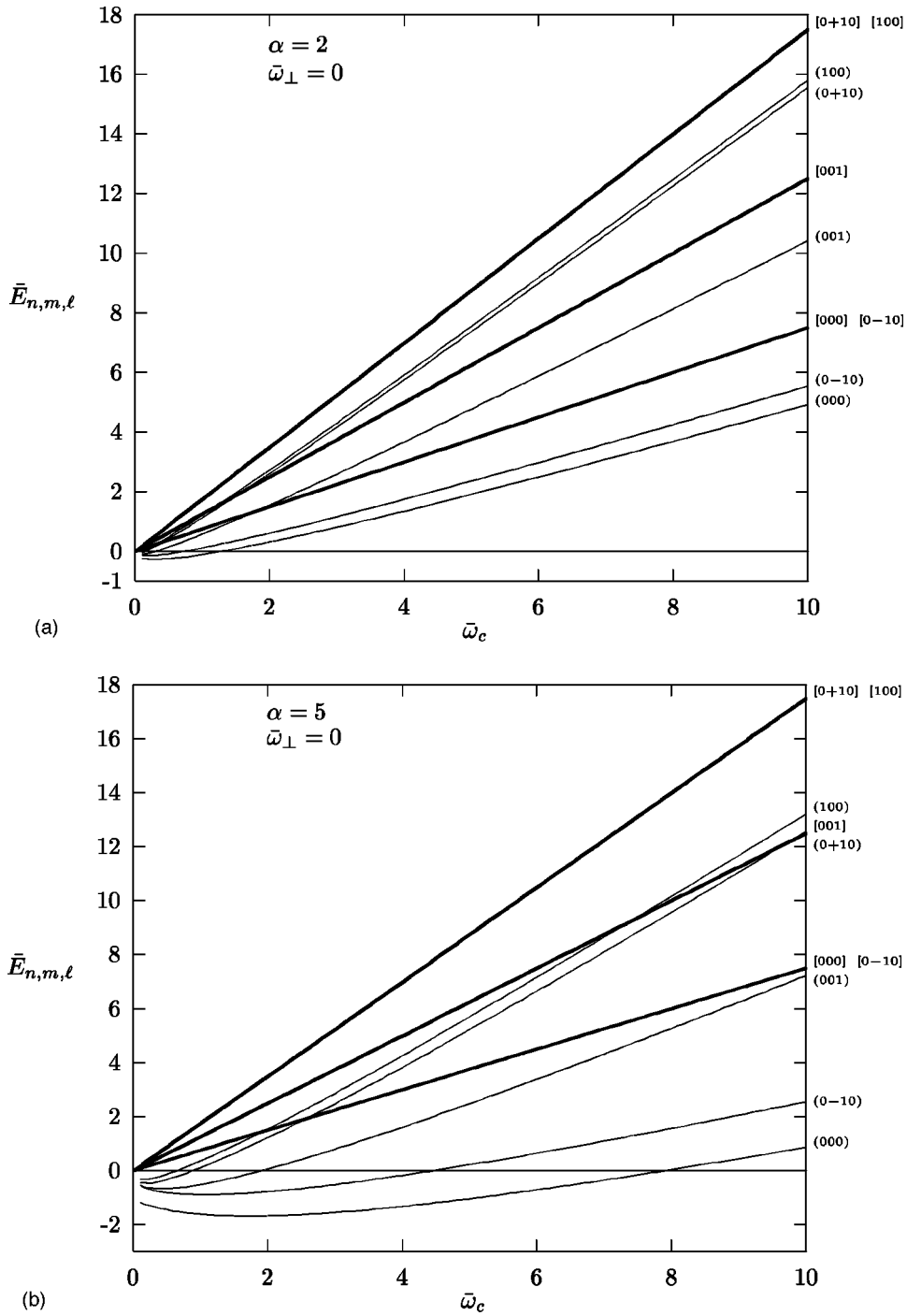


FIG. 1. Cyclotron frequency dependence of the magnetopolaron energy levels $\bar{E}_{n,m,l}$ in a quantum dot with an anisotropic parabolic confinement (a) at $\alpha=2$ and (b) at $\alpha=5$. The thick and thin solid lines represent the unperturbed $[n \mp ml]$ and perturbed $(n \mp ml)$ energy levels, respectively.

certain conditions, to the ground-state results of existing works, and gives also the first excited states in a magnetic field.

$$\text{A. } \bar{\Omega}^2 = \bar{\beta}^2 / \bar{\gamma}_{\mp}^2 = 1$$

This is the case that corresponds to taking $\bar{\omega} = \bar{\omega}_{\parallel}$ in Eq. (28), since $\bar{\beta} = \bar{\gamma}_{\mp}$, so one obtains the result

$$\begin{aligned} \bar{E}_{n,\mp m,l}(\bar{\beta}) = & \left(\frac{1}{2\bar{\beta}^2} + \frac{1}{2} \mu \bar{\omega}^2 \bar{\beta}^2 \right) \left(2n + m + l + \frac{3}{2} \right) \mp m \frac{\bar{\omega}_c}{2} \\ & - \alpha \frac{2}{\pi} \frac{1}{\bar{\beta}} I_{n \mp ml}(1). \end{aligned} \quad (29)$$

This is to be minimized with respect to $\bar{\beta}$. For $\alpha=0$, it can be easily seen that the variation with respect to $\bar{\beta}$ gives $\bar{\beta}^2$

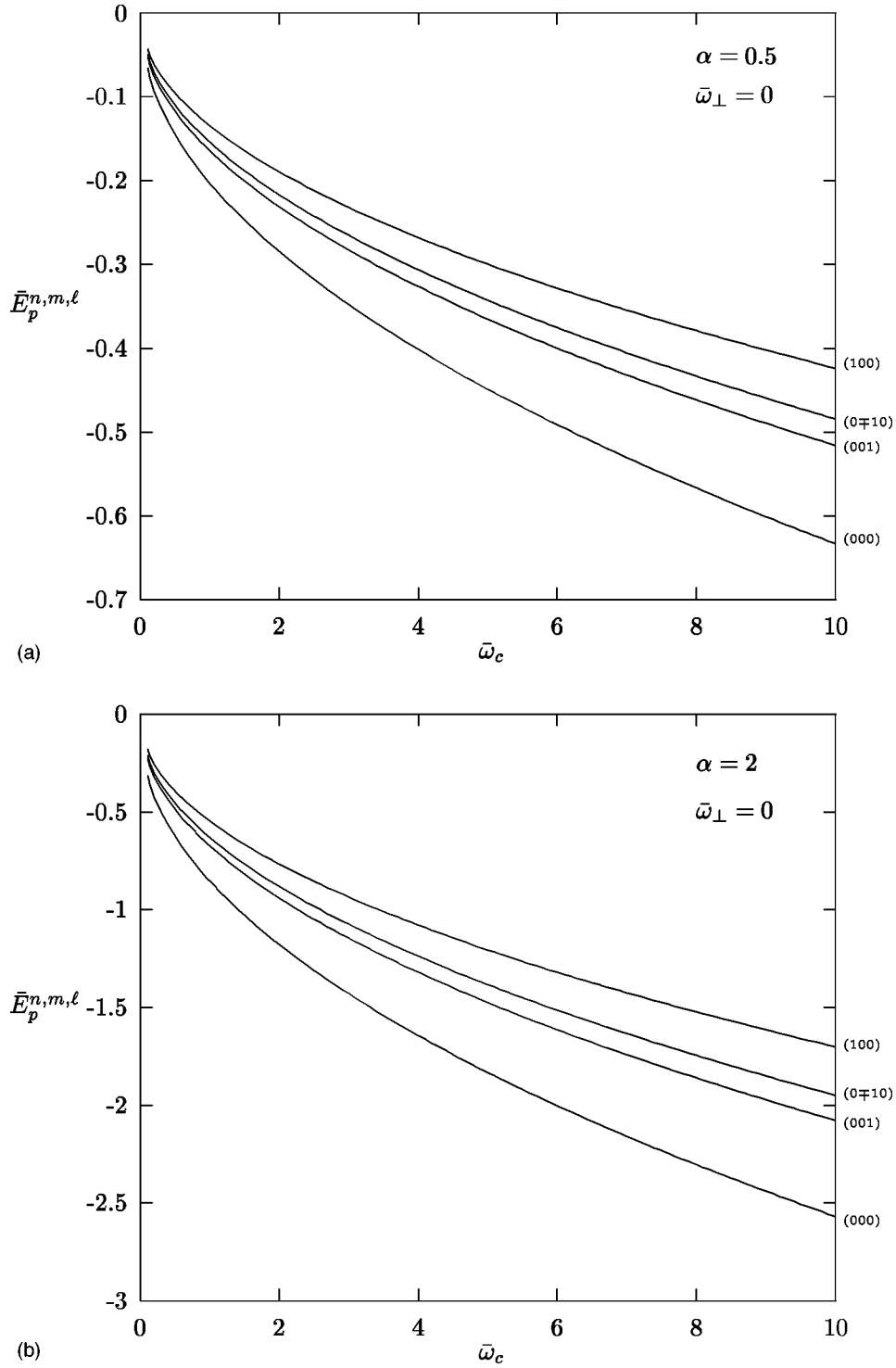


FIG. 2. Cyclotron frequency dependence of the magnetopolaron self-energies $\bar{E}_p^{n,m,l}$ in a quantum dot with an anisotropic parabolic confinement (a) at $\alpha=0.5$ and (b) at $\alpha=2$ for $\bar{\omega}_\perp=0$. (c) Same as (a), and (d) same as (b), but $\bar{\omega}_\perp=2$.

