Feynman-Haken path-integral approach for polarons in parabolic quantum wires and dots

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Within the framework of the Feynman-Haken (FH) variational path-integral theory, the expression for the ground-state energy of the electron and longitudinal-optical phonon system in parabolic quantum wires and dots with arbitrary electron-phonon coupling constant and confining potential strength is derived in a unified way with the use of a general effective potential. For quantum dots, due to high symmetry, a simple closed-form analytical expression for the Feynman energy can be obtained, and the analytical results in the extended-state and localized-state limit can be further derived. It is shown both analytically and numerically that the present FH results could be better than those obtained by the second-order Rayleigh-Schördinger perturbation theory and the Landau-Pekar strong-coupling theory for all cases, which, therefore, shows the effectiveness of the present approach. In quantum wires, it is found in numerical calculations that the binding of polarons is monotonically stronger as the effective wire radius in the whole coupling regime. Interestingly, when the confining potential of quantum wire is extremely strengthened, even in the weak- and intermediate-coupling regime, this system could exhibit some strong-coupling features. More importantly, it is proven strictly that a very recent result in the literature that ''the binding can be weaker than in bulk case at weak coupling'' is not an intrinsic property of this system. In quantum dots, it is found numerically that the polaron binding energy increases with the decrease in size of the dot and is much more pronounced in two dimensions (2D) than in 3D, while the relative polaronic enhancement is stronger in 3D than in 2D for not too weak electron-phonon coupling. [S0163-1829(98)01544-6]

I. INTRODUCTION

With the recent progress in microfabrication technology, such as molecular-beam epitaxy and nanolithography, it becomes possible to fabricate the synthetic polar semiconductor structures with low dimensionality, such as dielectric slabs, heterojunctions, quantum wells, quantum dots, and quantum wires. Two subjects of interest are the quantum wire,[1–4] which can be fabricated within low-nm size, and the quantum dot[5–8] which can be realized in both two- and three-dimensional (2D and 3D) systems, and can also be made as small as a few nm in size. These systems have attracted substantial attention due to the physical effects coming from their quasi-one-dimensionality (wires) and ultralow dimensionality (dots), which are useful for electronic and optoelectronic device applications. Recently, many investigations have been devoted to the effects of the electron-phonon interaction on various electronic properties of polar semiconductor quantum wires[9–37] and quantum dots.[11,38–47] One of the most significant observations that had been made within this context is that polaronic effects are extremely important in thin wires and small dots, and should, therefore, be taken into account when making devices with them.

Polarons in quantum wires or dots are markedly different from those in bulk materials, due to the presence of wire or dot potentials, which confine the motion of the carriers in the plane transverse to the wire axis or in all the spatial directions of dots. First, the confining potential may bring about much rich phonon modes,[9–17,38–40] such as confined phonon modes, interface phonon modes, etc. Second, even for the confining potential itself, there are so many types in the literature. It can be divided into three major types: the rectangular (or box) type,[12–15] cylindrical (or sphere) type,[11,16–23] and parabolic-type.[24–31,43–47] Further, it can also be characterized as finite[23] or infinite,[20] symmetric[17] or asymmetric.[24] A variety of phonon modes and various types of the wire potential have given rise to rich and varied investigations in this field in the last decade.

More recently, the sole effect of the interaction of electron and bulk longitudinal-optical (LO) phonons and polaronic properties in quantum wires and dots have been studied by a large number of authors.[18–37,41–46] Most of the papers are associated with the weak-coupling treatments. However, to our knowledge, only a few papers (e.g., Refs. 20 and 25) had been written on the polaronic effect over the whole coupling regime, which are also of great theoretical and practical importance. Except in Ref. 20, the general consensus is that the polaronic correction to the ground state is considerably stronger with the strength of the wire or dot confining potential. Therefore, high-degree confinement of quantum wires or dots should lead to the enhancement in the effective electron-phonon coupling. This would bring about the possibility that,

in spite of weak-polar coupling as in GaAs ($\alpha=0.07$); for instance, the polaron problem may show up as an intermediate- and strong-coupling feature. This is more pronounced in the II-VI compound semiconductors (e.g., CdS $\alpha=0.53$), where the electron-phonon coupling strength is almost in one order of magnitude larger than that in III-V materials. Consequently, the pure perturbation theory is not perfectly appropriate for a system with weak-coupling strength, which, however, could also exhibit intermediate-, even strong-coupling features through the variation of the confining potential strength. It is also evident that the Landau-Pekar (LP) theory[48] employed in Refs. 19, 29, and 44, which is only well suited in the strong-coupling limit, could not produce precise results for these systems. Thus, a theory that would be really suited for all coupling regimes simultaneously is imperative to provide some qualitative insight into the investigation on polarons in this system. On the other hand, such a universal theory may stimulate more experimental works on some materials with somewhat strong-coupling strengths, which will be helpful for better understanding of the role of the electron-LO phonon interactions in quantum wires or dots. For instance, recent progress in technology has already allowed the fabrication of nanosized and even atom-sized structures, including those with strong ionic substance, e.g., KBr/NaCl, KBr/RbCl, and NaCl/NaCl(001) monolayers.[49] In these materials, the electron-phonon coupling constant α is usually larger than one.

In the present paper, we will study the sole effect of the electron-LO phonon interactions on the ground-state energy of an electron in polar semiconductor quantum wires and dots with parabolic confinement for arbitrary coupling constants in a unified way, within the framework of the Feynman-Haken (FH) path-integral theory.[50–52] Such a choice for the confining potential, besides facilitating the derivations in the theory, is also, more importantly, close to the realistic case. Recently, Kash *et al.*[53] have observed some good evidences for the existence of a parabolic potential well in quantum wires produced by strain gradients using a patterned carbon stress. In addition, it is reasonable to consider the electron-phonon interaction with bulk phonons only, as far as there are no interfaces in these systems with the parabolic potential.

The remainder of this paper is organized as follows. In Sec. II we outline the theory of FH and derive the unified expression for the polaron energy over broad ranges of the confining potential of the quantum wire and dot, and arbitrary electron-phonon coupling strength. In the next section we also derive the energy expressions for polarons by means of the second-order Rayleigh-Schrödinger perturbation theory (RSPT) and the LP strong-coupling theory. In Sec. IV some analytical results for polarons in quantum dots are obtained analytically. Numerical results and some discussions are performed in Sec. V. The conclusions are summarized in the last section.

II. THEORY

The Hamiltonian describing the interaction of an electron and LO phonons in quantum wires and dots with parabolic potential can be, in a unified way, given by (in units of $m=\hbar=\omega_{\rm LO}=1$)

$$H=\frac{\mathbf{p}^2}{2}+V(\rho,z)+\sum_{\mathbf{k}} a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}+\sum_{\mathbf{k}} (v_{\mathbf{k}}a_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{r}}+\text{H.c.}), \tag{1}$$

where $\mathbf{r}=((\rho=x,y),z)$ and $\mathbf{p}$ are the position and momentum operators of the electron, and $V(\rho,z)=\frac{1}{2}\omega^2\rho^2+\frac{1}{2}\omega_z z^2$ is the confining potential. $\omega_z=0$ for quantum wires and $\omega_z=\omega$ for quantum dots, with ω being in units of $\omega_{\rm LO}$, measuring the confining strength of the parabolic potential, $a_k^{\dagger}$ and a_k are, respectively, the creation and annihilation operators of the LO phonons with the wave vector $\mathbf{k}=(\mathbf{k}_\rho,k_z)$,

$$|v_k|^2=\frac{2\sqrt{2}\pi\alpha}{\nu\mathbf{k}^2}, \tag{2}$$

with ν being the crystal volume and α being the electron-phonon coupling constant.

