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Impurity magnetopolaron in a parabolic quantum dot: the squeezed-state variational approach

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Abstract

We present a calculation of the ground-state binding energy of an impurity magnetopolaron confined in a three-dimensional (3D) parabolic quantum dot potential, in the framework of a variational approach based on two successive canonical transformations. First, we apply a displaced-oscillator type unitary transformation to diagonalize the relevant Fröhlich Hamiltonian. Second, a single-mode squeezed-state transformation is introduced to deal with bilinear terms arising from the first transformation. Finally, the parameters of these transformations together with the parameters included in the electronic trial wavefunction are determined variationally to obtain the ground-state binding energy of an impurity magnetopolaron confined in a 3D parabolic quantum dot potential. Our approach has two advantages: first, the displaced-oscillator transformation allows one to obtain results valid for whole range of electron–phonon coupling strength since it is a special combination of Lee–Low–Pines and Huybrechts (LLP–H) canonical transformations, and second, the later transformation improves all-coupling results. It has been shown that the effects of quadratic terms arising from the all-coupling approach are very important and should be taken into account in studying the size-dependent physical properties of nanostructured materials.

1. Introduction

With the use of advanced nanolithographic and epitaxial growth techniques [1], it is now possible to manufacture nanoscaled quantum confined systems such as quasi-two-dimensional (Q2D) quantum wells (QWs), quasi-one-dimensional (Q1D) quantum wires or quantum well wires (QWWs) and quasi-zero-dimensional (Q0D) quantum dots (QDs) [2, 3], with very low background impurity concentrations [4]. However, due to the fact that QDs are ultrasmall structures as compared to QWs or QWWs, the inclusion of a single impurity can dramatically affect the transport properties [4] as well as the electronic and optical properties of QDs in contrast to QWs or QWWs. Thus, a detailed knowledge of impurity effects on these physical properties is crucial in interpreting experimental findings such as emission and absorption

spectra, and photoluminescence spectra, and also in designing new nanostructured electronic and optoelectronic devices. Moreover, due to the reduction of the dimensionality of the system from 3D to Q0D, it is a well-known fact that electron–phonon interactions have more pronounced effects as compared to the bulk case [5]. Following the work of Erçelebi and Tomak [6] and Degani and Hipólito [7] in QW systems, the effects of electron–phonon coupling on impurity binding energies have been considered in various geometries such as in QWs [8], QWWs [9], and in spherical [10–12], parabolic [13, 14] and cylindrical QDs [15, 16]. Polaronic effects in QD systems with two [17] and N [18] electrons bound to a Coulomb impurity and with a Coulomb interacting electron–hole pair [19] have also been studied.

Since the existence of an external magnetic field has nonnegligible effects on above physical properties [1, 4] and provides both theoretical and experimental insight into these physical properties in nanostructured materials, a lot of work has also been devoted to the study of magnetic field effects in finite [20] and infinite [21] QWs, in parabolic [22, 23] QWWs and in 2D parabolic [24–26] QDs. In a previous work [27], where the adiabatic approach is employed, we have presented a comparative study of the effects of both quantum confinement and magnetic field on the ground-state and first-excited-state energies of an impurity magnetopolaron in a parabolic QDs, QWs and QWWs, and have concluded that the binding energies of an impurity magnetopolaron increase with increasing both the degree of spatial confinement and the magnetic field strength.

In this paper, a different unitary transformation scheme will be developed to diagonalize the well-known Fröhlich Hamiltonian describing an impurity magnetopolaron confined in a 3D parabolic QD potential. Our approach is based on a variational calculation with two successive unitary transformations. First, by a unitary transformation of displaced-oscillator type, which is a special combination of LLP–H canonical transformation, the relevant Fröhlich Hamiltonian is transformed into an effective Hamiltonian whose eigenvalues are completely equivalent to the original one, but which contains bilinear terms of phonon creation and annihilation operators as well as linear ones [28, 29]. This type of unitary transformation has been discussed in the literature from different points of view by many authors [30–36]. In particular, Ninno and Iadonisi [32] have provided a rigorous theoretical framework for the calculation of the position-dependent part of the phonon displacement arising from the relevant transformation, which is capable of describing the dynamics of electron–phonon interaction for the whole range of coupling constant. In the present work, to diagonalize the quadratic terms arising from this transformation, we introduce a single-mode squeezed-state transformation [37] as a second unitary transformation, which has been used before in the context of polaron theory [38, 39]. Finally, we have performed a variational calculation with the parameters included in the theory.

The layout of the present paper is as follows. The Fröhlich Hamiltonian describing an electron interacting with LO-phonons and bound to a hydrogenic impurity subjected to both a uniform magnetic field and a spatial confinement is introduced in the following section, and a diagonalization procedure for this Hamiltonian is employed. Section 3 is devoted to the discussion of some intermediate analytical results together with numerical ones for the ground-state binding energy of an impurity magnetopolaron and polaronic correction to this state. In section 4, we present our conclusions.

