Bound polaron in a cylindrical quantum wire of a polar crystal

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The impurity binding energy in a cylindrical quantum wire was studied by the variational approach. A two-parameter trial wave function was proposed to reflect the anisotropsy of the quantum wire. We have also derived the electron-phonon interaction Hamiltonians for the confined longitudinal optical phonon modes and the interface phonon (IO) modes in the cylindrical quantum wire. The influence of different phonon modes on the impurity binding energy was studied. Numerical calculation shows that the impurity binding energy increases greatly as the radius of the quantum wire decreases and is strongly modified by the electron-phonon interaction, especially by the electron-IO phonon interaction.

I. INTRODUCTION

The great progress in semiconductor nanotechnology, such as molecular-beam epitaxy, metal-organic chemical-vapor deposition, and chemical lithography, has made possible the realization of a wide variety of semiconductor heterostructures. Among which, the quantum-well wire (QWW) is of great interest to many authors. In the past decade, the study on the electronic structure, transport properties, excitonic and impurity levels, as well as impurity binding energies in the QWW has been carried out both experimentally[1–3] and theoretically.[4–6] Brown and Spector [6] studied the hydrogenlike impurities in a QWW, considering both the infinite and finite confined potential models. Villamil and Montenegro[4] investigated the binding and transition energies of the hydrogenlike donor impurity states with the influence of the magnetic field. One of the quantum-mechanical approaches being used in studying the impurity state in a QWW is the variational method. In the works mentioned above, the trial variational wave functions with one variational parameter were adopted. However, it is clear that the QWW system is not isotropic. A better variational wave function should be able to reflect this anisotropic nature of the QWW system. Actually, we have proposed two-parameter trial wave functions when we studied the quasi-two-dimensional systems (quantum wells).[7–9] Results showed that the two variational parameters, which reflect the anisotropy of the quantum-well structure, are quite different when the well is narrow. They are identical when the well is sufficiently wide, indicating that the system is now isotropic in nature. So, in the present paper, we will propose a two-parameter variational trial wave function to calculate the ground-state binding energy of an impurity in a cylindrical QWW.

It is also well known that the electron-optical phonon interaction plays an important role in the physical properties of the polar crystals. Research on the polaron effect on the quantum-well and quantum dot systems shows that the influence of the interface phonon could be enhanced and even become dominating as the dimensionality of the material reduces.[10,11] The polaron effect should not be ignored when studying the quantum wire systems. However, as far as we know, there is no paper devoted to the polaron or bound polaron properties in the quantum wire system. Of course, before investigating the polaron effect in a quantum wire, the phonon vibration modes in the quantum wire should be derived in advance. The electron-phonon interaction in a dielectric confined system was first studied by Lucas *et al.*[12] and Licari and Evrard[13] under the dielectric continuum model. Wendler[14] developed the framework of the theory of optical phonons and electron-phonon interaction for the spatially confined systems. Constantinou and Ridley[15] worked out the phonon modes in a $GaAs/Al_xGa_{1-x}As$ quantum wire. Recently, Wang and Lei[16] studied the scattering of electrons by different phonon modes in semiconductor nanostructures; Campos, Das Sarma, and Stroscio[17] also studied the influence of phonons on electron transport in a quantum wire. But the electron-phonon interaction Hamiltonians developed by Wang and Lei, and Campos, Das Sarma, and Stroscio are devoted to the many-electron processes of transport, so are not quite suitable for the situation being considered here. Recently, Li and Chen[18] obtained the phonon modes in a cylindrical quantum dot by using the dielectric continuum model. We shall use the dielectric continuum model to derive the confined longitudinal-optical (LO) phonon modes and the interface optical (IO) phonon modes as well as the Hamiltonians of their interaction with electrons.

It should be noted that the image potential induced by the charged particles may influence the properties of electrons in the quantum wire, especially when the quantum wire is narrow.[19,20] Wendler and Harbwig[21] studied the effect of the image potential on the binding energy of hydrogenic impu-

rities in semiconductor quantum wells. They took all image contributions (the mutual image potential between the hydrogenic impurity and the electron and the self-image potentials of the two particles) into consideration and concluded that the image potential effects on the hydrogenic donor binding energy are weak for donor positions in the center of the quantum well. Therefore, for simplicity, in the present work, we shall not consider the influence of image potential but focus our attention on that of the polaron effect on the impurity binding energy in a quantum wire.[4,6,9,22]

In the following, we will investigate the impurity binding energy in a cylindrical QWW, derive the free phonon Hamiltonians and the Fröhlich electron-phonon interaction Hamiltonians, and study the polaron effect on the impurity binding energy by taking both the confined LO modes and IO modes into consideration. We will first study the impurity ground-state binding energy in Sec. II, then derive the phonon Hamiltonians and the Fröhlich electron-phonon interaction Hamiltonians in Sec. III. The influence of different phonon modes on the impurity binding energy is studied in Sec. IV. In Sec. V is the numerical calculation and discussion. Finally, a brief summary is given in Sec. VI.

