Polaronic enhancement in the ground-state energy of an electron bound to a Coulomb impurity in a parabolic quantum dot

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Using the Feynman-Haken variational path-integral formalism we obtain the polaronic correction to the ground-state energy of an electron bound to a positive Coulomb impurity in a polar semiconductor quantum dot with parabolic confinement in both two and three dimensions. We perform calculations for the entire range of the electron-phonon coupling constant and the Coulomb binding parameter and for arbitrary confinement length. We apply our results to several semiconductor quantum dots and show that the quantum-dot enhancement in the polaronic correction in some of these dots can be very large. [S0163-1829(97)05615-4]

Ultralow-dimensional structures with quantum confinement in all the spatial directions are commonly referred to as quantum dots (see Ref. 1 for a review). With the recent developments in nanofabrication technology quantum dots can be realized in both two- and three-dimensional systems and can be made as small as a few nanometers in size. Interest in the subject of quantum dots is primarily twofold. First, the issues involved at the nanoscales are of fundamental importance because of the full quantum nature of the problem and thus have an intrinsic appeal. Secondly and probably more importantly the quantum-dot structures have tremendous potentiality of finding applications in microelectronic device technology because of their considerable design flexibility and very many novel physical effects.[2–6]

Recently much effort has also been directed towards exploring the polaronic properties of several semiconductor quantum dots.[7–14] It has been observed in this connection that the polaronic effects can be very large in these dots if their sizes are reduced to a few nanometers. More recently, the related problem of an optical polaron bound to a Coulomb impurity in a quantum dot has also been considered in the presence of a magnetic field.[15,16] Imperfections being a rule rather than an exception, such an impurity-bound polaron problem[17,18] is obviously more realistic and is therefore of much practical importance. In the present paper we purport to study the bound polaron problem in a quantum dot in the absence of a magnetic field and for the entire range of the electron-phonon coupling constant, the Coulomb binding parameter, and the confinement strength. We employ the Haken method[18–21] of using the Feynman path-integral formalism to obtain the ground-state (GS) energy of a bound polaron in a symmetric quantum dot with parabolic confinement in both two and three dimensions. We make an N-dimensional (ND) formulation and obtain results for both two- and three-dimensional dots as special cases. For the sake of mathematical simplicity we neglect the size quantization of phonons and model the relevant phonon modes by the corresponding bulk modes.

The Hamiltonian for a bound polaron in a parabolic quantum dot can be written as

$$H' = -\frac{\hbar^2}{2m}\nabla_{\vec{r}'}^2 + \frac{1}{2}m\sum_{i=1}^{N}\omega_{pi}^2 x_i'^2 - \frac{e^2}{\epsilon_\infty r'} + \hbar\omega_0\sum_{\vec{q}}\tilde{b}_{\vec{q}'}^{\dagger}\tilde{b}_{\vec{q}'} + \sum_{\vec{q}'}[\xi_{q'}(e^{i\vec{q}'\cdot\vec{r}'}-1)\tilde{b}_{\vec{q}'}^{\dagger} + \text{H.c.}], \tag{1}$$

where all vectors are N dimensional, $\vec{r}'$ is the position vector of the electron and m is its Bloch effective mass, ω_{pi} is the frequency of the confining potential in the ith direction, ω_0 is the longitudinal-optical- (LO) phonon frequency which is assumed to be dispersionless, $b_{\vec{q}}^{\dagger}(b_{\vec{q}})$ is the creation (annihilation) operator of a LO phonon of wave vector $\vec{q}$, and $\xi_{\vec{q}'}'$ is the electron-phonon interaction coefficient. We shall use the Feynman units in which the energy is scaled by $\hbar\omega_0$, length by r_0 where $r_0 = q_0^{-1}$, q_0 being an inverse length defined by $\hbar^2 q_0^2/m = \hbar\omega_0$, i.e., $q_0 = (m\omega_0/\hbar)^{1/2}$, volume by r_0^N, and wave vector by q_0. Such scalings are equivalent to setting $\hbar = m = \omega_0 = 1$. In these units, the Hamiltonian (1) reads

