Ground-state description for polarons in parabolic quantum wells

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Abstract.   Within the framework of Feynman–Haken variational path integral theory, for the first time, we calculate the ground-state energy of the electron and longitudinal-optical phonon system in parabolic quantum wells with respect to a general potential. We propose a simple expression for the Feynman energy, and compare it with those obtained by the second-order Rayleigh–Schrödinger perturbation theory and Landau–Pekar strong-coupling theory. It is shown both analytically and numerically that the results obtained from Feynman–Haken variational path integral theory can be better than those from the other two theories. We also find in numerical calculations that the binding energy of polarons becomes monotonically stronger as the effective well depth decreases in the whole coupling regime. More interestingly, the localization, which is caused by the effective potential, also can be perceived in the strong-coupling regime.

With the recent progress in micro-fabrication 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 the quantum well, which now can be fabricated within low-nanometre size. The properties of an electron confined in a quantum well (QW) have attracted much attention, since the quasi-two-dimensional (Q2D) polaron problem has become a reference problem for testing various theoretical models and approximation methods, and it can present a comparatively simple and realistic example for the interaction of a confined particle with quantized field. Some usual QW structures (e.g. GaAs, GdS) are composed of polar compounds, therefore the coupling of the electrons with polar-optical vibrations is in general important for determining the electron dynamics and has been studied a great deal [1–10].

   Considerable work has been done on the problem of polaron effects in QW structures, both theory [4–9] and experiment [10]. At the same time, many phonon modes [2–8], such as three-dimensional (3D) bulk optical (BO) modes, confined-slab BO phonon modes and interface phonon modes, and various confining potentials were included. However, most of the corresponding papers are associated with only the weak-coupling treatments or strong-coupling treatments. The general consensus is that the polaronic correction to the ground state increases considerably with the enhancement of the confining potential. Therefore, the high degree of confinement of these structures would always lead to the enhancement of the effective electron–phonon coupling. Consequently, the pure perturbation theory is not perfectly appropriate for the low-dimensional semiconductor structure with weak coupling

constant, since such systems could also exhibit some intermediate-, or even strong-coupling features through the variation of potential confinement and the decrease of dimensions.

So, a theory which would be really suited to all coupling regimes simultaneously is imperative to provide some qualitative insight into the investigations for polarons in this system. Furthermore, it will be helpful to understand the role of the electron–LO phonon interactions in such structures better, which is also of great theoretical and practical importance. The purpose of this paper is to generalize the previous Feynman–Haken (FH) path integral theory [11–13] to report the calculation of the ground-state energy for polarons in QWs with parabolic confinement in the whole coupling regime. Here, we will take into account only the non-screened interaction of the bulk LO phonon, not including the interface phonon modes and the nonparabolicity of the conduction band. Such choices cannot only facilitate the derivations in the theory; more importantly, can be much closer to realistic cases. Moreover, we may compare our calculations to the second-order Rayleigh–Schrödinger perturbation theory (RSPT) and Landau–Pekar (LP) strong-coupling theory.

The Hamilton for polarons in a parabolic quantum well can be written as

$$H = -\frac{1}{2}\nabla_r^2 + \frac{1}{2}\omega_z^2 z^2 + \sum_q a_q^+ a_q + \sum_q [\xi_q \exp(-i\boldsymbol{q} \cdot \boldsymbol{r})a_q^+ + \text{HC}] \tag{1}$$

where all vectors are three dimensions and the units have been chosen such as $\hbar = m = \omega_0 = 1$ (Feynman units), ω_0, the optical phonon frequency, is assumed to be dimensionless, $\boldsymbol{r}$ refers to the position vector of the electron, $\omega_z = \omega_{hz}/\omega_0$, ω_{hz} measures the confining strength of the parabolic potential for direction z, a_q^+ and a_q are the creation and annihilation operator for a LO phonon of wavevector $\boldsymbol{q}$ and for the three dimensional systems ξ_q is always given by [14]

$$|\xi_q|^2 = \frac{2^{3/2}\pi}{v q^2}\alpha \tag{2}$$

with v being the crystal volume, α being the electron–phonon coupling constant. Here we should mention that the phonon interactions have been already been eliminated.