2. IMPURITY BINDING ENERGY

Let us consider a polar semiconductor cylindrical quantum wire with radius R. It is convenient to adopt the cylindrical coordinate in this system. The impurity is located at ρ_i (taking the wire axis as the origin). Under the effective-mass approximation, the Hamiltonian of the system can be written as (neglecting the image effect)

$$H_e=-\frac{\hbar^2}{2m^*}\nabla^2-\frac{e^2}{\epsilon|\mathbf{r}-\mathbf{r}_i|}+V(\rho) \tag{1}$$

with

$$V(\rho)=\begin{cases}\infty, & \rho\geqslant R\\ 0, & \rho<R.\end{cases}$$

In order to construct an appropriate variational wave function, let us first consider the electron wave function in a cylindrical quantum wire with no impurity presented, i.e., find out the solution to the following Schrödinger equation: $(\rho<R)$

$$\frac{\hbar^2}{2m^*}\left[-\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)-\frac{\partial^2}{\partial z^2}\right]\psi(\rho,z)=E_0\psi(\rho,z). \tag{2}$$

The solution turned out to be

$$\psi(\rho,z)=R(\rho)\exp[iqz]\sim J_0(\sqrt{2m^*E_0/\hbar^2}\rho)\exp[iqz], \tag{3}$$

where $J_0(x)$ is the Bessel function of the zeroth order. The energy level is given by

$$E_0^l=\frac{\hbar^2(\chi_0^l)^2}{2m^*R^2}, \tag{4}$$

where χ_0^l is the lth zero of $J_0(x)$. For the ground state, $E_0^1=(\hbar\chi_0^1)^2/2m^*R^2$.

Based on the above result, considering the anisotropy of the quantum wire system, we propose a trial wave function with two variational parameters for Eq. (1):

$$\Phi(\rho,z)=NJ_0\left(\frac{\chi_0^1\rho}{R}\right)\exp[-\sqrt{\lambda^2|\rho-\rho_i|^2+\mu^2z^2}] \tag{5}$$

where λ and μ are variational parameters characterizing the anisotropy in the ρ and z directions. N is the normalized constant defined by

$$N^2\int\left[J_0\left(\frac{\chi_0^1\rho}{R}\right)\right]^2\times\exp[-2\sqrt{\lambda^2|\rho-\rho_i|^2+\mu^2z^2}]\rho\,d\rho\,d\varphi\,dz=1 \tag{6}$$

or

$$N^2\int\left[J_0\left(\frac{\chi_0^1\rho}{R}\right)\right]^2\frac{2\lambda|\rho-\rho_i|}{\mu}K_1(2\lambda|\rho-\rho_i|)\rho\,d\rho\,d\varphi=1 \tag{7}$$

where $K_1(x)$ is the second kind modified Bessel function of the first order.

The expectation value of H_e is given by

$$\langle\Phi(\rho,z)|H_e|\Phi(\rho,z)\rangle=T+U \tag{8}$$

with

$$\begin{aligned}T=&\frac{(\hbar\chi_0^1)^2}{4m^*R^2}-\frac{\hbar^2\lambda^2}{2m^*}+\frac{4\hbar^2\lambda^2N^2}{2m^*\mu}\int[J_0(\chi_0^1\rho/R)]^2K_0(2\lambda|\rho-\rho_i|)\rho\,d\rho\,d\varphi\\&-\frac{4\hbar^2\chi_0^1N^2\lambda^2}{2m^*\mu}\int J_0\left(\frac{\chi_0^1\rho}{R}\right)J_1\left(\frac{\chi_0^1\rho}{R}\right)K_0(2\lambda|\rho-\rho_i|)(\rho-\rho_i\cos\varphi)\rho\,d\rho\,d\varphi\\&+\frac{2\hbar^2\lambda N^2}{2m^*\mu}\int J_0\left(\frac{\chi_0^1\rho}{R}\right)\left[\frac{\chi_0^1}{R}J_1\left(\frac{\chi_0^1\rho}{R}\right)-\frac{(\chi_0^1)^2\rho}{2R^2}J_2\left(\frac{\chi_0^1\rho}{R}\right)\right]K_1(2\lambda|\rho-\rho_i|)|\rho-\rho_i|d\rho\,d\varphi\\&+\frac{\hbar^2(\mu^2-\lambda^2)}{2m^*}N^2\int\left[J_0\left(\frac{\chi_0^1\rho}{R}\right)\right]^2\mu^2z^2\frac{\exp[-2\sqrt{\lambda^2|\rho-\rho_i|^2+\mu^2z^2}]}{\lambda^2|\rho-\rho_i|^2+\mu^2z^2}\rho\,d\rho\,d\varphi\,dz\end{aligned} \tag{9}$$

and

$$U=-\frac{2N^2e^2}{\epsilon}\int\left[J_0\left(\frac{\chi_0^1\rho}{R}\right)\right]^2\frac{\exp[-2\sqrt{\lambda^2|\rho-\rho_i|^2+\mu^2z^2}]}{\sqrt{|\rho-\rho_i|^2+z^2}}\rho\,d\rho\,d\varphi\,dz\,. \tag{10}$$

The ground-state energy of the impurity state is obtained by minimizing the expectation value of the Hamiltonian H_e according to the variational parameters λ and μ:

$$E=\min_{\mu,\lambda}\langle\Phi(\rho,z)|H_e|\Phi(\rho,z)\rangle\,. \tag{11}$$

The impurity binding energy is given by

$$E_b=E_0^1-E=(\hbar\chi_0^1)^2/2m^*R^2-E\,. \tag{12}$$

3. THE ELECTRON-PHONON INTERACTION HAMILTONIAN

Before we proceed to investigate the influence of the electron-phonon interaction on the impurity, we should derive the phonon Hamiltonian as well as the electron-phonon interaction Hamiltonian for the cylindrical quantum wire first. This is also of practical interest to other phonon-attending processes such as the scattering of conducting electrons by phonons.