$$H = -\frac{1}{2}\nabla_{\vec{r}}^2 + \frac{1}{2}\sum_{i=1}^{N}\omega_i^2 x_i^2 - \frac{\tilde{\beta}}{r} + \sum_{\vec{q}}\tilde{b}_{\vec{q}}^{\dagger}\tilde{b}_{\vec{q}} + \sum_{\vec{q}}\{\xi_q(e^{-i\vec{q}\cdot\vec{r}}-1)\tilde{b}_{\vec{q}}^{\dagger} + \text{H.c.}\}, \tag{2}$$

where

$$\omega_i = \frac{\omega_{pi}}{\omega_0}, \quad \tilde{\beta} = \left(\frac{e^2}{\hbar\omega_0\epsilon_\infty}\right) \Big/ \left(\frac{\hbar}{m\omega_0}\right)^{1/2}, \qquad \xi_q = \xi_{q'}'/\hbar\omega_0. \tag{3}$$

For ξ_q we use the prescription of Peeters *et al.*[22] According to that prescription, ξ_q is given by

$$|\xi_q|^2 = \frac{\Gamma((N-1)/2)2^{N-(3/2)}\pi^{(N-1)/2}}{V_N q^{N-1}}\alpha. \tag{4}$$

To eliminate the impurity-phonon interaction we now apply the transformation, $b_{\vec{q}} = \tilde{b}_{\vec{q}} - \xi_q$. The Hamiltonian (2) then becomes

$$H = -\frac{1}{2}\nabla_{\vec{r}}^2 + \frac{1}{2}\sum_{i=1}^{N} \omega_i^2 x_i^2 - \frac{\beta}{r} + \sum_{\vec{q}} b_{\vec{q}}^{\dagger} b_{\vec{q}} + \sum_{\vec{q}} \{\xi_q (e^{-i\vec{q}\cdot\vec{r}} b_{\vec{q}}^{\dagger} + \text{H.c.}\}, \tag{5}$$

where $\beta = \tilde{\beta} - \sqrt{2}\alpha$. The above Hamiltonian without phonons corresponds to the impurity problem in a parabolic quantum dot which has been studied by Zhu *et al.*[23] by using an exact method. However, for polar semiconductor quantum dots the electron–optical-phonon interaction is expected to have sizable effects on the electronic properties and therefore the bound polaronic Hamiltonian (5) seems to be a better starting point. The transformation function relevant for the determination of the GS energy of the Hamiltonian (5) is given by the path integeral[24,25]

$$K_{00}(\vec{r}_b, t_b; \vec{r}_a, t_a) = \int D\vec{r}(t) e^S, \tag{6}$$

where the index 00 refers to the transition from a zero-phonon state to a zero-phonon state and S is a nonlocal classical action given by

$$S = \int \left(-\frac{1}{2}\dot{\vec{r}}^2 - \frac{1}{2}\sum \omega_i^2 x_i^2 + \frac{\beta}{r} \right) dt + \frac{1}{2}\sum_{\vec{q}} \int\int dt\, ds |\xi_q|^2 \exp\{i\vec{q}\cdot[\vec{r}(t) - \vec{r}(s)]\} \times \exp\{-|t-s|\}, \tag{7}$$

which is, however, not path integrable. Following the Haken method we therefore choose an effective trail action

$$S_{\text{eff}} = \int_{t_a}^{t_b} L_{\text{eff}} dt = \int_{t_a}^{t_b} \left[-\frac{1}{2}\dot{\vec{r}}^2 - V_{\text{eff}}(\vec{r}) \right] dt, \tag{8}$$

where $V_{\text{eff}}(\vec{r})$ is an effective potential which should be fairly close to the actual potential occurring in S and which should be exactly soluble. We shall specify the choice of V_{eff} later. If $\Phi_{j,\text{eff}}^{ND}$ and $E_{j,\text{eff}}^{ND}$ are, respectively, the eigenfunctions and eigenvalues of the quantum mechanical Hamiltonian H_{eff} corresponding to the classical Lagrangian L_{eff}, then the Feynman variational theorem yields

