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Relaxed and effective-mass excited states of a quantum-dot polaron

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The polaronic corrections to the first excited-state energies of an electron in a parabolic quantum dot are obtained variationally for the entire range of the electron-phonon coupling constant and for arbitrary confinement length using a canonical transformation method based on the Lee-Low-Pines-Gross formalism. Simple analytical results are obtained in some interesting limiting cases and for arbitrary values of the parameters the nature of the excited state is studied numerically. The theory is applied to two- and three-dimensional GaAs quantum dots to obtain information about the existence of both the effective mass and the relaxed excited states of a polaron in these systems. [S0163-1829(98)08028-X]

I. INTRODUCTION

Interest in the subject of quantum dots has continued unabated for more than a decade or so primarily for two reasons. Firstly, it has an intrinsic appeal because the natural length scales involved in it are of the order of a few nanometers where the quantum effects show up in their full glory and therefore the issues of interest in the quantum dot problems are of fundamental nature from the point of view of basic physics (see Ref. 1 for review). Secondly and perhaps more importantly, the quantum dot systems have very many new physical properties[2] and also have a lot of design flexibility which make them technologically very promising particularly from the point of view of microelectronic device applications.

One of the recent interests in the area of quantum dots has been to explore the electron-phonon interaction[3] effects on their electronic properties. A number of authors[4] have investigated in this connection the ground-state (GS) polaronic properties of several semiconductor quantum dots. However, to the knowledge of the present authors, only a very few calculations are available for the polaronic excited states of quantum dots. The excited-state calculations are important to understand the optical absorption properties of these systems. Zhu and Gu[5] have obtained the second-order Rayleigh-Schrödinger perturbative corrections to the first excited-state (ES) energy of an electron moving in a two-dimensional (2D) parabolic quantum dot. We have recently shown[6] that the second-order perturbative result for the first excited state polaronic correction can be obtained in a simple analytical form involving only Γ functions. This result is, however, valid for small values of the electron-phonon coupling constant α and for frequencies of the confining potential that are far away from the one at which the first excited state is unstable with respect to the emission of a longitudinal optical (LO) phonon. We have also presented recently a variational calculation for the ground- and excited-state polaronic energies for a quantum dot electron.[7] The aim of the present paper is to perform an improved variational calculation for the first excited-state polaronic energy in a symmetric quantum dot with parabolic confinement. We are able to extract from our calculation information about both the effective mass excited states and the relaxed excited states. We shall make an N-dimensional (ND) formulation for the sake of generality and obtain results for both the two- and three-dimensional dots as special cases. In our model a quantum dot embedded in a three-dimensional (3D) material with the motion of the dot electron confined in all the three spatial directions will be called a 3D quantum dot, while that embedded in a purely 2D (zero-thickness) system with the electron's motion confined in the two available directions will be referred to as a 2D quantum dot. For the sake of mathematical simplicity we shall neglect the size quantization of phonons and treat the relevant phonon modes within the framework of the Fröhlich model. This model is certainly not very rigorous for very small confinement lengths but still may serve as a good enough approximation to capture some of the most important electron-phonon interaction effects in polar quantum dots.

II. FORMULATION

The Hamiltonian for the ND (symmetric) parabolic quantum dot polaron problem can be written as

$$H=-\tfrac{1}{2}\nabla_r^2+\tfrac{1}{2}\omega^2r^2+\sum_{\vec{q}} b^\dagger_{\vec{q}}b_{\vec{q}}+\sum_{\vec{q}} (\xi_q e^{-\vec{q}\cdot\vec{r}}b^\dagger_{\vec{q}}+\text{H.c.}), \tag{1}$$

where all vectors are N dimensional and units have been chosen such that $\hbar=m=\omega_{\rm LO}=1$ (Feynman units), m being the Bloch effective mass of the electron, and $\omega_{\rm LO}$ the LO-phonon frequency, which is assumed to be dispersionless. In Eq. (1), $\vec{r}(x_1,x_2,\ldots,x_N)$ refers to the position vector of the electron, $\omega=\omega_h/\omega_{\rm LO}$, ω_h being the frequency of the confining parabolic potential, $b^\dagger_{\vec{q}}(b_{\vec{q}})$ is the creation (annihilation) operator for a LO-phonon of wave vector $\vec{q}$ and ξ_q is given by[8]

$$|\xi_q|^2=\left(\frac{\Gamma\left(\frac{N-1}{2}\right)2^{N-3/2}\pi^{(N-1)/2}}{V_Nq^{N-1}}\right)\alpha, \tag{2}$$

where V_N is the volume of the N-dimensional dot and α is the electron-phonon coupling constant.

