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VARIATIONAL CALCULATION ON GROUND-STATE ENERGY OF BOUND POLARONS IN PARABOLIC QUANTUM WIRES*

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Within the framework of Feynman path-integral variational theory, we calculate the ground-state energy of a polaron in parabolic quantum wires in the presence of a Coulomb potential. It is shown that the polaronic correction to the ground-state energy is more sensitive to the electron–phonon coupling constant than the Coulomb binding parameter, and it increases monotonically with decreasing effective wire radius. Moreover, compared to the results obtained by Feynman Haken variational path-integral theory, we obtain better results within the Feynman path-integral variational approach (FV approach). Applying our calculation to several polar semiconductor quantum wires, we find that the polaronic correction can be considerably large.

Keywords: polaron, path integral, quantum wire
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I. INTRODUCTION

With the recent progress in microfabrication technology, it has become possible to fabricate synthetic polar semiconductor structures with low dimensionality, such as dielectric slabs, heterojunctions, quantum wells, quantum dots and quantum wires. One subject of interest is quantum wires,[1−3] which now can be fabricated within nanometre size. These systems have attracted substantial attention due to the novel physical effects coming from their quasi-one-dimensionality (wires), which are useful for electronic and optoelectronic device applications.

Polarons in quantum wires are markedly different from those in bulk materials, due to the presence of wire potentials with the form $V(\rho = x, y)$, which confine the carriers motion in the ρ-plane transverse to the wire axis. The confining potential may bring out many rich phonon modes such as confined phonon modes, interface phonon modes, etc. Even for the confining potential itself, there are so many types: the rectangular, cylindrical and parabolic types. It can also be characterized as finite or infinite, symmetric or asymmetric. 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.[4−10]

Recently, much attention has been paid to the effect of the interaction of electron and bulk longitudinal-optical (LO) phonons and polaronic properties in quantum wires.[11−16] More recently, the Feynman path-integral variational approach (FV approach) has been reformulated to tackle polarons and bipolarons in parabolic quantum low-dimensional systems,[17] which is shown to be very effective in this field. As is well known, the Feynman path-integral variational approach is a very powerful one and better than all other approaches in the field of polaron problems. The main purpose of this paper is just to utilize this theory to study bound polarons in parabolic quantum wires.

II. FORMULA

The Hamiltonian describing bound polarons in a parabolic quantum wire can be written as (in units of $m = \hbar = \omega_{\rm LO} = 1$)

$$H = \frac{\boldsymbol{p}^2}{2} - \frac{\beta}{|\boldsymbol{r}|} + \sum_{\boldsymbol{k}} a^{+}_{\boldsymbol{k}} a_{\boldsymbol{k}} + \sum_{\boldsymbol{k}} [V_{\boldsymbol{k}} a_{\boldsymbol{k}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} + \mathrm{H.c.}] + V(\rho, z), \quad (1)$$

where $r(= \rho, z)$ and p are the position and the momentum operators of the electron, respectively, $V(\rho) = \frac{1}{2}\omega^2\rho^2$ is the confining potential of a quantum wire with ω being in units of $\omega_{\rm LO}$, measuring the confining strength of the parabolic potential, $a^{\dagger}_{\boldsymbol{k}}$ and $a_{\boldsymbol{k}}$ are, respectively, the creation and annihilation operators of

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the LO phonons with wave vector $\boldsymbol{k}$,

$$|v_{\boldsymbol{k}}|^2 = \frac{2\sqrt{2}\pi\alpha}{V\boldsymbol{k}^2}, \quad \beta = \frac{e^2}{\epsilon_0},$$

with V being the crystal volume, α and β being the electron–phonon coupling constant and Coulomb binding parameter. Here we should mention that the impurity–phonon interactions have already been eliminated.