2. Theory

An impurity magnetopolaron in a 3D parabolic QD potential is described by the Fröhlich Hamiltonian

$$H = H_{\mathrm{E}} + \sum_{\mathbf{q}} \hbar\omega_0 b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}} + \sum_{\mathbf{q}} \left(V_{\mathbf{q}} b_{\mathbf{q}} \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}} + \mathrm{H.c.} \right), \tag{1}$$

where

$$H_{\mathrm{E}} = \frac{1}{2\mu}\left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right)^2 - \frac{e^2}{\epsilon_0|\mathbf{r}|} + \frac{1}{2}\mu\omega_\bullet^2\mathbf{r}^2 \tag{2}$$

is the Hamiltonian of the electron–impurity subsystem. In equation (1), $\left|V_{\mathbf{q}}\right|^2 = (\hbar\omega_0)^2\, 4\pi\alpha r_0/Vq^2$ is the electron–phonon interaction amplitude, $b_{\mathbf{q}}^\dagger$ ($b_{\mathbf{q}}$) is the creation (annihilation) operator of an optical phonon with a wavevector $\mathbf{q}$ and an energy $\hbar\omega_0$, and $\mathbf{p}$ and $\mathbf{r}$ denote the electron momentum and position operators, respectively. α and r_0 are the electron–phonon coupling constant and polaron radius, respectively. In the absence of impurity, by choosing the symmetrical Coulomb gauge $\mathbf{A} = B(-y, x, 0)/2$ for the vector potential, equation (1) can then be written as a sum of Hamiltonians for an isotropic 3D harmonic oscillator in the lateral plane with mass μ and frequency $\omega^2 = (\omega_{\mathrm{c}}/2)^2 + \omega_\bullet^2$ and a term of $(\omega_{\mathrm{c}}/2)L_z$, where ω_{c} and $\omega_\bullet$ are the cyclotron frequency and the strength of spatial confinement, respectively.

In the first step, we carry out a unitary transformation of displaced-oscillator type:

$$U_1 = \exp\left\{\sum_{\mathbf{q}}\left[F_{\mathbf{q}}^*(\mathbf{r})b_{\mathbf{q}} - F_{\mathbf{q}}(\mathbf{r})b_{\mathbf{q}}^\dagger\right]\right\}, \tag{3}$$

which diagonalizes the phonon-related part of the Hamiltonian given by equation (1). We divide the transformed Hamiltonian into four parts as $\tilde{H} = U_1^{-1}HU_1 = H_{\mathrm{E}} + H_0 + H_1 + H_2$, each of which is given by

$$\begin{aligned}
H_0 &= \sum_{\mathbf{q}}\left[\frac{\hbar^2}{2\mu}\left|\nabla F_{\mathbf{q}}(\mathbf{r})\right|^2 + \hbar\omega_0|F_{\mathbf{q}}(\mathbf{r})|^2 + V_{\mathbf{q}}F_{\mathbf{q}}(\mathbf{r})\mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}} + V_{\mathbf{q}}^*F_{\mathbf{q}}^*(\mathbf{r})\mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{r}}\right],\\
H_1 &= \sum_{\mathbf{q}}\hbar\omega_0 b_{\mathbf{q}}^\dagger b_{\mathbf{q}} + \sum_{\mathbf{q}}\left\{\left[V_{\mathbf{q}}^*\mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{r}} + \frac{\hbar}{\mathrm{i}\mu}\left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right)\cdot\nabla F_{\mathbf{q}}(\mathbf{r}) + \hbar\omega_0 F_{\mathbf{q}}(\mathbf{r})\right]b_{\mathbf{q}}^\dagger + \mathrm{H.c.}\right\},\\
H_2 &= \sum_{\mathbf{q}}\sum_{\mathbf{q}'}\frac{\hbar^2}{2\mu}[2\nabla F_{\mathbf{q}}(\mathbf{r})\cdot\nabla F_{\mathbf{q}'}^*(\mathbf{r})b_{\mathbf{q}}^\dagger b_{\mathbf{q}'} - \nabla F_{\mathbf{q}}(\mathbf{r})\cdot\nabla F_{\mathbf{q}'}(\mathbf{r})b_{\mathbf{q}}^\dagger b_{\mathbf{q}'}^\dagger\\
&\qquad - \nabla F_{\mathbf{q}}^*(\mathbf{r})\cdot\nabla F_{\mathbf{q}'}^*(\mathbf{r})b_{\mathbf{q}}b_{\mathbf{q}'}],
\end{aligned} \tag{4}$$

respectively, with the help of the transformation rule

$$U_1^{-1}\left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right)U_1 = \mathbf{p} + \frac{e}{c}\mathbf{A} - \mathrm{i}\hbar\sum_{\mathbf{q}}\left[\nabla F_{\mathbf{q}}(\mathbf{r})b_{\mathbf{q}}^\dagger - \nabla F_{\mathbf{q}}^*(\mathbf{r})b_{\mathbf{q}}\right] + \frac{1}{2}\jmath(\mathbf{r}),$$

where

$$\jmath(\mathbf{r}) = -\mathrm{i}\hbar\sum_{\mathbf{q}}\left[F_{\mathbf{q}}^*(\mathbf{r})\nabla F_{\mathbf{q}}(\mathbf{r}) - F_{\mathbf{q}}(\mathbf{r})\nabla F_{\mathbf{q}}^*(\mathbf{r})\right]$$