$$E_{0,\text{exact}}^{ND} \leqslant E_{\text{FH}}^{ND} = \left\langle \phi_{0,\text{eff}}^{ND} \middle| \left(-\frac{1}{2}\nabla_{\vec{r}^2} + \frac{1}{2}\sum_i \omega_i^2 x_i^2 - \frac{\beta}{r} \right) \middle| \Phi_{0,\text{eff}}^{ND} \right\rangle - \sum_j \sum_{\vec{q}} \frac{|\langle \Phi_{j,\text{eff}}^{ND} | \xi_q e^{-i\vec{q}\cdot\vec{r}} | \Phi_{0,\text{eff}}^{ND} \rangle|^2}{E_{j,\text{eff}}^{ND} - E_{0,\text{eff}}^{ND} + 1} \tag{9}$$

where E_{FH}^{ND} is the Feynman-Haken variational energy which is an upper bound to the exact polaron GS energy $E_{0,\text{exact}}^{ND}$. Taking $V_{\text{eff}} = \frac{1}{2}\mu^4 r^2$ and assuming $\omega_1 = \omega_2 = \cdots \omega_N = \omega$ we finally obtain for a symmetric quantum dot

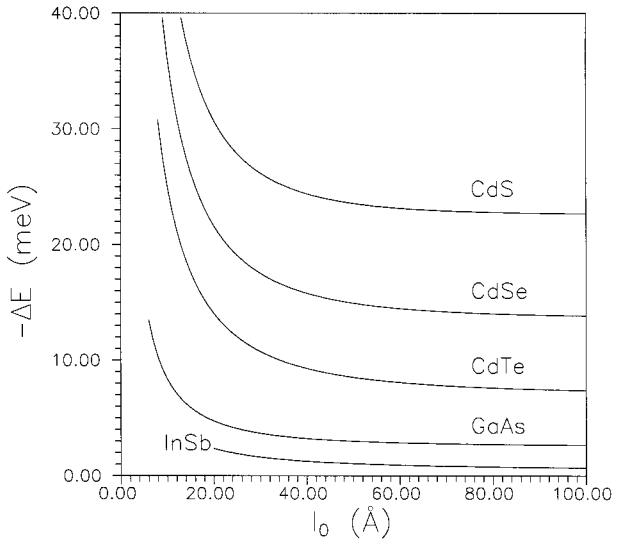

FIG. 1. Polaronic corrections, $-\Delta E$ (in meV) to the GS energy of an electron in InSb, GaAs, CdTe, CdSe, and CdS quantum dots with parabolic confinement in 3D, as a function of the confinement length l_0 (in angstroms).

$$E_{\text{FH}}^{ND} = \frac{N}{4Z} + \frac{N}{4l^4}Z - \frac{\Gamma((N-1)/2)}{\Gamma(N/2)}\beta\frac{1}{\sqrt{Z}} - \frac{\alpha\sqrt{\pi}}{2}\frac{\Gamma((N-1)/2)}{\Gamma(N/2)}\frac{1}{\sqrt{Z}}\frac{\Gamma(Z+1)}{\Gamma(Z+\frac{1}{2})}, \tag{10}$$

where $Z = 1/\mu^2$ and l is the dimensionless confinement length given by $l = l_0/r_0 = 1/\sqrt{\omega}$. Equation (10) has to be minimized numerically with respect to Z to obtain the variational Feynman-Haken GS energy for specific values of N.

In the absence of the electron-phonon interaction the energy of an impurity atom in a quantum dot can be written from Eq. (10) as

$$E_{\text{FH}}^{ND}(\alpha = 0) = \frac{N}{4Z'} + \frac{N}{4l^4}Z' - \frac{\Gamma((N-1)/2)}{\Gamma(N/2)}\beta\frac{1}{\sqrt{Z'}}, \tag{11}$$

where Z' has to be obtained from the equation

$$\frac{N}{4l^4}Z'^2 + \frac{1}{2}\frac{\Gamma((N-1)/2)}{\Gamma(N/2)}\beta Z'^{1/2} - \frac{N}{4} = 0. \tag{12}$$

The polaronic correction is then defined as

$$\Delta E = E_{\text{FH}}^{ND} - E_{\text{FH}}^{ND}(\alpha = 0), \tag{13}$$

which we obtain for both $N = 2$ and $N = 3$. As expected, in both 2D and 3D dots the polaronic effects are found to be more pronounced for larger values of α and β.

