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Bound Polaron in a Quantum Well Under an Electric Field *

Chen Weili and Xiao Jinglin†

(College of Physics and Electromechanics, Inner Mongolia University for Nationalities, Tongliao 028043, China)

Abstract: We conduct a theoretical study on the properties of a bound polaron in a quantum well under an electric field using linear combination operator and unitary transformation methods, which are valid in the whole range of electron-LO phonon coupling. The changing relations between the ground-state energy of the bound polaron in the quantum well and the Coulomb bound potential, the electric field strength, and the well width are derived. The numerical results show that the ground-state energy increases with the increase of the electric field strength and the Coulomb bound potential and decreases as the well width increases.

Key words: quantum well; bound polaron; ground-state energy; linear combination operator; electric field
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1 Introduction

In recent years, many theoretical and experimental investigations have been performed on the issue of the hydrogenic binding of an electron to a donor impurity confined within a low-dimensional heterostructure[1~3]. With the presence of shallow impurities in this material, the study of the electronic and optical properties of impurities in this system has an important role, and the electric field is an effective tool for studying the properties of impurities in a quantum well. The effect of an electric field on a donor in a quantum well has drawn the attention of several authors. Kasapoglu *et al*.[4] calculated variationally the ground state binding energy of a hydrogenic donor or impurity in a quantum well in the presence of crossed electric and magnetic fields applied tilted at an angle to the layers by using an appropriate coordinate transformation. Kasapoglu *et al*.[5] computed the binding energies of shallow donor impurities in differently shaped quantum wells under an applied electric field using a variational method. Liu *et al*.[6] calculated the ionization energy of a bound polaron confined to general step quantum wells in the presence of an electric field using a variational method. Huang *et al*.[7] calculated the ground state energy of an impurity by means of the LLP transformation in Ⅲ-Ⅴ and Ⅱ-Ⅵ quantum wells under electric fields. Aktas *et al*.[8] studied the ground state binding energy of a hydrogenic impurity in a coaxial cylindrical quantum well wire system subjected to an external electric field applied perpendicular to the symmetry axis of the wire system within a variational scheme. Li[9] studied the effects of an electric field on the subbands and binding energies of hydrogenic impurities in a GaAs-GaAlAs quantum well using the effective mass approximation. Many authors have studied the properties of donor impurities in quantum wells under an electric field. However, the linear combination operator and unitary transformation methods have seldom been used.

In this paper, we calculate the ground state energy of a bound polaron in a quantum well under an electric field using the linear combination operator and unitary transformation methods. We obtain the explicit dependence of the ground state energy of the bound polaron on the well width, the electric field strength, and the Coulomb bound potential.

2 Theory

We consider a QW in a polar semiconductor in the range of $|z| \leq L$ with infinite-height barrier material filling in the space in the region $|z| > L$. There is an electron coupled to a Coulomb impurity

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† Corresponding author. Email: xiaojlin@126.com
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located at the center of the well and interacting with the confined bulk LO-phonons and the electric field along the z direction. Using a Fröhlich-like Hamiltonian for the electron and LO-phonon interaction, the total Hamiltonian of the system[10] is

$$H = H_e + H_{LO} + H_{e\text{-}LO} + eFz \tag{1}$$

$$H_e = -\frac{\hbar^2}{2m}\nabla^2 + U(z) + V(z)$$

$$U(z) = \begin{cases} \infty, & |z| > L \\ 0, & |z| \leq L \end{cases}, \quad V(z) = -\frac{e^2}{4\pi K_0 \varepsilon_\infty r} \tag{2}$$

$$H_{LO} = \sum_w \hbar\omega_L a_w^+ a_w \tag{3}$$

$$H_{e\text{-}LO} = \sum_w Q_w (a_w + a_{-w}^+) e^{iw\cdot r} \tag{4}$$

where the spin effects are ignored. Here, K_0 is the permittivity of free space, m, ω_L are the band mass and the LO-phonon frequency, respectively. The vector $r = (\rho, z)$ is the position of the electron, and F is the electric field strength. In Eqs. (3) and (4), a_w^+, a_w are the phonon annihilation and creation operators, respectively. In Eq. (4),