is the current due to the displacement of the phonon field and therefore is required to be equal to zero [28]. At this stage, if one first constructs a trial wavefunction $|\Psi\rangle = |\mathbf{r}\rangle \otimes |0\rangle_{\mathrm{PH}}$ for the ground-state energy of $\tilde{H}$, where $|\mathbf{r}\rangle$ is the electronic part of the trial wavefunction and its coordinate representation is taken by

$$\Phi(\mathbf{r}) = \frac{\gamma_\perp\sqrt{\gamma_\parallel}}{\pi^{3/4}}\exp[-(\gamma_\perp^2\mathbf{r}_\perp^2 + \gamma_\parallel^2 z^2)/2], \tag{5}$$

and $|0\rangle_{\mathrm{PH}}$ is the phonon vacuum state, and then performs a minimization with respect to both the variational parameters arising from the phonon displacement $F_{\mathbf{q}}(\mathbf{r})$ given by the ansatz

$$F_{\mathbf{q}}(\mathbf{r}) = f_{\mathbf{q}}\exp[-\mathrm{i}(1-\lambda)\mathbf{q}\cdot\mathbf{r}], \tag{6}$$

and the variational parameters $\gamma_\perp$ and $\gamma_\parallel$ included in $\Phi(\mathbf{r})$, this minimum value, as will be shown later, yields all-coupling results. In fact, it is easy to check that the $\mathbf{r}$-dependent displaced-oscillator transformation, equation (3), together with such a choice of $F_q(\mathbf{r})$, equation (6), is completely equivalent to modified LLP transformations, i.e., to LLP–H transformations which were originally suggested by Lee *et al* [40] and then modified by Huybrechts [41] to extend this approach to all coupling strengths. As indicated in section 1, this kind of unitary transformation has been used widely in the context of polaron theory for achieving electron–phonon interactions in several systems such as free [34, 36], bound [28], magnetopolaron [32] and bipolaron [33] problems as well. Thus, the same effective Hamiltonian, equation (4), could also have been obtained by transforming equation (1) with $U_1' = \exp[-\mathrm{i}\lambda\mathbf{r}\cdot\sum_{\mathbf{q}}\mathbf{q}b_{\mathbf{q}}^\dagger b_{\mathbf{q}}]$ first and then with $U_1'' = \exp[\sum_{\mathbf{q}}(f_{\mathbf{q}}^* b_{\mathbf{q}} - f_{\mathbf{q}} b_{\mathbf{q}}^\dagger)]$, due to the fact that $U_1 = U_1' U_1''$, as also stated by Adamowski [29]. Therefore, equation (3) together with equation (6) yields all-coupling results, and reduces the results obtained from weak- and strong-coupling regimes at certain values of the variational parameter, since the variational parameter λ provides an interpolation scheme in that it is reduced to the well-known LLP method when $\lambda = 1$ and provides a good description in the extended state limit, whereas in the case of $\lambda = 0$, it is reduced to the Landau–Pekar method, which is an approach in the adiabatic case and is valid in the strong-coupling limit.

In the next step, in order to obtain more accurate results beyond those obtained by the LLP–H variational approach, it is necessary to include the effects of the non-diagonal terms of equation (4). This can be achieved by introducing the following single-mode squeezed-state transformation:

$$U_2 = \exp\left\{\tfrac{1}{2}\sum_{\mathbf{q}} G_{\mathbf{q}}\left[(b_{\mathbf{q}}^\dagger)^2 - (b_{\mathbf{q}})^2\right]\right\}, \tag{7}$$

which is suitable for the diagonalization of the quadratic phonon terms [37] in H_2. Furthermore, it can be easily seen that, under U_2 given by equation (7), the phonon annihilation and creation operators are transformed according to the rules $U_2^{-1} b_{\mathbf{q}} U_2 = b_{\mathbf{q}}\cosh G_{\mathbf{q}} + b_{\mathbf{q}}^\dagger \sinh G_{\mathbf{q}}$ and $U_2^{-1} b_{\mathbf{q}}^\dagger U_2 = b_{\mathbf{q}}^\dagger \cosh G_{\mathbf{q}} + b_{\mathbf{q}} \sinh G_{\mathbf{q}}$, respectively, which are in fact the well-known Bogoliubov canonical transformations. Hence, the transformed forms of H_1 and H_2 are straightforward, and the non-vanishing contribution to H_0 is found to be

$$\tilde{H}_2 = \sum_{\mathbf{q}}\left\{\left[\hbar\omega_0 + \frac{\hbar^2}{\mu}\left|\nabla F_{\mathbf{q}}(\mathbf{r})\right|^2\right]\sinh^2 G_{\mathbf{q}} - \frac{\hbar^2}{2\mu}[\nabla F_{\mathbf{q}}(\mathbf{r})\cdot\nabla F_{\mathbf{q}}(\mathbf{r}) + \nabla F_{\mathbf{q}}^*(\mathbf{r})\cdot\nabla F_{\mathbf{q}}^*(\mathbf{r})]\sinh G_{\mathbf{q}}\cosh G_{\mathbf{q}}\right\}. \tag{8}$$

