Polaronic effect on a bound polaron*

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Abstract: Feynman variational path-integral theory was used to obtain the ground-state energy of a polaron in a quantum well in the presence of a Coulomb potential for arbitrary values of the electron-phonon coupling constant α. Numerical and analytical results showed that the energy shift was more sensitive to α than to the Coulomb binding parameter (β) and increased with the decrease of effective quantum well width l_Z. It was interesting that due to the electronic confinement in the quasi-2D (quantum well) structures，the lower bound of the strong coupling regime was shifted to smaller values of α. Comparison of the polaron in the quantum well with that in the quantum wire or dot showed that the polaronic effect strengthened with decrease of the confinement dimension.

Key words: Bound polaron，Quantum well，Quantum wire，Quantum dot，Ground-state energy
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INTRODUCTION

Recent advances in fabrication technology aroused great interest in the physical properties of mesoscopic low-dimensional structures such as quasi-2D (quantum well)，quasi-1D (quantum wires) and quasi-0D (quantum dot) structures；most of which are made of ionic crystals and polar materials；for which reason，polaron phenomena can strongly influence the physical properties of such structures. Furthermore，due to the electronic confinement in the low-dimensional structures，strong-coupling regime can be realized at significantly small values of the electron-phonon interaction constant α (Zheng et al.，1994，1998；Ren et al.，1998；Chen et al.，1999).

Polarons in quantum wires or wells are markedly different from those in bulk materials，due to the presence of wire or well potentials，which confine the motion of the carriers in the plane transverse to the wire axis or along the well depth. More recently，the effective electron-phonon interaction of a polaron in quantum wires or wells were studied by a large number of authors. Most of their papers dealt with weak coupling treatments (Hai et al.，1993；Thilagam et al.，1994). However，a unified expression of the polaronic effect over the whole coupling regime has great theoretical and practical importance. Because high-degree confinement of quantum wires or wells should lead to enhancement of the effective electron-phonon coupling and bring about the possibility that in spite of weak-polar coupling such as that in GaAs ($\alpha=0.07$)，for instance，the polaron problem may show up as intermediate- or strong-coupling features (Chen et al.，1998；Pokatilov et al.，1999). In the present paper，we will give a unified formula to express the ground-state energy of a bound electron in quantum wells，which fit the whole coupling regime.

It is well known that Feynman developed a variational theory founded on the path integration which was successfully used to calculate the free polaron parameters，such as ground-state energy and effective mass，at arbitrary coupling regime (Feynman et al.，1955). There has been great advance in polaron research within the Feynman description of the polaron. For example，Haken

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calculated the ground-state energy of a polaron in the bulk crystal by introducing an effective potential within the framework of the Feynman path integral (Haken et al., 1957). Chen et al. in 2001 proposed a unified expression of the ground-state energy of a bound polaron in parabolic quantum dots and wires within the framework of Feynman theory. In this paper, we also employ Feynman theory to calculate the ground-state energy of a bound polaron in quantum well and found that our results were better than the results primarily obtained by Feynman-Haken theory or Laudau-Pekar theory. Finally, some new conclusions are made based on the numerical results.

CALCULATION

On the basis of Platzman's work on bound bulk polarons (Platzman et al., 1962), the Hamiltonian describing a bound polaron in a parabolic quantum well has the form (in units of $m=\hbar=\omega_{LO}=1$)

$$\boldsymbol{H} = \frac{\boldsymbol{p}^2}{2} - \frac{\beta}{|\boldsymbol{r}|} + \sum_k a_k^+ a_k + \sum_k [v_k a_k e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + v_k^* a_k^+ e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}] + V(\rho, z), \quad (1)$$

where $\boldsymbol{r}=(\rho(x,y),z)$ and $\boldsymbol{p}$ are the position and the momentum operators of the electron respectively, $V(\rho,z)=\frac{1}{2}\omega_z^2 z^2$ is the confining potential of quantum wells with ω_Z being in units of ω_{LO} measuring the confining strength of the potential, a_k^+ and a_k are respectively the creation and annihilation operators of the LO phonons with the wave vector k,

$$v_k^2 = \frac{2\sqrt{2}\pi\alpha}{k^2 V},$$
$$\alpha = \frac{e^2}{\hbar}\left(\frac{\boldsymbol{m}}{2\hbar\omega_{LO}}\right)^{1/2}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right),$$
$$\beta = \frac{e^2}{\hbar\omega_{LO}\varepsilon_\infty}\left(\frac{m\omega_{LO}}{\hbar}\right)^{1/2},$$

with V being the crystal volume, α and β are electron-phonon coupling constant and Coulomb binding parameter.