After integrating the path integral over the phonon coordinates, assuming that it is in its ground state, we can readily obtain the true action corresponding to Hamiltonian (1)

$$\begin{aligned} S = &-\frac{1}{2}\int_{t_a}^{t_b}\left(\frac{\mathrm{d}\boldsymbol{r}(t)}{\mathrm{d}t}\right)^2\mathrm{d}t + \frac{\alpha}{\sqrt{8}}\int_{t_a}^{t_b}\int_{t_a}^{t_b} \\ &\cdot\frac{\mathrm{e}^{-|t-s|}}{|\boldsymbol{r}(t)-\boldsymbol{r}(s)|}\mathrm{d}t\mathrm{d}s + \int_{t_a}^{t_b}\frac{\beta}{|\boldsymbol{r}(t)|}\mathrm{d}t \\ &-\frac{\omega^2}{2}\int_{t_a}^{t_b}\rho(t)^2\mathrm{d}t. \end{aligned} \tag{2}$$

We will choose a trial action as follows

$$\begin{aligned} S_1 = &-\frac{1}{2}\int_{t_a}^{t_b}\left(\frac{\mathrm{d}\boldsymbol{r}(t)}{\mathrm{d}t}\right)^2\mathrm{d}t - \frac{C_\rho}{2}\int_{t_a}^{t_b}\int_{t_a}^{t_b} \\ &\cdot\mathrm{e}^{-W_\rho|t-s|}\left|\rho(t)-\rho(s)\right|^2\mathrm{d}t\mathrm{d}s \\ &-\frac{C_z}{2}\int_{t_a}^{t_b}\int_{t_a}^{t_b}\mathrm{e}^{-W_z|t-s|}\left|z(t)-z(s)\right|^2\mathrm{d}t\mathrm{d}s \\ &-\frac{\lambda_\rho^2}{2}\int_{t_a}^{t_b}\rho(t)^2\mathrm{d}t - \frac{\lambda_z^2}{2}\int_{t_a}^{t_b}z(t)^2\mathrm{d}t. \end{aligned} \tag{3}$$

Here

$$\begin{aligned} \lambda_\rho^2 &= \lambda^2 + \omega^2, \\ \lambda_z^2 &= \lambda^2, \end{aligned} \tag{4}$$

and C_i, W_i, and λ are variational parameters. The Coulomb binding potential has been replaced by the term $\frac{1}{2}\lambda^2\boldsymbol{r}^2$, and the phonon field has been replaced by another particle of unknown mass bound harmonically to the electron with same symmetry.

Using the Jensen–Feynman inequality, the Feynman variational principle now reads

$$E_f \equiv E_1 - s' \geq E_0, \tag{5}$$

where E_0 is the true ground-state energy of the polaron and E_1 refers to that of the system, for which S_1 is the exact action,

$$E_1 = \lim_{t_b - t_a \to \infty}\frac{\ln\int_a^b \mathrm{e}^{S_1}\mathrm{D}\boldsymbol{r}(t)}{t_b - t_a}, \tag{6}$$

$$s' = \lim_{t_b - t_a \to \infty}\frac{\int_a^b (S - S_1)\mathrm{e}^{S_1}\mathrm{D}\boldsymbol{r}(t)}{(t_b - t_a)\int \mathrm{e}^{S_1}\mathrm{D}\boldsymbol{r}(t)}, \tag{7}$$

and

$$\begin{aligned} S - S_1 = &\frac{\alpha}{\sqrt{8}}\int_{t_a}^{t_b}\int_{t_a}^{t_b}\frac{\mathrm{e}^{|t-s|}}{|\boldsymbol{r}(t)-\boldsymbol{r}(s)|}\mathrm{d}t\mathrm{d}s \\ &+\frac{C_\rho}{2}\int_{t_a}^{t_b}\int_{t_a}^{t_b}\mathrm{e}^{-W_\rho|t-s|}\left|\rho(t)-\rho(s)\right|^2\mathrm{d}t\mathrm{d}s \\ &+\frac{C_z}{2}\int_{t_a}^{t_b}\int_{t_a}^{t_b}\mathrm{e}^{-W_z|t-s|}\left|z(t)-z(s)\right|^2\mathrm{d}t\mathrm{d}s \\ &+\int_{t_a}^{t_b}\frac{\beta}{|\boldsymbol{r}(t)|}\mathrm{d}t + \frac{\lambda^2}{2}\int_{t_a}^{t_b}r(t)^2\mathrm{d}t. \end{aligned} \tag{8}$$