After inserting equation (6) into H_0 in equation (4), and into equation (8), and performing some straightforward calculations, the final result for the total variational energy, including the electronic part, is found to be

$$\begin{aligned} E = {} & \left(\frac{\hbar^2}{2\mu}\gamma_\perp^2 + \frac{1}{2}\mu\omega^2\frac{1}{\gamma_\perp^2}\right) + \frac{1}{2}\left(\frac{\hbar^2}{2\mu}\gamma_\parallel^2 + \frac{1}{2}\mu\omega_\bullet^2\frac{1}{\gamma_\parallel^2}\right) - \frac{e^2}{2\pi^2\epsilon_0}\int\frac{\mathrm{d}^3\mathbf{k}}{k^2}\sigma(k) \\ & + \sum_{\mathbf{q}}\left[\left(\hbar\omega_0 + \frac{\hbar^2 q^2}{2\mu}(1-\lambda)^2\right)\left|f_q\right|^2 + V_q f_q \sigma(\lambda q) + V_q^* f_q^* \sigma(\lambda q)\right] \\ & + \sum_{\mathbf{q}}\left\{\left(\hbar\omega_0 + \frac{\hbar^2 q^2}{\mu}(1-\lambda)^2\left|f_{\mathbf{q}}\right|^2\right)\sinh^2 G_{\mathbf{q}}\right. \\ & \left. + \frac{\hbar^2 q^2}{2\mu}(1-\lambda)^2\sigma(2(1-\lambda)q)\left(f_{\mathbf{q}}^2 + f_{\mathbf{q}}^{*2}\right)\sinh G_{\mathbf{q}}\cosh G_{\mathbf{q}}\right\}, \end{aligned} \tag{9}$$

where $\sigma(\lambda\mathbf{q}) = \langle\exp(\mathrm{i}\lambda\mathbf{q}\cdot\mathbf{r})\rangle$, and $\langle\cdots\rangle$ denotes the expectation value with respect to electronic coordinates. In equation (9), we have used the identity $|\mathbf{r}|^{-1} = \int \mathrm{d}^3\mathbf{k}\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}/2\pi^2\mathbf{k}^2$. Equation (9) can be rewritten in dimensionless form by simply dividing both sides by $\hbar\omega_0$ and defining new dimensionless variational parameters $(\hbar/\mu\omega_0)^{1/2}\gamma_\perp = 1/\overline{\gamma}_\perp$ and $(\hbar/\mu\omega_0)^{1/2}\gamma_\parallel = 1/\overline{\gamma}_\parallel$ together with the functions

$$\begin{aligned}\mathcal{H}_\mathbf{q} &= 1 + 2r_0^2q^2(1-\lambda)^2\left|f_\mathbf{q}\right|^2,\\ \mathcal{J}_\mathbf{q} &= r_0^2q^2(1-\lambda)^2\sigma(2(1-\lambda)q)\left(f_\mathbf{q}^2 + f_\mathbf{q}^{*2}\right).\end{aligned} \tag{10}$$

Hence, we obtain

$$\begin{aligned}\overline{E} = &\left(\frac{1}{2\overline{\gamma}_\perp^2} + \frac{1}{2}\overline{\omega}^2\overline{\gamma}_\perp^2\right) + \frac{1}{2}\left(\frac{1}{2\overline{\gamma}_\parallel^2} + \frac{1}{2}\overline{\omega}_\bullet^2\overline{\gamma}_\parallel^2\right) - \frac{2}{\pi}\beta\frac{\overline{\gamma}_\parallel}{\overline{\gamma}_\perp^2}\mathbf{I}(\overline{\gamma}_\perp,\overline{\gamma}_\parallel)\\ &+ \sum_\mathbf{q}\{[1 + r_0^2q^2(1-\lambda)^2]|f_\mathbf{q}|^2 + \overline{V}_\mathbf{q}f_\mathbf{q}\sigma(\lambda q) + \overline{V}_\mathbf{q}^*f_\mathbf{q}^*\sigma(\lambda q)\\ &+ \mathcal{H}_\mathbf{q}\sinh^2 G_\mathbf{q} + \mathcal{J}_\mathbf{q}\sinh G_\mathbf{q}\cosh G_\mathbf{q}\},\end{aligned} \tag{11}$$

where $\beta = e^2/\epsilon_0\hbar\omega_0r_0$ and $\overline{V}_\mathbf{q} = V_\mathbf{q}/\hbar\omega_0$ are the binding energy parameter and the dimensionless electron–phonon interaction amplitude, respectively, and the integral $\mathbf{I}(\overline{\gamma}_\perp,\overline{\gamma}_\parallel)$ has the following form:

$$\mathbf{I}(\overline{\gamma}_\parallel/\overline{\gamma}_\perp) = \int_0^\infty x\mathrm{e}^{-x^2/2}\,\mathrm{d}x\int_0^\infty \mathrm{e}^{-y^2/2}\frac{\mathrm{d}y}{\left(\overline{\gamma}_\parallel/\overline{\gamma}_\perp\right)^2x^2 + y^2}.$$