$$Q_w = \left(\frac{\hbar\omega_L}{w}\right)\left(\frac{\hbar}{2m\omega_L}\right)^{1/4}\left(\frac{4\pi\alpha}{V}\right)^{1/2} \tag{5}$$

where

$$\alpha = \frac{e^2}{4\pi K_0 \hbar}\left(\frac{m}{2\hbar\omega_L}\right)^{1/2}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right) \tag{6}$$

where ε_0 and ε_∞ are the static and high-frequency dielectric constants, respectively, α is the Fröhlich coupling constant, and V is the volume of the semiconductor.

We expand the Coulomb bound potential in a series as follows:

$$\frac{1}{r} = \frac{4\pi}{V}\sum_w \frac{1}{w^2}\exp(-iw\cdot r) \tag{7}$$

Following Huybrechts, we also introduce the linear combination of the creation and annihilation operators b^+ and b to represent the momentum and position of the electron in the x-y plane:

$$\begin{gathered} p_j = \left[\frac{m\hbar\lambda}{2}\right]^{1/2}(b_j + b_j^+) \\ \rho_j = i\left[\frac{\hbar}{2m\lambda}\right]^{1/2}(b_j - b_j^+), \quad j = x, y \\ [b_j, b_j^+] = \delta_{ij} \end{gathered} \tag{8}$$

Here, λ is the vibration frequency, which is a variational parameter. We substitute Eq. (8) into Eq. (1) and then carry out the unitary transformations

$$\begin{gathered} U_1 = \exp\left(-i\sum_w w\cdot\rho\, a_w^+ a_w\right) \\ U_2 = \exp\left[\sum_w (f_w^* a_w^+ - f_w a_w)\right] \end{gathered} \tag{9}$$

where f_w^*, f_w are the variational parameters. We can easily obtain

$$\begin{aligned} H' = {} & \frac{\hbar\lambda}{2}\left(\sum_j b_j^+ b_j + 1\right) + \sum_w\left(\hbar\omega_L + \frac{a^2\hbar^2 w^2}{2m}\right)\times \\ & (a_w^+ + f_w^*)(a_w + f_w) + \frac{\hbar\lambda}{4}\sum_j (b_j^+ b_j^+ + b_j b_j) + \\ & \frac{P_z^2}{2m} + \sum_w (Q_w^*(a_{-w}^+ + f_{-w}^* + a_w + f_w)\exp(i\omega_z z) - \\ & \left(\frac{\hbar\lambda}{2m}\right)^2 \sum_w\sum_j \hbar w_j (b_j^+ + b_j)(a_w^+ + f_w^*)(a_w + f_w) - \\ & \sum_w \frac{4\pi e^2}{V\varepsilon_\infty w^2}\exp\left(-\frac{\hbar}{4m\lambda}w^2\right)\exp(-i\omega_z z)\times \\ & \exp\left(-\left(\frac{\hbar}{2m\lambda}\right)^2\sum_j w_j b_j^+\right)\exp\left(\left(\frac{\hbar}{2m\lambda}\right)^2\sum_j w_j b_j\right) + \\ & eFz + U(z) \end{aligned} \tag{10}$$

$$\begin{aligned} H_1'' = {} & \frac{1}{2m}\sum_w\sum_{w'}\hbar^2(a_w^+ + f_w^*)(a_{w'}^+ + f_{w'}^*)\times \\ & (a_w + f_w)(a_{w'} + f_{w'})\, w\cdot w' \end{aligned} \tag{11}$$

Equation (11) describes the interaction between phonons of different wave vectors in the recoil process when neglecting the recoil energy.

