A Fractional-Dimension Variational Approach for the Bound Polaron in Parabolic Quantum Wells*

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Abstract: The binding energy of a bound polaron in a finite parabolic quantum well is studied theoretically by a fractional-dimensional variational method. The numerical results for the binding energies of the bound polaron and longitudinal-optical phonon contributions in GaAs/$Al_{0.3}Ga_{0.7}$As parabolic quantum well structures are obtained as functions of the well width. It is shown that the binding energies of the bound polaron are obviously reduced by the electron-phonon interaction and the phonon contribution is observable and cannot be neglected.

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1 Introduction

Remarkable progress in device physics has made it possible to fabricate a wide variety of low-dimensional semiconductor systems. A great deal of effort has been devoted to the study of these structures because of their potential applications in a wide range of electronic and optoelectronic devices. One of the effects that has attracted a considerable amount of attention is the polaron effect[1~9].

A previous work studied the polaron problem in a parabolic quantum well (PQW) using the Lee-Low-Pines (LLP) variational method, considering the confined well and barrier longitudinal optical (LO) phonons as the slab and half-spacing modes similar to those used to treat the polaron problems in square quantum wells[2]. Hai et al.[3] considered an electron interacting with bulk LO phonons in a PQW and calculated the polaron energy and effective mass by a perturbation method. As an approximation, the interface optical phonon modes were omitted in the abovementioned papers because of the small difference between the well and barrier materials in the vicinity of the interfaces. Wang et al.[4] have recently discussed the electron-phonon effect on polarons in PQW structures and confirmed that the bulk LO phonon model is an acceptable approximation.

Of particular interest to the present work is the fractional-dimensional space approach proposed by He[10]. This simple and effective method has been used to treat the exciton states and polaron problems in low-dimension structures[11~14]. More recently, Wang et al[5] developed this approach to discuss the polaron effects on excitons in PQWs and obtained a surprisingly accurate estimation for the binding energy. However, to our knowledge, the bound polaron in PQW structures has rarely been discussed concretely.

In this paper, a fractional-dimensional model in combination with a LLP-like transformation and a variational treatment is developed to investigate the bound polaron in PQWs. A characteristic potential confinement length for the bound polaron in PQWs is introduced. We use a trial wave function with a fractional-dimensional variational parameter to calculate the binding energies of the bound polaron. As an example, the numerical results for the GaAs/$Al_{0.3}Ga_{0.7}$As PQW are given and discussed.

2 LLP-like transformation and fractional-dimensional space approach

Let us consider a PQW structure with well-width $2d$ generated by alternating multiple layers of GaAs and $Al_xGa_{1-x}As$ of varying thickness along the z-direction [1]. The relative thickness of the GaAs layers in the well decreases quadratically as the distance from the well center increases ($z = 0$). The barrier material is $Al_xGa_{1-x}As$. As an approximation, we assume the electron with the band mass of GaAs moves in the system and couples with a bulk optical phonon field. The Hamiltonian of the electron-phonon

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system then can be written as

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

The first term in Eq. (1) is the Hamiltonian of a bare electron and can be described within the framework of the isotropic effective mass approximation by

$$H_e = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{\varepsilon_\infty r} + V(z) \tag{2}$$

where ε_∞ is the high frequency dielectric constant, and the quantum well potential $V(z)$ is

$$V(z) = \begin{cases} \dfrac{V_0}{d^2}z^2, & |z| \leqslant d \\ V_0, & |z| > d \end{cases} \tag{3}$$

Here, V_0 is the well-depth for the electron and is determined by $V_0 = 0.6 \times 1250x$ (meV) for the GaAs/$Al_xGa_{1-x}As$ system.

The second term in Eq. (1) is the free-phonon-field Hamiltonian

$$H_{ph} = \sum_q \hbar\omega a_q^* a_q \tag{4}$$

where a_q^* and a_q are respectively the creation and annihilation operators of the LO-phonon with frequency ω and wave-vector q.

The last term in Eq. (1) stands for the electron-phonon interaction Hamiltonian and has the following form in the bulk-LO-phonons approximation[4,15]:

$$H_{e\text{-}ph} = \sum_q [V_q^* a_q^+ (e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} - 1) + \text{h.c.}] \tag{5}$$

where

$$V_q = i\left[\frac{2\pi e^2}{V} \times \frac{\hbar\omega}{q^2}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right)\right]^{1/2} \tag{6}$$

Carrying out two LLP-like unitary transformations

$$U_1 = \exp\left[-i\sum_q a_q^+ a_q \boldsymbol{q}\cdot\boldsymbol{r}\right) \tag{7}$$

and

$$U_2 = \exp\left[\sum_q (a_q^+ f_q - a_q f_q^*)\right] \tag{8}$$

the electron-phonon system Hamiltonian becomes

$$\begin{aligned} H^* &= U_2^{-1} U_1^{-1} H U_1 U_2 \\ &= H_e + \sum_q \left(\hbar\omega + \frac{\hbar^2 q^2}{2M}\right)(a_q^+ + f_q^*)(a_q + f_q) + \\ &\quad \sum_q [V_q (a_q + f_q)(1 - e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}) + \text{h.c.}] \end{aligned} \tag{9}$$

where the multi-phonon processes have been neglected in the mono-phonon approximation. The displacement amplitudes f_q and f_q^* will be variationally determined later.