We will use the dielectric continuum model and start with the electrostatic equations

$$\nabla\cdot\mathbf{D}=4\pi\rho_0(\mathbf{r}), \tag{13}$$

$$\mathbf{D}=\epsilon\mathbf{E}=\mathbf{E}+4\pi\mathbf{P}, \tag{14}$$

$$\mathbf{E}=-\nabla\phi(\mathbf{r}), \tag{15}$$

where $\rho_0(\mathbf{r})$ is the charge density. For free oscillation (i.e., $\rho_0=0$), we have

$$\epsilon\nabla^2\phi(\mathbf{r})=0. \tag{16}$$

A. Confined LO phonon modes

There are two solutions for Eq. (16). The first is $\epsilon=0$ inside the wire. Since

$$\epsilon(\omega)=\epsilon_\infty+\frac{\epsilon_0-\epsilon_\infty}{1-\omega^2/\omega_{\mathrm{TO}}^2} \tag{17}$$

$\epsilon(\omega)=0$ gives

$$\omega^2=\omega_{\mathrm{TO}}^2\frac{\epsilon_0}{\epsilon_\infty}=\omega_{\mathrm{LO}}^2, \tag{18}$$

in which we have made use of the Lyddane-Sachs-Teller relation, i.e., for the solution of $\epsilon(\omega)=0$, one obtained a bulk LO phonon vibration mode. The eigen function of the confined LO mode inside the wire can be chosen as

$$\phi_{ml}(r)=\begin{cases}C_{ml}J_m(Q_{ml}\rho)\exp[im\varphi]\exp[iq_zz], & \rho\leqslant R\\ 0, & \rho>R\end{cases} \tag{19}$$

where $J_m(x)$ is the Bessel function of the mth order, and $Q_{ml}=\chi_m^l/R$, where χ_m^l is the lth zero of $J_m(x)$.

The polarization vectors for the confined LO mode are

$$\begin{aligned}\mathbf{P}_{\mathrm{LO}}^{ml}&=\frac{1}{4\pi}\nabla\phi_{ml}(r)\\&=\frac{C_{ml}}{4\pi}\left\{\frac{1}{2}[J_{m-1}(Q_{ml}\rho)-J_{m+1}(Q_{ml}\rho)]Q_{ml}\mathbf{e}_\rho\right.\\&\quad+J_m(Q_{ml}\rho)\frac{im}{\rho}\mathbf{e}_\varphi\\&\quad\left.+J_m(Q_{ml}\rho)iq_z\mathbf{e}_z\right\}\mathbf{e}^{im\varphi}\mathbf{e}^{iq_zz}.\end{aligned} \tag{20}$$

To find the expression for the Hamiltonian of the free-phonon field, we start from the dynamic equations of motion of the crystal lattice:

$$\mu\ddot{\mathbf{u}}=-\mu\omega_0^2\mathbf{u}+e\mathbf{E}_{\mathrm{loc}}, \tag{21}$$

$$\mathbf{P}=ne\mathbf{u}+n\alpha\mathbf{E}_{\mathrm{loc}}, \tag{22}$$

where μ is the reduced mass of the ion pair and $\mathbf{u}=\mathbf{u}_+-\mathbf{u}_-$ is the relative displacement of the positive and negative ions, ω_0 is the frequency associated with the short-range force between ions, $\mathbf{E}_{\mathrm{loc}}$ is the local field at the position of the ions, n is the number of ion pairs per unit volume, and α is the electronic polarizability per ion pair.

The Hamiltonian of the free vibration is given by

$$H_{\mathrm{ph}}=\frac{1}{2}\int[n\mu\dot{\mathbf{u}}\cdot\dot{\mathbf{u}}+n\mu\omega_0^2\mathbf{u}\cdot\mathbf{u}-ne\mathbf{u}\cdot\mathbf{E}_{\mathrm{loc}}]d^3r. \tag{23}$$

Since

$$\mathbf{E}_{\mathrm{loc}}=-\frac{8}{3}\pi\mathbf{P} \tag{24}$$

we have

$$\mathbf{u}=\frac{1+\frac{8}{3}\pi n\alpha}{ne}\mathbf{P} \tag{25}$$

then we may write

$$\begin{aligned}H_{\mathrm{LO}}=\frac{1}{2}\int\left[n\mu\left(\frac{1+\frac{8}{3}\pi n\alpha}{ne}\right)^2\dot{\mathbf{P}}^*\cdot\dot{\mathbf{P}}\right.\\\left.+n\mu\omega_{\mathrm{LO}}^2\left(\frac{1+\frac{8}{3}\pi n\alpha}{ne}\right)^2\mathbf{P}^*\cdot\mathbf{P}\right]d^3r.\end{aligned} \tag{26}$$

Since

$$\int \mathbf{P}_{\mathrm{LO}}^{m'l'*}\cdot\mathbf{P}_{\mathrm{LO}}^{ml}d^3r=|C_{ml}|^2\frac{L}{8\pi}\left\{\frac{1}{2}(\chi_m^{l^2}+R^2q_z^2)J_{m+1}^2(\chi_m^l)\right\}\times\delta_{mm'}\delta_{ll'}\delta_{q_zq_z'}, \tag{27}$$

where L is the length of the quantum wire. If we choose C_{ml} to be

$$C_{ml}=\left(\frac{8\pi}{n\mu L}\right)^{1/2}\frac{ne}{1+\frac{8}{3}\pi n\alpha}\times\left\{\frac{1}{2}(\chi_m^{l^2}+R^2q_z^2)J_{m+1}^2(\chi_m^l)\right\}^{-1/2} \tag{28}$$

then P_{LO}^{ml} may form an orthonormal and complete set, which can be used to express $\mathbf{P}$ in

$$\mathbf{P}=\sum_{mlq_z}\left(\frac{\hbar}{\omega_{\mathrm{LO}}}\right)^{1/2}[a_{ml}(q_z)+a_{ml}^{\dagger}(q_z)]\mathbf{P}_{\mathrm{LO}}^{ml}(\mathbf{r}), \tag{29}$$

$$\dot{\mathbf{P}}=-i\sum_{mlq_z}(\hbar\omega_{\mathrm{LO}})^{1/2}[a_{ml}(q_z)-a_{ml}^{\dagger}(q_z)]\mathbf{P}_{\mathrm{LO}}^{ml}(\mathbf{r}). \tag{30}$$

