The effect of an anisotropic confinement on the ground-state energy of a polaron in a parabolic quantum dot

1998 J. Phys.: Condens. Matter 10 1495

(http://iopscience.iop.org/0953-8984/10/7/004)

J. Phys.: Condens. Matter **10** (1998) 1495–1503. Printed in the UK PII: S0953-8984(98)87505-X

The effect of an anisotropic confinement on the ground-state energy of a polaron in a parabolic quantum dot

Y Lépine and G Bruneau

Département de Physique et Groupe de Recherche sur la Physique et la Technologie des Couches Minces, Université de Montréal, CP 6128, Succursale 'Centre-Ville', Montréal, Québec, Canada, H3C 3J7

Received 8 September 1997, in final form 10 November 1997

Abstract. We study the ground-state energy of a large polaron in a quantum dot. The electron is treated as trapped in an anisotropic parabolic box while the coupling to bulk LO phonons is considered. An upper bound to the ground-state energy of the polaron is obtained using the Fock approximation of Matz and Burkey. With this treatment, we obtain variational results that are good to describe weak or strong electron–phonon coupling as well as the isotropic and the one- and two-dimensional confinement limits. The usual asymptotic limits are found for all of these cases. Numerical calculations carried out in order to study the validity of each of these limits as a function of the degree of anisotropy are presented. Also we discuss the effect that the anisotropy and the strength of the confining potential have on the self-energy of the polaron. We find that an anisotropic confinement is more effective as regards increasing the self-energy of the polaron than an isotropic confinement.

1. Introduction

A polaron results from the interaction between a carrier and the phonon excitations in a polar crystal. When its size is much larger than the lattice parameter, we have a large polaron. It is described by the Fröhlich Hamiltonian, which is based on the continuum and the effective-mass approximations [1]. The development of new growth techniques for epitaxial layers and nanometric methods enables the fabrication of quantum wells ('two-dimensional' structures), quantum wires ('one-dimensional' structures), and even quantum dots ('zero-dimensional' structures) in polar semiconductors to be achieved. This confinement of the carrier motion modifies the properties which are observed for three-dimensional materials [2]. It is of great interest to study the effect of confinement on the polaron properties in such structures in order to understand their electronic transport and optical properties.

Several studies have already been carried out on polarons in quantum dots. Zhu and Gu investigated a square dot-type confining potential; they dealt only with the case of weak coupling, using a perturbative method, and they stressed the importance of the phonon confinement in this case [3]. Klimin *et al* treated the bulk and interface vibrational modes and their respective contributions to the polaron effects for spherical quantum dots: the ground-state energy and the effective mass were obtained for weak coupling, using perturbation theory [4].

On the other hand, the harmonic confining potential model is of interest because it enables us to derive analytical results. It also makes it possible to avoid the difficulty of separating bulk and interface vibrations, since the interaction with interface phonons is ignored because of the absence of an abrupt interface [4]. This model can describe smooth interfaces and the consideration of just bulk phonons is a good first approximation for large dots or for dots whose two constituents have similar dielectric properties. This model was previously used by Yıldırım and Erçelebi [5, 6]. These authors developed two different approaches to tackle the weak- and strong-coupling limits separately. In the case of strong coupling, they rely on the Pekar formalism [6]; their variational model gives the self-energy and the effective mass of the polaron in both the two- and three-dimensional strong-coupling cases. For weak coupling [5], they use the second-order Rayleigh–Schrödinger perturbation theory (RSPT). Mukhopadhyay and Chatterjee [7] point out that this second-order RSPT correction to the ground-state polaron energy can be written as a simple expression involving only gamma functions. In reference [8], polaron states (the ground state and excited states) in a two-dimensional harmonic quantum dot are investigated, using again the second-order perturbation theory. The numerical results lead to the conclusion that there are increased polaronic effects in small quantum dots.