In this paper, we will employ the FH path-integral approach[50–52] to derive the ground-state energy expressions to these confined systems. Proceeding as outlined in Refs. 51 and 52, after integrating over the path integral over the phonon coordinates, assuming that they are in their ground state, we can readily obtain the true action corresponding to Hamiltonian (1),

$$S=\int_{t_a}^{t_b}dt[-\tfrac{1}{2}\dot{\mathbf{r}}^2-V(\rho,z)] +\tfrac{1}{2}\sum_{\mathbf{k}}\int_{t_a}^{t_b}\int_{t_a}^{t_b}|v_{\mathbf{k}}|^2e^{i\mathbf{k}\cdot[\mathbf{r}(\mathbf{t})-\mathbf{r}(\mathbf{s})]}e^{|t-s|}dt\,ds. \tag{3}$$

In the Feynman original approaches[50] one may choose a trial action

$$S_1=\int_{t_a}^{t_b}dt[-\tfrac{1}{2}\dot{\mathbf{r}}^2+K_1\rho^2+K_2z^2]-\tfrac{1}{2}C \times\int_{t_a}^{t_b}\int_{t_a}^{t_b}e^{-W|t-s|}|\mathbf{r}(t)-\mathbf{r}(s)|^2ds\,dt. \tag{4}$$

We shall, however, follow the procedure developed by Haken[51] in the treatment of the exciton-phonon problem and later applied to the bound polarons by Matsuura.[52] An advantage of this approach is that the strong-coupling feature of the system can be clearly characterized, which will be shown later. For the trial action S_1, we choose

$$S_1=\int_{t_a}^{t_b}dt\{-\tfrac{1}{2}\dot{\mathbf{r}}^2-V_{\rm eff}[\mathbf{r}(t)]\}=\int_{t_a}^{t_b}dt\,L_{\rm eff}, \tag{5}$$

where $V_{\rm eff}[\mathbf{r}(\mathbf{t})]$ is the effective trial potential to be chosen later. The corresponding quantum-mechanical Hamiltonian then satisfies

$$H_{\rm eff}\Phi_n^{\rm eff}(\mathbf{r})=[\tfrac{1}{2}\mathbf{p}^2+V_{\rm eff}(\mathbf{r})]\Phi_n^{\rm eff}(\mathbf{r})=E_n^{\rm eff}\Phi_n^{\rm eff}(\mathbf{r}), \tag{6}$$

where $\Phi_n^{\rm eff}(\mathbf{r})$ and $E_n^{\rm eff}$ are the wave function and ground-state energy of $H_{\rm eff}$. Therefore, the effective Dirac-Schwinger transformation function can be written as

$$K_{\rm eff}(r_b,t_b;r_a,t_a)=\int_a^b e^{S_1}D\mathbf{r}(\mathbf{t})$$
$$=\sum_n \Phi_n^{\rm eff}(\mathbf{r}_b)\Phi_n^{\rm eff*}(\mathbf{r}_a)e^{-E_n^{\rm eff}(t_b-t_a)}. \tag{7}$$

By Jensen-Feynman inequality, the Feynman variational principle now reads

$$E_0^{\rm exact}\leqslant E^F=E_0^{\rm eff}-s, \tag{8}$$

where $E_0^{\rm exact}$ is the exact ground-state energy corresponding to the true action (3),

$$s=\lim_{(t_b-t_a)\to\infty}\frac{\langle\langle S-S_1\rangle\rangle}{t_b-t_a}, \tag{9}$$

$\langle\langle S-S_1\rangle\rangle$ being given by

$$\langle\langle S-S_1\rangle\rangle=\frac{\int (S-S_1)e^{S_1}D\mathbf{r}(t)}{\int e^{S_1}D\mathbf{r}(t)}=C1+C2, \tag{10}$$

where

$$C1=\frac{\int_a^b\left\{\int_{t_b}^{t_a}[V_{\rm eff}(\mathbf{r})-V(\rho,z)]dt\right\}e^{S_1}D\mathbf{r}(t)}{\int_a^b e^{S_1}D\mathbf{r}(t)} \tag{11}$$

and

$$C2=\frac{\int_a^b\left\{\sum\Sigma_k\int_{t_a}^{t_b}\int_{t_a}^{t_b}\frac{1}{2}|v_k|^2e^{i\mathbf{k}\cdot[\mathbf{r}(\mathbf{t})-\mathbf{r}(\mathbf{s})]}e^{|t-s|}dt\ ds\right\}e^{S_1}D\mathbf{r}(t)}{\int e^{S_1}D\mathbf{r}(t)}. \tag{12}$$

According to the procedure of Ref. 51, both $C1$ and $C2$ can be calculated. To obtain $C1$, we should first calculate its numerator. We then can readily have

$$C1^{\rm num}=\int d\mathbf{r}(\mathbf{t})\int_{t_b}^{t_a}dt\ K_{\rm eff}(r_b,t_b;r_t,t)[V_{\rm eff}(\mathbf{r})$$
$$-V(\rho,z)]K_{\rm eff}(r_t,t;r_a,t_a). \tag{13}$$

Substituting Eq. (7) into Eq. (12), in the long-time limit, we get

$$C1^{\rm num}=(t_b-t_a)\Phi_0^{\rm eff}(\mathbf{r}_b)\Phi_0^{\rm eff*}(\mathbf{r}_a)e^{-E_0^{\rm eff}(t_b-t_a)}$$
$$\times\langle\Phi_0^{\rm eff}(\mathbf{r})|[V_{\rm eff}(\mathbf{r})-V(\rho,z)]|\Phi_0^{\rm eff}(\mathbf{r})\rangle. \tag{14}$$

In the same limit, the denominator of $C1$ reads

$$C1^{\rm den}=\Phi_0^{\rm eff}(\mathbf{r}_b)\Phi_0^{\rm eff*}(\mathbf{r}_a)e^{-E_0^{\rm eff}(t_b-t_a)}. \tag{15}$$

Thus, we obtain

$$C1=(t_b-t_a)\langle\Phi_0^{\rm eff}(\mathbf{r})|[V_{\rm eff}(\mathbf{r})-V(\rho,z)]|\Phi_0^{\rm eff}(\mathbf{r})\rangle. \tag{16}$$

In a similar way, we can get

$$C2=-(t_b-t_a)\sum_j\sum_{\mathbf{k}}\frac{|\langle\Phi_j^{\rm eff}(\mathbf{r})|[v_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{r}}]|\Phi_0^{\rm eff}(\mathbf{r})\rangle|^2}{E_0^{\rm eff}-E_j^{\rm eff}-1}. \tag{17}$$

By means of Eqs. (6) and (9), the inequality (8) becomes

$$E_0^{\rm exact}\leqslant E^F=I_1+I_2, \tag{18}$$

where

$$I_1=\langle\Phi_0^{\rm eff}(r)|[\tfrac{1}{2}\mathbf{p}^2+V(\rho,z)]|\Phi_0^{\rm eff}(\mathbf{r})\rangle \tag{19}$$

and

$$I_2=-\sum_j\sum_{\mathbf{k}}\frac{|\langle\Phi_j^{\rm eff}(\mathbf{r})|[v_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{r}}]|\Phi_0^{\rm eff}(\mathbf{r})\rangle|^2}{E_j^{\rm eff}-E_0^{\rm eff}+1}. \tag{20}$$

Equations (18)–(20) will yield the Feynman energy within the FH theory. It is to note that, if the effective potential $V_{\rm eff}(\mathbf{r})$ is chosen to be such a form that the corresponding Schrödinger equation can be analytically solved, substitution of the relevant energy eigenfunctions and eigenvalues into Eqs. (19) and (20) will produce the upper bound to the exact ground-state energy of the Hamiltonian (1).

It is interesting to find that Eqs. (18)–(20) will give the results of the second-order RSPT, if the effective potential $V_{\rm eff}(\mathbf{r})$ is exact, taken the confining potential $V(\rho,z)=\frac{1}{2}\omega^2\rho^2+\frac{1}{2}\omega_z z^2$. It follows that the second-order RSPT provides an upper bound to the exact ground-state energy. Furthermore, better upper bounds may be obtained by selecting the effective potential properly.

In this paper, according to the symmetry of the system studied, we will choose a variational effective potential as the following harmonic-oscillator-type, which is only isotropic in the ρ plane

$$V_{\rm eff}(\mathbf{r})=\tfrac{1}{2}\lambda_\rho^2\rho^2+\tfrac{1}{2}\lambda_z^2z^2, \tag{21}$$

where λ_ρ and λ_z are variational parameters to be determined. Obviously, the confining potential $V(\rho,z)=\frac{1}{2}\omega^2\rho^2+\frac{1}{2}\omega_z z^2$ is only a special form of Eq. (21) by setting $\lambda_\rho=\omega$ and λ_z

$=\omega_z$. Therefore, the second-order RSPT results should be covered in the following calculation based on Eq. (21) in principle.