$\mathbf{P}$ and $\dot{\mathbf{P}}$ are now quantum field operators. $a_{ml}^{\dagger}(q_z)$ and $a_{ml}(q_z)$ are the creation and annihilation operators for the LO phonon of the mlq_z mode. They satisfy

$$[a_{ml}(q_z),a_{m'l'}^{\dagger}(q_z')]=\delta_{mm'}\delta_{ll'}\delta_{q_zq_z'}, \tag{31}$$

$$[a_{ml}(q_z),a_{m'l'}(q_z')]=[a_{ml}^{\dagger}(q_z),a_{m'l'}^{\dagger}(q_z')]=0. \tag{32}$$

Then the Hamiltonian operator for the confined LO phonons will be

$$H_{\mathrm{LO}}=\sum_{mlq_z}\hbar\omega_{\mathrm{LO}}\left[a_{ml}^{\dagger}(q_z)a_{ml}(q_z)+\frac{1}{2}\right]. \tag{33}$$

The interaction Hamiltonian between the electron and the phonon field is

$$H_{e\text{-ph}}=-e\phi(\mathbf{r}). \tag{34}$$

$\phi(\mathbf{r})$ could be expanded in terms of the normal modes, so

$$H_{e\text{-LO}}=-\sum_{mlq_z}\left[\Gamma_{\mathrm{LO}}^{ml}(q_z)J_m\left(\frac{\chi_m^l\rho}{R}\right)\mathbf{e}^{im\varphi}\mathbf{e}^{-iq_zz}a_{ml}^{\dagger}(q_z)+\mathrm{H.c.}\right], \tag{35}$$

where

$$|\Gamma_{\mathrm{LO}}^{ml}|^2=\frac{4e^2\hbar\omega_{\mathrm{LO}}}{LJ_{m+1}^2(\chi_m^l)(\chi_m^{l^2}+R^2q_z^2)}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right). \tag{36}$$

B. Interface phonon modes

Another solution for Eq. (16) is

$$\nabla^2\phi(\mathbf{r})=0. \tag{37}$$

This will give the IO modes with $\epsilon\neq0$ inside the quantum wire. The solution for Eq. (37) is

$$\phi(\mathbf{r})=A_m\mathbf{e}^{im\varphi}\mathbf{e}^{iq_zz}\begin{cases}K_m(q_zR)I_m(q_z\rho), & \rho\leqslant R\\ I_m(q_zR)K_m(q_z\rho), & \rho>R\end{cases} \tag{38}$$

where $K_m(x)$ and $I_m(x)$ are the first and second kind modified Bessel functions, respectively. The boundary condition at $\rho=R$ is (suppose the material outside the quantum wire is nonpolar material with dielectric constant ϵ_d)

$$\epsilon(\omega)\frac{\partial\phi_1}{\partial\rho}=\epsilon_d\frac{\partial\phi_2}{\partial\rho}. \tag{39}$$

Then we get

$$\epsilon(\omega)=-\frac{I_m(q_zR)[K_{m-1}(q_zR)+K_{m+1}(q_zR)]}{K_m(q_zR)[I_{m-1}(q_zR)+I_{m+1}(q_zR)]}\epsilon_d. \tag{40}$$

The frequency of the IO vibration can be obtained through Eq. (17), i.e.,

$$\omega^2=\left[1+\frac{\epsilon_0-\epsilon_\infty}{\epsilon_\infty-\epsilon}\right]\omega_{\mathrm{TO}}^2. \tag{41}$$

The polarization field for the IO phonon modes are

$$\begin{aligned}\mathbf{P}_{\mathrm{IO}}^m&=\frac{1-\epsilon}{4\pi}\nabla[A_mK_m(q_zR)I_m(q_z\rho)\mathbf{e}^{im\varphi}\mathbf{e}^{iq_zz}]\\&=\frac{1-\epsilon}{4\pi}A_mK_m(q_zR)\left\{\frac{1}{2}q_z[I_{m-1}(q_z\rho)+I_{m+1}(q_z\rho)]\mathbf{e}_\rho+\frac{im}{\rho}I_m(q_z\rho)\mathbf{e}_\varphi+iq_zI_m(q_z\rho)\mathbf{e}_z\right\}\mathbf{e}^{im\varphi}\mathbf{e}^{iq_zz}.\end{aligned} \tag{42}$$

From Eqs. (21) and (22), we have

$$\mathbf{E}_{\mathrm{loc}}=\frac{\mu}{e}(\omega_0^2-\omega^2)\mathbf{u}, \tag{43}$$

$$\mathbf{u}=\frac{\mathbf{P}}{ne[1+(\alpha\mu/e^2)(\omega_0^2-\omega^2)]}. \tag{44}$$