In these units, the cyclotron frequency ω_c, the confinement frequency $\omega_\bullet$ and the associated confinement length $\ell_\bullet = (\hbar/\mu\omega_\bullet)^{1/2}$ all become dimensionless, and they can be expressed in terms of the LO-phonon frequency ω_0 and polaron radius $r_0 = (\hbar/2\mu\omega_0)^{1/2}$ in such a way that $\overline{\omega}_\mathrm{c} = \omega_\mathrm{c}/\omega_0$, $\overline{\omega}_\bullet = \omega_\bullet/\omega_0$ and $\overline{\ell}_\bullet = \ell_\bullet/r_0 = (2/\overline{\omega}_\bullet)^{1/2}$. By making use of equation (5), $\sigma(\lambda\mathbf{q})$ in equations (9)–(11) can easily be calculated in terms of hypergeometric functions as $\sigma(\lambda\mathbf{q}) = {}_1F_1(1,1;-\lambda^2q_\perp^2\overline{\gamma}_\perp^2/2){}_1F_1(1,1;-\lambda^2q_\parallel^2\overline{\gamma}_\parallel^2/2)$. Therefore, the minimization of equation (11) with respect to $f_\mathbf{q}$ and $G_\mathbf{q}$ yields two-coupled equations:

$$f_\mathbf{q} = \frac{\overline{V}_\mathbf{q}^*}{1 + r_0^2q^2(1-\lambda)^2F(q,\lambda;G_\mathbf{q})}\,{}_1F_1(1,1;-\lambda^2q_\perp^2\overline{\gamma}_\perp^2/2){}_1F_1(1,1;-\lambda^2q_\parallel^2\overline{\gamma}_\parallel^2/2), \tag{12a}$$

$$G_\mathbf{q} = \tfrac{1}{2}\tanh^{-1}\mathcal{J}_\mathbf{q}/\mathcal{H}_\mathbf{q}, \tag{12b}$$

respectively, with the solutions to equation (12*b*)

$$\sinh 2G_\mathbf{q} = \pm\frac{\mathcal{J}_\mathbf{q}}{\sqrt{\mathcal{H}_\mathbf{q}^2 - \mathcal{J}_\mathbf{q}^2}} \qquad \cosh 2G_\mathbf{q} = \pm\frac{\mathcal{H}_\mathbf{q}}{\sqrt{\mathcal{H}_\mathbf{q}^2 - \mathcal{J}_\mathbf{q}^2}}, \tag{13}$$

where the minus sign leads to exchanging the physical properties of $b_\mathbf{q}^\dagger$ and $b_\mathbf{q}$; only the plus sign solutions are taken into account for the minimization [37]. In equation (12*a*), we have introduced the abbreviation $F(q,\lambda;G_\mathbf{q}) = \cosh 2G_\mathbf{q} - \sigma(2\lambda q)\sinh 2G_\mathbf{q}$. To find an explicit expression for $f_\mathbf{q}$ we follow the continued fraction (CF) technique. First, we use equation (13) in equation (12*a*) to obtain the CF representation for $f_\mathbf{q}$ and repeat this procedure until we get a result which does not change with further iteration.

3. Results and discussion

Here, before starting to discuss the numerical results, we comment on a particular form of equation (11), i.e., in the limit of vanishing $G_\mathbf{q}$. This is the case that $F(q,\lambda;0) = 1$. In the

absence of magnetic field, one takes $\overline{\gamma}_{\perp} = \overline{\gamma}_{\parallel} = \overline{\gamma}$ due to restoring the spherical symmetry of the problem, and therefore one can easily see that, by substituting equation (12*a*) into equation (11), the total variational energy expression becomes

$$\overline{E} = \frac{3}{2}\left(\frac{1}{2\overline{\gamma}^2} + \frac{1}{2}\overline{\omega}_{\bullet}^2\overline{\gamma}^2\right) - \frac{2}{\pi}\frac{\beta}{\overline{\gamma}}\mathbf{I}(1) - \sum_{\mathbf{q}} \frac{\left|\overline{V}_{\mathbf{q}}\right|^2 \sigma^2(\lambda\mathbf{q})}{1 + r_0^2 q^2 (1-\lambda)^2}. \tag{14}$$

As usual, by converting the sum in equation (14) into an integral over $\mathbf{q}$ and using the result for $\mathbf{I}(1) = \sqrt{\pi/2}$ together with the help of the integral [42]

$$\int_0^{\infty} \frac{\mathrm{e}^{-\mu^2 x^2}}{x^2 + \eta^2}\,\mathrm{d}x = \frac{\pi}{2\beta}\left[1 - \Phi(\beta\eta)\right]\mathrm{e}^{\mu^2\eta^2},$$

where $\Phi(x) = (2/\sqrt{\pi})\int_0^x \exp(t^2)\,\mathrm{d}t$ is the probability integral, equation (14) becomes