By using Feynman variational principle, we can express the Feynman energy of a bound polaron confined in a parabolic well potential as follows

$$E_F = \lambda_\rho + \frac{\lambda_z}{2} + \frac{1}{2}\frac{(\lambda_\rho - v_{1\rho})^2(\lambda_\rho - v_{2\rho})^2}{\lambda_\rho^2(v_{1\rho}+v_{2\rho})} + \frac{1}{4}\frac{(\lambda_z - v_{1z})^2(\lambda_z - v_{2z})^2}{\lambda_z^2(v_{1z}+v_{2z})} - \frac{\alpha}{\sqrt{\pi}}\int_0^\infty e^{-t}\cdot \frac{1}{\sqrt{\chi_\rho(t)}}\frac{1}{\sqrt{1-\chi_z(t)/\chi_\rho(t)}}\cdot \arcsin(\sqrt{1-\chi_z(t)/\chi_\rho(t)})dt - \frac{2\beta}{\sqrt{\pi}}\cdot \frac{1}{\sqrt{f_{1\rho}+f_{2\rho}}}\frac{1}{\sqrt{1-(f_{1z}+f_{2z})/(f_{1\rho}+f_{2\rho})}}\cdot \arcsin\left(\sqrt{1-\frac{f_{1z}+f_{2z}}{f_{1\rho}+f_{2\rho}}}\right) - \frac{\lambda^2}{4}[2(f_{1\rho}+f_{2\rho})+(f_{1z}+f_{2z})], \quad (2)$$

where

$$x_\rho(t) = f_{1\rho}(1-e^{-v_{1\rho}t}) + f_{2\rho}(1-e^{-v_{2\rho}t})$$
$$x_z(t) = f_{1z}(1-e^{-v_{1z}t}) + f_{2z}(1-e^{-v_{2z}t}), \quad (3)$$

$$f_{1i} = \frac{1}{v_{1i}}\frac{v_i^2 - v_{1i}^2}{v_{2i}^2 - v_{1i}^2}, \quad f_{2i} = \frac{1}{v_{2i}}\frac{v_i^2 - v_{2i}^2}{v_{1i}^2 - v_{2i}^2}, \quad (4)$$

$$v_{1i,2i}^2 = \frac{1}{2}\{(1+M_i)v_i^2 + \lambda_i^2 \pm \sqrt{((1+M_i)v_i^2+\lambda_i^2)^2 - 4\lambda_i^2 v_i^2}\}, \quad (5)$$

where $i=\rho, z$, $\lambda_\rho^2=\lambda^2$; $\lambda_z^2=\lambda^2+\omega_z^2$. One can refer to ref. (Chen et al., 2001) for further details of derivations. Numerical results can be obtained from Eq. (2) by minimizing energy with respect to variational parameters M_i, v_i, λ, which are presented in the following.

DISCUSSION AND CONCLUSION

In order to calculate the effective electron-phonon interaction we should calculate the polaron energy shift of this system ($\Delta E = E_F - E_0$). we also need to have the energy E_0 of an electron in a quantum well without electron-phonon interaction. In Fig. 1(a), the polaron energy shifts ($-\Delta E$) are plotted versus α for different effective quantum well width $l_Z = 1/\sqrt{\omega_Z}$. Obviously, the electronic confinement becomes stronger with the decrease of l_Z. As shown in Fig. 1(a), the polaron energy shifts increase with increasing α and increase with the decrease of l_Z. If confinement is strong enough, even for small value of α, a considerably large energy shift could be found. So we can conclude that due to the electronic confinement in the low-dimensional structures, the intermediate- or strong-coupling regime can be realized at very weak electron-phonon interaction.