As a first step, following Feynman's [12] first procedure, 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).

$$S = \int_{t_a}^{t_b} dt \left[-\frac{1}{2}\nabla_r^2 + \frac{1}{2}\omega_z^2 z^2 \right] + \frac{1}{2}\sum_k \int_{t_a}^{t_b}\int_{t_a}^{t_b} |v_k|^2 e^{i\boldsymbol{k}\cdot(\boldsymbol{r}(t)-\boldsymbol{r}(s))} e^{|t-s|} dt\, ds. \tag{3}$$

Next, we will choose a path integral trial action to obtain a variational expression for the ground-state energy. We can follow the procedure developed by Haken [11] in the treatment of the exciton–phonon problem. The trial action s_1 can have the form as follows.

$$s_1 = \int_{t_a}^{t_b} dt \left[-\frac{1}{2}\nabla_r^2 - V_{eff}(r(t)) \right] = \int_{t_a}^{t_b} dt\, L_{eff} \tag{4}$$

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

$$H_{eff}\Phi_n^{eff}(\boldsymbol{r}) = \left[\frac{1}{2}\boldsymbol{P}^2 + V_{eff}(\boldsymbol{r}) \right]\Phi_n^{eff}(\boldsymbol{r}) = E_n^{eff}\Phi_n^{eff}(\boldsymbol{r}) \tag{5}$$

where E_0^{eff} and $\Phi_0^{eff}(\boldsymbol{r})$ are the ground-state energy and wavefunction of H_{eff}.

Similar to those in [12] and [13], we can obtain the FH energy as

$$E^{FH} = \langle \Phi_0^{eff}(\boldsymbol{r}) | \left[\frac{1}{2}P^2 + \frac{1}{2}\omega_z^2 z^2 \right] | \Phi_0^{eff}(\boldsymbol{r}) \rangle - \sum_j \sum_k \frac{|\langle \Phi_j^{eff} | v_k \, e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} | \Phi_0^{eff} \rangle|^2}{E_j^{eff} - E_0^{eff} + 1}. \tag{6}$$

It is to noted that, if the effective potential $V_{eff}(\boldsymbol{r})$ is chosen to be a form such that the corresponding Schrödinger equation can be analytically solved, substitution of the relevant energy eigenfunctions and eigenvalues into equation (6) will produce the upper bound to the exact ground-state energy of the Hamiltonian (1).

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 (xy-plane).

$$V_{eff}(\boldsymbol{r}) = \tfrac{1}{2}\lambda_\rho^2 \rho^2 + \tfrac{1}{2}\lambda_z^2 z^2 \tag{7}$$

where λ_ρ and λ_z are variational parameters to be determined. Such a form of $V_{eff}(\boldsymbol{r})$ is different from those in [11]–[13] and more suitable for the problem in quantum wells.

The energy eigenfunctions and eigenvalues corresponding to potential (7) are:

$$\phi_j(\boldsymbol{r}) = \left(\frac{\lambda_\rho \lambda_y^{1/2}}{\pi^{3/2} 2^{j_1+j_2+j_3} \, j_1! j_2! j_3!} \right)^{1/2} H_{j_1}(\sqrt{\lambda_\rho} x) H_{j_2}(\sqrt{\lambda_\rho} y) H_{j_3}(\sqrt{\omega_z} z)$$
$$\times \exp[-\tfrac{1}{2}\lambda_\rho^2 \rho^2 - \tfrac{1}{2}\lambda_z^2 z^2] \tag{8}$$

$$E_j^{eff} = (j_x + j_y + 1)\lambda_\rho + (j_z + \tfrac{1}{2})\lambda_z$$

where $H_n(\square)$ is the Hermite polynomial of order n. Then the first term of equation (6) becomes

$$I_1 = \frac{1}{2}\lambda_\rho + \frac{1}{4}\lambda_z + \frac{\omega_z^2}{4\lambda_z}. \tag{9}$$

If we use the transformation:

$$\frac{1}{E_j - E_0 + 1} = \int_0^\infty \exp[-(E_j - E_0 + 1)t] \, \mathrm{d}t \tag{10}$$

and the Slater sum rule for the Hermite polynomials:

$$\sum_n \frac{1}{2^n n!} H_n(\lambda x) H_n(\lambda x') \exp\left[-\frac{1}{2}\lambda^2(x^2 + x'^2) - 2np \right]$$
$$= \frac{\exp(p)}{\sqrt{2\sinh(2p)}} \exp\left\{ \left(-\frac{1}{4}\lambda^2 \right) [(x + x')^2 \tanh p + (x - x')^2 \coth p] \right\}. \tag{11}$$

Also, we can easily perform the summation over j_x, j_y and j_z in (6) respectively, then using

$$\sum_q \frac{\exp[i\boldsymbol{q}\cdot(\boldsymbol{r} - \boldsymbol{r'})]}{q^2} = \frac{v}{4\pi} \frac{1}{|\boldsymbol{r} - \boldsymbol{r'}|}. \tag{12}$$