We seek a variational solution of Eq. (1) for which we use a modification of the Lee, Low, and Pines (LLP) canonical transformation method first introduced by Gross[9] and later used by Takeguhara and Kasuya[10] for the 3D bound polaron problem. This method (which we shall refer to as the LLP-G method) admits a trivial generalization to N dimensions.[11] In this method one first employs the transformation

$$U(\vec{r})=\exp\left[\sum_{\vec{q}}\ \{f_{\vec{q}}(\vec{r})b^{\dagger}{}_{\vec{q}}-f^{*}_{\vec{q}}(\vec{r})b_{\vec{q}}\}\right], \tag{3}$$

where $f_q(\vec{r})$ is a function of both $\vec{q}$ and $\vec{r}$ and has to be obtained variationally. The transformed Hamiltonian reads

$$\begin{aligned}\tilde{H}&=U^{-1}HU\\&=\frac{1}{2}\Bigg[\hat{\vec{p}}^{2}+\sum_{\vec{q}}\ b^{\dagger}{}_{\vec{q}}\hat{\vec{p}}\cdot[\hat{\vec{p}},f_q(\vec{r})]-\sum_{\vec{q}}\ b_{\vec{q}}\hat{\vec{p}}\cdot[\hat{\vec{p}},f^{*}_q(\vec{r})]+\sum_{\vec{q}}\ b^{\dagger}{}_{\vec{q}}[\hat{\vec{p}},f_q(\vec{r})]\cdot\hat{\vec{p}}-\sum_{\vec{q}}\ b_{\vec{q}}[\hat{\vec{p}},f^{*}_q(\vec{r})]\cdot\hat{\vec{p}}\\&\quad+\sum_{\vec{q}\vec{q}'}\ b^{\dagger}{}_{\vec{q}}b^{\dagger}{}_{\vec{q}'}[\hat{\vec{p}},f_{\vec{q}}(\vec{r})]\cdot[\hat{\vec{p}},f_{q'}(\vec{r})]-\sum_{\vec{q}\vec{q}'}\ b^{\dagger}{}_{\vec{q}}b_{\vec{q}'}[\hat{\vec{p}},f_{\vec{q}}(\vec{r})]\cdot[\hat{\vec{p}},f^{*}_{\vec{q}'}(\vec{r})]-\sum_{\vec{q}\vec{q}'}\ b_{\vec{q}'}b^{\dagger}{}_{\vec{q}}[\hat{\vec{p}},f^{*}_{\vec{q}}(\vec{r})]\cdot[\hat{\vec{p}},f_{\vec{q}}(\vec{r})]\\&\quad+\sum_{\vec{q}\vec{q}'}\ b_{\vec{q}}b_{\vec{q}'}[\hat{\vec{p}},f^{*}_{\vec{q}}(\vec{r})]\cdot[\hat{\vec{p}},f^{*}_{\vec{q}'}(\vec{r})]\Bigg]+\tfrac{1}{2}\omega^{2}r^{2}+\sum_{\vec{q}}\ [b^{\dagger}{}_{\vec{q}}+f^{*}_{\vec{q}}(\vec{r})][b_{\vec{q}}+f_{\vec{q}}(\vec{r})]+\sum_{\vec{q}}\ \{\xi_q e^{-i\vec{q}\cdot\vec{r}}[b^{\dagger}{}_{\vec{q}}+f^{*}_{\vec{q}}(\vec{r})]+\text{H.c.}\},\end{aligned} \tag{4}$$

where $\hat{\vec{p}}=-i\vec{\nabla}_{\vec{r}}$ and we have used the condition

$$\sum_{\vec{q}}\ [f^{*}_{\vec{q}}(\vec{r})\vec{\nabla}f_{\vec{q}}(\vec{r})-f_{\vec{q}}(\vec{r})\vec{\nabla}f^{*}_{\vec{q}}(\vec{r})]=0, \tag{5}$$

which implies that the current due the displacement of the phonon field is zero in the bound state. The LLP-G variational energy is now written as

$$E^{ND}=\langle 0|\langle\phi^{\mathrm{ND}}(\vec{r})|\tilde{H}|\phi^{\mathrm{ND}}(\vec{r})\rangle|0\rangle, \tag{6}$$