In Figs. 1 and 2 we show the plot of $-\Delta E$ as a function of l_0 for a few selected quantum dots of polar semicondeuctors such as InSb, GaAs, CdTe, CdSe, and CdS. The material parameters used in the calculation are given in Table I. Figure 1 gives the behavior for the 3D dots while that for the 2D dots is shown in Fig. 2. Clearly for the same material and for the same value of the confinement length, the polaronic effect is stronger in a 2D dot than in a 3D dot. It is also clear that the polaronic effects exhibited by some of the dots are

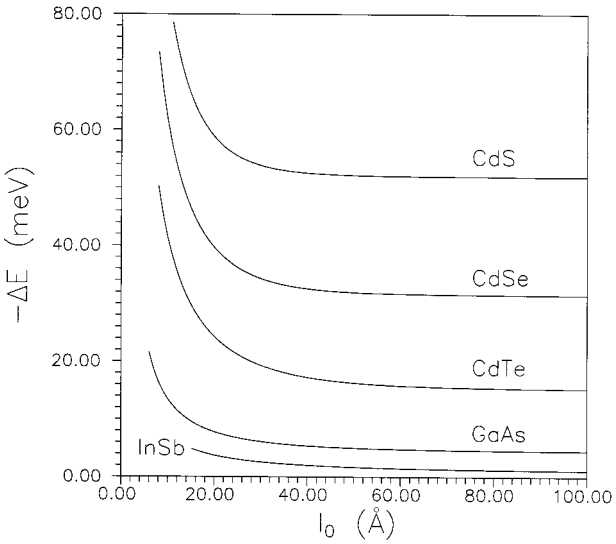

FIG. 2. Polaronic corrections, $-\Delta E$ (in meV) to the GS energy of an electron in InSb, GaAs, CdTe, CdSe, and CdS quantum dots with parabolic confinement in 2D as a function of the confinement length l_0 (in angstroms).

quite pronounced below a few nanometers. As the confinement length increases, the polaronic effect is, however, found to diminish significantly in both 2D and 3D dots over a small range of the confinement length after which ΔE varies rather slowly with the confinement length approaching asymptotically to the bulk limit.

In conclusion, we have studied the effect of electron–optical-phonon interaction on the motion of an electron bound to a positive Coulomb impurity in a symmetric polar semiconductor quantum dot with parabolic confinement in both two and three dimensions. We have employed the Feynman-Haken path-integral formalism which is known to yield quite accurate results for the polaron problems to obtain the polaronic correction to GS energy of the impurity-bound electron for the entire range of the electron-phonon coupling constant α and the Coulomb binding parameter β and for arbitrary confinement length. We observe that the polaronic corrections are more pronounced in a 2D dot than in a 3D dot of the same material for all values of the confinement length. We consider a few selected polar semiconductor quantum dots and demonstrate that the polaronic corrections increase as the confinement length decreases in both 2D and 3D dots and may become very large in some of these dots if the dot sizes are reduced below a few nanometers. We have, however, neglected in this work the effect of interaction of the electron with the interface phonons for the sake of mathematical simplicity. This probably restricts the validity of our results to dots of sizes larger than about 2 nm.

TABLE I. Material parameters for GaAs, CdS, CdSe, CdTe, and InSb (taken from Ref. 26).

	m (in units of bare electronic mass)	$\hbar\omega_0$ (in meV)	α	β
GaAs	0.066	36.7	0.068	0.5447
CdS	0.155	38.26	0.527	1.225
CdSe	0.130	26.576	0.460	1.238
CdTe	0.091	20.84	0.315	1.064
InSb	0.0138	24.46	0.022	0.2184

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