Then, we can integrate over the electron position vectors $\boldsymbol{r}$ and $\boldsymbol{r'}$ by transforming these vectors into the centre-of-mass vector $\boldsymbol{u} = (\boldsymbol{r} + \boldsymbol{r'})/2$ and the relative vectors $\boldsymbol{v} = \boldsymbol{r} - \boldsymbol{r'}$, then the second term of equation (6) is simplified to:

$$I_2 = -\int_0^\infty \mathrm{d}t \, e^{-t} \alpha \sqrt{\frac{\lambda_z}{\pi(1 - e^{-\lambda_z t})}} \frac{\tan^{-1}\sqrt{x - 1}}{\sqrt{x - 1}} \tag{13}$$

where

$$x = \frac{\lambda_z(1 + \coth(\lambda_z t/2))}{\lambda(1 + \coth(\lambda t/2))}. \tag{14}$$

Finally the FH energy reads,

$$E^{FH} = I_1 + I_2. \tag{15}$$

So far, for given α and ω_z, one can obtain the ground-state energy of Hamiltonian (1) by minimizing equation (15) with respect to λ_ρ and λ_z. It should be pointed out that this Feynman energy expression (15) is suitable for the entire range of electron–phonon coupling constant α, and the strength of the confining potential ω_z.

In order to calculate the polaronic correction to the ground-state energy of this system, we also need to have the energy in a quantum well without electron–phonon interaction. Obviously, it can be obtained from equation (9) by finding out the optimal fit to λ_ρ and λ_z, where the polaronic energy correction is just corresponding to the difference between these two cases.

Physically, it is expected that the polaronic energy correction $-\Delta E$ is more pronounced for larger electron–phonon coupling constant α. This is consistent with our numerical results displayed in figure 1, where we plot the variation of the polaron binding energy ΔE^{FH} as the function of effective well depth $l = 1/\sqrt{\omega_z}$ for different values of α. It is also found that the value of ΔE^{FH} is more sensitive to the value of α and decreases with larger l.
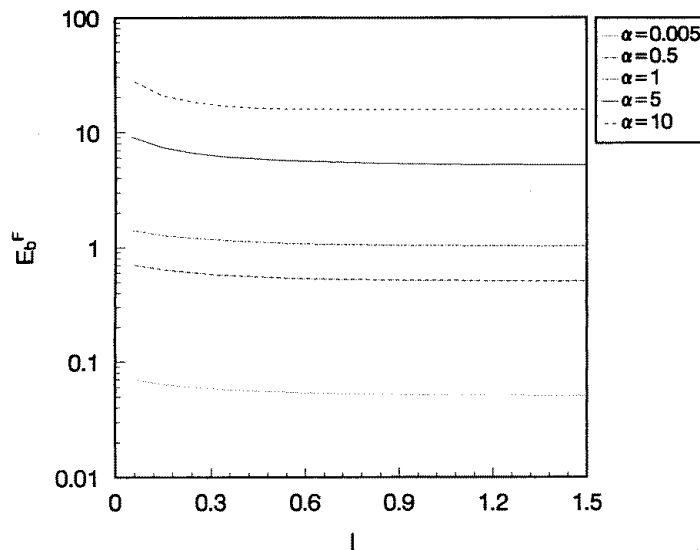

Figure 1. The binding energy of polarons in quantum wells within the FH path integral theory as a function of the effective well depth l at $\alpha = 0.005, 0.5, 1, 5$ and 10.

To show the effectiveness of this approach, we will also study this system within the well known Landau–Pekar (LP) variational theory [15] and the second-order RSPT.

Firstly, the strong-coupling bound polarons in quantum wells can be investigated by the LP variational scheme. Alternatively, we proceed to give a more concise representation of this scheme. The adiabatic polaron ground state can be given through the following product ansatz

$$|\cdots\rangle = \phi(\mathbf{r})|A\rangle = \frac{\lambda_\rho(\lambda_z)^{1/2}}{\pi^{3/4}} \, \mathrm{e}^{-(\lambda_\rho^2\rho^2+\lambda_z^2z^2)/2} \, \mathrm{e}^{(\sum_q f_q b_q^+ + \mathrm{HC})}|0\rangle \tag{16}$$

where $|0\rangle$ is the unperturbed zero phonon state satisfied for all $\mathbf{k}$, λ_ρ and λ_z are the variational parameters, they will be determined variationally.

