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Effect of electron–phonon interaction on the impurity binding energy in a quantum wire

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Abstract

The effect of electron–optical phonon interaction on the hydrogenic impurity binding energy in a cylindrical quantum wire is studied. By using Landau and Pekar variational method, the Hamiltonian is separated into two parts which contain phonon variable and electron variable, respectively. A perturbative-variational technique is then employed to construct the trial wave function for the electron part. The effect of confined electron–optical phonon interaction on the binding energies of the ground state and an excited state are calculated as a function of wire radius. Both the electron-bulk optical phonon and electron-surface optical phonon coupling are considered. It is found that the energy corrections of the polaron effects on the impurity binding energies increase rapidly as the wire radius is shrunk, and the bulk-type optical phonon plays the dominant role for the polaron effects.

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1. Introduction

During the past decades the development of the epitaxial crystal growth techniques such as molecular-beam epitaxy and metal–organic chemical vapor deposition has made the growth of the quasi-two-dimensional (quantum well) or quasi-one-dimensional (quantum wire) [1–4] systems possible with controllable well thickness or wire radius. These quantum structures have been applied to many semiconductor devices, such as high-electron-mobility transistors. Recent progresses in growth and fabrication techniques have been able to fabricate the quantum wires with radii less than 100 Å. Theoretically, the electronic properties of a hydrogenic impurity in the quantum well [5–8] and the quantum wire [9–16] have been studied by many authors. The impurity binding energies of a quantum wire with infinite or finite potential barrier [9] and with different shapes of the cross-section [10–12] have been discussed. The effect of location [10–12] of impurities with respect to the wire axis was also studied previously. The emission line for quantum wires was observed [17] to be two to three times broader than that of quantum wells

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and with 6–10 meV higher binding energy. It is expected that the same properties in quantum wells were further improved by the reduction of dimensionality to quasi-one-dimensional quantum wires.

The physics of impurity states in quantum wire is very interesting because specific properties can be easily achieved by varying the wire radius. An electron bound to an impurity on the axis of the quantum wire behaves like a bounded three-dimensional electron when the boundary is far away. However, as the wire radius is reduced, the electron confinement due to the potential barrier becomes very important. Especially in the quantum wire with infinitely high potential wall, the total energy of the electron may change from negative to positive at a certain radius and finally diverges to infinity as the radius approaches zero. Furthermore, it is well known that the reduction of dimensionality increases the effective strength of the Coulomb interaction. The binding energy E_b of the ground state of a hydrogenic impurity in N-dimension is given by $E_b = [2/(N-1)]^2 R_y^*$, where $R_y^* = \mu e^4/2\varepsilon^2\hbar^2$ is the effective Rydberg. Hence the dramatic change in the binding energy may serve as a clear signal for variation in the effective dimension of the quantum wire.

It is known that an electron weakly bound to a hydrogen impurity in a polar semiconductor will interact with the phonons of the host semiconductor. In the past decade, many authors have studied the polaron effect on the binding energy of impurity or exciton in quantum well [18–26]. Recently, the electron–phonon effect on the binding energy of the donor impurity in a quantum wire with rectangular cross-section was reported [27–29]. It was found the polaron effect on the binding energy becomes sizeable as the electron gets more deeply bound. The polaron shifts in donor energy levels are found to be of the order of 10% in a weakly polar system. In studying the polaron effect on the impurity binding energy, most of the previous works considered the interaction of the electron and bulk optical (BO) phonon only. However, in ionic crystal, the motion of an electron near the surface may be affected very much by the surface longitudinal optical (SO) phonon [30]. An electron may be trapped at the surface by the electron–SO phonon interaction. Besides, the electron–phonon interaction Hamiltonian in the previous works was valid only for the bulk. Therefore, we will choose the Hamiltonian derived by Li and Chen [31], who considered the confined phonon modes in the cylindrical quantum dot.

Most of the previous approaches concentrating on the polaron effect on the ground state of an impurity in a quasi-one-dimensional wire employ the variational method or perturbation method. Since the construction of variational trial wave functions is entirely based on physical intuition, the estimation of the accuracy of the result obtained from variational approach is very difficult. Furthermore, the perturbation method is only a good access to those systems with very small perturbation in most cases. Therefore, it would be most desirable to have an alternative approach which is not only simple but also efficient to the quantum wire problem. In this work, we employ a simple approximation treatment which combines the spirit of both variational principle and perturbational approach to study the effect of electron–phonon interaction on the ground-state binding energy of a hydrogenic impurity located inside a quantum wire.