$=1/\bar{\omega}$ which yields $\bar{E}_{n,\mp m,l}=[2n+m+l+(3/2)]\bar{\omega} \mp m(\bar{\omega}_c/2)$; for the zero-magnetic-field case, $\bar{\omega}_\perp$ becomes equal to $\bar{\omega}_\parallel$, and from Eq. (29) it should also be noted that $\bar{E}_{n,\mp m,l}$ reduces to the $\bar{E}_{n,l}=(2n+1)\bar{\omega}_\perp+[l+(1/2)]\bar{\omega}_\perp$, which is the well-known energy eigenvalue of a 3D isotropic oscillator. In the presence of a magnetic field, and further on the assumption that $\bar{\omega}_\perp=0$, we come to the result $\bar{E}_{n,\mp m,l}=[n+(m \mp m)/2+(1/2)]\bar{\omega}_c+[l+(1/2)](\bar{\omega}_c/2)$, which is

the energy eigenvalues of an electron moving in a homogeneous magnetic field and a 1D parabolic potential.

When $\alpha \neq 0$, minimization of Eq. (29) with respect to $\bar{\beta}$ results in a fourth-order equation for $\bar{\beta}$,

$$\bar{\beta}^4 + e_{n \mp ml}(\alpha, \bar{\omega})\bar{\beta} - g(\bar{\omega}) = 0, \quad (30)$$

where $g(\bar{\omega}) = 1/\bar{\omega}^2$ and

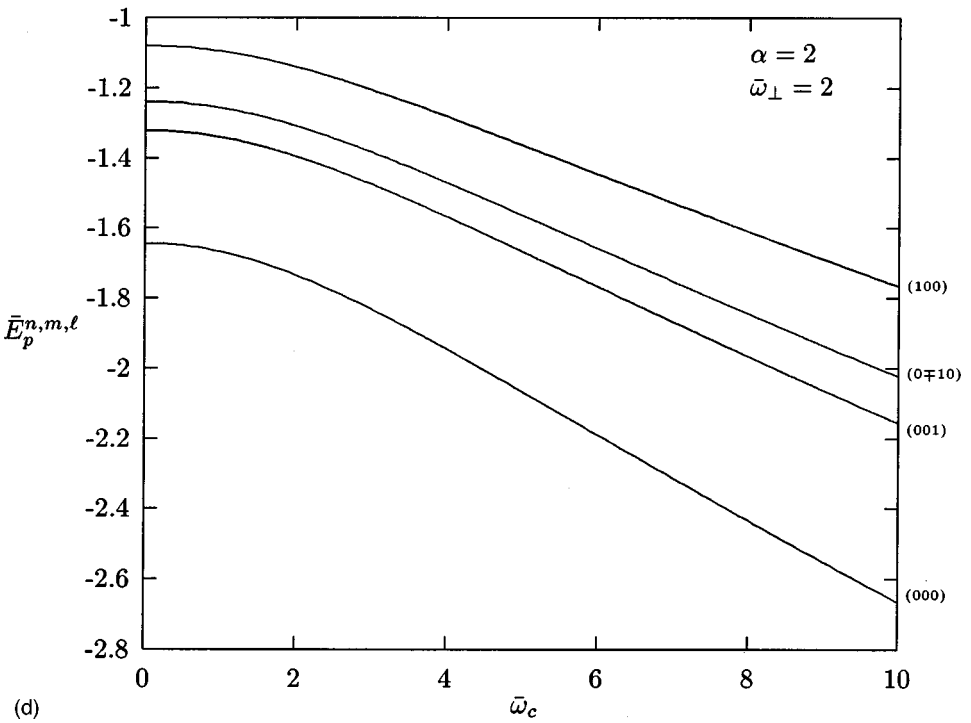
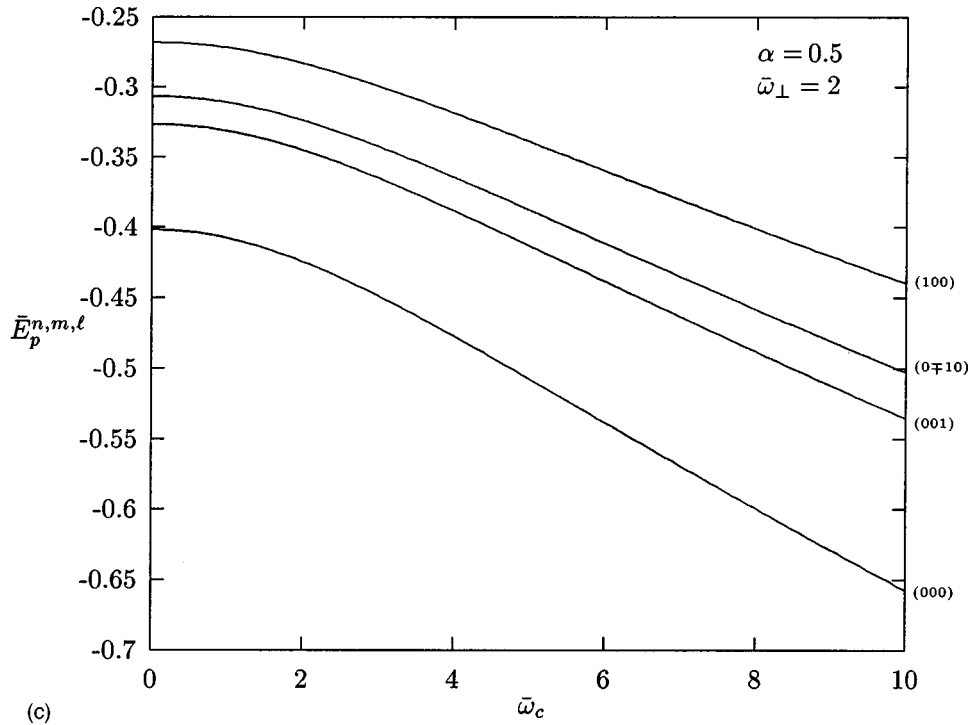


FIG. 2. (Continued).

$$e_{n\bar{+}ml}(\alpha, \bar{\omega}) = \frac{2\alpha}{\pi} I_{n\bar{+}ml}(1) \left/ \left[4 \left(2n + m + l + \frac{3}{2} \right) \bar{\omega}^2 \right] \right. \quad (31)$$

This can be solved analytically in terms of α and $\bar{\omega}$ for certain values of $(n, \bar{+}m, l)$. The solutions to Eq. (30) give two imaginary and two real roots. As the former roots can be omitted, one of the real roots gives minimized energies that we used in our calculation, and the second one has not been

considered since it gives maximum energies. The real root giving the minimized energies can be easily found as

$$\beta(\alpha, \bar{\omega}) = \frac{1}{2} \left\{ -[a_{n\bar{+}ml}(\alpha, \bar{\omega})]^{1/2} + [-a_{n\bar{+}ml}(\alpha, \bar{\omega}) + \frac{1}{2} c_{n\bar{+}ml}(\alpha) \bar{\omega}^{-2} [a_{n\bar{+}ml}(\alpha, \bar{\omega})]^{-1/2}]^{1/2} \right\}, \quad (32)$$