One can easily derive the LP energy as follows.

$$E^{LP} = \frac{1}{2}\lambda_\rho + \frac{1}{4}\lambda_z + \frac{\omega_z^2}{4\lambda_z} - \frac{\alpha}{\sqrt{\pi}} \frac{\sqrt{\lambda_\rho}}{B} \sin^{-1}(B) \tag{17}$$

where $B = \sqrt{1 - \lambda_\rho/\lambda_z}$, and λ_ρ and λ_z are the variational parameters.

For convenience, we introduce the relative difference, η, for the polaronic energy correction ΔE obtained by these two variational approaches: FH and LP methods.

$$\eta = \frac{\Delta E^{FH} - \Delta E^{LP}}{\Delta E^{FH}}. \tag{18}$$

In figure 2, we plot the values of η as a function of the effective well depth l for coupling constants α. It is obvious that the polaronic energy correction obtained in FH path integral theory is considerably larger than those from LP theory. The trend is more substantial not only with the decrease of the coupling constant α but also with the increase of the effective well depth l. When $l \to 0$, the difference between these two theories becomes minute. Probably, this is just because the electron–phonon coupling is extremely strengthened for the quantum wells in this limit, and LP theory is known to be more suitable for the strong-coupling or strong-Coulomb-binding limit. Overall, we find the FH path integral theory is superior to the famous LP theory.
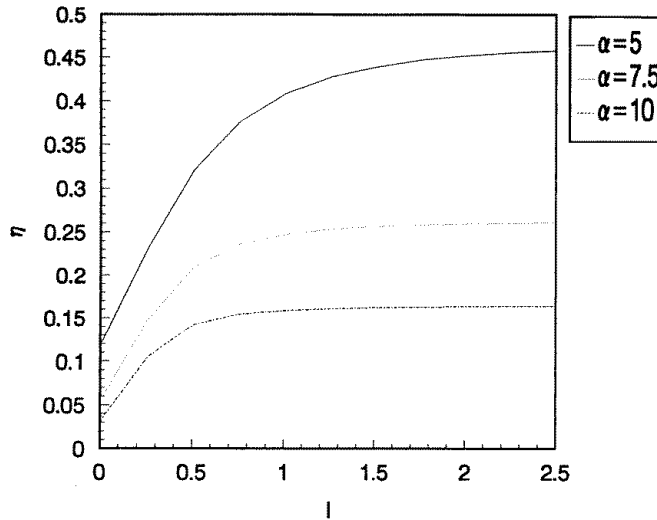

Figure 2. The relative difference between results for binding energy of polarons in quantum wells within the FH theory and LP theory, $\eta = (\Delta E^{FH} - \Delta E^{LP})/\Delta E^{FH}$, as a function of the effective well depth l at $\alpha = 5, 7.5, 10$.

Next, we will compare RSPT with FH path integral theory for quantum wells as well as LP theory. Obviously, the ground-state energy E^{PT_2} in the second-order RSPT can be straight forwardly deduced from (15) by setting $\lambda_\rho = 0$, and $\lambda_z = \omega_z$. It has the form exactly like the following.

$$E^{PT_2} = \frac{1}{2}\omega_z - \alpha\sqrt{\frac{\omega_z}{\pi}} \int_0^\infty dt \, \frac{e^{-t}}{\sqrt{1 - e^{-\omega_z t}}} \frac{\tan^{-1}\sqrt{x' - 1}}{\sqrt{x' - 1}} \tag{19}$$

where $x' = \frac{1}{2}\omega_z t[1 + \coth(\frac{1}{2}\omega_z t)]$.

Similarly, we can introduce the relative difference, η', for the polaronic energy correction ΔE obtained by these two theories: FH path integral theory and the second-order RSPT