$$\overline{E} = \frac{3}{2}\left(\frac{1}{2\overline{\gamma}^2} + \frac{1}{2}\overline{\omega}_{\bullet}^2\overline{\gamma}^2\right) - \sqrt{\frac{2}{\pi}}\frac{\beta}{\overline{\gamma}} - \frac{\alpha}{1-\lambda}\exp\left[\frac{\lambda^2\overline{\gamma}^2}{(1-\lambda)^2}\right]\mathrm{erfc}\left(\frac{\lambda\overline{\gamma}}{1-\lambda}\right), \tag{15}$$

in which $\mathrm{erfc}(x)$ is the complementary error function. It can be easily seen that equation (15), in the absence of impurity, reduces to the previously obtained result in the article by Sahoo [34], provided that one takes the variational parameters as λ and $1-a$ instead of γ and λ, respectively, and uses the confinement length as $\ell = 1/\sqrt{2}\lambda$ in Fröhlich units. One can also check that the asymptotic limits of equation (15) yield

$$\overline{E} = \frac{3}{2}\left(\frac{1}{2\overline{\gamma}^2} + \frac{1}{2}\overline{\omega}_{\bullet}^2\overline{\gamma}^2\right) - \sqrt{\frac{2}{\pi}}\frac{\beta}{\overline{\gamma}} - \begin{cases} \alpha/\sqrt{\pi}\overline{\gamma} & \text{for } \lambda = 1, \\ \alpha & \text{for } \lambda = 0, \end{cases} \tag{16}$$

which are completely equivalent to the results of strong- and weak-coupling regimes, respectively. In the former case, i.e., $\lambda = 1$, minimization with respect to $\overline{\gamma}$ yields a fourth-order equation

$$\overline{\omega}_{\bullet}^2\overline{\gamma}^4 + \frac{2(\sqrt{2}\beta + \alpha)}{3\sqrt{\pi}}\overline{\gamma} - 1 = 0,$$

which can be solved analytically as is done in [27]. However, instead of discussing its analytical solutions, we will present its asymptotic solutions to provide insight about the qualitative behaviour of the ground-state energy of an impurity magnetopolaron in a 3D parabolic QD potential. First, in the case of strong electron–phonon interaction and weak spatial confinement, one gets the solution $\overline{\gamma} = 3\sqrt{\pi}/2(\sqrt{2}\beta + \alpha)$, and hence on replacing this result back into equation (16) this yields the energy

$$\overline{E} = \frac{27}{16}\frac{\overline{\omega}_{\bullet}^2}{(\sqrt{2}\beta + \alpha)^2} - \frac{(\sqrt{2}\beta + \alpha)^2}{3\pi},$$

which reduces to the well-known strong coupling result $-\alpha^2/3\pi$ in the absence of impurity and spatial confinement. Second, in the case of a strong spatial confinement but weak electron–phonon coupling and binding parameter, one obtains the solution $\overline{\gamma}^2 = 1/\overline{\omega}_{\bullet}$, which gives rise to the energy

$$\overline{E} = \frac{3}{2}\overline{\omega}_{\bullet} - \sqrt{\frac{\overline{\omega}}{\pi}}(\sqrt{2}\beta + \alpha), \tag{17}$$

which is the sum of the ground-state energy of a 3D isotropic oscillator with frequency $\overline{\omega}_{\bullet}$ and the contributions from impurity and electron–phonon interaction in the weak coupling regime. Due to the fact that, setting $\lambda = 0$, minimization of equation (16) yields again a fourth-order equation in $\overline{\gamma}$, one can easily see that, in the case of a strong spatial confinement

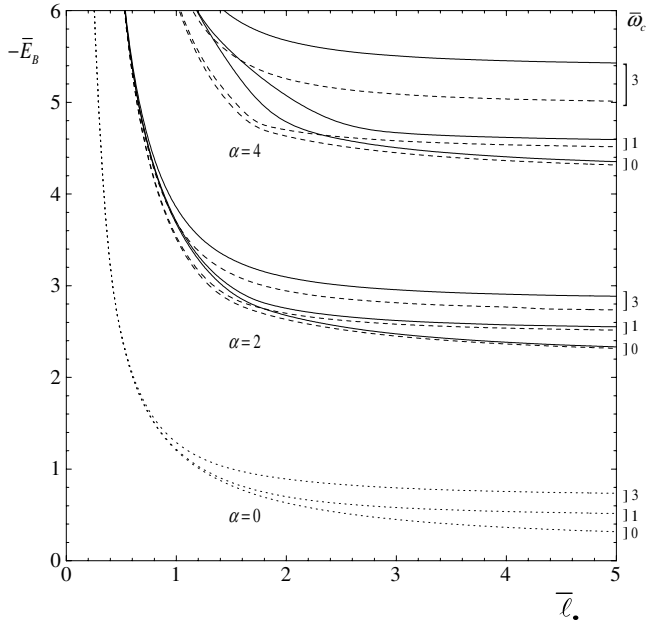

Figure 1. Binding energy of an impurity magnetopolaron as a function of confinement length $\ell_\bullet = \ell/r_0 = \sqrt{2/\overline{\omega}}$ for various values of magnetic field and electron–phonon coupling strength at $\beta = 1$. While the dashed curves represent the results of the all-coupling approach, the squeezing effect on the binding energy is denoted by the solid curves. The three dotted curves at the bottom refer to the unperturbed impurity binding energy, i.e., in the absence of electron–phonon interaction.

but a weak binding parameter, equation (16) exhibits a minimum when $\overline{\gamma}^2 = 1/\overline{\omega}_\bullet$, leading to equation (17) again.