In the following variational calculations, we assume a low-temperature limit, i.e. the zero-phonon state, and we choose the ground wave-function

$$|\psi\rangle = \Phi(z)\,|0\rangle \tag{12}$$

where $|0\rangle$ is the zero-phonon state of the phonon field, and $\Phi(z)$ describes the z-direction wave function in an infinite one-dimensional square well, which is given by[11]

$$\Phi(z) = \begin{cases} N(\beta)\exp[-\beta(z/L + 1/2)]\cos(\pi z/L), & |z| < L/2 \\ 0, & |z| \gg L/2 \end{cases} \tag{13}$$

where β is a variational parameter determined by minimizing the total energy, and $N(\beta)$ is the normalization constant which is easily obtained by the relation

$$N^2(\beta) = 4\beta(\beta + \pi^2)[L\pi^2(1 - e^{-2\beta})]^{-1} \tag{14}$$

Thus we obtain the expectation value of system as

$$\begin{aligned} E = {} & \langle\psi|H'|\psi\rangle = \frac{\hbar\lambda}{2} + \\ & \sum_w\left(\hbar\omega_L + \frac{\hbar^2 w^2}{2m}\right)|f_w^*|^2 + \sum_w (Q_w(f_w + f_{-w}^*)) - \\ & \sum_w \frac{4\pi e^2}{V\varepsilon_\infty w^2}\exp\left(-\frac{\hbar}{4m\lambda}w^2\right) + \\ & \left\langle\Phi(z)\left|\frac{P_z^2}{2m} + eFz\right|\Phi(z)\right\rangle \end{aligned} \tag{15}$$

Using the variational method, we get

$$f_w^* = -\frac{Q_w}{\hbar\omega_L + \frac{\hbar^2 w^2}{2m}} \tag{16}$$

Substituting Eq. (18) into Eq. (17), we have

$$E(\lambda,\beta) = \frac{\hbar\lambda}{2} - \hbar\omega_0\alpha - \beta_0\sqrt{\lambda} + \frac{\hbar^2(\pi^2-\beta^2)}{2mL^2} + |e|FL\left(\frac{1}{2\beta} + \frac{\beta}{\beta^2+\pi^2} - \frac{1}{2}\coth\beta\right) \tag{17}$$

where

$$\beta_0 = \frac{e^2}{2K_0\varepsilon_0\pi^2}\sqrt{\frac{m\pi}{\hbar}}$$

Performing the variation of $E(\lambda,\beta)$ with respect to λ,β, we obtain

$$\sqrt{\lambda} = \frac{\beta_0}{\hbar} \tag{18}$$

$$F = \frac{-\beta\hbar^2}{meL^3\left(-\frac{1}{2\beta^2} + \frac{\pi^2-\beta^2}{(\pi^2+\beta^2)^2} + \frac{2e^{-2\beta}}{(1-e^{-2\beta})^2}\right)} \tag{19}$$

Substituting Eqs. (18) and (19) into Eq. (17), we finally obtain the ground state energy of a weak-coupling bound polaron in a quantum well within an electric field, i.e.

$$E_0 = -\frac{\beta_0^2}{2\hbar} - \alpha\hbar\omega_0 + |e|FL\left(\frac{1}{2\beta} + \frac{\beta}{\beta^2+\pi^2} - \frac{1}{2}\coth\beta\right) + \frac{(\pi^2-\beta)\hbar^2}{2mL^2} \tag{20}$$

3 Results and discussion

We numerically calculate the ground state energy of a weak-coupling bound polaron in a GaAs quantum well with an applied longitudinal electric field. The corresponding parameters for GaAs[12] are: $\varepsilon_0 = 12.83$, $\varepsilon_\infty = 10.9$, $\hbar\omega_0 = 36.7\text{meV}$, $m = 0.067m_0$, where m_0 is the free electron mass, and the electron-phonon coupling constant is $\alpha = 0.067$.