$$\eta' = \frac{\Delta E^{FH} - \Delta E^{PT_2}}{\Delta E^{PT_2}}. \tag{20}$$

The results are shown in figure 3. It is clearly shown that ΔE^{FH} is really higher than ΔE^{PT_2} in all cases. After careful inspection of this figure, it is not different to find that: (1) In the weak-coupling limit (i.e. $\alpha < 3$), the results from FH path integral theory are in good agreement with those from the RSPT. (2) In the intermediate-coupling regime (i.e. $\alpha = 3, 4, 5$), there exists a critical well depth l_c. Below l_c, the difference between the two calculated binding energies becomes substantially larger when l decreases. In contrast, above l_c, the difference is so small that it can be neglected. Here we can find the RSPT is also very effective. (3) The relative polaronic energy decreases monotonically with the well depth l and changes very slowly as the well depth l asymptotically approaches the bulk limit. We can perceive the localization, which is caused by the effective potential (in the form (7)).
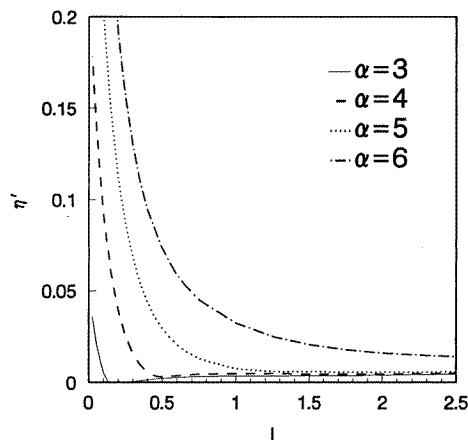

Figure 3. The relative difference between results for binding energy of polarons in quantum wells within the FH theory and RSPT, $\eta' = (\Delta E^{FH} - \Delta E^{PT_2})/\Delta E^{PT_2}$, as a function of the effective well depth l at $\alpha = 3, 4, 5, 6$.

So far, we have shown that the path integral theory can produce better results than the second-order RSPT and LP variational theory can do in the whole coupling regime.

Finally, we will address a very important problem, which is relevant to the appearance of the critical well depth l_c. This form is especially reasonable in the strong-coupling regime. The polaron wavefunction should be localized in all directions with a factor $\sim e^{-\lambda^2 r^2}$ owing to the strong coupling. This has been shown in the strong-coupling LP theory [15] and the modified one [16]. More interesting, the effective potential also exists in the intermediate- and weak-coupling cases. In figure 4, we present the variation of effective transverse spatial extent $\xi_\rho (\xi_\rho = 1/\sqrt{\lambda_\rho})$ as a function of well depth l at different α. We can perceive that for $\alpha \leqslant 5$, all curves diverge at the critical well depth l_c, which just corresponds to the vanish of the transverse part $\frac{1}{2}\lambda_\rho \rho^2$. Whether this part takes effect or not depends only on the values α and l. The ξ_ρ remains finite for $\alpha > 5$ and arbitrary l. This is just because the strong-coupling features exist as well in these systems even without the effective potential. Moreover, it is very clear in all the curves that ξ_ρ reduces with the shrinkage of the quantum

well. In other words, the transverse part $\frac{1}{2}\lambda_\rho\rho^2$ in the effective potential (7) is strengthened with the enhancement of the well confining potential; so is the longitudinal part. Thus, the strength of the well potential is equivalent to the enhancement of the effective electron–phonon coupling, which is consistent with the general trend in the literature.
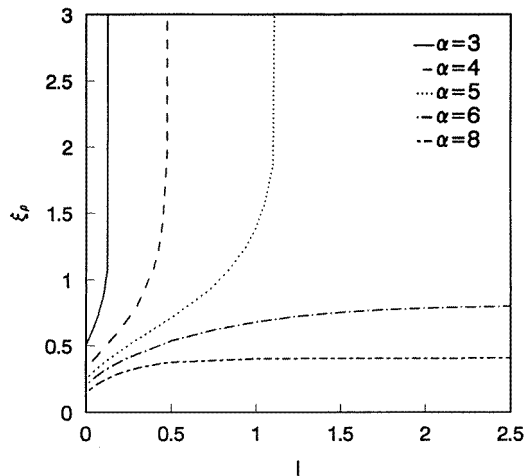

Figure 4. The variation of effective transverse spatial extent $\xi_\rho(\xi_\rho = 1/\sqrt{\lambda_\rho})$ as a function of well depth l at $\alpha = 3, 4, 5, 6, 8$.

In summary, we have studied the polaronic effect of quantum wells within the framework of FH variational path integral theory. By selecting a more general harmonic-type effective potential, we have derived a concise expression for the ground-state energy of this system. We observe that the polaronic energy correction is more sensitive to the electron–phonon coupling constant than the other parameters. Moreover, compared to the results obtained by LP variational theory and the second-order RSPT, the present variational results are more effective and accurate. More interestingly, by numerical calculation, we can perceive the transition from two-dimensional free polarons to quantum wells, and then to three-dimensional free polarons in the weak-coupling regime.

Finally, we should point out the present derivation can be easily extended to more complicated polar semiconductor structures, such as the interface phonon mode in the GaAs/AlGaAs, which is known to be a strong scattering mechanism. This work is in progress.

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