Then Eq.(7) can be divided into four parts

$$s' = \mathrm{I} + \mathrm{II} + \mathrm{III} + \mathrm{IV}. \tag{9}$$

Next, we will calculate the terms in the above equation one by one. First we consider I,

$$\begin{aligned} \mathrm{I} = &\lim_{\tau\to\infty}\frac{\alpha}{(t_b-t_a)\sqrt{8}}\int_{t_a}^{t_b}\int_{t_a}^{t_b} \\ &\cdot<\frac{1}{|\boldsymbol{r}(t)-\boldsymbol{r}(s)|}>\mathrm{e}^{-|t-s|}\mathrm{d}t\mathrm{d}s \\ = &\lim_{\tau\to\infty}\frac{\alpha}{(t_b-t_a)\sqrt{8}}\int_{t_a}^{t_b}\int_{t_a}^{t_b}\Big[\int\frac{\mathrm{d}^3\boldsymbol{k}}{2\pi^2k^2} \\ &\cdot<\exp\{\mathrm{i}\boldsymbol{k}\cdot[\boldsymbol{r}(t)-\boldsymbol{r}(s)]\}>\Big]\mathrm{e}^{-|t-s|}\mathrm{d}t\mathrm{d}s. \end{aligned} \tag{10}$$

One has to calculate

$$\begin{aligned} &<\exp\{\mathrm{i}\boldsymbol{k}\cdot[\boldsymbol{r}(\delta)-\boldsymbol{r}(\sigma)]\}> \\ =&\frac{\int_a^b\exp\{\mathrm{i}\boldsymbol{k}\cdot[\boldsymbol{r}(\delta)-\boldsymbol{r}(\sigma)]\}\cdot\mathrm{e}^{S_1}\mathrm{D}\boldsymbol{r}(t)}{\int_a^b\mathrm{e}^{S_1}\mathrm{D}\boldsymbol{r}(t)} = \frac{A_1}{A_2}, \end{aligned} \tag{11}$$

where

$$\begin{aligned} A_1 = &\int\exp\Big\{-\frac{1}{2}\int_{t_a}^{t_b}\left(\frac{\mathrm{d}\boldsymbol{r}(t)}{\mathrm{d}t}\right)^2\mathrm{d}t \\ &-\frac{C_\rho}{2}\int_{t_a}^{t_b}\int_{t_a}^{t_b}\mathrm{e}^{-W_\rho|t-s|}\left|\rho(t)-\rho(s)\right|^2\mathrm{d}t\mathrm{d}s \\ &-\frac{C_z}{2}\int_{t_a}^{t_b}\int_{t_a}^{t_b}\mathrm{e}^{-W_z|t-s|}\left|z(t)-z(s)\right|^2\mathrm{d}t\mathrm{d}s \\ &-\frac{\lambda_\rho^2}{2}\int_{t_a}^{t_b}\rho(t)^2\mathrm{d}t - \frac{\lambda_z^2}{2}\int_{t_a}^{t_b}z(t)^2\mathrm{d}t \\ &+\int_{t_a}^{t_b}g_{\boldsymbol{k}}(t)\cdot\boldsymbol{r}(t)\mathrm{d}t\Big\}\mathcal{D}\boldsymbol{r}(t), \end{aligned} \tag{12}$$

$$A_2 = \int \exp\Big\{ -\frac{1}{2}\int_{t_a}^{t_b}\left(\frac{\mathrm{d}\boldsymbol{r}(t)}{\mathrm{d}t}\right)^2 \mathrm{d}t - \frac{C_\rho}{2}\int_{t_a}^{t_b}\int_{t_a}^{t_b} \mathrm{e}^{-W_\rho|t-s|}\,|\rho(t)-\rho(s)|^2\,\mathrm{d}t\mathrm{d}s - \frac{C_z}{2}\int_{t_a}^{t_b}\int_{t_a}^{t_b} \mathrm{e}^{-W_z|t-s|}\,|z(t)-z(s)|^2\,\mathrm{d}t\mathrm{d}s - \frac{\lambda_\rho^2}{2}\int_{t_a}^{t_b}\rho(t)^2\mathrm{d}t - \frac{\lambda_z^2}{2}\int_{t_a}^{t_b} z(t)^2\mathrm{d}t\Big\}\mathrm{D}\boldsymbol{r}(t), \quad (13)$$

with

$$g_{\boldsymbol{k}}(t) = \mathrm{i}\boldsymbol{k}[\delta(t-\delta)-\delta(t-\sigma)]. \quad (14)$$