where $|0\rangle$ is the unperturbed zero-phonon state and $\phi^{ND}(\vec{r})$ is a real function of the electronic coordinates. Variation of Eq. (6) with respect to $f^{*}_{\vec{q}}(\vec{r})$ now leads to the following equation for $f_{\vec{q}}(\vec{r})$:

$$\left\{\left[\frac{\hat{\vec{p}}^{2}}{2},f_{\vec{q}}(\vec{r})\right]+f_q(\vec{r})\right\}\phi^{\mathrm{ND}}(\vec{r})=-\xi_q e^{-i\vec{q}\cdot\vec{r}}\phi^{\mathrm{ND}}(\vec{r}). \tag{7}$$

Eq. (6) then assumes the following form:

$$\begin{aligned}E^{ND}=&-\langle\phi^{\mathrm{ND}}|\tfrac{1}{2}\nabla^{2}|\phi^{ND}\rangle+\tfrac{1}{2}\omega^{2}\langle\phi^{\mathrm{ND}}|r^{2}|\phi^{\mathrm{ND}}\rangle\\&+\tfrac{1}{2}\sum_{\vec{q}}\ \{\xi^{*}_q\langle\phi^{\mathrm{ND}}|e^{i\vec{q}\cdot\vec{r}}f_{\vec{q}}(\vec{r})|\phi^{\mathrm{ND}}\rangle+\text{H.c.}\}.\end{aligned} \tag{8}$$

To proceed further we have to make a choice for the function $\phi^{\mathrm{ND}}(\vec{r})$. Choosing ϕ^{ND} to be the eigenfunction of a trial Hamiltonian H_t, i.e.,

$$H_t\phi^{\mathrm{ND}}_j(\vec{r})\equiv\left[\frac{\vec{p}^{2}}{2}+V(r)\right]\phi^{ND}_j(\vec{r})=\mathcal{E}^{ND}_j\phi^{ND}_j(\vec{r}), \tag{9}$$

we can solve Eq. (7) to obtain

$$f_{\vec{q}}(\vec{r})\phi^{\mathrm{ND}}_j(\vec{r})=-\sum_{j'}\ \frac{\langle\phi^{\mathrm{ND}}_{j'}|\xi_q e^{-i\vec{q}\cdot\vec{r}}|\phi^{ND}_j\rangle}{(\mathcal{E}^{ND}_{j'}-\mathcal{E}^{ND}_j+1)}|\phi^{\mathrm{ND}}_{j'}\rangle, \tag{10}$$

which, when substituted in Eq. (8) leads to

$$\begin{aligned}E^{\mathrm{ND}}_j=&\langle\phi^{ND}_j|(-\tfrac{1}{2}\nabla^{2}_{\vec{r}}+\tfrac{1}{2}\omega^{2}r^{2})|\phi^{ND}_j\rangle\\&-\sum_{\vec{q}}\ \sum_{j'}\ \frac{|\langle\phi^{ND}_{j'}|\xi_q e^{-i\vec{q}\cdot\vec{r}}|\phi^{ND}_j\rangle|^{2}}{(\mathcal{E}^{\mathrm{ND}}_{j'}-\mathcal{E}^{ND}_j+1)}.\end{aligned} \tag{11}$$

For the GS ($j=0$) the LLP-Gross energy (11) is identical with the Feynman-Haken path-integral expression and if the trial potential $V(r)$ is chosen as $\frac{1}{2}\omega^{2}r^{2}$ then Eq. (11) will give the second-order Rayleigh-Schrödinger perturbative result. The LLP-Gross method has, however, a few advantages over the path-integral method. First, in addition to the GS it also gives the excited states and, secondly, in this approach it is easy to improve on the result obtained from Eq. (11) by including the off-diagonal terms of the reduced Hamiltonian $\tilde{H}$ either by perturbation theory or by employing the higher-order Tamm-Dancoff approximation on $\tilde{H}$, which will incorporate the correlation between successively emitted virtual phonons.