The energy eigenfunctions and eigenvalues corresponding to potential (21) are

$$\Phi_j^{\rm eff}(\mathbf{r})=\left(\frac{\lambda_\rho\lambda_z^{1/2}}{\pi^{3/2}2^{j_x+j_y+j_z}j_x!j_y!j_z!}\right)^{1/2}\times H_{j_x}(\sqrt{\lambda_\rho}x)H_{j_y}(\sqrt{\lambda_\rho}y)H_{j_z}(\sqrt{\lambda_z}z)e^{-(\lambda_\rho\rho^2/2+\lambda_z z^2/2)},$$
$$E_j^{\rm eff}=(j_x+j_y+1)\lambda_\rho+(j_z+\tfrac{1}{2})\lambda_z, \tag{22}$$

where $H_n(\ )$ is the Hermite polynomial of order n. Now Eq. (19) yields

$$I_1=\tfrac{1}{2}\lambda_\rho+\tfrac{1}{4}\lambda_z+\frac{\omega^2}{2\lambda_\rho}+\frac{\omega_z^2}{4\lambda_z}. \tag{23}$$

Using the transformations

$$\frac{1}{E_j^{\rm eff}-E_0^{\rm eff}+1}=\int_0^\infty e^{-(E_j^{\rm eff}-E_0^{\rm eff}+1)t}dt, \tag{24}$$

and the Slater sum rule for the Hermitian polynomials

$$\sum_n \frac{1}{2^n n!}H_n(\lambda x)H_n(\lambda x')\exp[-\tfrac{1}{2}\lambda^2(x^2+x'^2)-2np]$$
$$=\frac{e^p}{\sqrt{2\sinh(2p)}}\exp\{-\tfrac{1}{4}\lambda^2[(x+x')^2\tanh(p)+(x-x')^2\coth(p)]\}, \tag{25}$$

one can perform the summation over j_i $(i=x,y,z)$ in Eq. (20) easily. Then using

$$\sum_{\mathbf{k}}\frac{e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}}{k^2}=\frac{\nu}{4\pi}\frac{1}{|\mathbf{r}-\mathbf{r}'|}, \tag{26}$$

one can integrate over the electron position vectors $\mathbf{r}$ and $\mathbf{r}'$ by transforming these vectors into center-of-mass vector $\mathbf{u}=(\mathbf{r}+\mathbf{r}')/2$ and relative vectors $\mathbf{v}=\mathbf{r}-\mathbf{r}'$, and finally have

$$I_2=-\frac{\alpha}{2\sqrt{\pi}}\int_0^\infty dt\ e^{-t}\frac{\sqrt{\lambda_z}}{\sqrt{1-e^{-\lambda_z t}}}\frac{1}{\sqrt{1-\mathcal{R}}}\ln\left(\frac{1+\sqrt{1-\mathcal{R}}}{1-\sqrt{1-\mathcal{R}}}\right), \tag{27}$$

with

$$\mathcal{R}=\frac{\lambda_z[1+\coth(\lambda_z t/2)]}{\lambda_\rho[1+\coth(\lambda_\rho t/2)]}. \tag{28}$$

For later use, we now write the Feynman energy completely in terms of Eqs. (18), (23), and (27),

$$E^F=\tfrac{1}{2}\lambda_\rho+\tfrac{1}{4}\lambda_z+\frac{\omega^2}{2\lambda_\rho}+\frac{\omega_z^2}{4\lambda_z}-\frac{\alpha}{2\sqrt{\pi}}\times\int_0^\infty dt\ e^{-t}\frac{\sqrt{\lambda_z}}{\sqrt{1-e^{-\lambda_z t}}}\frac{1}{\sqrt{1-\mathcal{R}}}\ln\left(\frac{1+\sqrt{1-\mathcal{R}}}{1-\sqrt{1-\mathcal{R}}}\right). \tag{29}$$

It should be pointed out that this Feynman energy expression (29) could be suited for all coupling constant α and arbitrary strength of the confining potential ω.

In the weak-coupling limit, the condition that the confining potential is stronger than the electron-phonon interaction is always met, so the variational parameter λ_ρ and λ_z could be mainly determined by Eq. (29) without the fifth term in the right-hand side,

$$\lambda_\rho=\omega,\quad \lambda_z=\omega_z. \tag{30}$$

As a result, we easily have

$$E^{\omega c}=\omega+\frac{1}{2}\omega_z-\frac{\alpha}{2\sqrt{\pi}}\times\int_0^\infty dt\ e^{-t}\frac{\sqrt{\omega_z}}{\sqrt{1-e^{-\omega_z t}}}\frac{1}{\sqrt{1-\mathcal{R}_{\rm wc}}}\ln\left(\frac{1+\sqrt{1-\mathcal{R}_{\rm wc}}}{1-\sqrt{1-\mathcal{R}_{\rm wc}}}\right), \tag{31}$$

with

$$\mathcal{R}_{\omega c}=\frac{\omega_z[1+\coth(\omega_z t/2)]}{\omega[1+\coth(\omega t/2)]}.$$

This weak-coupling result will be shown to be just identical to the second-order RSPT results in the next section.

For quantum wires, setting $\omega_z=0$, the above equation can be slightly transformed into

$$E_{\rm QW}^{\omega c}=\omega-\frac{\alpha}{2\sqrt{\pi}}\int_0^\infty dt\ \frac{e^{-t}}{\sqrt{t}}\frac{1}{\sqrt{1-\mathcal{R}'}}\ln\left(\frac{1+\sqrt{1-\mathcal{R}'}}{1-\sqrt{1-\mathcal{R}'}}\right), \tag{32}$$

with

$$\mathcal{R}'=\frac{1}{\frac{1}{2}\omega t[1+\coth(\omega t/2)]}.$$

For quantum dots, since $\omega_z=\omega$, we can get a very simple closed-form analytical expression for the Feynman energy in the weak-coupling limit

$$E_{\rm QD}^{\omega c}=\frac{3}{2}\omega-\frac{\alpha}{\sqrt{\omega}}\frac{\Gamma\left(\frac{1}{\omega}\right)}{\Gamma\left(\frac{1}{\omega}+\frac{1}{2}\right)}, \tag{33}$$

which is no other than the second-order RSPT result for $N=3$ obtained by Mukhopadhyay and Chatterjee.[43]

Moreover, for comparison, we will study these systems within the second-order RSPT for weak coupling and the LP variational theory for strong coupling as well in the next section.

III. STANDARD WEAK- AND STRONG-COUPLING THEORY

A. Second-order perturbation theory

The second-order RSPT correction to the ground-state energy due to the electron-LO phonon interaction in Hamiltonian (1) is given by

$$\Delta E=-\sum_j \sum_{\mathbf{k}} \frac{|\langle\Phi_j(\mathbf{r})|[v_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{r}}]|\Phi_0(\mathbf{r})\rangle|^2}{E_j-E_0+1}, \quad (34)$$

where the energy eigenfunctions $\Phi_j(\mathbf{r})$ and eigenvalues E_j are corresponding to the confining potential $V(\rho,z)=\frac{1}{2}\omega^2\rho^2+\frac{1}{2}\omega_z z^2$. The difference between Eqs. (34) and (20) is that the energy eigenfunctions and eigenvalues are corresponding to a different potential $V(\rho,z)$ and $V_{\rm eff}(\mathbf{r})$, respectively. The ground-state energy $E^{\rm PT2}$ in the second-order RSPT, therefore, can be straightforwardly derived from Eq. (29) by setting $\lambda_\rho=\omega$ and $\lambda_z=\omega_z$, and has exactly the form (31). Note that the same results can be derived in slightly different ways. It should be stressed again that $E^{\rm PT2}$ is the upper bound to the true ground-state energy due to the Feynman variational principle Eq. (8), which will be useful for subsequent discussions.

In the bulk limit, i.e., $\omega\to 0$, one can easily obtain 3D free-polaron ground-state energy as $-\alpha$. This is just the well-known results obtained by many authors (see Ref. 54 and references therein).

Here, we should mention that, although the second-order RSPT is a standard method in polarons physics, such a unified energy expression for polarons in both quantum wires and quantum dots within this theory as Eq. (31), which explicitly consists of only a one-dimensional integral has not been reported before, to the best of our knowledge.