Since the three space coordinates in the above path integrals are completely separable, it is sufficient to evaluate

$$A_{1i} = \int \exp\Big\{ -\frac{1}{2}\int_{t_a}^{t_b}\left(\frac{\mathrm{d}r_i(t)}{\mathrm{d}t}\right)^2 \mathrm{d}t - \frac{C_i}{2}\int_{t_a}^{t_b}\int_{t_a}^{t_b} \mathrm{e}^{-W_i|t-s|}\,|r_i(t)-r_i(s)|^2\,\mathrm{d}t\mathrm{d}s - \frac{\lambda_i^2}{2}\int_{t_a}^{t_b} r_i(t)^2\mathrm{d}t + \int_{t_a}^{t_b} g_i(t)r_i(t)\mathrm{d}t\Big\}\mathrm{D}r_i(t), \quad (15)$$

$$A_{2i} = \int \exp\Big\{ -\frac{1}{2}\int_{t_a}^{t_b}\left(\frac{\mathrm{d}r_i(t)}{\mathrm{d}t}\right)^2 \mathrm{d}t - \frac{C_i}{2}\int_{t_a}^{t_b}\int_{t_a}^{t_b} \mathrm{e}^{-W_i|t-s|}\,|r_i(t)-r_i(s)|^2\,\mathrm{d}t\mathrm{d}s - \frac{\lambda_i^2}{2}\int_{t_a}^{t_b} r_i(t)^2\mathrm{d}t\Big\}\mathrm{D}r_i(t). \quad (16)$$

One can easily obtain

$$A_{1i} = \exp\left\{\frac{1}{2}\int_0^\tau g_i(t)\overline{r_i}(t)\mathrm{d}t\right\}, \qquad A_{2i} = 1, \quad (17)$$

$$\overline{r_i}(t) = \frac{1}{2}\int_0^\tau [f_{1i}(1-\mathrm{e}^{-v_{1i}|t-t'|}) + f_{2i}(1-\mathrm{e}^{-v_{2i}|t-t'|})]g_i(t')\mathrm{d}t' + c, \quad (18)$$

where

$$f_{1i} = \frac{1}{v_{1i}}\frac{W_i^2-v_{1i}^2}{v_{2i}^2-v_{1i}^2}, \quad f_{2i} = \frac{1}{v_{2x}}\frac{W_i^2-v_{2i}^2}{v_{1i}^2-v_{2i}^2},$$
$$v_{1i,2i}^2 = \frac{1}{2}\{(v_i^2+\lambda_i^2) \pm \sqrt{(v_i^2+\lambda_i^2)^2-4\lambda_i^2W_i^2}\},$$
$$v_i^2 = W_i^2+4C_i/W_i, \quad i=\rho,z. \quad (19)$$

Thus we have

$$< \exp\{\mathrm{i}k_i[r_i(\delta)-r_i(\sigma)]\} > = \exp\left\{\mathrm{i}\frac{1}{2}k_i[\overline{r_i}(\delta)-\overline{r_i}(\sigma)]\right\}. \quad (20)$$

So one can readily obtain

$$< \exp\{k_i[r_i(\delta)-r_i(\sigma)]\} > = \exp\Big\{ -\frac{1}{2}[f_{1i}(1-\mathrm{e}^{v_{1i}|\delta-\sigma|}) + f_{2i}(1-\mathrm{e}^{v_{2i}|\delta-\sigma|})]k_i^2\Big\}. \quad (21)$$

Combining all three coordinates results in

$$< \exp\{\mathrm{i}\boldsymbol{k}\cdot[\boldsymbol{r}(\delta)-\boldsymbol{r}(\sigma)]\} > = \exp\Big(-\frac{1}{2}\{[f_{1\rho}(1-\mathrm{e}^{-v_{1\rho}|\delta-\sigma|}) + f_{2\rho}(1-\mathrm{e}^{-v_{2\rho}|\delta-\sigma|})]k_\rho^2 + [f_{1z}(1-\mathrm{e}^{-v_{1z}|\delta-\sigma|}) + f_{2z}(1-\mathrm{e}^{-v_{2z}|\delta-\sigma|})]k_z^2\}\Big). \quad (22)$$