Following Eq. (23), we obtain the Hamiltonian for the IO phonon

$$H_{\mathrm{IO}}=\frac{1}{2}\int d^3r\left[n\mu\left(\frac{1}{ne[1+(\alpha\mu/e^2)(\omega_0^2-\omega^2)]}\right)^2\dot{\mathbf{P}}^*\cdot\dot{\mathbf{P}}+n\mu\omega^2\left(\frac{1}{ne[1+(\alpha\mu/e^2)(\omega_0^2-\omega^2)]}\right)^2\mathbf{P}^*\cdot\mathbf{P}\right]. \tag{45}$$

Since

$$\int \mathbf{P}_{\mathrm{IO}}^{m*}\cdot\mathbf{P}_{\mathrm{IO}}^{m'}d^3r=\frac{(1-\epsilon)^2q_zRL}{16\pi}A_m^2K_m^2(q_zR)I_m(q_zR)\times\left[\frac{q_zR}{2(m-1)}[I_{m-2}(q_zR)-I_m(q_zR)]+\frac{q_zR}{2(m+1)}([I_m(q_zR)-I_{m+2}(q_zR)]\right]\delta_{mm'}\delta_{q_zq_z'}. \tag{46}$$

We may choose A_m to be

$$|A_m|^2=\frac{n^2e^2[1+(\alpha\mu/e^2)(\omega_0^2-\omega^2)]^2}{n\mu(1-\epsilon)^2}\times\frac{16\pi}{LK_m^2(q_zR)I_m(q_zR)q_zR[I_{m-1}(q_zR)-I_{m+1}(q_zR)]}, \tag{47}$$

or

$$|A_m|^2=\frac{4\omega^2}{LK_m^2(q_zR)I_m(q_zR)q_zR[I_{m-1}(q_zR)-I_{m+1}(q_zR)]}\times\left[\frac{1}{\epsilon-\epsilon_0}-\frac{1}{\epsilon-\epsilon_\infty}\right] \tag{48}$$

in which we have made use of the following relations:[13]

$$\omega_p^2=4\pi ne^2/\mu, \tag{49}$$

$$1-\frac{4}{3}\pi n\alpha=\frac{\omega_p}{\omega_{\mathrm{TO}}}\frac{1}{\sqrt{\epsilon_0-\epsilon_\infty}}, \tag{50}$$

$$1+\frac{8}{3}\pi n\alpha=\frac{\omega_p}{\omega_{\mathrm{TO}}}\frac{\epsilon_\infty}{\sqrt{\epsilon_0-\epsilon_\infty}}. \tag{51}$$

Then $\mathbf{P}_{\mathrm{IO}}^m$ may form an orthonormal and complete set. We may express $\mathbf{P}$ as

$$\mathbf{P}=\sum_{mq_z}\left(\frac{\hbar}{\omega}\right)^{1/2}[b_m(q_z)+b_m^\dagger(q_z)]\mathbf{P}_{\mathrm{IO}}^m, \tag{52}$$

$$\dot{\mathbf{P}}=-i\sum_{mq_z}(\hbar\omega)^{1/2}[b_m(q_z)-b_m^\dagger(q_z)]\mathbf{P}_{\mathrm{IO}}^m, \tag{53}$$

where $b_m^\dagger(q_z)$ and $b_m(q_z)$ are the creation and annihilation operators of the IO phonon with frequency ω. They satisfy

$$[b_m(q_z),b_{m'}^\dagger(q_z')]=\delta_{mm'}\delta_{q_zq_z'}, \tag{54}$$

$$[b_m(q_z),b_{m'}(q_z')]=[b_m^\dagger(q_z),b_{m'}^\dagger(q_z')]=0. \tag{55}$$

The Hamiltonian operator for the IO phonons is

$$H_{\mathrm{IO}}=\sum_{mq_z}\hbar\omega\left[b_m^\dagger(q_z)b_m(q_z)+\frac{1}{2}\right]. \tag{56}$$

Following Eq. (34) we get

$$H_{e\text{-IO}}=-\sum_{mq_z}[\Gamma_{\mathrm{IO}}^m(q_z)\mathbf{e}^{im\varphi}\mathbf{e}^{-iq_zz}b_m^\dagger(q_z)+\mathrm{H.c.}]\times\begin{cases}K_m(q_zR)I_m(q_z\rho), & \rho\leqslant R\\ I_m(q_zR)K_m(q_z\rho), & \rho>R\end{cases} \tag{57}$$

where

$$|\Gamma_{\mathrm{IO}}^m|^2=\frac{4e^2\hbar\omega}{LK_m^2(q_zR)I_m(q_zR)q_zR[I_{m-1}(q_zR)+I_{m+1}(q_zR)]}\times\left(\frac{1}{\epsilon-\epsilon_0}-\frac{1}{\epsilon-\epsilon_\infty}\right). \tag{58}$$

IV. THE BOUND POLARON BINDING ENERGY

Now we consider the polaron effect on the impurity (which is known as bound polaron) state. The Hamiltonian of the system can be written as

$$H=H_e+H_{\mathrm{ph}}+H_{e\text{-ph}}, \tag{59}$$

where H_e, which is the impurity Hamiltonian, is given in Eq. (1). The second term is the phonon Hamiltonian:

$$H_{\mathrm{ph}}=H_{\mathrm{LO}}+H_{\mathrm{IO}}=\sum_{mlq_z}\hbar\omega_{\mathrm{LO}}[a_{ml}^\dagger(q_z)a_{ml}(q_z)+\tfrac{1}{2}]+\sum_{mq_z}\hbar\omega[b_m^\dagger(q_z)b_m(q_z)+\tfrac{1}{2}]. \tag{60}$$