In Fig. 1(b), we display the variation of $-\Delta E$ as function of Coulomb binding parameter (β) for different well width. It is interesting to find that $-\Delta E$ increases much more slowly as β increases compared with Fig. 1(a). So the value of $-\Delta E$ is more sensitive than β to the value of α and decreases with the increase of l_Z.

In Fig. 2(a) and (b), the polaron energy shifts are plotted versus l_Z for different α or β. It is demonstrated in these figures that polaron energy shift increases with the strengthening of the confinement. This is not difficult to understand. When a confinement is increasing, the interaction of the phonon and the electron is pronounced so that the effective polaronic effect is strengthened.

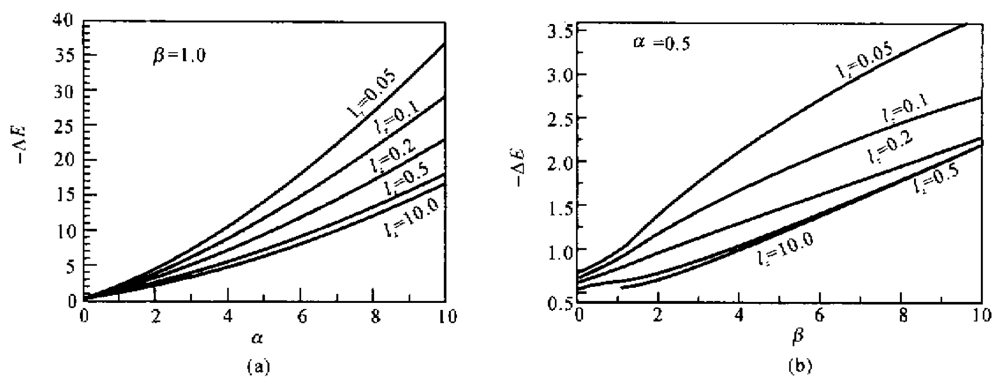

Fig. 1 The polaron energy shift ($-\Delta E$) as a function of (a) and (b) β in different well width: $l_Z = 0.05 \sim 10.0$ (in Feynman units).

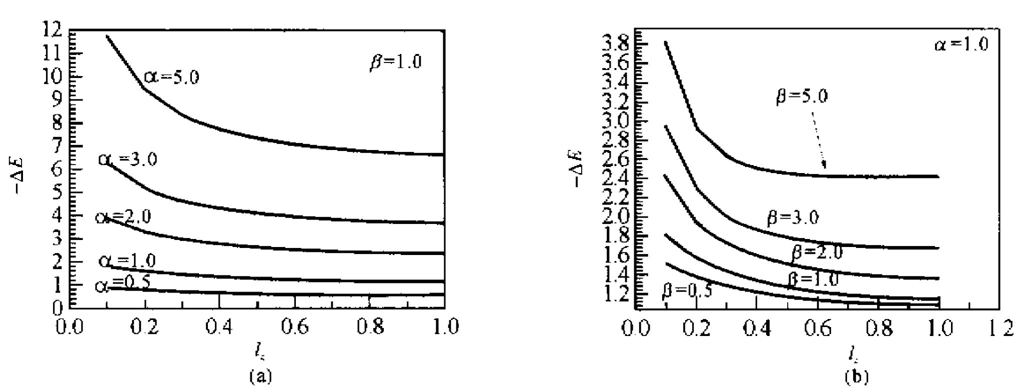

Fig. 2 Plots of the polaron energy shift versus quantum well width
(a) $\beta = 1.0$ α:0.5−5.0; (b) $\alpha = 1.0$ β:0.5−5.0

In Fig. 3, we plot the polaron energy shift as a function of α or l_Z(R) with polaron in quantum well, quantum wire or quantum dot. we compare the polaron in the quantum well (l_Z) with the polaron in the quantum wire or dot (R) (Chen et al., 2001) and find that the polaron energy shift becomes larger as polaron in quantum well is changed to polaron in quantum wire or dot. So we conclude that effective electron-phonon coupling is strengthened as the dimension of the confinement is reduced.