Inserting this back into Eq.(10), we have

$$\mathrm{I} = \frac{\alpha}{\sqrt{\pi}}\int_0^\infty \mathrm{e}^{-t}\frac{1}{\sqrt{\chi_z(t)}} \cdot \frac{1}{\sqrt{1-\frac{\chi_\rho(t)}{\chi_z(t)}}}\tanh^{-1}\left(\sqrt{1-\frac{\chi_\rho(t)}{\chi_z(t)}}\right)\mathrm{d}t, \quad (23)$$

where

$$\chi_\rho(t) = f_{1\rho}(1-\mathrm{e}^{-v_{1\rho}t}) + f_{2\rho}(1-\mathrm{e}^{-v_{2\rho}t}),$$
$$\chi_z(t) = f_{1z}(1-\mathrm{e}^{-v_{1z}t}) + f_{2z}(1-\mathrm{e}^{-v_{2z}t}). \quad (24)$$

In order to calculate II, we can expand both sides of Eq.(20), equate the coefficients of k_i^2, and obtain

$$< [\boldsymbol{r}(\delta)-\boldsymbol{r}(\sigma)]^2 > = 2[f_{1\rho}(1-\mathrm{e}^{-v_{1\rho}|\delta-\sigma|}) + f_{2\rho}(1-\mathrm{e}^{-v_{2\rho}|\delta-\sigma|})] + [f_{1z}(1-\mathrm{e}^{-v_{1z}|\delta-\sigma|}) + f_{2z}(1-\mathrm{e}^{-v_{2z}|\delta-\sigma|})]. \quad (25)$$

From Eq.(8), we have

$$\mathrm{II} = \lim_{\tau\to\infty}\frac{2C_\rho}{2\tau}\int_0^\tau\int_0^\tau [f_{1\rho}(1-\mathrm{e}^{-v_{1\rho}|t-s|}) + f_{2\rho}(1-\mathrm{e}^{-v_{2\rho}|t-s|})]\mathrm{e}^{-W|t-s|}\mathrm{d}t\mathrm{d}s + \lim_{\tau\to\infty}\frac{C_z}{2\tau}\int_0^\tau\int_0^\tau [f_{1z}(1-\mathrm{e}^{-v_{1z}|t-s|}) + f_{2z}(1-\mathrm{e}^{-v_{2z}|t-s|})]\mathrm{e}^{-W|t-s|}\mathrm{d}t\mathrm{d}s = \frac{1}{2}\frac{v_\rho^2-W_\rho^2}{v_{2\rho}+v_{1\rho}} + \frac{1}{4}\frac{v_z^2-W_z^2}{v_{2z}+v_{1z}}. \quad (26)$$

To calculate III, we could take similar procedures in the calculation of I by transforming

$$\frac{1}{|\boldsymbol{r}(t)|} = \int\frac{\mathrm{d}^3\boldsymbol{k}}{2\pi k^2}\exp[\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}(t)]. \quad (27)$$

The classical path can be obtained as follows

$$\frac{\mathrm{d}^2\overline{r_i}(t)}{\mathrm{d}t^2} = 2C_i \int_0^\tau \mathrm{e}^{-W_i|t-s|}[\overline{r_i}(t) - \overline{r_i}(s)]\mathrm{d}s + \lambda^2\overline{r_i}(t) - g_i'(t), \quad (28)$$

$$g_i'(t) = \mathrm{i}k_i\delta(t-\sigma).$$

The solution of Eq.(28) can be obtained as

$$\overline{r_i}(t) = \frac{1}{2}[f_{1i}(\mathrm{e}^{-v_{1i}|t-\sigma|} - \mathrm{e}^{-v_{1i}|\sigma|}) + f_{2i}(\mathrm{e}^{-v_{2i}|t-\sigma|} - \mathrm{e}^{-v_{2i}|\sigma|})]\mathrm{i}k_i. \quad (29)$$

Combining all three coordinates yields

$$\begin{aligned} &< \exp\{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}(\sigma)\} > \\ &= \exp\Big(-\frac{1}{4}\{[f_{1\rho}(1-\mathrm{e}^{-v_{1\rho}|\sigma|}) \\ &\quad + f_{2\rho}(1-\mathrm{e}^{-v_{2\rho}|\sigma|})]k_\rho^2 \\ &\quad + [f_{1z}(1-\mathrm{e}^{-v_{1z}|\sigma|}) + f_{2z}(1-\mathrm{e}^{-v_{2z}|\sigma|})]k_z^2\}\Big). \end{aligned} \quad (30)$$