B. Landau-Pekar strong-coupling theory

The strong-coupling polarons in quantum wires and dots can also be investigated by the LP variational scheme.[48] Alternatively, we here proceed to give a more concise representation of this scheme. The adiabatic polaron ground state can be given through the following product ansatz:

$$|\ \rangle=\phi(\mathbf{r})|A\rangle, \quad (35)$$

where the electron part $\phi(\mathbf{r})$ is chosen as the following product of two Gaussian-type wave functions in transverse and longitudinal coordinates:

$$\phi(\mathbf{r})=\varphi(\rho)\chi(z),$$
$$\varphi(\rho)\sim e^{-\lambda_1\rho^2/2}, \quad \chi(z)\sim e^{-\lambda_2 z^2/2}, \quad (36)$$

with λ_1 and λ_2 being variational parameters to be determined, and $|A\rangle$ is the phonon coherent state,

$$|A\rangle=\exp\left(\sum_k [f(k)a_k^\dagger-f^*(k)a_k]\right)|0\rangle, \quad (37)$$

here $f(\mathbf{k})$ and $f^*(\mathbf{k})$ will be determined variationally, $|0\rangle$ is the unperturbed zero phonon state satisfying $a_k|0\rangle=0$ for all $\mathbf{k}$.

To find the optimal fit to $f(\mathbf{k})$ and $f^*(\mathbf{k})$, we should minimize the expectation value of the Hamiltonian (1) that describes a polaron confined in a parabolic potential $V(\rho,z)=\frac{1}{2}\omega^2\rho^2+\frac{1}{2}\omega_z z^2$ in the trial state (35) $\langle\ |H|\ \rangle$, which has the following functional form:

$$E[f(\mathbf{k}),f^*(\mathbf{k})]$$
$$=\tfrac{1}{2}\lambda_1+\tfrac{1}{4}\lambda_2+\frac{\omega^2}{2\lambda_1}+\frac{\omega_z^2}{4\lambda_2}+\sum_{\mathbf{k}} f^*(k)f(k)$$
$$+\sum_{\mathbf{k}}\left\{v_{\mathbf{k}}\exp\left[-\left(\frac{k_\rho^2}{4\lambda_1}+\frac{k_z^2}{4\lambda_2}\right)\right]f(k)+\text{H.c.}\right\}, \quad (38)$$

and get

$$f(\mathbf{k})=-v_k^*\exp\left[-\left(\frac{k_\rho^2}{4\lambda_1}+\frac{k_z^2}{4\lambda_2}\right)\right],$$
$$f^*(\mathbf{k})=-v_k\exp\left[-\left(\frac{k_\rho^2}{4\lambda_1}+\frac{k_z^2}{4\lambda_2}\right)\right]. \quad (39)$$

Inserting these back into Eq. (38), we finally have strong-coupling energy as

$$E^{\rm LP}=\frac{1}{2}\lambda_1+\frac{1}{4}\lambda_2+\frac{\omega^2}{2\lambda_1}+\frac{\omega_z^2}{4\lambda_2}-\frac{\alpha}{\sqrt{\pi}}\frac{\sqrt{\lambda_1}}{\sqrt{(\lambda_1/\lambda_2)-1}}$$
$$\times\ln[\sqrt{(\lambda_1/\lambda_2)-1}+\sqrt{\lambda_1/\lambda_2}]. \quad (40)$$

It is interesting to note from both Eqs. (29) and (40) that, for the finite value of ω and in the limit of $\alpha\to\infty$, λ_ρ approaches λ_z in Eq. (29) and λ_1 approaches λ_2 in Eq. (40). Then, both equations can be reduced to

$$E^{\rm LP}=\frac{3}{4}\lambda+\frac{\omega^2}{2\lambda}-\frac{\alpha}{\sqrt{\pi}}\sqrt{\lambda}. \quad (41)$$

Further, if setting $\omega=0$ (i.e., bulk case), the ground-state energy reads

$$E^{\rm LP}=-\frac{1}{3\pi}\alpha^2, \quad (42)$$

which is no other than the well-known strong-coupling results for 3D free polarons.[48,55,56]

So far, we have proven that the present FH path-integral method can reproduce the results in both the weak- and strong-coupling limit obtained by standard perturbation theory and strong-coupling theory, respectively. It is also expected that the present approach can produce good results for polarons in both quantum wires and dots with arbitrary coupling strength and confining potential. These will be demonstrated in the numerical calculations performed in Sec. V.

IV. ANALYTICAL RESULTS FOR QUANTUM DOTS

Obviously, for quantum wires with the potential of axial symmetry, the expressions of the Feynman energy (29) cannot be reduced anymore. For quantum dots, however, due to a confining potential with sphere symmetry, we can obtain a simple closed-form analytical expression for the Feynman energy by setting $\omega_z=\omega$,

$$E^F=\frac{3}{4}\lambda+\frac{3\omega^2}{4\lambda}-\frac{\alpha}{\sqrt{\lambda}}\frac{\Gamma\left(\frac{1}{\lambda}\right)}{\Gamma\left(\frac{1}{\lambda}+\frac{1}{2}\right)}. \tag{43}$$

For later use, Eq. (43) is also extended to those for polarons in multidimensional quantum dots

$$E^F=\frac{N}{4}\lambda+\frac{N\omega^2}{4\lambda}-\frac{\sqrt{\pi}\alpha}{2\sqrt{\lambda}}\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\frac{\Gamma\left(\frac{1}{\lambda}\right)}{\Gamma\left(\frac{1}{\lambda}+\frac{1}{2}\right)}. \tag{44}$$

More interestingly, we can discuss two limiting cases by Eq. (44).

A. Extended-state solutions

In the limit $\alpha\to 0$ and $\omega\to 0$, it can be noted from Eq. (44) that there exists an extended-state solution, i.e., $\lambda\to 0$. Thus, Eq. (44) reduces to

$$E^F=\frac{N}{4}\lambda+\frac{N\omega^2}{4\lambda}-\frac{\sqrt{\pi}\alpha}{2}\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\left(1+\frac{\lambda}{8}\right). \tag{45}$$

Minimizing the above energy with respect to λ gives

$$E^F=-\frac{\sqrt{\pi}}{2}\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\alpha+\frac{N}{2}\omega\left(1-\frac{\sqrt{\pi}}{4N}\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\alpha\right)^{1/2}. \tag{46}$$

Utilizing $\sqrt{1-x}\approx 1-x/2$ for small x, we can obtain the same weak-confinement limit results by the second-order RSPT method.[43]

In the limit of $\omega\to 0$, we will get

$$E^F=-\frac{\sqrt{\pi}}{2}\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\alpha, \tag{47}$$

which is just the well-known second-order perturbation result for free N-dimensional polarons obtained by many authors.[57]

B. Localized-state solutions

We also have the localized-state solution from Eq. (44), i.e., $\lambda\to\infty$, if either $\alpha\to\infty$ or $\omega\to\infty$. In this limit, one can show that

$$\frac{\Gamma\left(\frac{1}{\lambda}\right)}{\Gamma\left(\frac{1}{\lambda}+\frac{1}{2}\right)\sqrt{\lambda}}=\frac{\sqrt{\lambda}}{\sqrt{\pi}}\left(1+\frac{2\ln 2}{\lambda}\right). \tag{48}$$

Thus, Eq. (44) reduces to

$$E^F=\frac{N}{4}\lambda+\frac{N\omega^2}{4\lambda}-\frac{\alpha}{2}\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\sqrt{\lambda}\left(1+\frac{2\ln 2}{\lambda}\right). \tag{49}$$

In principle, minimizing the above energy with respect to λ would yield the Feynman energy in the localized state. However, it is obvious that one could not obtain a simple analytical expression for this energy. Only in some extreme cases, one can get the analytical results.