It is obvious from these results that equation (11) together with equations (12*a*) and (12*b*) not only provides the results for the ground-state binding energy of an impurity magnetopolaron in a 3D parabolic QD valid in the whole range of electron–phonon coupling strengths, but also improves them. To reveal this, we have plotted the ground-state binding energy of an impurity magnetopolaron $\bar{E}^{\mathrm{B}} = \bar{E}(\alpha, \beta; \overline{\omega}) - \bar{E}(0, 0; \overline{\omega})$ and the polaronic correction to the ground-state energy $\Delta\bar{E} = \bar{E}(\alpha, \beta; \overline{\omega}) - \bar{E}(0, \beta; \overline{\omega})$, in figures 1 and 2 respectively.

In figure 1, we have presented a comparison of both the magnetic field and size dependence of the binding energy that have been obtained within the squeezed-state approach with all-coupling results. It can be clearly seen from the figure that (i) switching the electron–phonon interaction on leads to the enhancement of the binding energy of the impurity, (ii) application of a uniform magnetic field yields a further increase in the binding energy and (iii) as the strength of the electron–phonon interaction, α, increases, the corrections to the binding energy due to the squeezing become quite large as compared to those obtained in the all-coupling approach. Another important feature revealed in the figure is the fact that the introduction of a magnetic field enhances this correction. Furthermore, squeezing effects are enhanced by decreasing the size of the QD, i.e., by increasing the strength of spatial confinement.

In figure 2, we have plotted the polaronic correction to the ground-state energy of an impurity in a parabolic QD as a function of the confinement length for $\beta = 1$ and 3. From the figure, we see that the polaronic correction is more pronounced for $\beta = 3$ than for $\beta = 1$, and that it is increased with decreasing the size of the QD. The inset shows the dependence of

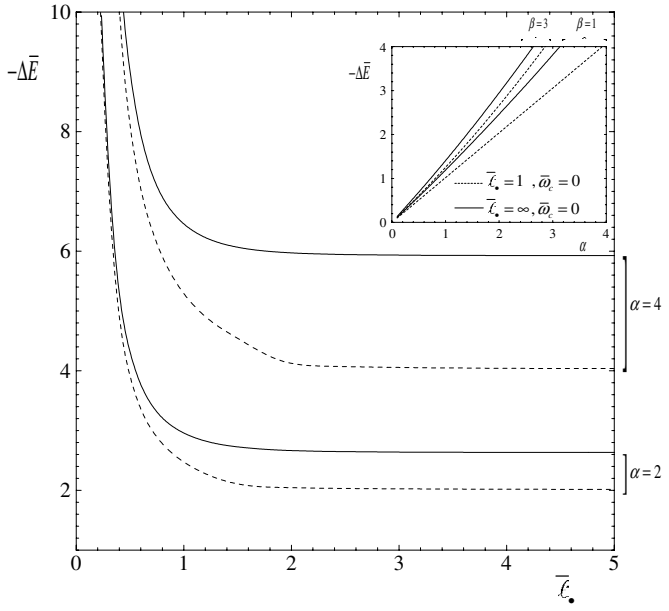

Figure 2. Polaronic correction to the ground-state of an impurity as a function of confinement length $\ell_\bullet$ for $\overline{\omega}_c = 0$. The dashed and solid curves refer to $\beta = 1$ and 3, respectively.

the polaronic correction on α, and reveals the effect of quantum confinement on the polaronic correction to the ground-state of an impurity for different values of β.

Finally, for $\beta = 1$, to illustrate how the computed variational parameters λ, $\overline{\gamma}_\perp$ and $\overline{\gamma}_\parallel$ change with both spatial confinement length and magnetic field, and in particular to clarify how λ plays a crucial role in the interpolation between two different regimes, we present the dependences of these parameters on the confinement length for three different values of magnetic field at $\alpha = 4$, in figure 3. For comparison, the results for $\alpha = 2$ are also displayed in the inset. From the figure and the inset, one can draw the following qualitative conclusions. First, for the zero magnetic field the two variational parameters $\overline{\gamma}_\perp$ and $\overline{\gamma}_\parallel$ coincide, and they both exhibit a tendency to decrease with decreasing the confinement length $\overline{\ell}_\bullet$, i.e., with increasing the strength of spatial confinement, even in the presence of a magnetic field. Second, while the introduction of a magnetic field ($\overline{\omega}_c = 1$) leads to the two curves for $\overline{\gamma}_\perp$ and $\overline{\gamma}_\parallel$ splitting significantly at larger values of confinement length, for a stronger magnetic field ($\overline{\omega}_c = 3$), however, they are positioned much closer to each other. We also note that, since $\lambda = 0$ at the spatial region defined by ($\overline{\ell}_\bullet > 2$) for $\overline{\omega}_c \leqslant 1$ at $\alpha = 2$ and ($\overline{\ell}_\bullet > 2.2$) for $\overline{\omega}_c \leqslant 1$ at $\alpha = 4$, the intermediate coupling theory is valid, while outside these regions the all-coupling variational approach is needed due to the nonzero λ. Finally, as the strength of confinement increases with decreasing confinement length, quantum size effects become important, leading to abrupt changes in all curves because increasing the strength of quantum confinement strengthens the electron–phonon interaction. In other words, the curves for $\overline{\gamma}_\perp$ and $\overline{\gamma}_\parallel$ for $\overline{\omega}_c \leqslant 1$ show a steplike decrease, while λ exhibits a steplike increase for $\overline{\omega}_c \leqslant 1$ around $\overline{\ell}_\bullet \sim 2$, indicating again the need for the use of the all-coupling variational approach for QDs whose sizes are of the order of the radius of a few polarons. Furthermore, at small $\overline{\ell}_\bullet$, for which quantum size effects are more significant, the curves for $\overline{\gamma}_\perp$ and $\overline{\gamma}_\parallel$ for every value of magnetic field fall roughly as $1/\overline{\omega}$ or $\overline{\ell}_\bullet/\sqrt{2}$.