with

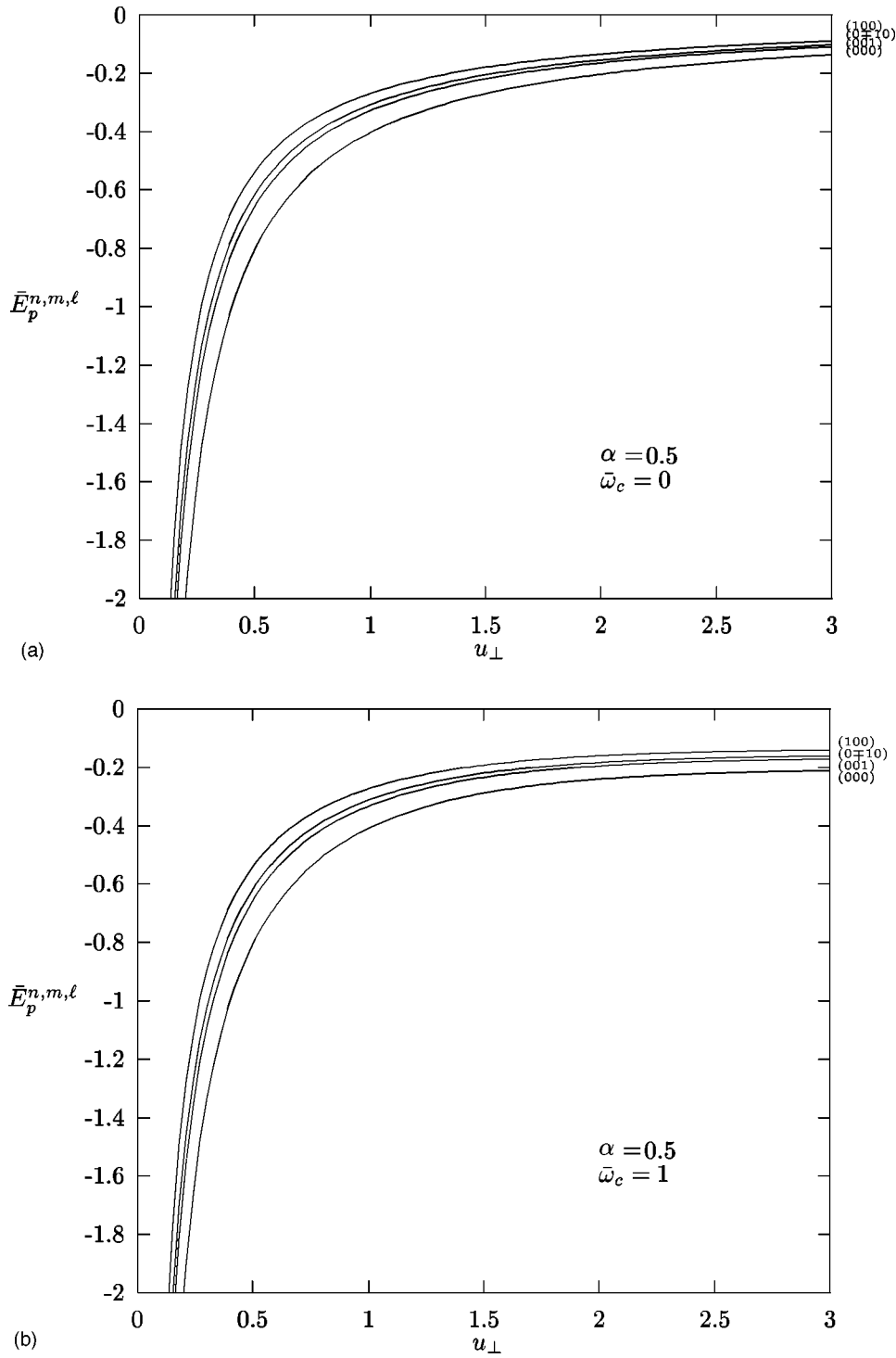


FIG. 3. The magnetopolaron self-energies $\bar{E}_p^{n,m,l}$ as a function of confinement length u_\perp (a) in the absence of a magnetic field and (b) at $\bar{\omega}_c=1$, for $\alpha=0.5$.

$$a_{n\mp ml}(\alpha, \bar{\omega}) = -16 \times 2^{1/3} b_{n\mp ml}^{-1}(\alpha, \bar{\omega}) + (12 \times 2^{1/3} \bar{\omega}^2)^{-1} b_{n\mp ml}(\alpha, \bar{\omega}), \quad (33)$$

$$b_{n\mp ml}(\alpha, \bar{\omega}) = \{27 \times 4 c_{n\mp ml}^2(\alpha) \bar{\omega}^2 + [729 \times 16 c_{n\mp ml}^4(\alpha) \bar{\omega}^4 + 442368 \times 64 \bar{\omega}^6]^{1/2}\}^{1/3},$$

in which $c_{n\mp ml}(\alpha) = 4 \bar{\omega}^2 e_{n\mp ml}(\alpha, \bar{\omega})$. By substituting Eq. (32) back into Eq. (29), and using the results for $I_{n\mp ml}(1)$

which are evaluated in Appendix A for different values of three quantum numbers (n, m, l), one obtains the analytical results for the ground state and the excited states of the problem.

For the ground-state energy in the absence of a magnetic field, Eq. (29) reduces to the energy obtained by Lépine and Bruneau,⁸ who recently showed that their results for the ground-state energy are valid for any strength of electron-phonon coupling, by comparing them with those of Yıldırım and Erçelebi,²² who also studied the problem in weak- and

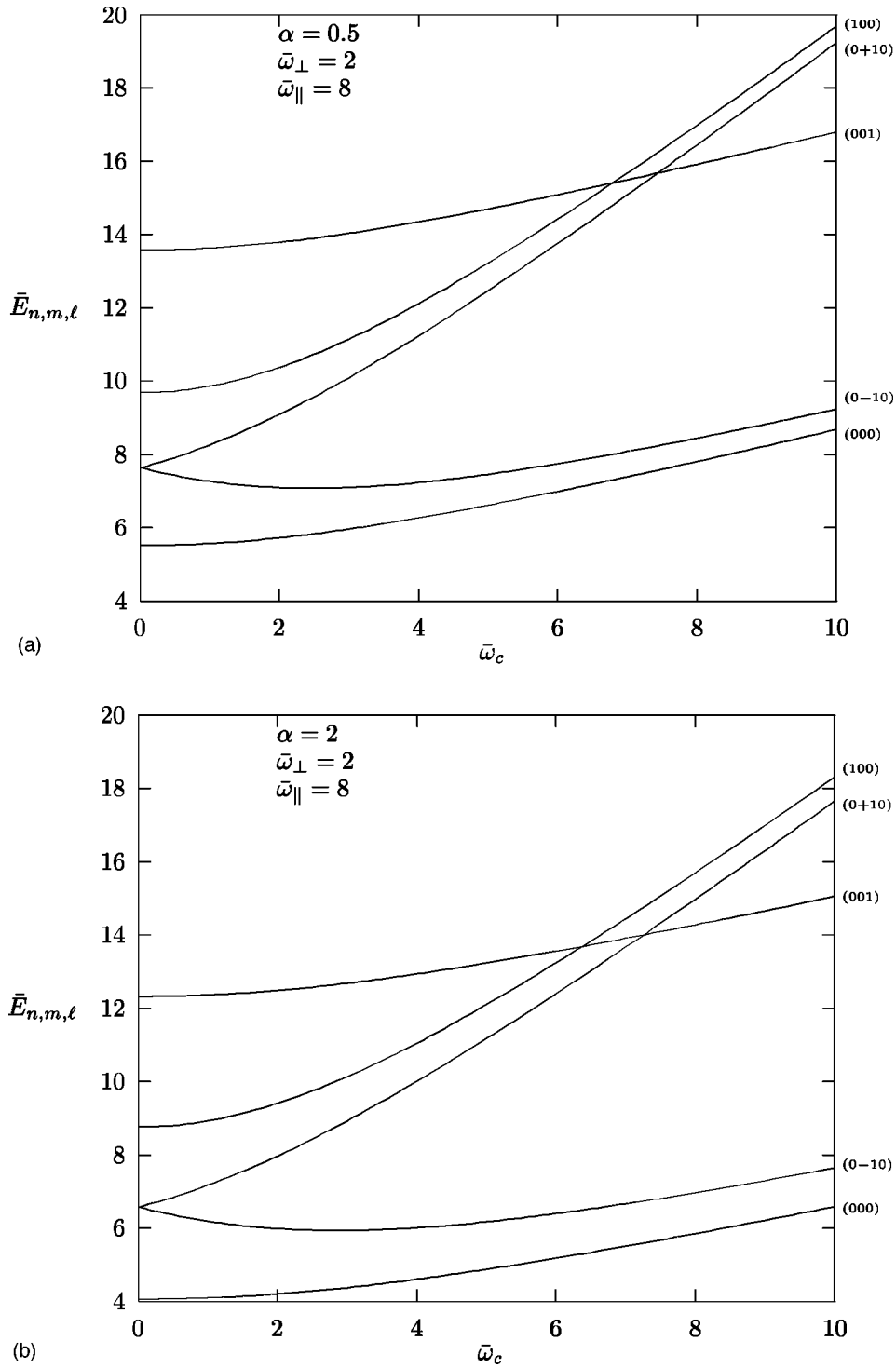


FIG. 4. Cyclotron frequency dependence of the magnetopolaron self-energies $\bar{E}_p^{n,m,l}$ in a quantum dot with an anisotropic parabolic confinement (a) at $\alpha=0.5$ and (b) at $\alpha=2$, for $\bar{\omega}_\perp=2$ and $\bar{\omega}_\parallel=8$.