The third term is the electron-phonon interaction Hamiltonian given by

$$H_{e\text{-ph}}=H_{e\text{-LO}}+H_{e-\mathrm{IO}} \tag{61}$$

in which $H_{e\text{-LO}}$ and $H_{e\text{-IO}}$ are given by Eqs. (34) and (57), respectively. We will use the variational method in our calculation. The trial wave function is chosen to be

$$|\Psi\rangle=\Phi(\rho,z)S|0\rangle. \tag{62}$$

$\Phi(\rho,z)$ is given in equation (5), $|0\rangle$ is the phonon vacuum state, while S is defined by

$$S=\exp\left(\sum_{mlq_z}[f_{ml}^{\mathrm{LO}}(q_z)a_{ml}^\dagger(q_z)-f_{ml}^{\mathrm{LO}*}(q_z)a_{ml}(q_z)]+\sum_{mq_z}[f_m^{\mathrm{IO}}(q_z)b_m^\dagger(q_z)-f_m^{\mathrm{IO}*}(q_z)b_m(q_z)]\right). \tag{63}$$

The unitary operator S transforms the phonon operator as follows:

$$S^\dagger a_{ml}^\dagger(q_z)S=a_{ml}^\dagger(q_z)+f_{ml}^{\mathrm{LO}*}(q_z), \tag{64}$$

$$S^\dagger a_{ml}(q_z)S=a_{ml}(q_z)+f_{ml}^{\mathrm{LO}}(q_z). \tag{65}$$

$$S^\dagger b_m^\dagger(q_z)S=b_m^\dagger(q_z)+f_m^{\mathrm{IO}*}(q_z), \tag{66}$$

$$S^\dagger b_m(q_z)S=b_m(q_z)+f_m^{\mathrm{IO}}(q_z). \tag{67}$$

The expectation value of H is

$$\langle\Psi|H|\Psi\rangle = T+U+\sum_{ml q_z}|f_{ml}^{\mathrm{LO}}(q_z)|^2+\sum_{m q_z}|f_m^{\mathrm{IO}}(q_z)|^2 + \sum_{ml q_z}\left[\Gamma_{\mathrm{LO}}^{ml}(q_z)\langle\Phi(\rho,z)|J_m\left(\frac{\chi_m^l\rho}{R}\right)\times\mathbf{e}^{im\varphi}\mathbf{e}^{-iq_z z}|\Phi(\rho,z)\rangle+\mathrm{H.c.}\right]+\sum_{m q_z}[\Gamma_{\mathrm{IO}}^{m}(q_z)\times\langle\Phi(\rho,z)|g(q_z,\rho)\mathbf{e}^{im\varphi}\mathbf{e}^{-iq_z z}|\Phi(\rho,z)\rangle+\mathrm{H.c.}] \tag{68}$$

where

$$g(q_z,\rho)=\begin{cases}K_m(q_zR)I_m(q_z\rho), & \rho\leqslant R\\ I_m(q_zR)K_m(q_z\rho), & \rho>R.\end{cases} \tag{69}$$

Minimizing $\langle\Psi|H|\Psi\rangle$ with respect to $f_{ml}^{\mathrm{LO}*}(q_z)$ and $f_m^{\mathrm{IO}*}(q_z)$, respectively, one obtains

$$f_{ml}^{\mathrm{LO}}(q_z)=-\Gamma_{ml}^{\mathrm{LO}}(q_z)\langle\Phi(\mathbf{r})|J_0\left(\frac{\chi_m^l}{R}\rho\right)\mathbf{e}^{im\varphi}\mathbf{e}^{-iq_z z}|\Phi(\mathbf{r})\rangle, \tag{70}$$

$$f_m^{\mathrm{IO}}(q_z)=-\Gamma_m^{\mathrm{IO}}(q_z)\langle\Phi(\mathbf{r})|g(q_z,\rho)\mathbf{e}^{im\varphi}\mathbf{e}^{-iq_z z}|\Phi(\mathbf{r})\rangle. \tag{71}$$

Inserting Eqs. (70) and (71) into Eq. (68), we get

$$\langle\Psi|H|\Psi\rangle = T+U-\Delta E_{\mathrm{LO}}-\Delta E_{\mathrm{IO}} \tag{72}$$

with

$$\Delta E_{\mathrm{LO}}=\sum_{ml q_z}\frac{1}{\hbar\omega_{\mathrm{LO}}}|\Gamma_{ml}^{\mathrm{LO}}(q_z)|^2\times\left|\langle\Phi(\mathbf{r})|J_0\left(\frac{\chi_m^l}{R}\rho\right)\mathbf{e}^{im\varphi}\mathbf{e}^{-iq_z z}|\Phi(\mathbf{r})\rangle\right|^2 \tag{73}$$

and

$$\Delta E_{\mathrm{IO}}=\sum_{m q_z}\frac{1}{\hbar\omega}|\Gamma_m^{\mathrm{IO}}(q_z)|^2\times|\langle\Phi(\mathbf{r})|g(q_z,\rho)\mathbf{e}^{im\varphi}\mathbf{e}^{-iq_z z}|\Phi(\mathbf{r})\rangle|^2. \tag{74}$$

T and U are defined in Eqs. (9) and (10), respectively. The ground-state energy of the system is calculated by Eq. (72):

$$E=\min_{\lambda,\mu}\langle\Psi|H|\Psi\rangle. \tag{75}$$

Similar to Sec. II, the impurity binding energy with phonon contribution is given by

$$E_b=E_0^1-E=(\hbar\chi_0^1)^2/2m^*R^2-E \tag{76}$$

but the meaning of E is not the same as that in Eq. (12)