In this paper we study a polaron in a quantum dot: the electron is trapped in an anisotropic parabolic potential and only the coupling to the bulk LO phonons is taken into account. The main advantage of our formalism is that it gives the self-energy of the polaron, in a unified way, for both the strong- and weak-coupling limits and for the one-dimensional (1D), two-dimensional (2D) and three-dimensional (3D) confinements. It also provides us with the possibility of investigating all of the intermediate cases. As a first step, in section 2, we present the Fröhlich Hamiltonian and the Fock approximation of Matz and Burkey [9] applied to the present case. We discuss the model used to describe the confined polaron. In section 3, we derive the self-energy of the polaron and the corresponding asymptotic behaviours. Finally we present the numerical results in section 4.

2. The formalism

To describe a polaron in a parabolic quantum well, the effective-mass approximation is used for the electron. The lattice, described in the framework of the harmonic approximation, is considered as a continuum. Periodic boundary conditions are chosen over a cube of volume V. The resulting Hamiltonian is written (in dimensionless form) as the sum of the free-particle Hamiltonians and of their interaction [1]:

$$H = H_0 + H_{int} \tag{1}$$

$$H_0 = \hat{p}^2 + \sum_{\boldsymbol{k}} a^\dagger_{\boldsymbol{k}} a_{\boldsymbol{k}} + V(\boldsymbol{r}) \tag{2}$$

$$H_{int} = \sum_{\boldsymbol{k}} (V_k a_{\boldsymbol{k}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} + V_k^* a^\dagger_{\boldsymbol{k}} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}) \tag{3}$$

where $V(\boldsymbol{r})$ is the confining potential and $a^\dagger_{\boldsymbol{k}}, a_{\boldsymbol{k}}$ are the annihilation and creation operators for a LO phonon of wave vector $\boldsymbol{k}$. Also,

$$V_k = -\frac{\mathrm{i}}{k}\left(\frac{4\pi\alpha r_0^3}{V}\right)^{1/2} \tag{4}$$

$$\alpha = \left(\frac{e^2}{2r_0\hbar\omega_{LO}}\right)(\epsilon_\infty^{-1} - \epsilon_0^{-1}) \tag{5}$$

$$r_0 = \left(\frac{\hbar}{2m^*\omega_{LO}}\right)^{1/2} \tag{6}$$

where α is the electron–phonon coupling constant and ω_{LO} is the longitudinal optical phonon frequency (taken as $\omega_{LO} = 1$ in equations (2) and (3)). m^* is the electron effective mass and ϵ_∞ and ϵ_0 are the high-frequency and static dielectric constants, respectively. r_0 is the unit of length and is a measure of the polaron radius.

Starting from this Hamiltonian, a Green's function equation-of-motion approach in the framework of the Fock approximation of Matz and Burkey is used to obtain the ground-state energy [9]. The theory is valid at zero temperature and, not being perturbative, for any coupling or confining strength. A non-linear effective Schrödinger equation is derived in which the ground state is approached via a complete set of eigenstates. We then obtain from this equation an upper bound for the polaron ground-state energy (E_0) in terms of a variational model spectrum, $\{\Psi_n(\boldsymbol{r})\}$:

$$E_0 = \int \Psi_0^*(\boldsymbol{r}) H_0 \Psi_0(\boldsymbol{r})\ \mathrm{d}^3r + \sum_n \sum_{\boldsymbol{k}} |V_k|^2 \int \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(r-r')} \frac{\Psi_n(\boldsymbol{r})\Psi_n^*(\boldsymbol{r}')}{E_0 - E_n - 1} \Psi_0(\boldsymbol{r}')\Psi_0^*(\boldsymbol{r})\ \mathrm{d}^3r\ \mathrm{d}^3r' \tag{7}$$

where $\boldsymbol{k}$ is the 3D phonon wave vector, and $\boldsymbol{r}$ the 3D electron position. For the confinement potential ($V(\boldsymbol{r})$), we choose an anisotropic harmonic potential, with spring constant Ω along the directions x and y, and K along the z-axis:

$$V(\boldsymbol{r}) = \Omega^4\rho^2 + K^4 z^2 \tag{8}$$

where

$$\rho^2 = x^2 + y^2. \tag{9}$$

Thus, we can describe a 3D polaron ($\Omega = K = 0$), a 2D polaron ($\Omega = 0$ and $K \to \infty$), a 1D polaron ($\Omega \to \infty$ and $K = 0$), and a polaron in a quantum dot (Ω and $K \neq 0$). For the model potential, we use an anisotropic harmonic potential, with variational spring constants β and γ:

$$H_m = \hat{p}^2 + \beta^4\rho^2 + \gamma^4 z^2. \tag{10}$$

Its eigenvalues and eigenfunctions are well known. This Hamiltonian is used to generate the variational spectrum $\psi_n(\boldsymbol{r})$ used in equation (7).

The complete spectrum summation is done using the Slater sum rule [10]. After integration, we find the ground-state energy:

$$E_0 = \beta^2 + \frac{\gamma^2}{2} + \frac{\Omega^4}{\beta^2} + \frac{K^4}{2\gamma^2} - \sqrt{\frac{2}{\pi}}\alpha F \tag{11}$$

where F is given by

$$F = \gamma \int_0^\infty \mathrm{d}t\ \frac{\mathrm{e}^{-t}}{\sqrt{1 - \mathrm{e}^{-2\gamma^2 t}}} \frac{\tan^{-1}\sqrt{\xi}}{\sqrt{\xi}} \qquad \text{for } \gamma \geqslant \beta \tag{12}$$

or by

$$F = \gamma \int_0^\infty \mathrm{d}t\ \frac{\mathrm{e}^{-t}}{\sqrt{1 - \mathrm{e}^{-2\gamma^2 t}}} \frac{\tanh^{-1}\sqrt{-\xi}}{\sqrt{-\xi}} \qquad \text{for } \gamma \leqslant \beta. \tag{13}$$

In these equations, ξ is given by

$$\xi = \frac{\gamma^2(1 - \mathrm{e}^{-2\beta^2 t})}{\beta^2(1 - \mathrm{e}^{-2\gamma^2 t})} - 1. \tag{14}$$

β and γ are determined by minimizing E_0. Equation (11) reduces to the energy found by Yıldırım and Erçelebi who studied the same anisotropic harmonic confining potential in the weak-coupling [5] and strong-coupling limits [6]. Our result is however valid for any strength of electron–phonon coupling.

3. Asymptotic limits

At this stage, it is of interest to study the asymptotic limits of equation (11). This is done for the cases of strong ($\alpha \gg 1$) and weak ($\alpha \ll 1$) coupling and for both isotropic and anisotropic confining potentials. In the following, the different limits refer to the dimensionality of the polaron. More precisely, the 1D limit refers to a 2D confinement. The 2D limit refers to a 1D confinement and the 3D limit refers to the absence of confinement.

3.1. The isotropic limit

In the isotropic case, $\Omega = K$. The energy minimization gives $\beta = \gamma$. In the strong-coupling limit (α or $K \gg 1$), the electron wavefunction is strongly localized and $\beta \gg 1$. The ground-state energy then reduces to

$$E_0 = \frac{3\beta^2}{2} + \frac{3K^4}{2\beta^2} - \sqrt{\frac{2}{\pi}}\alpha\beta. \tag{15}$$

This equation has to be minimized with respect to β. If the effect of confinement is much stronger than that of polarization ($K \gg \alpha$), we find that the energy is that of the 3D harmonic oscillator, lowered by a correction linear in α, due to a static lattice polarization around the average position of the electron:

$$E_0 = 3K^2 - \sqrt{\frac{2}{\pi}}\,\alpha K. \tag{16}$$

However, if the confinement effects are smaller than the polarization effects ($K \ll \alpha$), the ground-state energy is that of a self-trapped 3D polaron in the strong-coupling limit [2, 9], corrected by the harmonic potential energy associated with an electron located at an average distance determined by the self-trapping radius:

$$E_0 = -\frac{\alpha^2}{3\pi} + \frac{27\pi K^4}{4\alpha^2}. \tag{17}$$

If the electron–phonon coupling strength is weak ($\alpha \ll 1$), and in the limit of strong confining potentials ($K \gg 1$), we find that the ground-state energy of the system is given by equation (16): it corresponds to an harmonic oscillator with a small polarization correction. In the low-confinement limit (α and $K \ll 1$), the ground-state corresponds to a polaron bound in a harmonic potential. Two corrections are present: a self-energy shift ($-\alpha$) and an effective-mass correction

$$E_0 = -\alpha + \frac{3K^2}{\sqrt{m^*}} \tag{18}$$

with

$$\sqrt{m^*} = \frac{1}{1 - \alpha/12} \tag{19}$$

or

$$m^* \approx \frac{1}{1 - \alpha/6}. \tag{20}$$

This expression corresponds to a 3D Fröhlich polaron bound to a harmonic potential, as studied using second-order perturbation theory [1, 5]. Note that for all of these isotropic limits the effect of large confinements is to increase the self-energy of the polaron (defined as the ground-state energy minus the elastic energy ($E_0 - 3K^2$)).

3.2. The 1D limit: 2D confinement ($\Omega \gg K$)

In the anisotropic case ($\Omega \neq K$) the minimization gives $\beta \neq \gamma$. In the following, we consider two limiting cases: the 2D confinement ($\Omega \gg K$) and the 1D confinement ($\Omega \ll K$). For the 2D confinement, i.e. when $\Omega \gg K$, the polaron has a one-dimensional character. It is well known that the one-dimensional Fröhlich ground-state energy diverges in the absence of a phonon Debye cut-off. Consequently, we expect this energy to diverge when Ω increases. A consequence of this divergence is that the polaron self-energy increases rapidly with the two-dimensional confinement.

We first study the strong-coupling case ($\alpha \gg 1$). For $\Omega \gg \alpha \gg K$, we obtain

$$E_0 = 2\Omega^2 - \frac{\alpha^2 \ln^2(\Omega)}{\pi}. \tag{21}$$

This is the 2D harmonic energy to which is added a self-energy correction that reflects the lattice polarization induced by the oscillating electron. This energy diverges logarithmically with Ω as it should for a 1D limit. For $\Omega \gg K \gg \alpha$, we find

$$E_0 = 2\Omega^2 + K^2 - \alpha K \sqrt{\frac{2}{\pi}} \ln(2\Omega/K). \tag{22}$$

This is the harmonic energy with a perturbative polarization correction. Note again the logarithmic behaviour of the polarization correction.

For weak coupling (α and $K \ll 1$ and $\Omega \gg 1$), we find

$$E_0 = 2\Omega^2 + K^2 - \frac{3}{2}\alpha \ln 2 - \alpha \ln \Omega + \frac{\alpha}{2}\sqrt{\pi}\gamma_{\mathrm{Euler}}. \tag{23}$$

In this limit, the correction due to the lattice polarization is linear in α and diverges in the 1D limit ($\Omega \gg K$) as it should.

3.3. The 2D limit: 1D confinement ($K \gg \Omega$)

This is the limit when $K \gg \Omega$. As the electron is confined in one direction, the polaron has a 2D character. We first consider the strong-coupling limit ($\alpha \gg 1$). For $K \gg \Omega \gg \alpha$, we obtain

$$E_0 = K^2 + 2\Omega^2 - \alpha\Omega\sqrt{\frac{\pi}{2}}. \tag{24}$$

This is the harmonic energy to which a polarization term adjusted to the average position of the electron is added. For $K \gg \alpha \gg \Omega$, we obtain

$$E_0 = K^2 - \frac{\alpha^2 \pi}{8} + \frac{8\Omega^4}{\pi\alpha^2}. \tag{25}$$

The first term of this equation is the 1D harmonic energy while the second term is the self-energy of a strong-coupling 2D Fröhlich polaron [6, 11]. The last term is a correction to these energies, due to the smaller harmonic coupling in the xy-plane.