By means of the third term of Eq.(8), we have

$$\begin{aligned} \mathrm{III} &= \lim_{\tau\to\infty}\frac{\beta}{\tau}\int_0^\tau \Big[\int \frac{\mathrm{d}^3\boldsymbol{k}}{2\pi^2k^2}\exp\Big(-\frac{1}{4}\{[f_{1\rho}(1 \\ &\quad - \mathrm{e}^{-v_{1\rho}t}) + f_{2\rho}(1-\mathrm{e}^{-v_{2\rho}t})]k_\rho^2 \\ &\quad + [f_{1z}(1-\mathrm{e}^{-v_{1z}t}) + f_{2z}(1-\mathrm{e}^{-v_{2z}t})]k_z^2\}\Big)\Big]\mathrm{d}t \\ &= \frac{2\beta}{\sqrt{\pi}}\frac{1}{\sqrt{f_{1z}+f_{2z}}}\cdot\frac{1}{\sqrt{1-\dfrac{f_{1\rho}+f_{2\rho}}{f_{1z}+f_{2z}}}} \\ &\quad \cdot\tanh^{-1}\left(\sqrt{1-\frac{f_{1\rho}+f_{2\rho}}{f_{1z}+f_{2z}}}\right). \end{aligned} \quad (31)$$

Proceeding as before, we can easily obtain

$$\begin{aligned} \mathrm{IV} &= \lim_{\tau\to\infty}\frac{\lambda^2}{2\tau}\int_0^\tau < \boldsymbol{r}(t)^2 > \mathrm{d}t \\ &= \frac{\lambda^2}{4}[2(f_{1\rho}+f_{2\rho}) + (f_{1z}+f_{2z})]. \end{aligned} \quad (32)$$

We can find E_1 by differentiating Eq.(6) with respect to C_i, this leads to

$$\frac{\mathrm{d}E_{1i}}{\mathrm{d}C_i} = \lim_{\tau\to\infty}\frac{\int\frac{\mathrm{d}s_1}{\mathrm{d}C_i}\mathrm{e}^{S_1}\mathrm{D}\boldsymbol{r}(t)}{\tau\int\mathrm{e}^{S_1}\mathrm{D}\boldsymbol{r}(t)} = \frac{1}{W_i(v_{2i}+v_{1i})}. \quad (33)$$

Integrating the above equation straightforwardly under the boundary condition that if $C_i = 0$ (no electron–phonon interaction along i direction in the system corresponding to action S_1), $E_{1i} = \frac{1}{2}\lambda_i$, gives

$$E_1 = (v_{1\rho}+v_{2\rho}-W_\rho) + \frac{1}{2}(v_{1z}+v_{2z}-W_z). \quad (34)$$

Finally, we can present the Feynman energy of bound polarons confined in a parabolic potential $V(\rho) = \frac{1}{2}\omega^2\rho^2$ by the use of Eqs.(5), (23), (26), (31), (32) and (34) as follows

$$\begin{aligned} E_{\mathrm{F}} &= (v_{1\rho}+v_{2\rho}-W_\rho) + \frac{1}{2}(v_{1z}+v_{2z}-W_z) \\ &\quad - \frac{1}{2}\frac{v_\rho^2-W_\rho^2}{v_{2\rho}+v_{1\rho}} - \frac{1}{4}\frac{v_z^2-W_z^2}{v_{2z}+v_{1z}} \\ &\quad - \frac{\lambda^2}{4}[2(f_{1\rho}+f_{2\rho}) + (f_{1z}+f_{2z})] \\ &\quad - \frac{\alpha}{\sqrt{\pi}}\int_0^\infty \mathrm{e}^{-t}\frac{1}{\sqrt{\chi_z(t)}}\frac{1}{\sqrt{1-\dfrac{\chi_\rho(t)}{\chi_z(t)}}} \\ &\quad \cdot\tanh^{-1}\left(\sqrt{1-\frac{\chi_\rho(t)}{\chi_z(t)}}\right)\mathrm{d}t \end{aligned} \quad (35)$$

$$\begin{aligned} &\quad - \frac{2\beta}{\sqrt{\pi}}\frac{1}{\sqrt{f_{1z}+f_{2z}}}\cdot\frac{1}{\sqrt{1-\dfrac{f_{1\rho}+f_{2\rho}}{f_{1z}+f_{2z}}}} \\ &\quad \cdot\tanh^{-1}\left(\sqrt{1-\frac{f_{1\rho}+f_{2\rho}}{f_{1z}+f_{2z}}}\right), \end{aligned} \quad (36)$$

where all parameters are corresponding to those of Eq.(19) with the same values in all three coordinates.