strong-coupling limits. In order to see this, from Eq. (29) one writes the ground-state energy in the following form:

$$\bar{E}_{000}(\bar{\beta}) = \frac{3}{2} \left(\frac{1}{2\bar{\beta}^2} + \frac{1}{2}\bar{\omega}^2\bar{\beta}^2 \right) \mp m \frac{\bar{\omega}_c}{2} - \frac{\alpha}{\sqrt{\pi}} \frac{1}{\bar{\beta}}, \quad (34)$$

where we have used $I_{000}(1) = \sqrt{\pi}/2$ (see Appendix A). Equation (34) is exactly the same as Eq. (15) in Ref. 8, provided that one substitutes the variational parameter $\bar{\beta}$ with $1/\sqrt{2}\bar{\beta}$

and $\bar{\omega}/2$ with K^2 . In Ref. 8, Eq. (34) is minimized with respect to $\bar{\beta}$, and a special form of Eq. (31) was obtained and solved approximately for some asymptotic limits. While our analytical treatment allows us to find the excited-state energies in addition to the ground-state ones as a function of $\bar{\omega}$, together with Eq. (32) it also unifies all expressions for the ground-state energy found by other authors,^{8,22} not only in any strength of electron-phonon interaction coupling but also in a nonzero magnetic field. Furthermore it gives excited-

state energies in any coupling strengths and in a magnetic field.

It is well known that the Landau levels of an unperturbed electron in a uniform magnetic field are no longer linear in a cyclotron frequency $\bar{\omega}_c$ which is proportional to the magnetic field when the electron-phonon interaction is switched on. As expected, they are also shifted by an amount of polaron self-energy, and bend up when the magnetic field increases. We observe these properties in Fig. 1, that shows the ground- and first-excited-state energies of the polaron corresponding to the various combinations of three different quantum numbers $(n, \mp m, l)$ as a function of $\bar{\omega}_c$ for $\alpha=2$ and 5, at $\bar{\omega}_\perp=0$. Since the confinement frequency $\bar{\omega}_\perp$, expressed in terms of the LO-phonon frequency ω_0 , is directly related to the dimensionless confinement length $u_\perp=l_\perp/r_0=\sqrt{2/\bar{\omega}_\perp}$, the case for $\bar{\omega}_\perp=0$ defines a 2D magnetopolaron with one-dimensional confinement along the z axis with a confinement frequency $(\bar{\omega}_c/2)$, which itself depends on B . Hence, as B increases, the magnetopolaron is strongly localized in two dimensions, and therefore effectively becomes a 2D system in which the polaronic effects are enhanced. In order to understand the influence of the electron-phonon interaction on electronic levels, we have also plotted unperturbed energy levels of an electron by thick solid lines in the same figure. By comparison of Figs. 1(a) and 1(b), one observes that the difference in energy levels increases with increasing electron-phonon coupling strength α . For a more detailed study, we also present plots that show a variation of the polaron self-energies for different $(n, \mp m, l)$ with $\bar{\omega}_c$ for some values of α and $\bar{\omega}_\perp$ in Fig. 2. A first observation from these figures appears to show that the polaron self-energy for the ground state is the largest and appears to lie below the others, as expected. One also notices that the polaron self-energies for different quantum numbers $(n, \mp m, l)$ increase with increasing electron-phonon coupling strength by comparison of Figs. 2(a) and 2(b) with Fig. 2(c) and 2(d), and with decreasing confinement length l_\perp by comparison of Fig. 2(a) with Fig. 2(c), and Fig. 2(b) with Fig. 2(d). In Fig. 3, we demonstrate the dependence of polaron self-energies for different quantum numbers $(n, \mp m, l)$ on the dimensionless confinement length u_\perp for some fixed values of $\bar{\omega}_c$ and α . It should be noted that the polaron self-energies for different $(n, \mp m, l)$ increase with decreasing confinement length l_\perp . The case $\bar{\omega}_c=0$ has also been interpreted by the authors of Ref. 8 for several values of electron-phonon coupling strength α .

$$\text{B. } \bar{\Omega}^2 = \bar{\beta}^2 / \bar{\gamma}_\mp^2 < 1$$

With this condition, $\bar{\beta}^2 < \bar{\gamma}_\mp^2$, one has to minimize Eq. (28) with respect to both $\bar{\beta}$ and $\bar{\gamma}_\mp$. This yields two coupled equations which have complicated dependencies on α , $\bar{\omega}_c$, $\bar{\omega}_\parallel$, $\bar{\omega}_\perp$, and $I_{n\mp ml}(\bar{\Omega})$ for the relevant variational parameters, so that it seems impossible to solve them; however, if one can use the values $\bar{\beta}^2=1/\bar{\omega}_\parallel$ and $\bar{\gamma}_\mp^2=1/\bar{\omega}$ corresponding to $\alpha=0$ as a first approximation, then Eq. (28) takes the form

$$\begin{aligned} \bar{E}_{n,\mp m,l} = & (2n+m+1)\bar{\omega} + \left(l + \frac{1}{2}\right)\bar{\omega}_\parallel \mp m \frac{\bar{\omega}_c}{2} \\ & - \alpha \frac{2}{\pi} \frac{\bar{\omega}}{\sqrt{\bar{\omega}_\parallel}} I_{n\mp ml}(\bar{\Omega}). \end{aligned} \quad (35)$$

In Appendix A, we present the details of calculation of the integrals $I_{n\mp ml}(\bar{\Omega})$ involved in Eq. (35) for some values of (n, m, l) . From Eqs. (A10) and (A11), the integral appearing in the evaluation of the ground state is found to be

$$I_{000}(\bar{\Omega}) = \frac{1}{\bar{\Omega} \sqrt{1-\bar{\Omega}^2}} \arctan \left[\frac{\sqrt{1-\bar{\Omega}^2}}{\bar{\Omega}} \right]. \quad (36)$$

We note that the ground-state energy obtained by substitution of Eq. (36) into Eq. (35) yields the result of Yıldırım and Erçelebi,²² provided that one replaces $\bar{\gamma}_\mp^2$ by $1/\lambda_1$ and $\bar{\beta}^2$ by $1/\lambda_2$; it also gives 2D limit (1D confinement) results of Ref. 22 by substitution of relevant parameters with the parameters defined there, in the absence of magnetic field. So our result for the ground-state energy is consistent with that from Refs. 8 and 22, and also includes the magnetic-field dependence. For this limit we can easily obtain the first-excited-state energies. This requires evaluating certain integrals, which can be obtained from Eqs. (A10) and (A12)–(A16) and are of the following forms:

$$I_{0\mp 10}(\bar{\Omega}) = -\frac{3\sqrt{\pi}}{32}\Lambda^2 + \frac{3\sqrt{\pi}}{16}\Lambda + \left[1 - \frac{1}{2}\Lambda + \frac{3}{16}\Lambda^2\right]I_{000}, \quad (37)$$

$$\begin{aligned} I_{001}(\bar{\Omega}) = & -\frac{3\sqrt{\pi}}{8} - \frac{\sqrt{\pi}}{4}\bar{\Omega}^2 + \left[1 + \bar{\Omega}^2\Lambda + \frac{3}{4}\bar{\Omega}^4\Lambda^2\right]I_{000} \\ & - \frac{\sqrt{\pi}}{2}\bar{\Omega}^2\Lambda \left[1 + \frac{1}{2}\bar{\Omega}^2 + \frac{3}{4}\bar{\Omega}^2\Lambda\right], \end{aligned} \quad (38)$$

$$\begin{aligned} I_{100}(\bar{\Omega}) = & \left[1 - \Lambda + \frac{9}{8}\Lambda^2 - \frac{15}{16}\Lambda^3 + \frac{105}{256}\Lambda^4\right]I_{000} \\ & + \frac{\sqrt{\pi}}{2}\Lambda \left[\frac{9}{16} - \frac{23}{32}\Lambda + \frac{170}{256}\Lambda^2 - \frac{105}{256}\Lambda^3\right], \end{aligned} \quad (39)$$

where we have defined $\Lambda = 1/(1-\bar{\Omega}^2)$. Inserting Eqs. (37)–(39) together with Eq. (36) into Eq. (35) yields the ground- and first-excited-state energies of the polaron. They are plotted in Fig. 4. as a function of cyclotron frequency ($\bar{\omega}_c$) for two different values of α at fixed confinement frequencies $\bar{\omega}_\parallel$ and $\bar{\omega}_\perp$. Here the increase of electron-phonon interaction