For the weak-coupling limit (α and $\Omega \ll 1$ and $K \gg 1$), we find

$$E_0 = K^2 - \frac{\pi}{2}\alpha + \frac{2\Omega^2}{\sqrt{m^*}} \tag{26}$$

$$m^* = \frac{1}{(1 - \pi\alpha/8)}. \tag{27}$$

The first term of this expression is the elastic energy of an electron in a 1D harmonic potential. The second term is simply the self-energy of a 2D polaron [2] while the last term corresponds to the elastic energy of a 2D polaron bound to a harmonic potential. Note that the effective mass has been renormalized to the 2D polaron effective mass [11]. This result was previously found by Yıldırım and Erçelebi [5] using perturbation theory and by Thilagam and Singh [12] who used a variational approach.

4. Numerical calculations

In order to obtain some idea of the effects of the confinement on the polaron self-energy over the whole range of confinement strength, we compute the ground-state energy (E_0) from equations (12) and (13), after a minimization with respect to β and γ. We then plot the resulting polaron self-energy (E_p), i.e. E_0 minus the confinement potential ($E_0 - K^2 - 2\Omega^2$), as a function of the different parameters. A useful parameter is the confinement length defined as the root mean square position of the electron resulting from the harmonic confinement alone. It is

$$L_z = \langle z^2 \rangle^{1/2} = 1/(\sqrt{2}K) \tag{28}$$

for the z-direction and

$$L_\rho = \langle \rho^2 \rangle^{1/2} = 1/\Omega \tag{29}$$

for the radial direction. In the present system of units, the polaron quantum radius is equal to one. We thus expect the effect of confinement to be more important when L_z or L_ρ becomes smaller than 1.

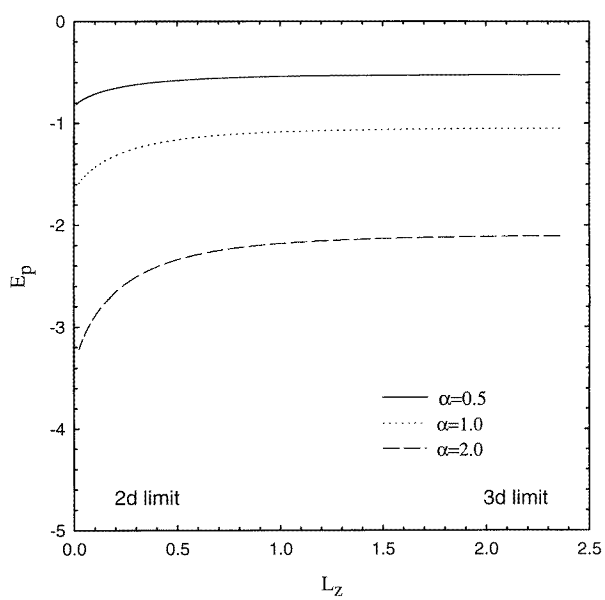

Figure 1. The self-energy of the polaron ($E_0 - K^2 - 2\Omega^2$) as a function of L_z, for $L_\rho = 2.0$ ($\Omega = 0.5$) and $\alpha = 0.5$, 1.0 and 2.0.

In figure 1, we plot the polaron self-energy (E_p) as a function of L_z, keeping Ω equal to a constant value (0.5) or $L_\rho = 2.0$, a value for which the confinement length is twice the size of the polaron radius. For large values of L_z, we have an anisotropic 3D polaron, while, as L_z decreases, the polaron increases its localization in the z-direction. Asymptotically, we get a two-dimensional polaron. We observe that the absolute value of the self-energy increases sharply as the anisotropy is increased through the increase of the confinement, up to its finite asymptotic 2D limit when L_z goes to zero. This enhancement of the self-energy is important only when the confinement length becomes smaller than the polaron radius ($L_z < 1$). We find the same overall behaviour at different electron–phonon coupling strengths. The effect of 1D confinement is thus to enhance the effect of electron–phonon interaction.