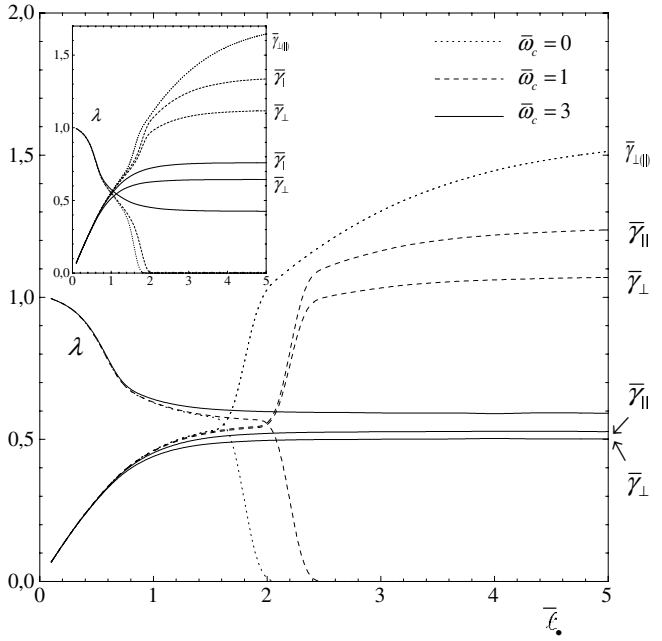

Figure 3. The variational parameters λ, $\overline{\gamma}_{\perp}$ and $\overline{\gamma}_{\|}$ that are determined by requiring equation (11) to be a minimum as a function of the confinement length for three different values of magnetic field for $\beta = 1$ and $\alpha = 4$. The inset shows the case for $\beta = 1$ and $\alpha = 2$.

4. Conclusion

In accordance with the purposes of the paper, which were (i) to obtain the ground-state energy of an impurity magnetopolaron in a 3D parabolic QD and hence polaronic contributions to this energy, within the framework of all-coupling regime, and (ii) to improve them, we have introduced a different unitary transformation scheme to diagonalize the relevant Fröhlich Hamiltonian. Since the first transformation employed here allows one to analyse both the size and the magnetic field dependence of the impurity magnetopolaron binding energy, it gives rise to terms that are proportional to the bilinear forms of the phonon creation and annihilation operators as well as the linear ones. Besides achieving an all-coupling approximation scheme for an impurity magnetopolaron in a 3D parabolic QD, we have analysed the effects of these quadratic terms on the impurity binding energy by introducing a single-mode squeezed state transformation. Our results show that the corrections to the binding energy due to the inclusion of such terms strongly depend on the size of the QD and the strength of the magnetic field. We have concluded that these terms give rise to a considerable increase in the binding energy with increasing both the strength of magnetic field and the spatial confinement length, and thus they should be taken into account in analysing the polaronic effects in QDs whose size are of the order of the radius of a few polarons.

We have considered the effects of the interaction of an electron with bulk-type LO-phonons on the binding energy of a hydrogen-like impurity placed symmetrically on the centre of a 3D parabolic QD by introducing a single-mode squeezed state transformation in addition to the usual LLP–H transformations, and have not taken into account the effects of interaction with surface optical-type (SO) phonons and deviation of the impurity from the dot centre. However, it has been very recently shown that

(i) for any value of coupling and for small binding strength the total electron–phonon interaction energy depends weakly on the impurity position and has a maximum when the impurity is at the centre of the dot, and that this maximum shifts inside the dot as the binding strength increases [35], and
(ii) the effects of the electron–LO phonon interaction are more significant than that the effects of the electron–SO phonon interaction in small QDs [12], but the contribution of the SO phonon to the impurity binding energy increases as the impurity shifts away from the centre while that of the LO phonon decreases in large QDs [11].

Since such effects, as is well-known, may become important, depending on both the size of the QD and material parameters, further investigations of these points should be made within the framework of our approach.

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