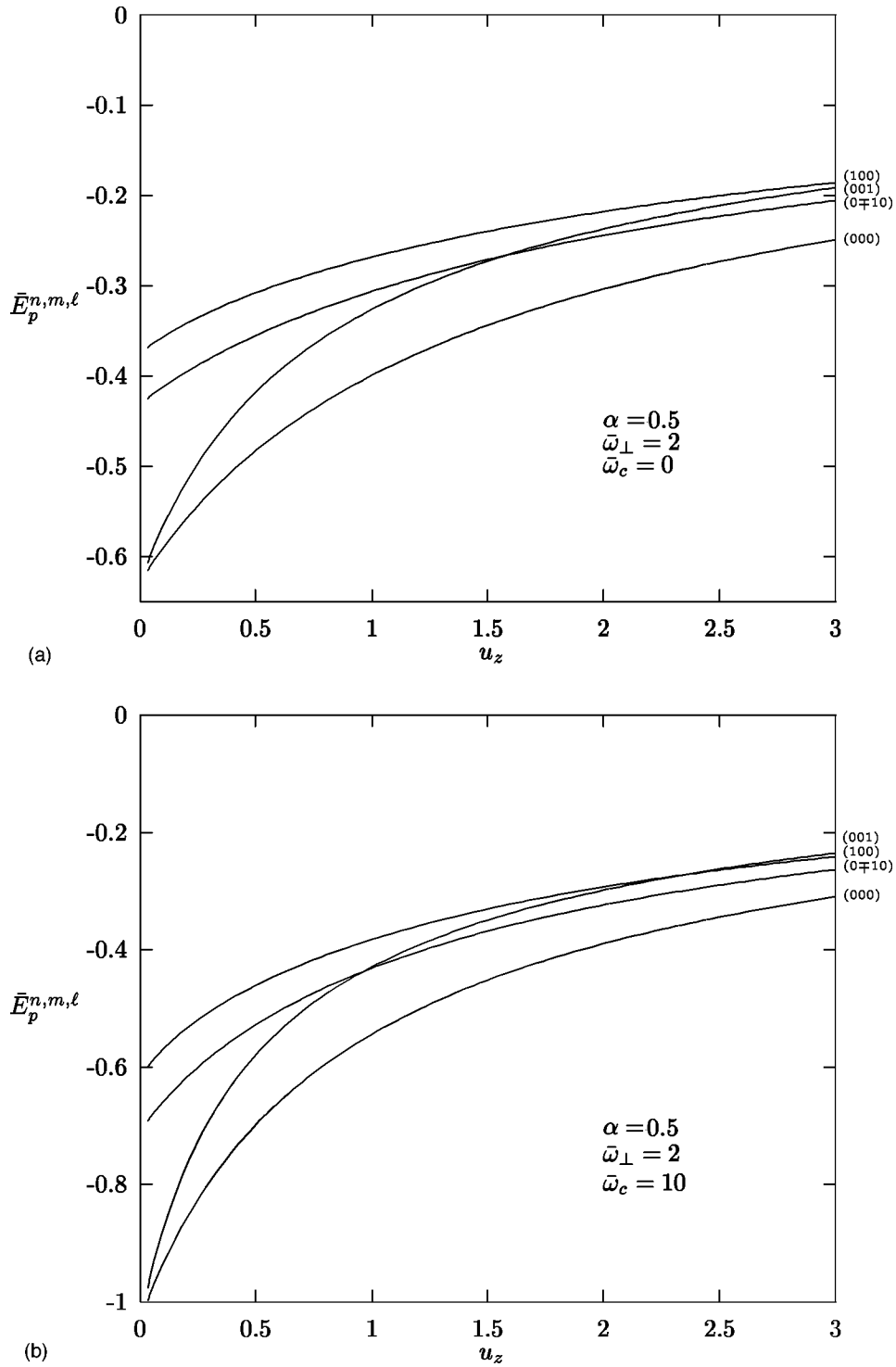


FIG. 5. The magnetopolaron self-energies $\bar{E}_p^{n,m,l}$ as a function of confinement length u_z (a) for $\bar{\omega}_\perp=2$ and $\bar{\omega}_c=0$ and (b) for $\bar{\omega}_\perp=2$ and $\bar{\omega}_c=10$, at $\alpha=0.5$. (c) Same as (a), and (d) same as (b), but $\alpha=2$.

causes a lowering in energy levels for the same reasons as pointed out above. For comparison, the polaron self-energies for the ground and first excited states are also plotted in Fig. 5 as a function of confinement length u_z for two different values of α and $\bar{\omega}_c$ at a fixed confinement frequency $\bar{\omega}_\perp$. One can easily observe that the polaron self-energies increase not only with increasing electron-phonon interaction by comparison of Figs. 5(a) and 5(b) with 5(c) and 5(d), but also with increasing cyclotron frequency due to the fact that

electron is localized in the xy plane perpendicular to the magnetic field, by comparison of Figs. 5(a) and 5(c) with 5(b) and 5(d);

$$C. \bar{\Omega}^2 = \bar{\beta}^2 / \bar{\gamma}_\mp^2 > 1$$

By using Eqs. (B1) and (B2), one obtains the value of the integral appearing in the calculation of the ground state in this case as

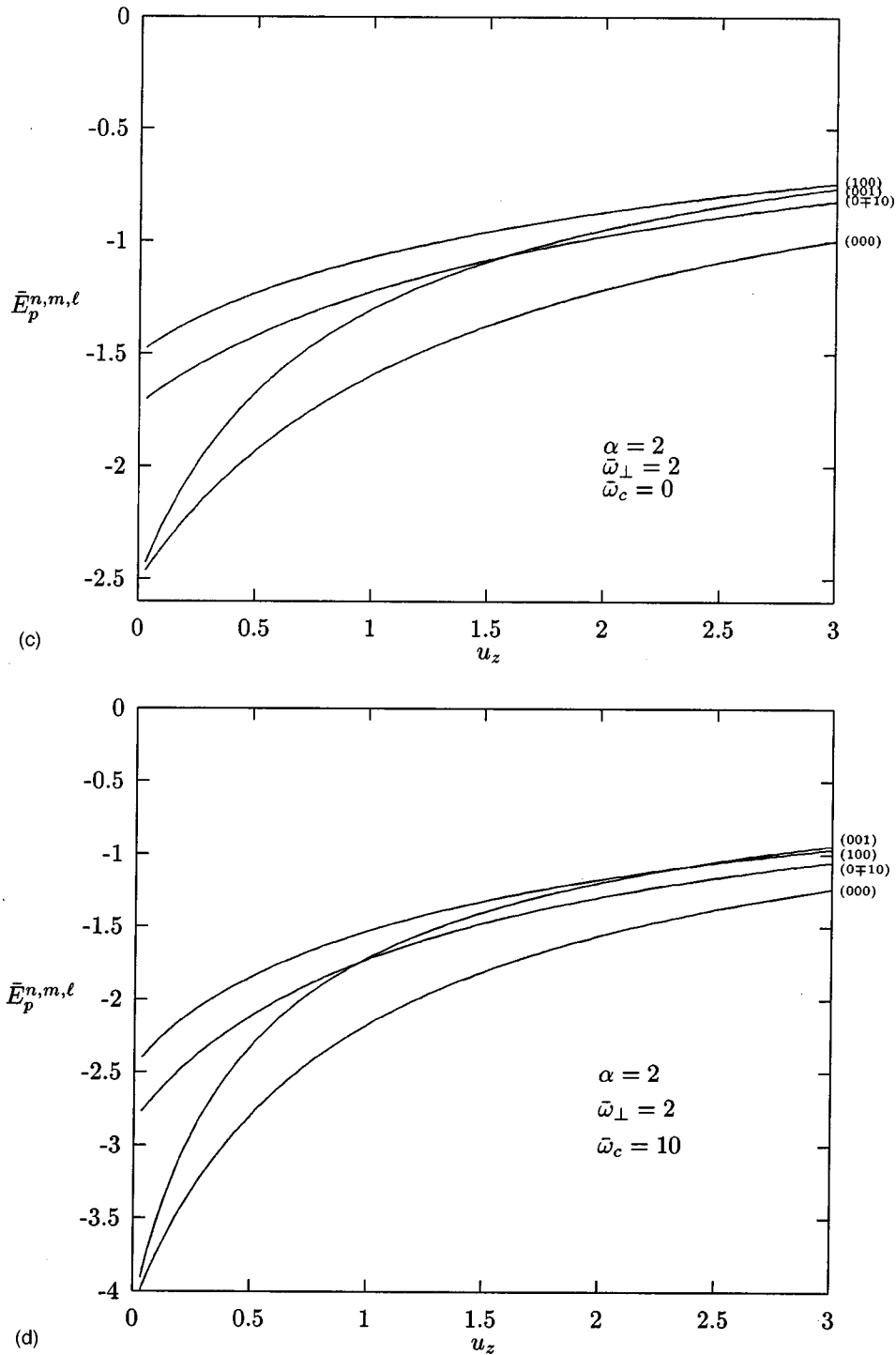


FIG. 5. (Continued).