III. RESULTS AND DISCUSSION

To evaluate Eq. (11) we choose the trial potential as $V(r)=\frac{1}{2}\mu^{4}r^{2}$. Then $\phi^{ND}_j(\vec{r})$ and $\mathcal{E}^{ND}_j$ are given by

$$\begin{aligned}\phi^{\mathrm{ND}}_j(\vec{r})=&\left(\frac{\mu^{N}}{\pi^{N/2}2^{j_1+j_2+\cdots+j_N}j_1!j_2!\cdots j_N!}\right)^{1/2}\\&\times H_{j_1}(\mu x_1)\cdots H_{j_N}(\mu x_N)e^{-(\mu^{2}/2)r^{2}},\end{aligned} \tag{12}$$

$$\mathcal{E}_j^{ND}=\left(j_1+j_2+\cdots+j_N+\frac{N}{2}\right)\mu^2, \tag{13}$$

where $H_{j_i}(\mu x_i)$ is the Hermite polynomial. Equation (11) finally reads, for the first excited state $(j=1)$,

$$E_1^{ND}=\left(\frac{N+2}{4}\right)\mu^2+\left(\frac{N+2}{4l^4}\right)\frac{1}{\mu^2}-\frac{\alpha}{4N}\mu\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\times\int_0^\infty dt\; e^{-(1-\mu^2)t}\left\{\frac{(2N-1)e^{-\mu^2 t}}{(1-e^{-\mu^2 t})^{1/2}}-1\right\}+\frac{\alpha}{4}\frac{\Gamma\left(\frac{N-1}{2}\right)}{N\Gamma\left(\frac{N}{2}\right)}\frac{\mu}{(\mu^2-1)}, \tag{14}$$

where l is the dimensionless confinement length given by $l=l_o/r_o=1/\sqrt{\omega}$, where $l_o=(\hbar/m\omega_h)^{1/2}$ and $r_o=(\hbar/m\omega_{\mathrm{LO}})^{1/2}$. Equation (14) has to be minimized with respect to μ to obtain the first excited-state polaron energy. This has to be done, in general, numerically and for specific values of N. We shall be interested in $N=2$ and $N=3$. It may be noted that the energy expression (14) has a singularity at $\mu=1$, which corresponds to the instability of the excited state with respect to the emission of a phonon. Before discussing the numerical results, we shall present some interesting limiting cases for arbitrary N.

a. Extended-state solutions $(\mu\to 0)$. In this limit, $l\to\infty$ and $\alpha\to 0$, and we can use the asymptotic relation

$$z^{b-a}\frac{\Gamma(z+a)}{\Gamma(z+b)}\quad \widetilde{z\rightarrow\infty}\quad 1+\frac{(a-b)(a+b-1)}{2z}, \tag{15}$$

so that Eq. (14) can be approximately written as

$$E_1^{ND}=\left(\frac{N+2}{4}\right)\mu^2+\left(\frac{N+2}{4l^4}\right)\frac{1}{\mu^2}-\frac{\alpha\sqrt{\pi}}{2}\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\left[1+\left(\frac{N+2}{8N}\right)\mu^2\right]. \tag{16}$$

Minimizing Eq. (16) with respect to μ yields

$$\mu^2=\frac{1}{l^2\left[1-\frac{\alpha\sqrt{\pi}}{4N}\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\right]^{1/2}}, \tag{17}$$

and therefore Eq. (16) reduces to

$$E_1^{ND,\mathrm{EMES}}=-\frac{\alpha\sqrt{\pi}}{2}\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}+\left(\frac{N+2}{2}\right)\frac{1}{l^2}\left[1-\frac{\alpha\sqrt{\pi}}{4N}\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\right]^{1/2}, \tag{18}$$

which is the effective mass excited state (EMES) result.[12] As we have already pointed out, the first excited-state energy (14) has a singularity at $\mu=1$. Therefore the minima corresponding to the effective mass excited-state would occur on the left side of the singularity. The situation described by Eq. (18) is that of an undisturbed weak-coupling polaron (at least to first order) sitting at the first excited level of the confining parabolic potential of the quantum dot.

b. Localized state limit $(\mu\to\infty)$. In this limit one can show that

$$\frac{\Gamma\left(\frac{1}{\mu^2}+1\right)}{\Gamma\left(\frac{1}{\mu^2}+\frac{1}{2}\right)}\simeq\frac{\left(1+\frac{2}{\mu^2}\ln 2\right)}{\sqrt{\pi}}. \tag{19}$$