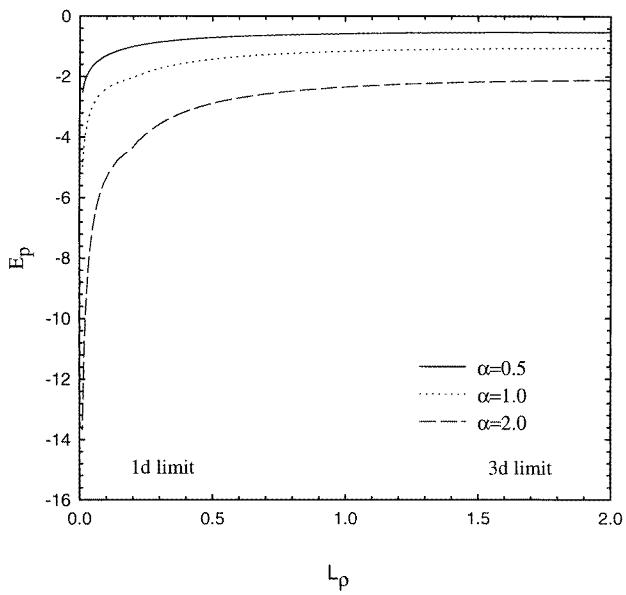

Figure 2. The self-energy of the polaron ($E_0 - K^2 - 2\Omega^2$) as a function of L_ρ, for $L_z = 2.0$ ($K = 0.35$) and $\alpha = 0.5$, 1.0 and 2.0.

In figure 2, we look at the effect of a 2D confinement. We plot the polaron self-energy (E_p) as a function of L_ρ, keeping K equal to a constant value (0.35) or $L_z = 2.0$. This value is such that the confinement length is twice the polaron radius. For large values of L_ρ, we have an anisotropic 3D polaron, while for small values of the confinement length, we asymptotically have a 1D polaron. The confinement length is then smaller than the polaron radius ($L_\rho < 1$). We observe that, as the confinement increases in the xy-plane, the absolute value of the polaron self-energy increases rapidly as L_ρ decreases, with the expected logarithmic divergence for strong confinement. This behaviour is enhanced as the electron–phonon coupling strength increases. The effect of a 2D confinement is thus to dramatically increase the effect of the electron–phonon interaction.

We have also plotted, in figure 3, the polaron self-energy as a function of the coupling parameter α, for different strengths of the 2D confining potential ($\Omega = 1.0$ ($L_\rho = 1.0$), $\Omega = 5.0$ ($L_\rho = 0.2$) and $\Omega = 10.0$ ($L_\rho = 0.1$)), keeping K equal to 1.0 ($L_z = 0.71$). For small coupling, the self-energy goes to zero as it should. As the coupling increases, we observe a rapid increase in the polaron self-energy. This increase is proportionally larger for a larger confinement because we then approach the 1D limit. This confirms again the idea that a confinement increases the self-energy of the polaron and that the effect is larger for a higher degree of anisotropy.

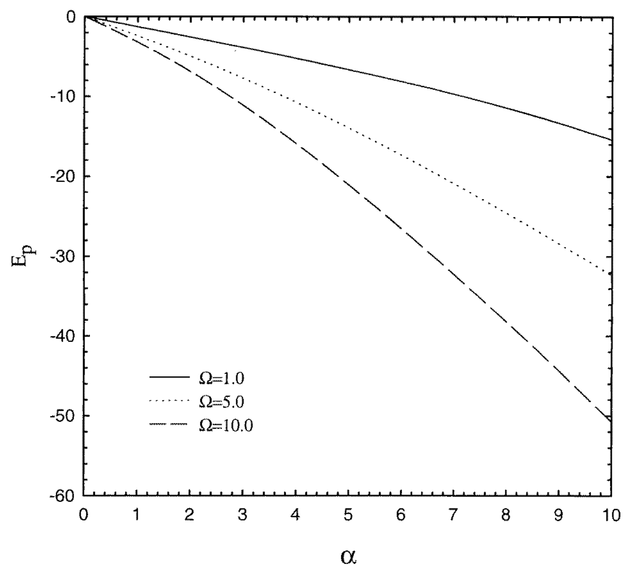

Figure 3. The self-energy of the polaron ($E_0 - K^2 - 2\Omega^2$) as a function of α, for $K = 1.0$ and $\Omega = 1.0$, 5.0 and 10.0.