$$I_{000}(\bar{\Omega}) = \frac{\sqrt{\pi}}{2} \frac{1}{\bar{\Omega} \sqrt{\bar{\Omega}^2 - 1}} \ln[\bar{\Omega} + \sqrt{\bar{\Omega}^2 - 1}], \quad (40)$$

which differs from Eq. (36). Exactly the same results hold for the integrals $I_{0\mp 10}(\bar{\Omega})$, $I_{001}(\bar{\Omega})$, and $I_{100}(\bar{\Omega})$ as for the previous case, provided that now one uses Eq. (40) for $I_{000}(\bar{\Omega})$ instead of Eq. (36). So, in this limit, we find the ground- and the first-excited-state energies by inserting Eqs. (37)–(39) together with Eq. (40) into Eq. (35). They exhibit

the same behavior under the variation of cyclotron frequency and of electron-phonon coupling strength at fixed confinement frequencies $\bar{\omega}_{\parallel}$ and $\bar{\omega}_{\perp}$ (Fig. 6). In order to understand better how polaron self-energies for the ground and the first excited states are influenced by the change of confinement length u_{\perp} , we plot them in Fig. 7.

IV. CONCLUSION

In this paper, we have performed a variational calculation to obtain the ground- and first-excited-state energies of a

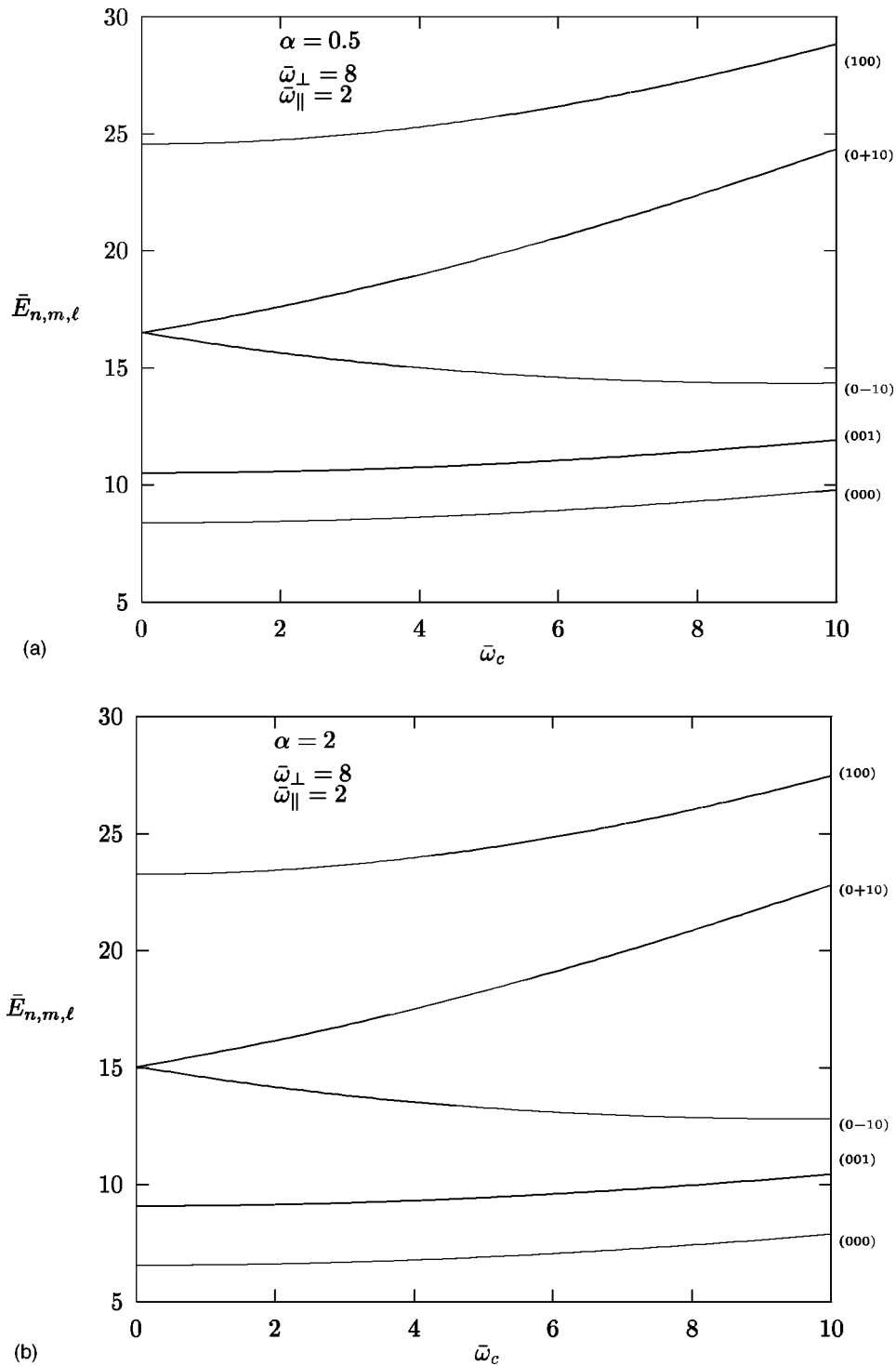


FIG. 6. Cyclotron frequency dependence of the magnetopolaron energy levels $\bar{E}_{n,m,l}$ in a quantum dot with an anisotropic parabolic confinement (a) at $\alpha=0.5$ and (b) at $\alpha=2$, for $\bar{\omega}_\perp=8$ and $\bar{\omega}_\parallel=2$.

polaron in a parabolic QD. It is assumed that the electron-interface-LO-phonon interaction can be negligible in comparison with bulk LO phonons. The ground-state energies in zero magnetic fields have reduced to the results obtained by other methods. The first-excited-state energies are also obtained, but to our knowledge there exists no study with which we can compare our results. The present method is valid for intermediate coupling strength. Therefore, our results can be experimentally realized for semiconductor dots, such as CuCl and CdSe.

A QD may have many electrons, changing from a few electrons to a thousand. Electron-electron interaction that may be important in certain problems can be negligible in some cases. For example, it was shown that magneto-optical absorption lines by many electrons do not differ from those of only one electron.¹⁹ In the present approach we have neglected these interactions for the sake of simplifying our calculations. The confinement lengths u_\perp and u_z are expressed in terms of the polaron radius r_0 and are dimensionless. Only the values of u_\perp and u_z larger than unity are meaningful,