In the limit $\alpha\to\infty$ and for finite ω, the value of λ is mainly determined by the first and last terms in the right-hand side of Eq. (49). Inserting the resultant λ back into Eq. (49) we arrive at

$$E^F=-\frac{1}{4N}\left[\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\right]^2\alpha^2-N\ln 2+\frac{N^3\omega^2}{4\alpha^2}\left[\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\right]^2. \tag{50}$$

It is to note that the first terms in the right-hand side of Eq. (50) is no other than the strong-coupling results for the ground-state energy of free multidimensional polarons[48]

In the other case, i.e., in the limit $\omega\to\infty$ and finite α, the value of λ is only determined by the first two term in the right-hand side of Eq. (49). In a similar way, we have

$$E^F=\frac{N}{2}\omega-\frac{\alpha}{2}\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\left(\sqrt{\omega}+\frac{2\ln 2}{\sqrt{\omega}}\right). \tag{51}$$

Interestingly, one may find that Eq. (51) can also be given by the second-order RSPT in the strong-confinement limit ($\omega\to\infty$).[43]

Finally, we would like to point out that the present localized-state solutions (49) can also be obtained from the LP results. To prove this, one can readily have the LP energy by extending Eq. (40) to the case for polarons in multidimensional quantum dots

$$E^{\mathrm{LP}}=\frac{N}{4}\lambda+\frac{N\omega^2}{4\lambda}-\frac{\alpha}{2}\frac{\Gamma\left(\frac{N-1}{2}\right)}{\Gamma\left(\frac{N}{2}\right)}\sqrt{\lambda}, \tag{52}$$

which is just identical to Eq. (49) in the limit $\lambda \to \infty$. This good agreement may demonstrate the correctness of our derivation.

V. NUMERICAL RESULTS AND DISCUSSIONS

Generally speaking, for arbitrary electron-coupling strength and confinement potential of quantum wires (or dots), we may calculate the ground-state energy of the Hamiltonian (1) by minimizing the Feynman energy E_F in Eq. (29) [or Eq. (44)] numerically. One of the important physical observables to be evaluated in this field is the binding energy of polarons, which is defined as the difference of the ground-state energy of the confined system in the presence and absence of the electron-phonon interaction. For later use, we define the effective radius R of quantum wires or dots as

$$R = \frac{1}{\sqrt{\omega}}. \tag{53}$$

We will present some numerical results and discussions for quantum wires and dots, respectively, in the following two subsections.

A. Quantum wires

First of all, we would like to mention a recent paper[20] by Ercelebi and Senger. In that paper, within a perturbation-variational scheme proposed previously by Devreese *et al.*[58] in the treatment of polarons bound to a Coulomb center and later successfully applied to bipolarons,[59] the authors have calculated the binding energy and the effective mass of polarons in a cylindrical quantum wire with infinite potential boundary. The key results obtained is that ''at weak coupling, the binding energy of the polaron can be smaller and its mass less inertial compared with the bulk case when the wire is made narrow.'' Evidently, this is an exceptional result that is contrary to the general trend that the electron-phonon interaction is inherently stronger in systems of lower dimensionality.

We notice that the model Hamiltonian in Ref. 20 is the same as Hamiltonian (1) in the present paper, except for slightly different wire potentials that topologically have the same shape. Alternatively, in the absence of the electron-phonon coupling, the energy eigenvalues of the electron in these two confining potentials are positive and separated. Therefore, in our opinion, the essential features of polarons confined in quantum wires with these two potentials should be qualitatively consistent.

Motivated by that paper, let us plot the curves for the polaron binding energy E_b^F, which are obtained numerically from Eq. (29), vs the effective wire-radius R, at coupling constants ranging from extreme small value $\alpha = 0.005 - 1.0$ in Fig. 1. Unfortunately, at weak coupling, we have not found any sign to exhibit this exceptional feature displayed in that paper, but the behaviors of all the curves are just consistent with the general trend.

We next present the results from the second-order RSPT. Because the E_b^{PT2} is proportional to α, one can immediately notice that the curves of $E_b^{\mathrm{PT2}}/\alpha$ vs R, at weak coupling, are independent of α and, therefore, exhibit the same behavior, which is shown in Fig. 2. Clearly, the second-order RSPT results also agree with the general trend, i.e., the binding is monotonically stronger as the wire radius R decreases.

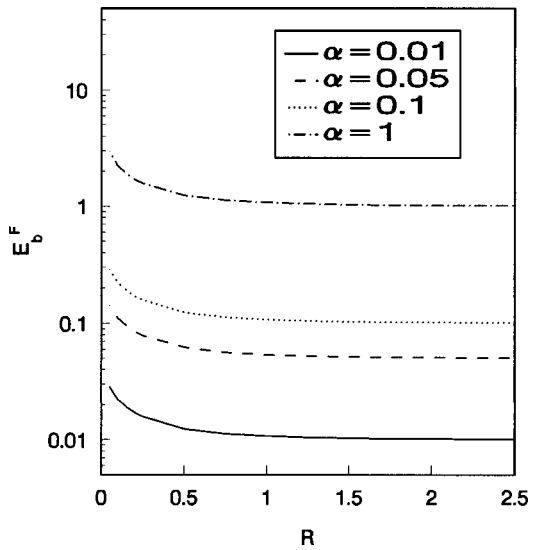

FIG. 1. The binding energy E_b^F of polarons in quantum wires within the FH path-integral theory, as a function of the effective wire-radius R at $\alpha = 0.01$, 0.05, 0.1, and 1.

As stated previously, the results for the ground-state energy by the second-order RSPT are upper bounds to the true ground-state energy. Thus, even one can obtain the exact results of the ground-state energy of polarons in quantum wire, which may push the E_b vs R curves to the higher position, the values of E_b for any R is, absolutely, not lower than α, the value of E_b in bulk limit $R \to \infty$. Thus, we have strictly shown that the key result in Ref. 20 is unreasonable and the general conclusion is still qualitatively right.

We think that the result obtained in Ref. 20 is only an artifact produced by the variational scheme, which is quite poor at weak and intermediate coupling,[60] rather than an in-

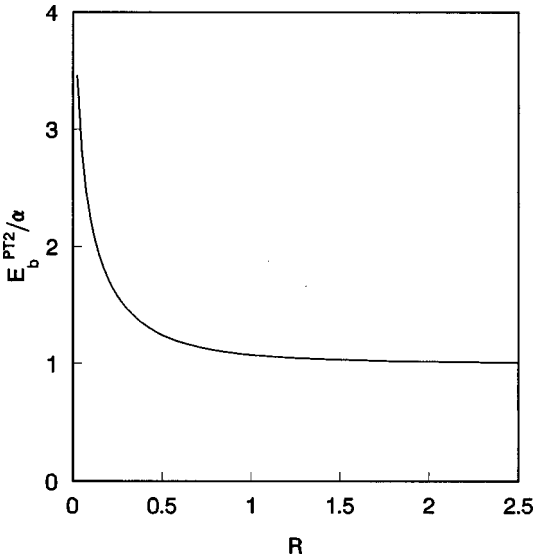

FIG. 2. The binding energy of polarons in quantum wires E_b^{PT2} in units of α, within the second-order RSPT as a function of the effective wire-radius R.

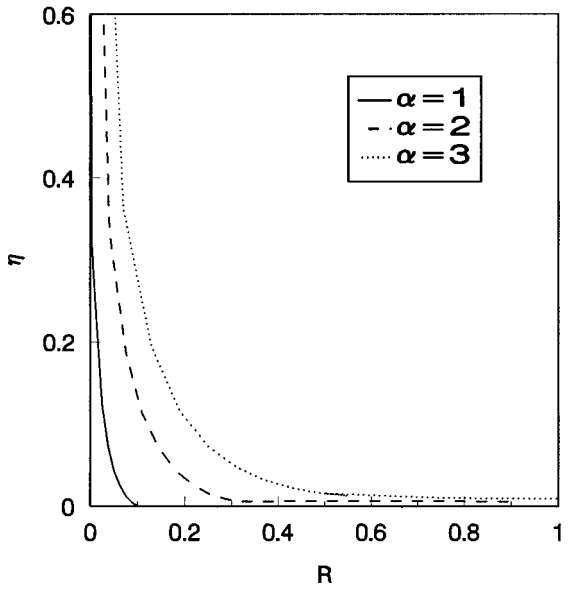

FIG. 3. The relative difference between results for binding energy of polarons in quantum wires within the FH theory and the second-order RSPT $\eta=(E_b^F-E_b^{\mathrm{PT2}})/E_b^{\mathrm{PT2}}$, as a function of the effective wire-radius R at $\alpha=1$, 2, and 3.

trinsic property of the polarons confined in quantum wires. The crucial reason yielding this exceptional and incorrect conclusion is that the scheme adopted could lead to the overestimation of the ground-state energy of the system at least for $0<\alpha\leqslant 3$. This point is clearly shown from Figs. 2 and 3 in Ref. 20. In the bulk limit, i.e., $R\rightarrow\infty$, in the regime $0<\alpha\leqslant 3$, the polaron ground-state energy is, surprisingly, much higher than $-\alpha$, the well-known results of free polarons within many approximate theories, such as the perturbation theory, the Lee-Low-pines theory, and the Feynman path-integral method (see Ref. 54).