5. Conclusion

In this paper, we have obtained an analytical variational expression for the ground-state energy of a Fröhlich polaron confined in an anisotropic parabolic well. This expression is valid for any coupling strength or any degree of confinement, in the framework of the Fröhlich Hamiltonian. The different asymptotic limits of our result permit us to reproduce the expressions found by other authors for small or large electron–phonon coupling and for different degrees of confinement. Our treatment unifies these results and describes the cases intermediate between the limiting cases. It also allows the investigation of the effect of an anisotropic confinement.

We have found that a confinement increases the self-energy of the polaron and that an anisotropic confinement is more effective in producing that effect than an isotropic confinement. In particular, a two-dimensional confinement leading to a one-dimensional polaron increases the self-energy logarithmically while a one-dimensional confinement leading to a two-dimensional polaron leads to an increased constant self-energy. This increase can be associated with a reduction of the electron phase space, an effect similar to the localization induced in the strong-coupling regime.

It is of interest to note the analogy between the harmonic two-dimensional confinement and the electron localization resulting from the application of a magnetic field. In the strong-field regime, the electron behaves as a one-dimensional polaron with the associated logarithmic divergence in the self-energy [13]. The physical picture is then the same as in the present model. This can be seen easily by comparing equations (23)–(29) with the corresponding equations of reference [13] which treats the bulk polaron in a constant magnetic field in the framework of the Fock approximation. The addition of a magnetic field to the present model would be of interest in the study of cyclotron resonance in quantum dots.

To summarize, we have shown that the effect of an anisotropic harmonic confinement was to increase the self-energy of the polaron. This increase is important when the confinement length becomes smaller than the polaron radius as shown from numerical calculations. It is also more important for a two-dimensional confinement than for a one-dimensional one. In this context, it is important to note that when the confinement length becomes of the order of the lattice parameter (this can be the case for a high magnetic field), the Fröhlich Hamiltonian is no longer valid, and that corrections to the effective mass and to the continuum dielectric approximation must be taken into account.

Acknowledgments

This work was partly supported by the National Research Council of Canada (NSERC) and by le Fonds pour la Formation de Chercheurs et l'aide à la Recherche.

References

[1] Devreese J T 1972 *Polarons in Ionic Crystals and Polar Semiconductors* (Amsterdam: North-Holland) pp 1–40
[2] Das Sarmas S and Mason B A 1985 *Ann. Phys., NY* **163** 78
[3] Zhu K-D and Gu S-W 1992 *J. Phys.: Condens. Matter* **4** 1291
[4] Klimin S N, Pokatilov E P and Fomin V M 1994 *Phys. Status Solidi* b **184** 373
[5] Yıldırım T and Erçelebi A 1991 *J. Phys.: Condens. Matter* **3** 4357
[6] Yıldırım T and Erçelebi A 1991 *J. Phys.: Condens. Matter* **3** 1271
[7] Mukhopadhyay S and Chatterjee A 1995 *Phys. Lett.* **204A** 411
[8] Zhu K-D and Gu S-W 1992 *Phys. Lett.* **163A** 435
[9] Matz D and Burkey B C 1971 *Phys. Rev.* B **3** 3847
[10] Rainville E D 1967 *Special Functions* 4th edn (New York: Macmillan) p 198
[11] Hai G-Q, Peeters F M and Devreese J T 1990 *Phys. Rev.* B **42** 11 063
[12] Thilagam A and Singh J 1994 *Phys. Rev.* B **9** 13 583
[13] Lépine Y and Matz D 1976 *Can. J. Phys.* **54** 1979