Figures 1 and 2 describe the variation of the ground state energy of the weak-coupling bound polaron versus the electric field strength with different Coulomb potentials and well widths. The two figures clearly show the influence of the electric field on the ground state energy. In Fig. 1, the ground state energy of the bound polaron in the well is plotted as a function of the electric field strength for different Coulomb potentials $\beta_0 = 4$, $\beta_0 = 5$ and the well width $L = 10\text{nm}$. This shows that the absolute value of the ground state energy of the bound polaron increases monotonically with increasing electric field strength, and the two lines are almost parallel. Figure 2 shows for the well widths $L = 10\text{nm}$ and $L = 15\text{nm}$ and the Coulomb potential $\beta_0 = 4$ that the absolute value of the ground state energy of the bound polaron in the well also increases monotonically with the increasing of the electric field strength, and changes rapidly with electric field strength in the case of the wider well. For an electric field strength of $F = 0$, the two lines almost intersect, because if $F = 0$ the third term in Eq. (20) equals zero, and the value of the ground state energy is decided by the others.

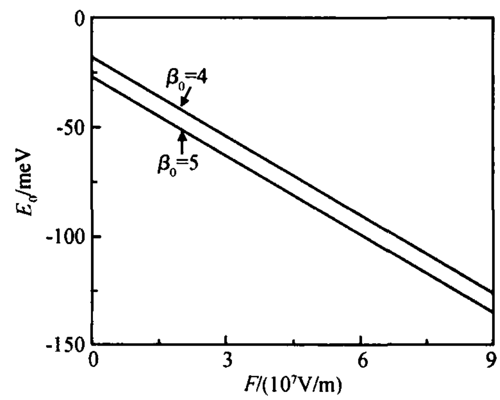

Fig. 1　Ground state energy E_0 of the bound polaron versus the electric field strength F for two Coulomb potentials $\beta_0 = 4$ and $\beta_0 = 5$

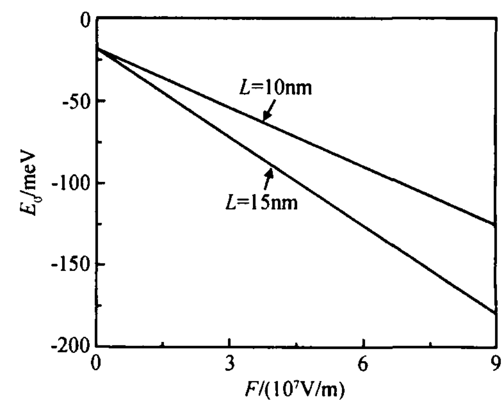

Fig. 2　Ground state energy E_0 of the bound polaron versus the electric field strength F for two well widths $L = 10\text{nm}$ and $L = 15\text{nm}$

As shown in Figs. 3 and 4, there are significant corrections to the ground state energy of the weak-coupling bound polaron versus the well width. From Fig. 3, we can see that the absolute value of the ground state energy decreases with increasing well width L for different Coulomb potentials β_0 =

4, β_0 = 5 and a given variational parameter β = 70. In Fig. 4, we also see that the absolute value of the ground state energy decreases with increasing well width for two different variational parameters β = 70 and β = 30. In Figs. 3 and 4, when the well width is small, the absolute value of the ground state energy decreases sharply and finally becomes flat. In Fig. 3 the two curves almost coincide with each other as the well width reaches small values, and when the well width is large, they are almost parallel. The reverse is true in Fig. 4, in which the two curves almost coincide with each other as the well width becomes large.

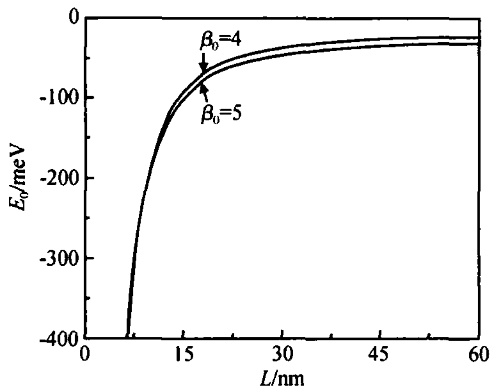

Fig. 3 Ground state energy E_0 of the bound polaron versus the well-width L for different Coulomb potentials β_0