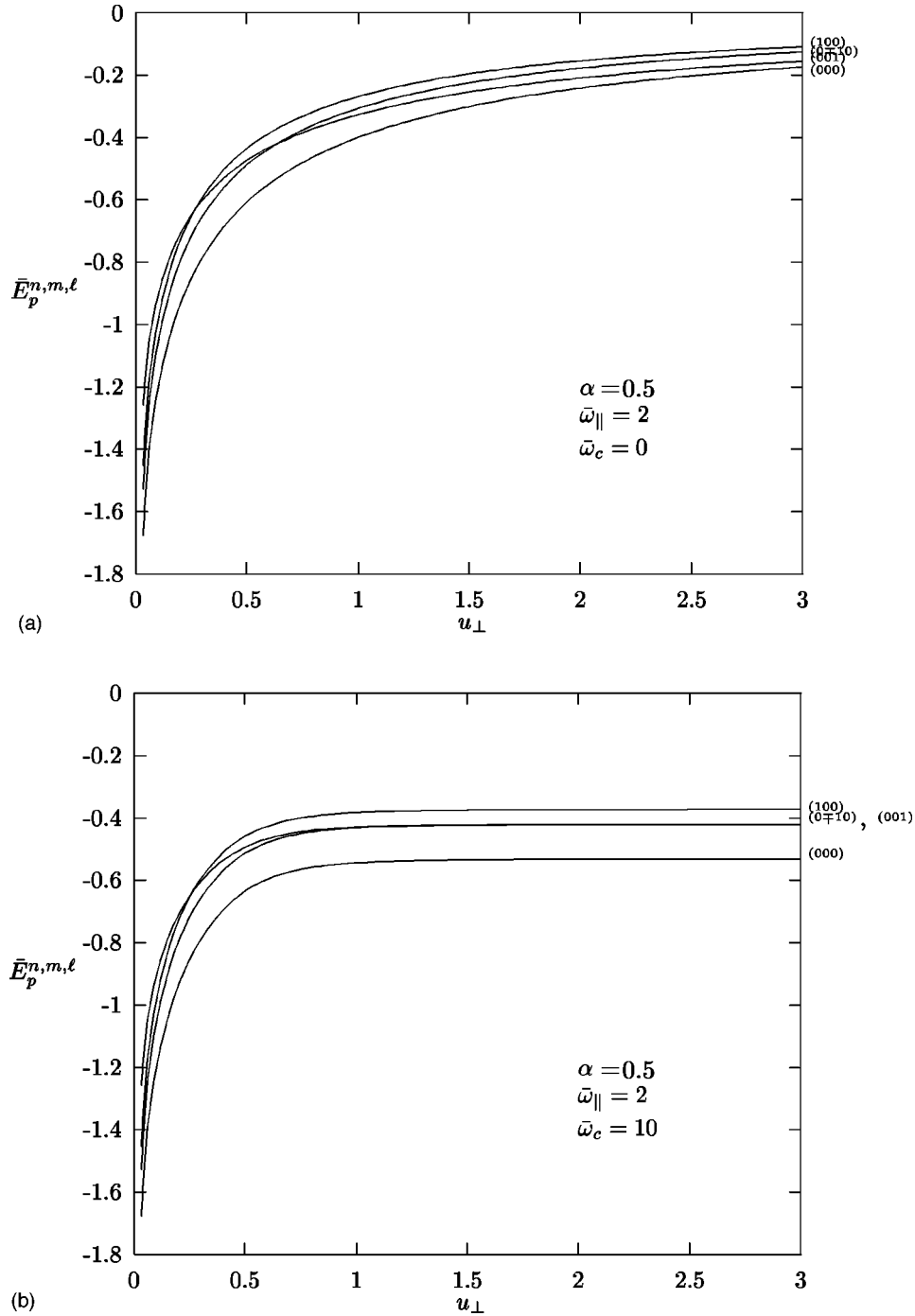


FIG. 7. The magnetopolaron self-energies $\bar{E}_p^{n,m,\ell}$ as a function of confinement length u_\perp (a) for $\bar{\omega}_\parallel = 2$ and $\bar{\omega}_c = 0$ and (b) for $\bar{\omega}_\parallel = 2$ and $\bar{\omega}_c = 10$, at $\alpha = 0.5$. (c) Same as (a), and (d) same as (b), but $\alpha = 2$.

since the Fröhlich Hamiltonian is valid in the continuum approximation.

In summary, we have analytically calculated the ground and first excited states of the magnetopolaron in an anisotropic QD. We have observed that effects of the electron-phonon interaction, besides those of confinement in all directions, have a great importance in analyzing the localization properties of the electron. Furthermore, the presence of a magnetic field makes these effects more prominent, as can be observed from the figures.

ACKNOWLEDGMENT

This work was supported in part by the Scientific and Technical Research Council of Turkey (TUBITAK) under TBAG Project No. 1654.

APPENDIX A

In this and in Appendix B we evaluate the integral given in Eq. (28), i.e.,

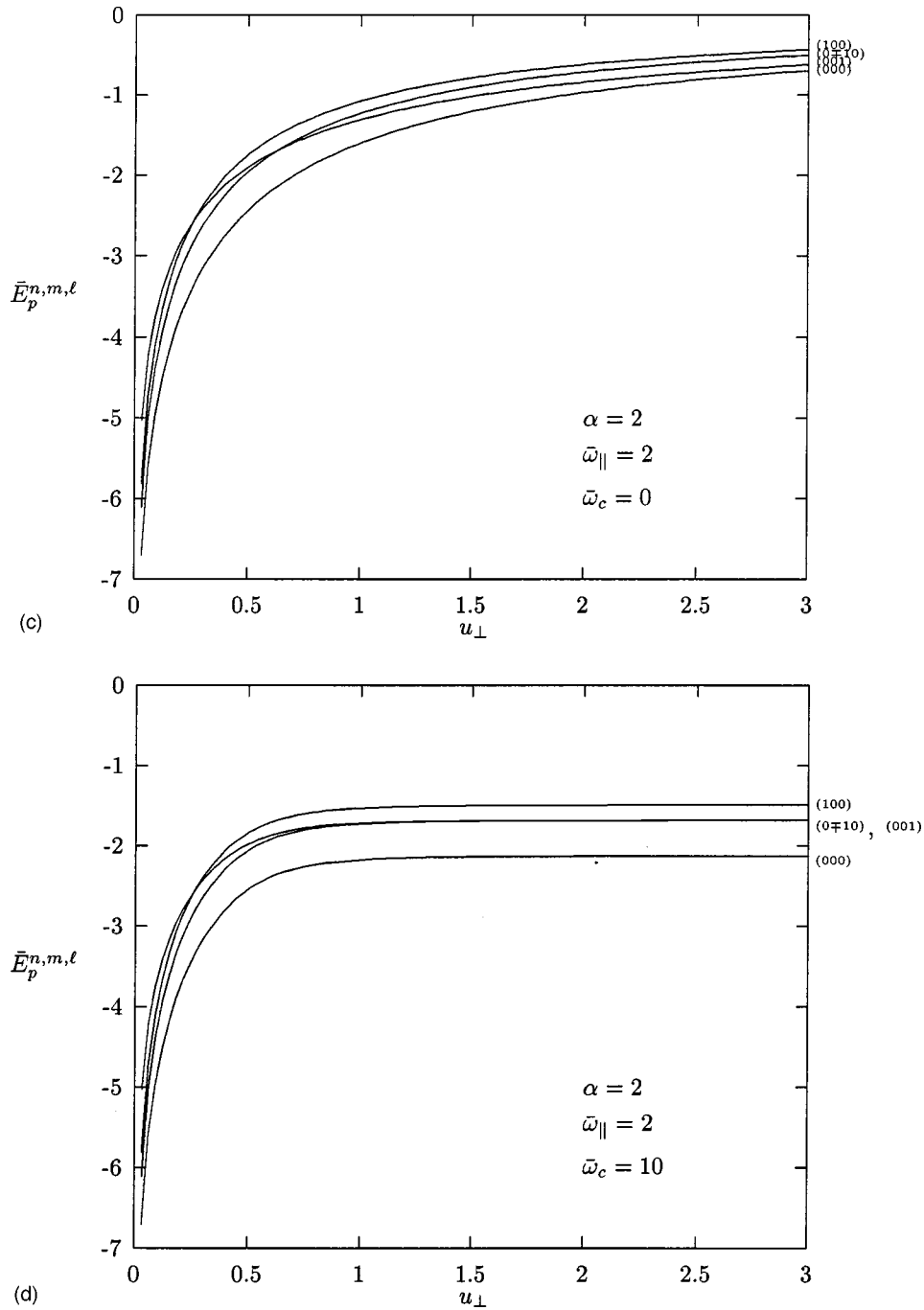


FIG. 7. (Continued).

$$I_{nml}(\bar{\Omega}) = \int_0^\infty x dx |\rho_{nm}(x^2/2)|^2 \int_0^\infty dy \frac{e^{-y^2}}{\bar{\Omega}^2 x^2 + y^2} L_l^2(y^2), \tag{A1}$$

for different values of three quantum numbers (n, m, l) and $\bar{\Omega}$, which we require in the text. First we will consider the case of $\bar{\Omega}^2 = 1$. If we use the following integral, with this choice of the parameter $\bar{\Omega}$, over the variable y and for $l=0$ in Eq. (A1),²³

$$I_0(\mu, \beta) = \int_0^\infty dy \frac{e^{-\mu^2 y^2}}{y^2 + \beta^2} = [1 - \Phi(\beta\mu)] \frac{\pi}{2\beta} e^{\beta^2 \mu^2}, \tag{A2}$$

in which $\Phi(\beta\mu) = (2/\sqrt{\pi}) \int_0^{\beta\mu} dt \exp(-t^2)$ is the well-known probability integral, then we obtain

$$I_{nm0}(1) = \frac{\pi}{2} \int_0^\infty dx |\rho_{nm}(x^2/2)|^2 [1 - \Phi(x)] e^{x^2}. \tag{A3}$$