Thus in the localized-state limit Eq. (14) becomes

$$E_1^{ND}=\left(\frac{N+4}{2}\right)\mu^2+\left(\frac{N+2}{4l^4}\right)\frac{1}{\mu^2}-\frac{\alpha}{2}\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\left(1-\frac{1}{4N}\right)\frac{(2\ln 2+\mu^2)}{\mu}, \tag{20}$$

where μ has to be obtained from

$$\left(\frac{N+2}{2}\right)\mu^4-\left(\frac{N+2}{2}\right)\frac{1}{l^4}-\frac{\alpha}{2}\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\times\left(1-\frac{1}{4N}\right)(\mu^3-2\mu\ln 2)=0. \tag{21}$$

In the limit of strong electron-phonon coupling and weak confinement, Eq. (21) can be approximately solved to yield

$$\mu=\frac{\alpha}{(N+2)}\left(1-\frac{1}{4N}\right)\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}, \tag{22}$$

so that Eq. (20) reads

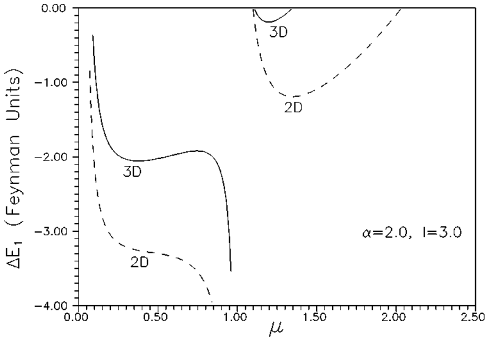

FIG. 1. Polaronic corrections, ΔE_1 (in Feynman units) to the ES energy of an electron in 2D and 3D quantum dots for $\alpha=2$ and $l=3$ as a function of the variational parameter μ.

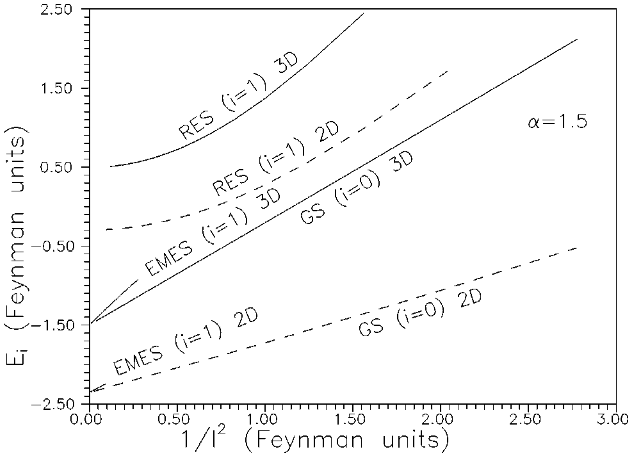

FIG. 2. EMES and RES energies (in Feynman units) of a polaron as a function of $1/l^2$ (in Feynman units) for $\alpha=1.5$ in 2D and 3D quantum dots. The GS polaron energies are also shown for the sake of comparison.

$$E_1^{ND,\mathrm{RES}}=-\frac{\alpha^2}{4(N+2)}\left(1-\frac{1}{4N}\right)^2\left(\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\right)^2+\frac{(N+2)^3}{4\alpha^2 l^4}\frac{1}{\left(1-\frac{1}{4N}\right)^2}\left\{\frac{\Gamma(N/2)}{\Gamma\left(\frac{N-1}{2}\right)}\right\}^2-(N+2)\ln 2, \tag{23}$$

which is the first relaxed-excited-state (RES) energy in the limit of large α and weak confinement. Even without the last term Eq. (23) is lower than the corresponding result that could be obtained by using the Landau-Pekar method[13] with the Gaussian function as the trial function. It may be recalled that in the case of GS, the LLP-G (or the Feynman-Haken path-integral) expression (without the log term) is the same as the Landau-Pekar result.

In the limit of strong confinement ($l\rightarrow 0$) and small electron-phonon coupling ($\alpha\rightarrow 0$), Eq. (21) can be approximately solved by dropping the third term to give

$$\mu^2=\frac{1}{l^2}, \tag{24}$$

and thus in this limit the first relaxed-excited-state energy is given by

$$E_1^{ND,\mathrm{RES}}=\frac{(N+2)}{2l^2}-\frac{\alpha}{2}\left(1-\frac{1}{4N}\right)\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\left(\frac{1}{l}+2l\ln 2\right), \tag{25}$$

which is the second-order perturbative result for strong confinement. Since the first relaxed-excited-state energy expressions (23) and (25) are obtained for large values of μ, the minima corresponding to these energies will be on the right side of the singularity. It may be mentioned that the LLP-G method cannot produce an excited state of the effective mass type in the localized-state limit, even for the ground-state energy. Thus our results may not be very accurate in the limit of weak confinement and strong electron-phonon coupling where one might probably expect effective mass type states.