V. RESULT AND DISCUSSION

B. Impurity binding energy

We performed numerical calculation on the impurity binding energy with Eqs. (8)–(11). In Fig. 1, we plotted the impurity binding energy (solid line) as a function of the radius of the QWW (R), the impurity is at the center. We chose the effective atomic unit so that the unit of length is the effective Bohr radius $a_0^*=\epsilon\hbar^2/m^*e^2$ and the unit of energy is the effective Rydberg $R_g=m^*e^4/2\hbar^2\epsilon^2$, which are about 100 Å and 5.25 meV, respectively, for GaAs. We can see from Fig. 1 that the impurity binding energy declines as the radius of the QWW R increases, and approaches 1 R_g, which is the three-dimensional limit, when the radius of the QWW is quite large. The variational parameters μ and λ changes with changing R (see Fig. 2). They are not the same until the radius R is sufficiently large (see the curve of μ/λ in Fig. 2) indicating that the system of QWW is not isotropic in most of the cases. The ratio μ/λ increases quickly as the radius R reduces, showing that the system is approaching the one-dimensional limit as the radius of the QWW reduces. In Fig. 3 we compare our results with that of Brown and Spector,[6] which was obtained based on a one-parameter trial wave function. We could see that for the quantum wire with large radius, the two methods give the same value for the impurity binding energy. However, when the quantum wire is narrow, the difference between the two methods becomes obvious. Our method gives a larger impurity binding energy (about 6% higher than that of Brown and Spector), or, a lower impurity ground-state energy. According to the variational principle of quantum mechanics, the present method gives a better result. So it is quite necessary to adopt biparameter variational trial wave function for the low-dimensional systems such as the quantum wire and quantum-well structures. In Fig. 4, we plotted the impurity binding energy as a function of the impurity position; the radius of the QWW is 1 a_0^*. One could find out that the impurity binding energy decreases as the impurity shifts away from the center. We have also plotted the impurity binding energy as a function of the radius R when the impurity positions at $\rho_i=0.5R$ (see

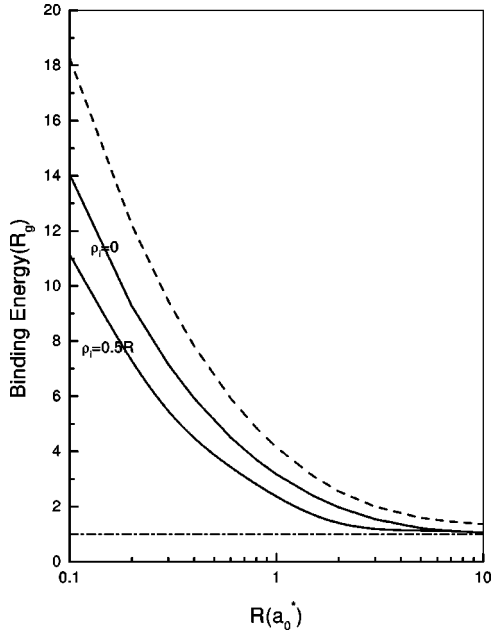

FIG. 1. The binding energies of impurity, without phonon contribution (solid curves); and bound polaron, i.e, with phonon contribution (dashed curve) as functions of the radius of the quantum wire.

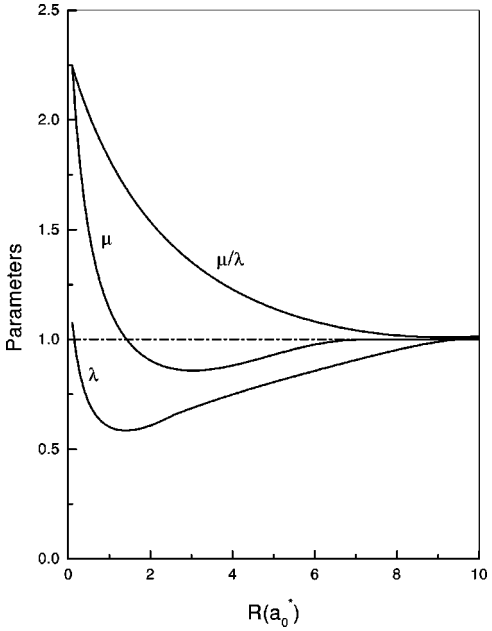

FIG. 2. Variational parameters as functions of the radius of the quantum wire.

Fig. 1). We could see that the binding energy is smaller for an off-center impurity compared with that when the impurity is at the center of the quantum wire. However, this difference vanishes when R is large, showing that the system is now three dimensional in nature, consequently the translational symmetry holds.

B. Bound polaron binding energy

The calculation of the bound polaron binding energy was carried out for a free-standing QWW of GaAs. The parameters of the wire material are $m^*=0.067m_0$ (m_0 is the free-electron mass), $\hbar\omega_{\mathrm{LO}}=36.25$ meV, $\hbar\omega_{\mathrm{TO}}=33.29$ meV, $\epsilon_0=13.18$, $\epsilon_\infty=10.89$. The impurity binding energy with the influence of the LO and IO phonons, which is also called the bound polaron binding energy, is calculated as a function of the radius R. In order to show the phonon influence on the impurity binding energy, we plotted the bound polaron binding energy (dashed curve; $\rho_i=0$) together with that without phonon contribution in Fig. 1. We have to convert the energy unit from meV to R_g so that they are comparable. Results show that the phonon influence becomes stronger as radius R decreases. The phonon contribution to the binding energy could reach as high as 23.1% at very narrow GaAs QWW. It should be noted that the coupling between the electron and