The remaining integral over x in Eq. (A3) can be easily performed by means of the integral identity²³

$$I(p, q) = \int_0^\infty dx [1 - \Phi(px)] x^{2q-1} = \frac{\Gamma\left(q + \frac{1}{2}\right)}{2\sqrt{\pi} p^{2q}}. \tag{A4}$$

By using the various values of ρ_{nm} given by Eqs. (19) and (A4), one finds the following results:

$$I_{000}(1) = \frac{\sqrt{\pi}}{2}, \quad I_{0\mp 10}(1) = \frac{23\sqrt{\pi}}{60}, \quad I_{100}(1) = \frac{423\sqrt{\pi}}{1260}. \tag{A5}$$

In order to find the result of the remaining integral required in the text, i.e., $I_{001}(1)$, one has to consider the integral

$$I_{001}(1) = \int_0^\infty x dx e^{-x^2} \int_0^\infty dy \frac{e^{-y^2}}{x^2 + y^2} (1 - y^2)^2, \tag{A6}$$

where the value of ρ_{00} given in Eq. (19) and $L_1(y^2) = (1 - y^2)$ are used. To evaluate the integral over y in Eq. (A6) one also needs the relations

$$I_2(\mu, \beta) = -\frac{1}{2\mu} \frac{\partial}{\partial \mu} I_0(\mu, \beta) = \int_0^\infty y^2 dy \frac{e^{-\mu^2 y^2}}{y^2 + \beta^2} = \frac{\sqrt{\pi}}{2\mu} - \frac{\pi\beta}{2} e^{\beta^2 \mu^2} [1 - \Phi(\beta\mu)] \tag{A7}$$

and

$$I_4(\mu, \beta) = -\frac{1}{2\mu} \frac{\partial}{\partial \mu} I_2(\mu, \beta) = \int_0^\infty y^4 dy \frac{e^{-\mu^2 y^2}}{y^2 + \beta^2} = \frac{\sqrt{\pi}}{4\mu^3} - \frac{\sqrt{\pi}}{2} \frac{\beta^2}{\mu} + \frac{\pi}{2} \beta^3 e^{\beta^2 \mu^2} [1 - \Phi(\beta\mu)], \tag{A8}$$

which are derived by repeated differentiation partially of Eq. (A2) with respect to the parameter μ . On substituting these and Eq. (A2) in Eq. (A6), one obtains the integrals over x , which have the same structure as in Eq. (A4). So the result is

$$I_{001}(1) = \frac{98\sqrt{\pi}}{240}. \tag{A9}$$

In the following we will evaluate Eq. (A1) for the case of $\bar{\Omega}^2 < 1$. As we have done above, we start with the case $l = 0$, so that Eq. (A1) can be written in the form

$$I_{nm0}(\bar{\Omega}) = \int_0^\infty x dx |\rho_{nm}(x^2/2)|^2 \int_0^\infty dy \frac{e^{-y^2}}{\bar{\Omega}^2 x^2 + y^2} = \frac{\pi}{2\bar{\Omega}} \int_0^\infty dx |\rho_{nm}(x^2/2)|^2 [1 - \Phi(\bar{\Omega}x)] e^{\bar{\Omega}^2 x^2}, \tag{A10}$$

again by using Eq. (A2). If the values of ρ_{nm} for different values of n and m given in Eq.(19) are replaced into Eq. (A10), one first needs to use the integral²³

$$I_0(\mu) = \int_0^\infty dz [1 - \Phi(z)] e^{-\mu^2 z^2} = \frac{1}{\sqrt{\pi}} \frac{\arctan \mu}{\mu}; \tag{A11}$$

furthermore, the other integrals to be appeared in calculation can be obtained from Eq. (A11), by repeated differentiation partially of Eq. (A11) with respect to the parameter μ :

$$I_2(\mu) = -\frac{1}{2\mu} \frac{\partial}{\partial \mu} I_0(\mu) = \int_0^\infty z^2 dz [1 - \Phi(z)] e^{-\mu^2 z^2} = \frac{1}{2\sqrt{\pi}} \left[\frac{\arctan \mu}{\mu^3} - \frac{1}{\mu^2(1 + \mu^2)} \right], \tag{A12}$$

$$I_4(\mu) = -\frac{1}{2\mu} \frac{\partial}{\partial \mu} I_2(\mu) = \int_0^\infty z^4 dz [1 - \Phi(z)] e^{-\mu^2 z^2} = \frac{1}{4\sqrt{\pi}} \left[\frac{3 \arctan \mu}{\mu^5} - \frac{3}{\mu^4(1 + \mu^2)} - \frac{2}{\mu^2(1 + \mu^2)^2} \right], \tag{A13}$$

$$I_6(\mu) = -\frac{1}{2\mu} \frac{\partial}{\partial \mu} I_4(\mu) = \int_0^\infty z^6 dz [1 - \Phi(z)] e^{-\mu^2 z^2} = \frac{1}{8\sqrt{\pi}} \left[\frac{15 \arctan \mu}{\mu^7} - \frac{15}{\mu^6(1 + \mu^2)} - \frac{10}{\mu^4(1 + \mu^2)^2} - \frac{8}{\mu^2(1 + \mu^2)^3} \right], \tag{A14}$$

$$I_8(\mu) = -\frac{1}{2\mu} \frac{\partial}{\partial \mu} I_6(\mu) = \int_0^\infty z^8 dz [1 - \Phi(z)] e^{-\mu^2 z^2} = \frac{1}{16\sqrt{\pi}} \left[\frac{105 \arctan \mu}{\mu^9} - \frac{105}{\mu^8(1 + \mu^2)} - \frac{70}{\mu^6(1 + \mu^2)^2} - \frac{56}{\mu^4(1 + \mu^2)^3} - \frac{48}{\mu^2(1 + \mu^2)^4} \right], \tag{A15}$$

which on substitution into Eq. (A10) give the results used in the text. Finally, for $I_{001}(\bar{\Omega})$, we evaluate the integral

$$I_{001}(1) = \int_0^\infty x dx e^{-x^2} \int_0^\infty dy \frac{e^{-y^2}}{\bar{\Omega}^2 x^2 + y^2} (1 - y^2)^2 \tag{A16}$$

by means of Eqs. (A7) and (A8) together with the help of Eqs. (A14) and (A15); hence one finds the result used in the text.

APPENDIX B

In Appendix A we require the result of integral (A10), in which the conditions $\bar{\Omega}^2 = 1$ and $\bar{\Omega}^2 < 1$ are imposed, respectively. Here we must evaluate it by considering the integral

$$I_0(\mu) = \int_0^\infty dz [1 - \Phi(\beta z)] e^{\mu^2 z^2} z^{\nu-1} \\ = \frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\sqrt{\pi\nu\beta^\nu}} {}_2F_1\left(\frac{\nu}{2}, \frac{\nu+1}{2}; \frac{\nu}{2} + 1; \frac{\mu^2}{\beta^2}\right), \quad (\text{B1})$$

but now we have the condition $\bar{\Omega}^2 > 1$, so that $\mu^2 = 1 - (1/\bar{\Omega}^2) < 1$. In Eq. (B1) ${}_2F_1$ is the well-known hypergeometric function. For $n=m=0$, it can be easily shown that Eq. (A10) results in

$$I_{000}(\bar{\Omega}) = \frac{\sqrt{\pi}}{2} \frac{1}{\bar{\Omega}^2} {}_2F_1\left(\frac{1}{2}, 1; \frac{3}{2}; \mu^2\right) = \frac{\sqrt{\pi}}{2} \frac{1}{\bar{\Omega}^2} \frac{\ln\left(\frac{1+\mu}{1-\mu}\right)}{2\mu}, \quad (\text{B2})$$

where we have used ${}_2F_1\left(\frac{1}{2}, 1; \frac{3}{2}; \mu^2\right) = \ln[(1+\mu)/(1-\mu)]/2\mu$.²⁴ In attempting to evaluate Eq. (A10) for values n and m different from zero, and also Eq. (A16) under the condition $\bar{\Omega}^2 > 1$ with $n=m=0$, one needs to evaluate integrals concerning ${}_2F_1$ with different arguments such as ${}_2F_1\left(\frac{3}{2}, 2; \frac{5}{2}; \mu^2\right)$, ${}_2F_1\left(\frac{5}{2}, 3; \frac{7}{2}; \mu^2\right)$ and so on. In handling this kind of integrals, it is necessary to use an important identity²⁴

$$\frac{d}{dz} {}_2F_1(a, b; c; z) = \frac{ab}{c} {}_2F_1(a+1, b+1; c+1; z).$$

Finally, we obtain the previous results, Eqs. (37)–(39), as in the case of $\bar{\Omega}^2 < 1$, but with different $I_{000}(\bar{\Omega})$ given by Eq. (B2).

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