Now, we will concentrate on comparing the Feynman results based on Eq. (29) with those obtained within the second-order RSPT [Eq. (32)] and the LP variational theory [Eq. (40)] with $\omega_z=0$ to assess the effectiveness of the FH theory for polarons in quantum wires.

It is expected theoretically that the Feynman binding energy E_b^F should be not lower than E_b^{PT2} by the second-order RSPT due to the more general form of the effective potential (21). As an example to show this prediction, in Fig. 3, we plot the relative difference between the Feynman results and the second-order RSPT results for the polaron binding energy $\eta=(E_b^F-E_b^{\mathrm{PT2}})/E_b^{\mathrm{PT2}}$, as a function of the effective wire radius R at different coupling constants $\alpha=1$, 2, and 3.

It is clearly shown that E_b^F is really higher than E_b^{PT2} in all cases. After careful inspection of this figure, it is not difficult to find: (1) For given α in the weak- and intermediate-coupling regime, there exists a critical wire radius R_c. Below R_c, the difference between the two calculated binding energies become larger substantially when R further decreases. On the contrary, above R_c, the difference is so small that it can be negligible, one can say both methods produce equally good results. (2) The R_c becomes smaller with the decrease of α. Then, in the weak-coupling limit, these two curves will coincide with each other. The existence of R_c will be explained later.

Next, it is the nature that we compare the Feynman results with those by the LP strong-coupling theory within Eq. (40). In Fig. 3 we give the relative difference between the Feynman results and the LP results for the polaron binding energy $\eta'=(E_b^F-E_b^{\mathrm{LP}})/E_b^{\mathrm{LP}}$, as a function of the effective wire radius R. Except in the strong-confinement limit (i.e., $\omega\rightarrow\infty$), E_b^F is higher than E_b^{LP}, and this trend is more substantial with the decrease of the coupling constant α. The difference between the results by these two approaches should disappear not only in the strong-coupling limit, but also in the strong-confinement limit due to the fact that the high-degree confinement of quantum wires would also result in the enhancement of the electron-phonon coupling.

So far, we have shown that for polarons in quantum wires with parabolic confinement, the FH path-integral theory can produce better results than the second-order RSPT and the LP variational theory in the whole coupling regime.

Now, we address a very important problem that is relevant to the appearance of the critical wire radius R_c. It is recalled in Sec. II that we have taken the effective potential as the form (21), which includes both the transverse and longitude part of the coordinate. In the strong-coupling regime this form is reasonable, because even without the confining potential, owing to strong phonon-coupling strength, the polaron wave function should be localized in all directions with a factor $\sim e^{-\lambda^2\mathbf{r}^2}$ or $\sim e^{-\lambda^2|\mathbf{r}|}$. This has been evidently shown in the strong-coupling LP theory[48] and its modified one.[55] But in the weak-coupling regime, in terms of the wire potential with $\omega_z=0$, polarons could move freely along the wire axis, and it seems difficult to imagine that polarons would be localized along the wire axis. So one might think this effective potential might be unreasonable for weak coupling.

Fortunately, it is not always that case. Before proceeding with any discussions, we will calculate the effective longitudinal spatial extent ξ_z alone the wire axis, which is defined as

$$\xi_z=\frac{1}{\sqrt{\lambda_z}}, \tag{54}$$

where λ_z is obtained by minimizing Eq. (29) with respect to λ_ρ and λ_z. In principle, the effective transverse spatial extent ξ_ρ is smaller than ξ_z owing to the confining potential.

Figure 4 presents the variation of ξ_z as the a function of the effective wire radius R at different α. It is very clear in all curves that ξ_z reduces with the shrink of the quantum wire. In other words, the longitudinal part $\lambda_z^2 z^2/2$ in the effective potential (21) is strengthened with the enhancement of the wire confining potential, so does the transverse part. Thus, the strength of the wire potential is equivalent to the enhancement of the effective electron-phonon coupling, which is consistent with the general trend in the literature.

More interestingly, for $\alpha\leqslant 5$, all the curves diverge at a critical wire radius R_c. Note that the divergence corresponds to the vanishes of the longitudinal part $\lambda_z^2 z^2/2$ in the effective potential (21). Whether the longitudinal part in effective potential should exist or not depends only on the values of α and R. Therefore, as a unified variational theory to deal with this system in the whole coupling regime, this general form (21) of the effective potential remains naturally reasonable.

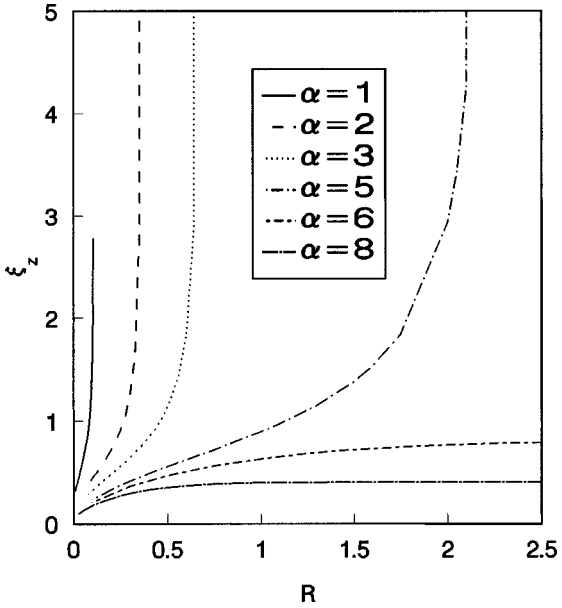

FIG. 4. The longitudinal spatial extent ξ_z in quantum wires within the FH theory as a function of the effective wire-radius R at $\alpha=1$, 2, 3, 5, 6, and 8.

Now, it is very important to link these discussions to Fig. 3. R_c's in Figs. 3 and 4 have the same meaning and are nearly identical. Below R_c, ξ_z becomes finite (i.e., λ_z becomes larger than 0), and the system would show some strong-coupling features coming from the highly confining potential of quantum wires. Thus, the results of the second-order, which is only exact in the weak-coupling limit, are quite poor. Conversely, above R_c, no strong-coupling features show up (ξ_z diverges), and the weak-coupling perturbative results are then still good approximate ones.

It is also interesting to note that, for $\alpha \geqslant 6$, the ξ_z remains finite for arbitrary R. This is because the system itself has some strong-coupling features even without the wire confining potential, which is also consistent with the above discussions.

Finally, we should compare the present FH results for polaron binding energy in parabolic quantum wires with those for the same system obtained recently by Pokatilov *et al.*, who used two approaches: (i) Feynman variational principle (FVP) and (ii) interpolation variational theory (IVT) (see Ref. 25), which are exhibited in Fig. 5. R^* in Ref. 25 and in this figure differs from R by a factor $\sqrt{2}$ due to the definition of the polaron radius. It is interesting to note that our results lie inbetween those by FVP and IVT approaches in the whole-coupling regime. It is clear that our results are not as good as those by FVP. As the effective wire radius decreases, our results become more and more close to FVP results. More interestingly, from the highest curves we can see that our results are in good agreement with FVP results for the small wire radius and large coupling constant.