c. Numerical results. The first excited-state polaronic correction to the quantum dot electron energy can be defined as

$$\Delta E_1=E_1^{ND}-\frac{(N+2)}{2l^2}, \tag{26}$$

which as a function of μ would have in general two minima, one corresponding to the EMES that can occur for $\mu<1$ and the other corresponding to the RES that can occur for $\mu>1$. As we have already mentioned, the first effective mass excited state describes a situation in which we have an undisturbed polaron in the first excited state of the confining potential of the quantum dot. The relaxed excited states occur when the localization potential for the electron arises from the combined effect of the lattice polarization and the parabolic potential. It should, however, be pointed out that for the excited-state polaronic level to exist, ΔE_1 should be negative. We have studied the variation of ΔE_1 as a function

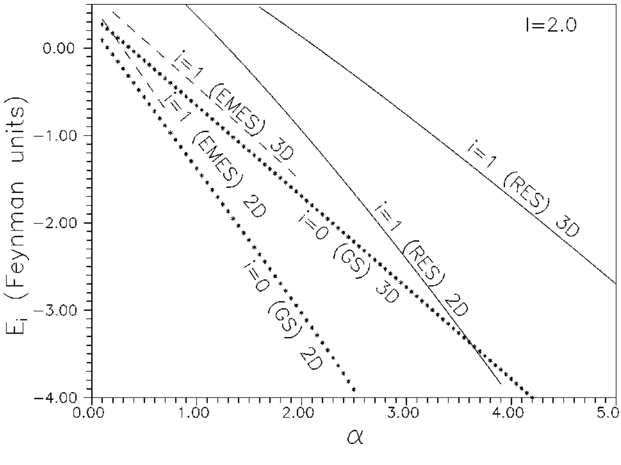

FIG. 3. EMES and RES energies (in Feynman units) of a polaron as a function of α for $l=2$ in both 2D and 3D quantum dots. The GS energies are also shown for the sake of comparison.

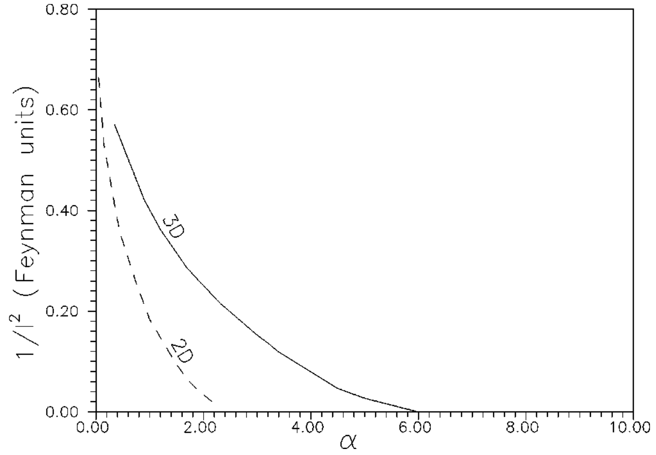

FIG. 4. The curve giving the critical values of α and $1/l^2$ (in Feynman units) below which EMES would exist in 2D and 3D quantum dots.

of μ for both 2D and 3D dots for various sets of values of α and l. The typical behavior is shown in Fig. 1 where we have taken $\alpha=2$ and $l=3$. It is clear that, in two dimensions, ΔE_1 has only one minimum corresponding to the RES while, in three dimensions, ΔE_1 has two minima, one corresponding to the EMES and the other to the RES, the EMES being, as expected, lower in energy. For $\alpha=2$ and $l=1$ we find that in both two and three dimensions, ΔE_1 shows only one minimum that occurs for $\mu>1$, implying that the first excited states in these cases are of the RES type. For $\alpha=2$ and $l=7$ we find that, in two dimensions, ΔE_1 shows two minima, one giving the EMES energy correction and the other giving the first RES energy correction. In three dimensions also we find that there are two minima in the $\Delta E_1-\mu$ curve, but the minimum for $\mu>1$ gives a positive polaronic energy correction and is therefore not acceptable. For $\alpha=0.5$ and $l=5.0$ we find that the the first excited state is of the EMES type in both 2D and 3D dots. We would like to add here that when the minimum of the $\Delta E_1-\mu$ curve is very close to the singularity, the energies obtained are not very accurate. Therefore in such cases even if we may obtain a small positive value for ΔE_1, the relaxed excited states may still possibly exist.