III. RESULTS AND DISCUSSION

Physically, it is expected that the polaronic energy correction $(-\Delta E)$ is more pronounced for large electron–phonon coupling constant α and Coulomb binding parameters β. This is consistent with our numerical results displayed in Figs.1(a) and 1(b), where we plot the variation of $-\Delta E$ as a function of α and β, respectively, for different effective wire radius $R = 1/\sqrt{\omega}$. It is also found that the value of $-\Delta E$ is more sensitive to the value of α than that of β and decreases with the increase of R. This may be due to the strong confining potential of quantum wire that causes the interaction of electron and phonon more intensive than the Coulomb binding potential does.

To show the effectiveness of this approach, we will also study this system within the well-known Feynman–Haken(FH) variational path-integral theory, one can easily derive the FH energy as follows[18]

$$\begin{aligned} E^{\mathrm{FH}} &= \frac{1}{2}\lambda_\rho + \frac{1}{4}\lambda_z + \frac{\omega^2}{2\lambda_\rho} - \frac{\beta}{\pi^{1/2}}\frac{\sqrt{\lambda_z}}{A}\ln\left(\frac{1+A}{1-A}\right) \\ &\quad - \frac{\alpha}{2\sqrt{\pi}}\int_0^\infty \mathrm{d}t\,\mathrm{e}^{-t}\frac{\sqrt{\lambda_z}}{\sqrt{1-\mathrm{e}^{-\lambda_z t}}}\frac{1}{\sqrt{1-B}} \\ &\quad \times\ln\left(\frac{1+\sqrt{1-B}}{1-\sqrt{1-B}}\right), \end{aligned} \quad (37)$$

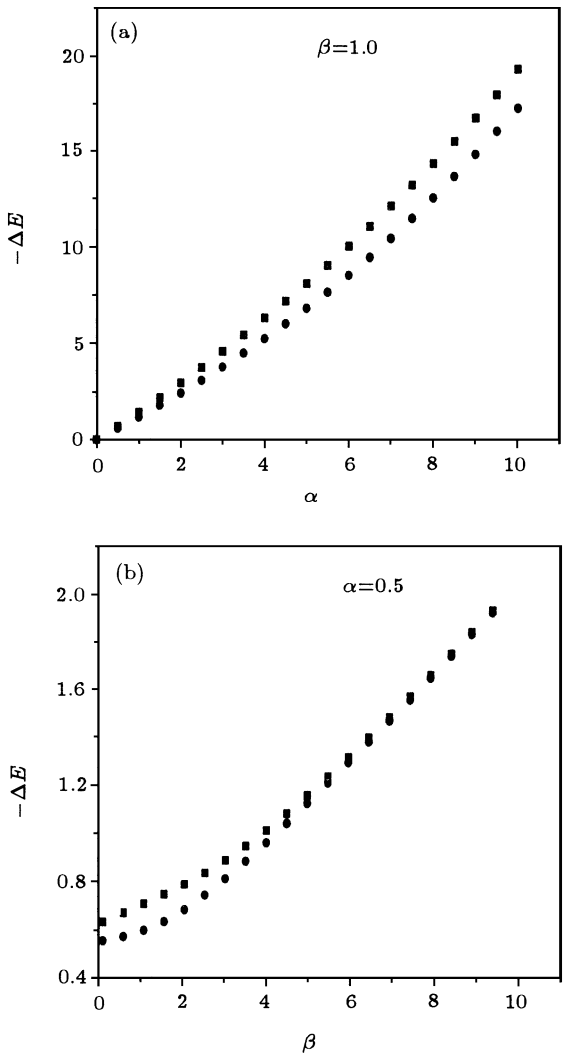


Fig.1. The polaronic energy $-\Delta E^{\mathrm{F}}$ by the FV approach as a function of (a) α and (b) β for two effective wire radius: R=0.5 (square dots) and R=1.0 (circle dots) (in Feynman units).

where $A = \sqrt{1-\frac{\lambda_z}{\lambda_\rho}}, B = \frac{\lambda_z\,(1+\coth(\lambda_z t/2))}{\lambda_\rho\,(1+\coth(\lambda_\rho t/2))}, \lambda_\rho$ and λ_z are variational parameters. For convenience, we introduce the relative difference, η, between the polaronic energy corrections $-\Delta E$ obtained by the two variational approaches: FV approach and FH variational path-integral theory,

$$\eta = \frac{\Delta E^{\mathrm{F}} - \Delta E^{\mathrm{FH}}}{\Delta E^{\mathrm{F}}}.$$

In Fig.2, we plot the value of η as a function of the effective wire radius R for coupling constant α and Coulomb binding parameters β, which are in the range of parameters of practical materials. It is shown that the polaronic energy correction obtained in Feynman path-integral variational approach (FV approach) is considerably larger than that obtained within the FH theory. From the viewpoint of variational principle, FV approach is, therefore, superior to the famous FH path-integral approach.