The appearance of a plateau in the weak-coupling regime in the present results can be obviously interpreted by Fig. 6 where we have simultaneously presented the variations of polaron binding energy and the effective longitudinal spatial extent along the wire axis ξ_z with coupling-constant α. As discussed before, as far as ξ_z is infinite, the FH results would agree well with the second-order RSPT results that the value

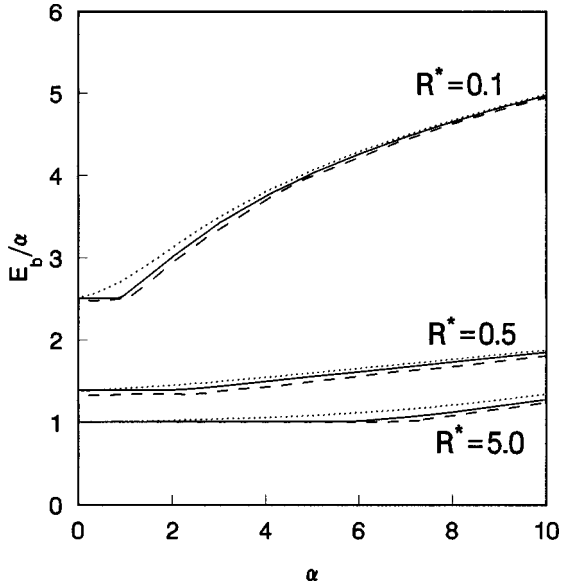

FIG. 5. Comparison of the present results (solid lines) for the dimensionless binding energy E_b/α of polarons in quantum wires and the FVP ones (dotted lines) (Ref. 25) and IVT ones (dashed lines) (Ref. 25) as a function of the coupling-constant α for the different effective wire-radius $R^*=0.1$, 0.5 and 5 (here $R^*=\sqrt{2}R$).

of E_b/α is independent of α. Therefore, for given wire-radius R, the value of E_b/α is not sensitive to α until ξ_z becomes finite.

B. Quantum dots

First, it is also natural to compare the present results for the binding energy of polarons in quantum dots with those by the second-order RSPT used in Ref. 43 and the LP strong-

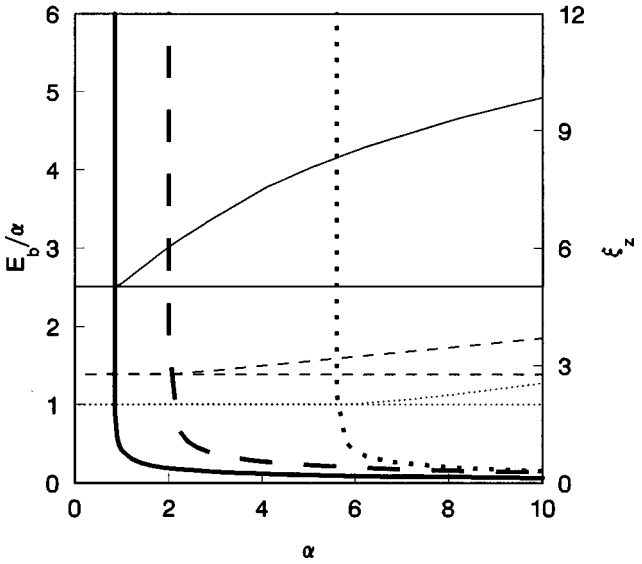

FIG. 6. The dimensionless binding energy E_b/α (thin lines) of polarons and the longitudinal spatial extent ξ_z (thick lines) within the FH theory as a function of the coupling constant α for different effective wire radius $R^*=0.1$ (solid lines), 0.5 (dashed lines), and 5 (dotted lines) (here $R^*=\sqrt{2}R$ and the horizontal thin lines gives the second-order RSPT results for E_b/α).

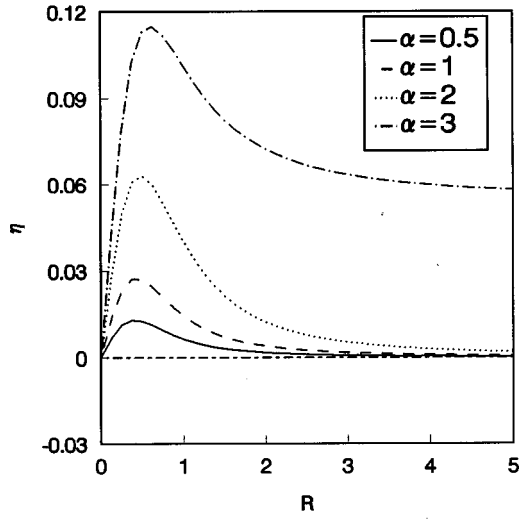

FIG. 7. The relative difference between the results for the binding energy within the FH theory and the second-order RSPT $\eta=(E_b^F-E_b^{\mathrm{PT2}})/E_b^{\mathrm{PT2}}$, as a function of the effective dot radius R at different coupling constants $\alpha=0.5$, 1, 2, and 3 in 2D.

coupling theory employed in Ref. 44, to assess the effectiveness of this approach for polarons in quantum dots. As discussed in the last subsection, it is also expected theoretically that the present results should be better than the results by these two approaches, which will be shown in the following numerical results.

In Fig. 7, we plot the relative difference between our results and the the second-order RSPT results for the binding energy of polarons in quantum dots, $\eta=(E_b^F-E_b^{\mathrm{PT2}})/E_b^{\mathrm{PT2}}$, as a function of effective dot radius R, at different coupling constants α in 2D. It is clearly shown that the present ground-state energy E_F is really lower than or equal to E_{PT2} in all cases. In the limit of $\alpha\rightarrow 0$, the present results are in good agreement with the second-order RSPT results. As α increases, the difference between the two calculated energies becomes larger and larger, and more interestingly, this trend is more pronounced while the confinement length R is around 0.5–1. For instance, at $\alpha=3$, the maximum value $\eta_{\max}$ is as high as about 12%.

After careful inspection of this figure, it is not difficult to find that the present results also agree well with the second-order RSPT results in the strong-confinement limit, i.e., $R\rightarrow 0$ for finite α. This may be attributed to the fact that both of these theories could produce the same strong-confinement results as shown in Eq. (51) in Sec. III. The totally different limiting dependence of η on the effective radius in this figure for dots and in Fig. 3 for wires, in our opinion, is originated from the intrinsically different confining potentials.

Figure 8 displays the relative difference of the Feynman results and those by the LP strong-coupling theory within Eq. (52) for 2D polarons in dots. All the curves in this figure and in Fig. 9 for wires show similar behavior, and, therefore, similar discussions may be made and are not presented again.

Next, we shall discuss in some depth the effect of dimensionality on the polaron properties in quantum dots by studying it in 2D and 3D, which have also been performed in Ref.

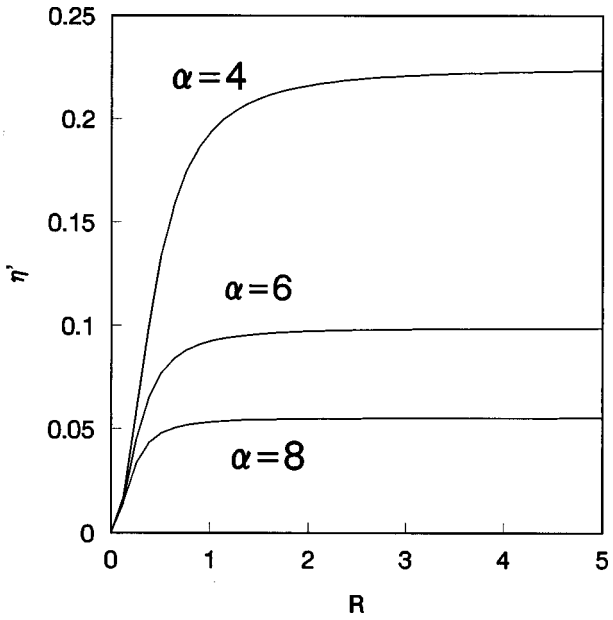

FIG. 8. The relative difference between the results for the binding energy of polarons in 2D dots within the FH theory and the LP theory $\eta'=(E_b^F-E_b^{\mathrm{LP}})/E_b^{\mathrm{LP}}$, as a function of the effective dot radius R at $\alpha=4$, 6, and 18.

43 and are of practical importance as well for the reason that quantum dots can be technologically realized in both 2D and 3D systems.