We obtain both the EMES and the RES energies ($E_1^{\mathrm{EMES}}, E_1^{\mathrm{RES}}$) as a function of $1/l^2$ for $\alpha=1.5$ in both two and three dimensions. The results are shown in Fig. 2, where we have also shown the behavior of the GS polaron energy (E_0) for the sake of comparison. In Fig. 3 we plot E_o, E_1^{EMES} and E_1^{RES}, as a function of α for $l=2$ for both two- and three-dimensional dots. It is evident from all these figures that the difference between the GS energy and the first RES energy is always greater than an LO-phonon energy. It can also be noticed that for a particular value of α the EMES ceases to exist below a certain value of the confinement length. Again, for a given value of l the EMES exists only if α does not exceed a particular value. We show this behavior more elaborately in Fig. 4, for both 2D and 3D dots. The regions, lying below the 2D and the 3D curves, give in the respective dimensions the parts of the parameter space where effective mass excited states would exist.

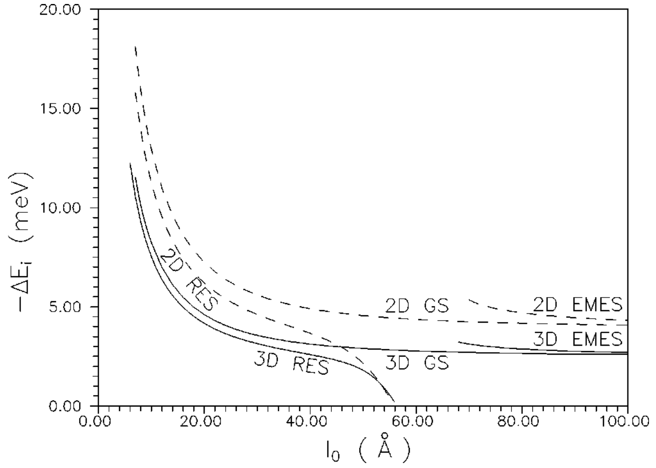

FIG. 5. Polaronic corrections, $-\Delta E_1$ (in meV) to the ES energy of an electron in 2D and 3D GaAs quantum dots as a function of the confinement length l_o (in Å). The GS energies are also shown for the sake of comparison.

We can easily apply our theory to realistic quantum dots. As an example we show in Fig. 5. the behavior of $-\Delta E_1$ for 2D and 3D GaAs quantum dots. The GS polaronic corrections to the electron energy are also shown for comparison. The material parameters used in the calculation have been taken from Ref. 14. One can notice that for large values of the confinement length the first excited state of a polaron in a GaAs quantum dot is of the effective mass type. However, if the dot size is small, the first excited state of the polaron can be described by a relaxed excited state. It is also evident from the figure that both the GS and the ES energy corrections to the energy of an electron in a GaAs quantum dot due to the polaronic interaction can be quite large if the dot sizes are sufficiently small. Furthermore, the difference between the GS and ES polaronic self-energy corrections can also be quite significant for small dots, particularly in two dimensions.

IV. CONCLUSION

In conclusion, we have performed an improved variational calculation to obtain the first excited-state energy of a polaron in a symmetric parabolic quantum dot in both two and three dimensions. We have obtained results for all values of the electron-phonon coupling constant and for arbitrary confinement length. We have shown that in some interesting limiting cases simple analytical results can be obtained. Our calculation provides information about both the effective mass and the relaxed excited states. We have shown that for a given value of α the nature of the first excited state of a polaron in a quantum dot depends crucially on the confinement length. We have observed that the difference between the GS and the first RES energies is always greater than an LO-phonon energy for all the cases we have investigated. We have finally applied our results to two- and three-dimensional GaAs quantum dots for which we find that the first excited state is of the effective mass type if the dot size is large while for a small dot the first excited state is described by a relaxed excited state. We have shown that, as in the case of the GS, the polaronic corrections to the excited-state energy of a quantum dot electron can also be quite large if the dot sizes are reduced to a few nanometers. We furthermore observe that the difference between the GS and the ES polaronic self-energy corrections can be quite significant for small dots, particularly in two dimensions. This might have some important effects on the optical absorption properties of polar semiconductor quantum dots. These investigations are in progress and will be reported in due course.

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