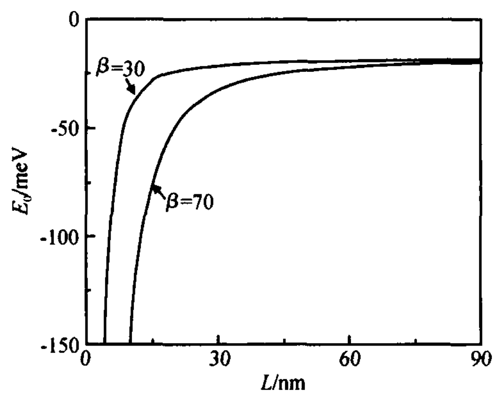

Fig. 4 Ground state energy E_0 of the bound polaron versus the well-width L for variational parameter β

The dependence of the ground state energy of the weak-coupling bound polaron in the quantum well on the variational parameter in the wavefunction is given in Fig. 5 for different Coulomb potentials β_0 = 4, β_0 = 5 and the well width L = 10nm. It is obvious that the absolute value of the ground state energy will rapidly become large as the variational parameter increases.

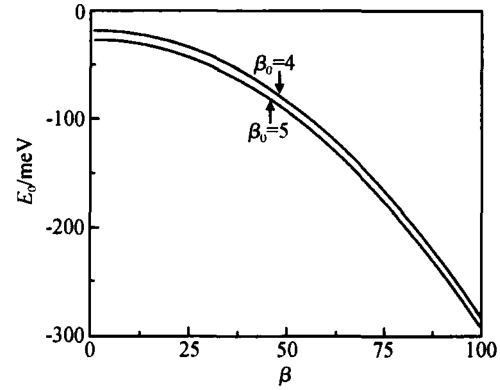

Fig. 5 Ground state energy E_0 of the bound polaron versus the variational parameter β for different Coulomb potentials

We plot the values of the ground state energy of the weak-coupling bound polaron in the quantum well versus the Coulomb potential β_0 with different electric field strengths: $F = 1 \times 10^7$, 4×10^7 V/m and the well width L = 10nm, as shown in Fig. 6. We observe that the absolute value of the ground state energy increases as the Coulomb potential β_0 increases for a given electric field. From Eq. (18), we can see that the vibration frequency is proportional to the square of the Coulomb potential β_0, so the influence of the vibration frequency on the ground state energy becomes stronger.

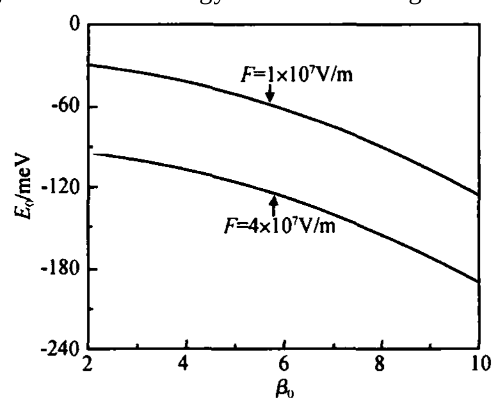

Fig. 6 Ground state energy E_0 of the bound polaron versus Coulomb potentials β_0 for different electric field strengths F

4 Conclusion

Using the linear combination operator and unitary transformation methods, we have calculated, the ground state energy of a weak-coupling bound polaron in a quantum well under an electric field along the z direction. We obtained the explicit dependence of the ground state energy of the bound polaron on the well width, the electric field strength, and the Coulomb bond potential, respectively. The ground-state energy increases with the increase of the electric field strength and the Coulomb potential, and it decreases as the well width increases.

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电场中束缚极化子 *

陈伟丽　肖景林†

(内蒙古民族大学物理与机电学院, 通辽　028043)

摘要: 采用线性组合算符及幺正变换方法研究了电场对量子阱弱耦合束缚极化子的性质的影响. 推导出量子阱中束缚极化子的基态能量和库仑束缚势、电场和阱宽的变化关系. 数值计算结果表明, 基态能量因电场和库仑束缚势的不同而不同, 随电场和库仑束缚势的增大而增大, 随阱宽的增大而迅速减小.

关键词: 量子阱; 束缚极化子; 基态能量; 线性组合算符; 电场

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†通信作者. Email: xiaojlin@126.com

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