We present the binding energy of 2D and 3D polarons in quantum dots as a function of the effective dot radius R with two typical coupling constants $\alpha=1$ and 7 in Fig. 10. It is clearly shown that the polaronic effect is substantially strengthened with contracting the quantum dot in both 2D and 3D. It is also noticed that the binding is stronger in 2D

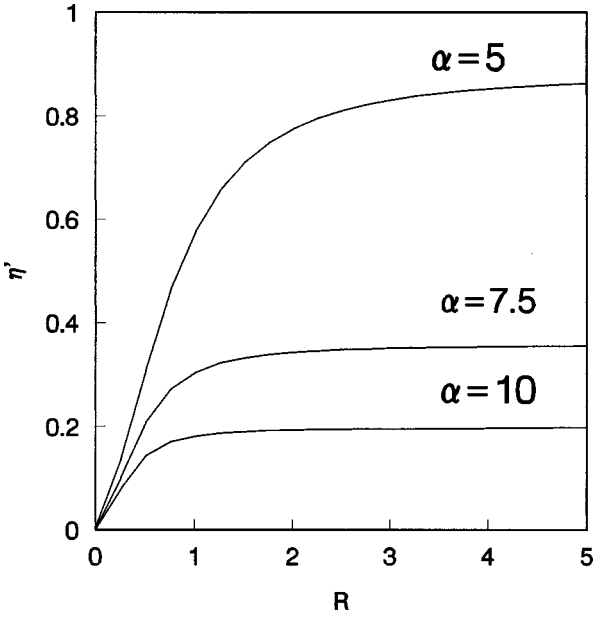

FIG. 9. The relative difference between results for the binding energy of polarons in quantum wires within the FH theory and the LP theory $\eta'=(E_b^F-E_b^{\mathrm{LP}})/E_b^{\mathrm{LP}}$, as a function of the effective wire-radius R at $\alpha=5$, 7.5, and 103.

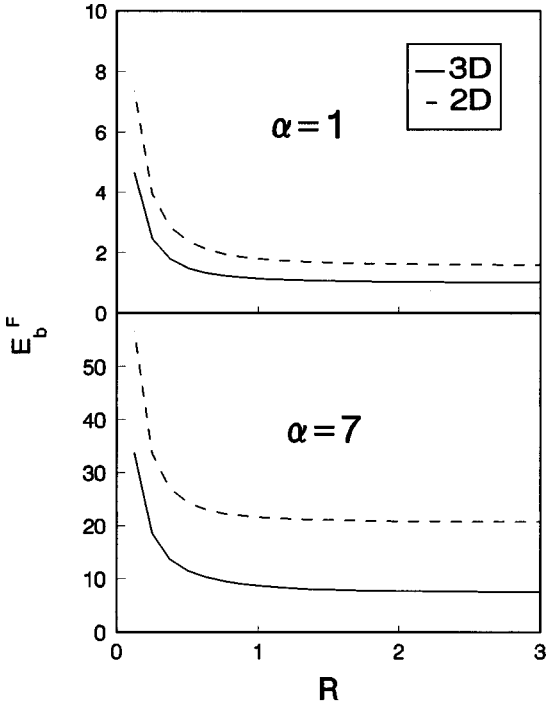

FIG. 10. The binding energy E_b^F of polarons in quantum dots within the FH theory as a function of the effective dot radius R at $\alpha=1$ and 7 in 2D and 3D.

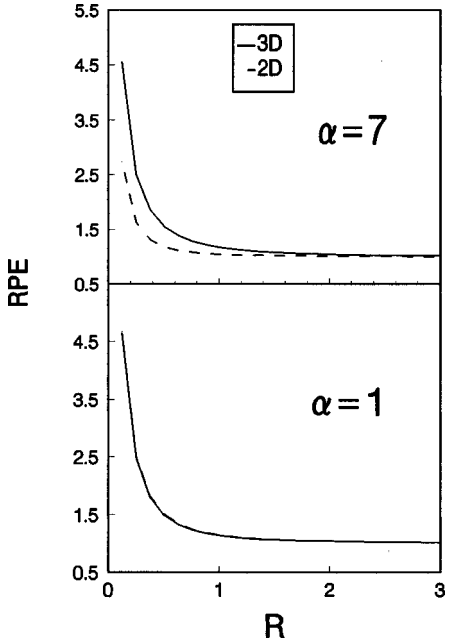

FIG. 11. The RPE to the ground-state energy of an electron in a quantum dot within the FH theory as a function of the effective dot radius R at $\alpha=1$ and 7 in 2D and 3D.

than in 3D, and this trend is more pronounced with the increase of the coupling constant. This is consistent with the previous weak-coupling results.

In order to qualify the effect of confinement on the polaronic effect more precisely, we will calculate the relative polaronic enhancement in quantum dots with respect to the corresponding bulk value

$$\mathrm{RPE}=\frac{E_b(R)}{E_b(R\rightarrow\infty)}. \tag{55}$$

The numerical results are displayed in Fig. 11. It is observed that, at the weak coupling, the variation of the relative polaronic enhancement (RPE) with the effective dot radius R is independent of the dimensionality. This is consistent with the previous results of the weak-coupling perturbation theory.[43] But as the coupling constant α increases, our results indicate that the variation of RPE with R become sensitive to the dimensionality when the dot is made narrow. This conclusion cannot be made by the second-order RSPT approach.[43]

It is also interesting to note from Fig. 11 that the RPE is stronger in 3D than in 2D, while the electron-phonon coupling is not too weak, contrary to the absolute binding energy $E_b(R)$ presented in Fig. 10. $E_b(R\rightarrow\infty)$ in Eq. (54) is the ground-state energy of multidimensional bulk polarons. Since $\mathrm{RPE}^{3D}\geqslant\mathrm{RPE}^{2D}$ is always met for arbitrary α shown in Fig. 11, we can deduce that, with the reduced dimensionality, although polaronic effects both in quantum dots and in bulk systems become stronger, the enhancement of the former one is not as substantial as the latter one.

We would like to mention the work of Klimin, Pokatilov, and Fomin,[11] where the authors have carried out the exact separation of bulk and interface vibrational excitations in the confined system for the first time to our knowledge, and obtained the fundamental results for the polaron ground-state energy as well as for the effective mass. Our results for the binding energy of polarons in quantum dots qualitatively agree with those for the polaronic shift of the electron levels due to the bulklike phonon contribution for symmetrical electron states ($l=0$) in dotlike objects having spherical shapes [cf. *b* curves of Fig. 2(a) in Ref. 11].

V. CONCLUSIONS

In this paper, we have generalized the previous FH variational path-integral theory to investigate the polaronic effects in both quantum wires and quantum dots with parabolic potential in the whole electron-phonon coupling regime and confining potential strength in a unitary way. For quantum dots, due to higher symmetry compared to quantum wires, a simple closed-form analytical expression for the Feynman energy can be obtained and the analytical results in the extended-state and localized-state limit can be further arrived. In order to test the validity of this theory, we have performed comparisons of the present results with those obtained by the standard second-order RSPT, the LP strong-coupling theory, as well as recently more advanced investigation performed by Pokatilov *et al.*, within the FVP and IVT approaches.

On the basis of the obtained analytical and numerical results, the main conclusions are summarized as follows.

(1) The FH variational path-integral theory can produce better results for polarons in both quantum wires and quantum dots than the second-order RSPT, LP strong-coupling theory does for arbitrary α and confining potential strength. In addition, the present results for polarons in quantum wires lie inbetween the recent results obtained by Pokatilov *et al.*, within the FVP and IVT approaches.

(2) The binding is monotonically stronger as the decrease of the effective radius R of the quantum wires or dots in the

whole coupling regime, not only at weak coupling.

(3) By selecting a very general form of effective potential needed in the variational path-integral theory, it is shown systematically that the strength of the wire potential is equivalently the enhancement of the effective electron-phonon coupling. Further, it is found that, because of the highly confining potential of quantum wires, this system could even exhibit some strong-coupling features in the weak- and intermediate-coupling regime. Then the weak coupling of the second-order RSPT fails to describe the ground-state of this system, but the universal variational path-integral theory is still a very powerful one.

(4) In a strict meaning, it is shown that the exceptional results in a recent paper (Ref. 20) are not an intrinsic property of polarons confined in quantum wires, and is only an artifact produced by a variational scheme, which is quite poor at weak coupling.

(5) It is found that the polaronic effect in quantum dots is enhanced with lowering dimensionality. Furthermore, as the coupling constant increases, the value of the RPE becomes dependent on both the dimensionality and the coupling constant, different from the previous conclusions by the second-order RSPT approach. Interestingly, the RPE is found to be larger in 3D than in 2D if the coupling strength is not too weak.

Finally, it should be pointed out that the present approach is also well suited for the problem of bound polarons in these confined systems with parabolic potential. These extensions are in progress.

ACKNOWLEDGMENTS

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