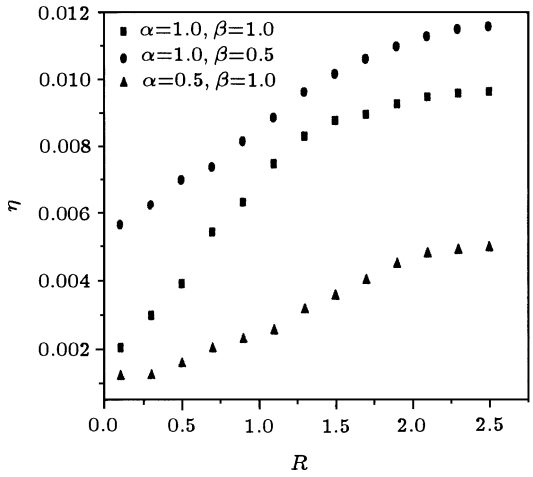


Fig.2. The relative difference between results for the polaronic energy correction within the FH theory and FV approach, η, as a function of the wire radius R for different values of α and β (in Feynman units).

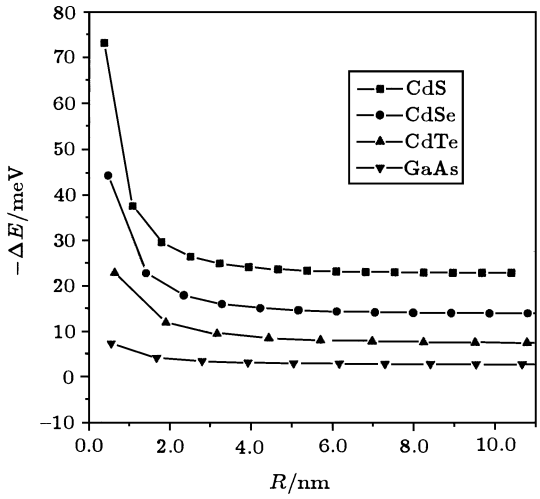


Fig.3. The polaron energy correction, $-\Delta E$ (in meV) within the Feynman path-integral variational theory as a function of the effective wire radius R (in nm) in CdS, CdSe, CdTe and GaAs quantum wires with parabolic potential.

Finally, we apply our calculations to several semiconductor quantum wires, such as CdS, CdSe, CdTe and GaAs, which are shown in Fig.3. The material parameters used in the calculation are given in Table 1, which are quoted from Ref.[19]. It is clear that the polaronic effects are quite pronounced in these materials when R is below a few nanometres. The polaronic effect decreases monotonically with R and changes very slowly as R approaches asymptotically to the bulk limit. We also find that the magnitude of the polaronic correction is predominantly determined

by the electron–phonon coupling constant α and the optical phonon energy, and only slightly influenced by the Coulomb binding parameters β. This also agrees with the previous result obtained by other authors.[18]

Table 1. Some parameters of CdS, CdSe, CdTe and GaAs (ω_{LO} is in units of bare electron mass).

Material	m	ω_{LO}	α	β
CdS	0.155	38.26	0.527	1.225
CdSe	0.130	26.58	0.460	1.238
CdTe	0.091	20.84	0.315	1.064
GaAs	0.066	36.7	0.068	0.5447

In summary, we have studied the polaronic effect of an electron bound to a positive Coulomb impurity in quantum wires within the Feynman variational path-integral theory. Compared to the results obtained by the FH variational theory, the present variational results are more accurate. We observe that the polaronic energy correction is more sensitive to the electron–phonon coupling constant than to the Coulomb binding parameters. We consider a few selected polar semiconductor quantum wires and show that the polaronic energy correction is substantial when the effective wire radius is taken below a few nanometres.

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