We now use a variational method to calculate the ground state energy of the bound polaron. The ground state wave function of the electron-phonon system is chosen as

$$|\Psi\rangle = |\phi(\boldsymbol{r})\rangle |0\rangle \tag{10}$$

where $|0\rangle$ is the zero-phonon state, and $|\phi(\boldsymbol{r})\rangle$ is a trial wave function for the ground state and will be determined by a fractional-dimensional variational treatment. Then, the variational energy of the bound polaron can be calculated as

$$\begin{aligned} E &= \langle 0 | \langle \phi(\boldsymbol{r}) | H^* | \phi(\boldsymbol{r})\rangle | 0\rangle \\ &= E_0 + \sum_q f_q^* f_q \left(\hbar\omega + \frac{\hbar^2 q^2}{2m}\right) + \\ &\quad \sum_q [V^*(q) f_q + \text{h.c.}] \end{aligned} \tag{11}$$

where

$$E_0 = \langle \phi(\boldsymbol{r}) | H_e | \phi(\boldsymbol{r})\rangle \tag{12}$$

$$V(q) = \langle \phi(\boldsymbol{r}) | V_q (1 - e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}) | \phi(\boldsymbol{r})\rangle \tag{13}$$

Solving the minimum equation

$$\frac{\partial E}{\partial f_q} = \frac{\partial E}{\partial f_q^*} = 0 \tag{14}$$

gives the displacement amplitudes f_q and f_q^*

$$f_q = -\frac{V^*(q)}{\hbar\omega + \hbar^2 q^2/2m} \tag{15a}$$

and

$$f_q^* = -\frac{V(q)}{\hbar\omega + \hbar^2 q^2/2m} \tag{15b}$$

Substituting Eqs. (15a) and (15b) into Eq. (12), we obtain the variational energy

$$E = E_0 - \sum_q \frac{|V(q)|^2}{\hbar\omega + \hbar^2 q^2/2m} \tag{16}$$

The ground state energy of the bound polaron is then determined by minimizing Eq. (16).

The electron part of the wave function is complicated to express in an analytic form. He[10] proposed the fractional-dimension model to study excitons in confined systems. We calculate variationally the ground state energy of the bound polaron by linking the LLP-like transformations with the fractional-dimension model. We choose the trail wave function in Eq. (10) similar to the 3D form:

$$\phi(r) = \sqrt{\frac{1}{\pi\lambda^3}}\exp\left(-\frac{r}{\lambda}\right) \tag{17}$$

where λ is the variational parameter. The variational energy of the bound polaron in a 3D system is

$$E_0^{(3)} = \langle \phi(r) | -\nabla^2 - 2/r | \phi(r)\rangle = \frac{1}{\lambda^2} - \frac{2}{\lambda} \tag{18}$$

The energy is measured in the 3D Rydberg and the length in 3D Bohr radius. Extending this expression into the fractional-dimension model, the ground state energy of the bound polaron can be written as the D-dimensional space form[5]:

$$E_0^{(D)} = \frac{1}{\lambda^2} - \frac{2}{\lambda(1 - e^{-L}/2)} \tag{19}$$

In Eq. (19), L is the characteristic potential confinement length in the z-direction, which is determined by minimizing the variational energy of the electron

$$E(a) = \langle \Psi(z) | H | \Psi(z)\rangle \tag{20}$$

The Hamiltonian and the trial wave function for the ground state of an electron moving in the finite PQW is:

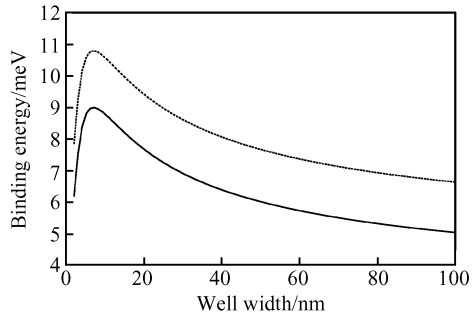

Fig. 1　Binding energies of the bound polaron with (solid line) and without phonon contributions (dashed line) as functions of the well-width in the finite PQW

$$H = -\frac{\hbar^2}{2m}\times\frac{\partial^2}{\partial z^2} + V(z) \tag{21}$$

$$\Psi(z) = \left(\sqrt{\frac{2}{\pi}}\times\frac{1}{a}\right)^{1/2}\exp(-z^2/a^2) \tag{22}$$

where a is the variational parameter and can be chosen as the characteristic potential confinement length, namely

$$L = a$$

According to the discussion above, substituting Eq. (17) into Eqs. (12) and (13) and then into Eq. (16), the variational energy of the bound polaron in the fractional- dimensional model is:

$$E(\lambda) = \frac{1}{\lambda^2} - \frac{2}{\lambda[1-(1/2)e^{-L}]} - \alpha\hbar\omega\,\frac{2}{\pi}\int_0^\infty \mathrm{d}x\,\frac{1}{1+x^2}\left[1-\frac{16}{[4+(\lambda u x)^2]^2}\right]^2 \tag{23}$$

where $u = (2m\omega/\hbar)^{1/4}$, and $\alpha = (me^2/\hbar^2 u)(1/\varepsilon_\infty - 1/\varepsilon_0)$ is the electron-phonon coupling constant.

The ground state energy of the bound polaron is then

$$E = \min_{\lambda} E(\lambda) \tag{24}$$

The binding energy of the bound polaron E_b is defined by

$$E_b = E_{free} - E \tag{25}$$

In Eq. (25), E_{free} is the energy of the polaron and can be calculated by the method used in Ref. [4].

3　Numerical results and discussion

The binding energies of the bound polaron in the $GaAs/Al_{0.3}Ga_{0.7}As$ PQW have been computed by using Eqs. (23) ~ (25). The parameters used in our calculation are as follows[16]: $m_e = 0.0665m_0$, $\hbar\omega = 36.25$meV, $\varepsilon_0 = 13.18$, $\varepsilon_\infty = 10.89$. The numerical results are illustrated in Figs. 1 and 2.

Figure 1 plots the curves of the binding energies of the bound polaron with and without phonon contributions, respectively, as functions of the well-width in the finite $GaAs/Al_{0.3}Ga_{0.7}As$ PQW. The binding energies of the bound polaron increase with the well-width at the beginning, rapidly reach maxima at around 7nm, and finally approach the 3D values when the well-width is large enough. Moreover, the binding energies are reduced by the electron-phonon interaction because of the phonon screening on the Coulomb potential. The shift of the binding energies caused by the electron-phonon coupling is around 20% ~ 30% for the calculated system. Therefore, the electron-phonon coupling effect is observable and should be considered in discussing the electronic states in PQWs.

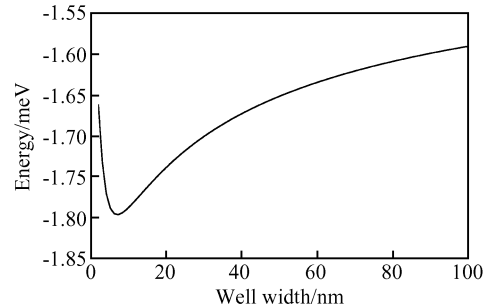

Fig. 2　Contribution of LO phonons to the binding energy of the bound polaron as a function of the well-width in the finite PQW

To clarify the effect of electron-phonon interaction, Figure 2 illustrates the contribution of LO phonons to the binding energy of the bound polaron in the same system as a function of the well-width. The electron-phonon coupling effect first increases and achieves a maximum (around 1.79meV) at around 7nm as the well-width increases, and drops slowly. It is understood that the penetration of the electron wave function into the barriers becomes important when the well is narrow enough, and the electron-phonon coupling effect is reduced to the binding energy.

4　Conclusion

In summary, we have extended a fractional-dimensional method in combination with a LLP-like transformation and a variational treatment to calculate the binding energy of a bound polaron in finite parabolic quantum wells. The numerical results for the $GaAs/Al_{0.3}Ga_{0.7}As$ parabolic quantum well are obtained and discussed. The binding energies of the bound polaron and the phonon contribution reach their maxima as the well-width increases. The binding energy of the bound polaron is reduced by the electron-phonon interaction, and the phonon contribution is observable and cannot be neglected.

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抛物量子阱中的束缚极化子:分维变分方法*

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摘要: 采用分维变分方法讨论了有限深抛物量子阱中束缚极化子的束缚能,得到了束缚能随阱宽的变化关系,并给出了声子对束缚能的贡献随阱宽的变化曲线.数值计算的结果表明,束缚极化子的束缚能随阱宽的增大存在一极大值,电子-声子的相互作用使束缚极化子的束缚能显著降低,声子的贡献不可忽略.

关键词: 束缚极化子; 束缚能; 抛物量子阱
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