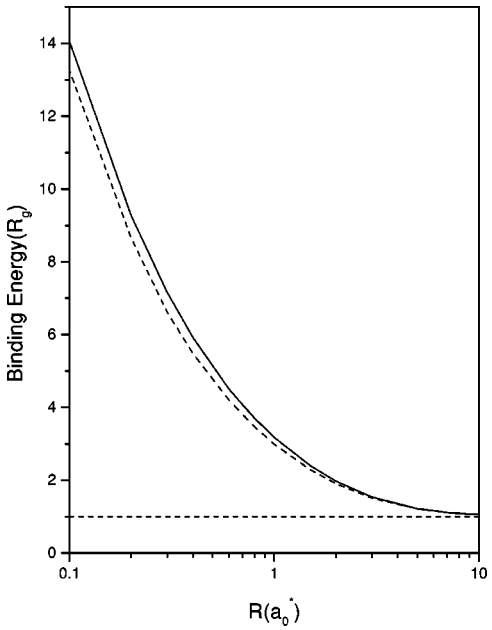

FIG. 3. The impurity binding energy calculated by using different variational trial wave functions. Solid line, this work; dashed line, Brown and Spector.

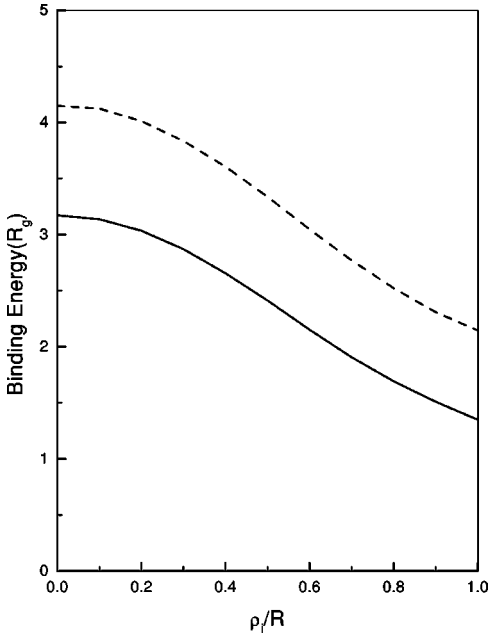

FIG. 4. Binding energies of: impurity (solid curve) and bound polaron (dashed curve) as functions of the impurity position at $R=1a_0^*$.

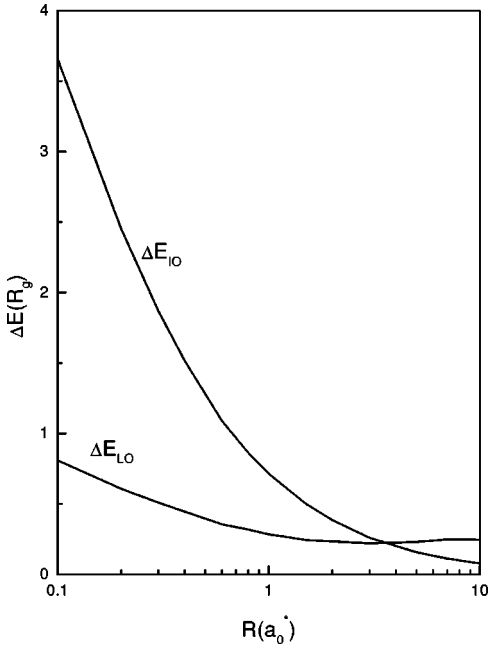

FIG. 5. Contributions of different phonon modes to the bound polaron binding energy as functions of the quantum wire.

phonons is considered to be weak in GaAs. So it is important for us to pay attention to the influence of phonon on the physical properties of the QWW structure. Or we may say that there is no ''weak coupling'' between the electron and phonons in the QWW systems. In order to find out the roles of different phonon modes in the total phonon contributing to the bound polaron binding energy, we plotted the contributions of different phonon modes separately in Fig. 5. We can see from Fig. 5 that the contribution of the IO phonons (ΔE_{IO}) plays an important role in the bound polaron binding energy, especially when the QWW is narrow. ΔE_{IO} increases quickly as the radius R reduces. As the radius R gets smaller, the interface of the QWW gets closer to the electron, hence the interface phonons impose greater influence on the electron, resulting in a stronger coupling. In comparison with that of the IO phonon, the contribution of confined LO phonon to the impurity binding energy is far less important. It does not change a lot when the radius R changes. When R is very large, the influence of IO phonons becomes very weak and the influence of the LO phonon becomes dominant, which is just the case of three dimensional bulk material.

VI. SUMMARY

In this paper, we have calculated the ground-state energy and binding energy of an impurity in a cylindrical quantum well wire. In order to reflect the anisotropy of the QWW system, we adopted a two-parameter trial wave function for the variational calculation. Results show that the binding energy of the impurity increases greatly as the radius of the QWW reduces. The change of the variational parameters with R indicates that for the low-dimensional systems, it is necessary to take the anisotropic nature of the system into consideration when constructing the variational trial wave functions. In order to investigate the influence of optical phonon on the impurity binding energy, we derived the phonon Hamiltonian and the Fröhlich Hamiltonians of the electron-phonon interaction for the confined LO phonon modes and the interface phonon modes. Calculations on the GaAs QWW shows that the phonon-electron interaction may strongly influence the impurity binding energy. For a very narrow GaAs QWW, the contribution of electron-phonon interaction to the impurity binding energy may be up to as much as 23%. Calculations also show that as the radius of the QWW reduces, the influence of the interface phonon becomes a dominant factor influencing the impurity binding energy.

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