In Fig. 4, we plot the value of E as a function of α or β which are in the range of parameters of practical materials. It is shown that energy obtained in the Feynman variational (FV) approach is smaller than that obtained within the

Feynman-Haken (FH) theory or Laudau-Pekar (LP) theory (Ren et al., 1999; Chatterjee et al., 1990). From the viewpoint of variational principle, FV approach is therefore superior to the famous FH path integral approach or LP theory.

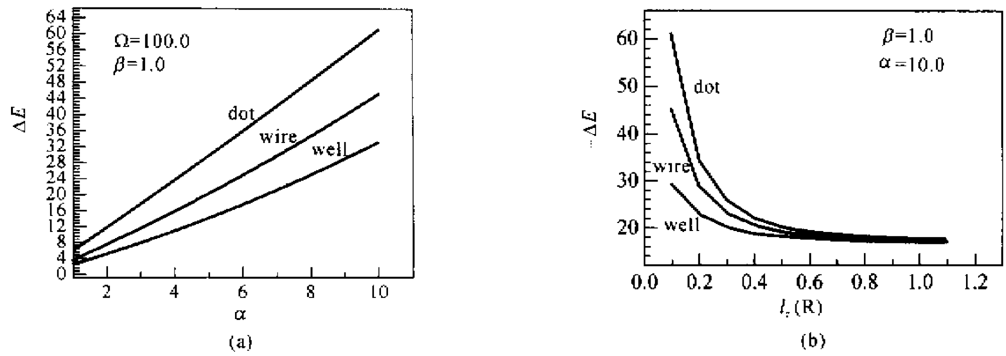

Fig. 3 Plots of the polaron energy shift versus α or $l_Z(R)$ with polaron in quantum well, quantum wire or quantum dot. (a) $\beta = 1.0$, $\Omega = 100.0$; (b) $\beta = 1.0$, $\alpha = 10.0$

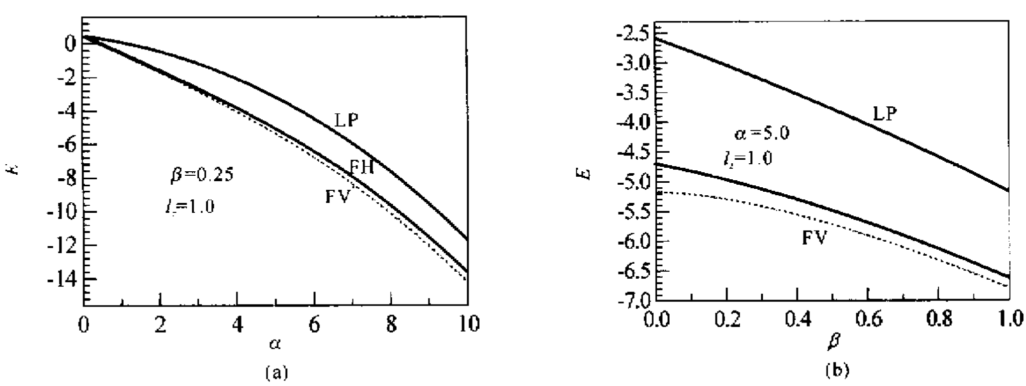

Fig. 4 Feynman energy obtained by Feynman path-integration (FV) or Feynman-Haken theory (FH) or Landau-Pekar theory (LP) as a function of (a) α (b) β.

CONCLUSIONS

In summary, by using of the Feynman variational principle, we obtained a unified expression for the ground-state energy of a bound polaron in a parabolic quantum well, which fit the whole electron-phonon coupling regime. It was found that the present results are better than those by Feynman-Haken path-integral theory and Laudau-Pekar strong-coupling theory.

Further numerical results showed that the energy shift increases as the electron-phonon interaction constant α increases and increase with the increase of confinement. The polaron effect is enhanced by confinement so much that the intermediate- or strong-coupling regime can be realized at significantly small values of coupling constant α. Finally, we compared the polaron in the quantum well with the polaron in the quantum wire or dot and found that the polaronic effect is strengthened as the dimension of the confinement is reduced.

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