2. Theory

Consider now a hydrogenic impurity located on the axis of a rigid wall cylindrical quantum wire with a radius d. The Hamiltonian of the impurity electron interacting with the phonon can be expressed as

$$H = H_e + H_b + H_{e\text{-}b} + H_{sp} + H_{e\text{-}sp}, \tag{1}$$

where H_e is the electronic part of the Hamiltonian

$$H_e = -\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) - \frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial z^2} - \frac{e^2}{\varepsilon r} + V(\rho). \tag{2}$$

$V(\rho)$ is the confining potential which is assumed as

$$V(\rho) = \begin{cases} 0 & \text{for } \rho \leqslant d, \\ \infty & \text{for } \rho > d \end{cases} \tag{3}$$

and ε and μ are the dielectric constants of the well and the effective mass of the electron. Recently, Li and Chen [31] have derived the confined longitudinal-optical phonon and surface phonon modes

of a free-standing cylindrical quantum dot of radius d and height $2D$. We will follow their Hamiltonian and let D approach infinity, such that the dot system can become a quantum wire. Therefore, H_b is the bulk phonon Hamiltonian which can be expressed as

$$H_b = \sum_{n,l} \hbar\omega_{LO} a_{nl}^{\dagger} a_{nl}, \tag{4}$$

where $\hbar\omega_{LO}$ is the dispersionless bulk optical (BO) phonon energy, $a_{nl}^{\dagger}(a_{nl})$ is the creation (annihilation) operator for BO phonon. $H_{e\text{-}b}$ is the interaction between the electron and BO phonon which can be expressed as

$$H_{e\text{-}b} = \sum_n J_0\left(\frac{\chi_n}{d}\rho\right)\left[\sum_{l=1,3,\ldots} V_{nl}\cos\left(\frac{l\pi}{2D}z\right) \times (a_{nl} + a_{nl}^{\dagger}) + \sum_{l=2,4,\ldots} V_{nl}\sin\left(\frac{l\pi}{2D}z\right)(a_{nl} + a_{nl}^{\dagger})\right] \tag{5}$$

with

$$V_{nl} = \frac{1}{V}\frac{4\pi e^2\hbar\omega_{LO}}{[(\chi_n/d)^2 J_2^2(\chi_n) + (l\pi/2D)^2 J_1^2(\chi_n)]} \times\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right), \tag{6}$$

where J_m is the mth-order Bessel function, χ_n is the nth-root of J_0, and $V = 2\pi d^2 D(D \to \infty)$ is the crystal volume. H_{sp} is the surface optical phonon (SO) phonon Hamiltonian which can be expressed as

$$H_{sp} = \sum_n \hbar\omega_{sp} B_n^{\dagger} B_n, \tag{7}$$

where $\hbar\omega_{sp}$ is the surface optical (SO) phonon energy, $B_n^{\dagger}(B_n)$ is the creation (annihilation) operator for SO phonon. $H_{e\text{-}sp}$ is the interaction between electron and SO phonon:

$$H_{e\text{-}sp} = \sum_{n=2,4,\ldots} \Gamma_n I_0\left(\frac{n\pi}{2D}\rho\right)\cos\left(\frac{n\pi}{2D}z\right)(B_n^{\dagger} + B_n) \tag{8}$$

with

$$\Gamma_n^2 = \frac{1}{S}\frac{4\pi e^2\hbar\omega_{sp}}{Dk_n[I_0^2(k_n d) - I_2(k_n d)I_0(k_n d)]} \times\left(\frac{1}{\varepsilon(\omega_{sp}) - \varepsilon_0} - \frac{1}{\varepsilon(\omega_{sp}) - \varepsilon_\infty}\right), \tag{9}$$

$$\omega_{sp}^2 = \left[1 + \frac{\varepsilon_0 - \varepsilon_\infty}{\varepsilon_\infty - \varepsilon(\omega_{sp})}\right], \tag{10}$$

$$\varepsilon(\omega_{sp}) = \frac{-I_0(k_n d)K_1(k_n d)}{K_0(k_n d)I_1(k_n d)}, \tag{11}$$

where $k_n = n\pi/2D$, and $S = \pi d^2$. I_m and k_m are, respectively, the mth-order modified Bessel function of the first and second kind.

Following Landau and Pekar's variational approach [32], the trial wave function can be written as

$$|\Psi\rangle = \Phi(r)U_b U_s|0\rangle, \tag{12}$$

where $\Phi(r)$ depends only on the electron coordinate, and $|0\rangle$ is the phonon vacuum state defined by $b_q|0\rangle = 0$, $a_q|0\rangle = 0$, and U is a unitary transformation given by

$$U_b = \exp\left(\sum_{nl}(a_{nl}^{\dagger} f_{nl} - a_{nl} f_{nl}^{*})\right), \tag{13}$$

$$U_s = \exp\left(\sum_n (B_n^{\dagger} g_n - B_n g_n^{*})\right). \tag{14}$$

where f_{nl} and g_n are the variational function and the unitary operators U_b and U_s transform the bulk phonon and surface phonon operators as follows:

$$U_b^{\dagger} a_{nl}^{\dagger} U_b = a_{nl}^{\dagger} + f_{nl}^{\dagger}, \tag{15}$$

$$U_b^{\dagger} a_{nl} U_b = a_{nl} + f_{nl}, \tag{16}$$

$$U_s^{\dagger} B_n^{\dagger} U_s = B_n^{\dagger} + g_n^{\dagger}, \tag{17}$$

$$U_s^{\dagger} B_n U_s = B_n + g_n. \tag{18}$$

The parameters f_{nl}, f_{nl}^{*}, g_n, g_n^{*} can be obtained by minimizing the $\langle|H|\rangle$ with respect to the parameters f_{nl}, f_{nl}^{*}, g_n, g_n^{*}. Then, the expectation value

$\langle H\rangle$ turns out to be

$$\langle H\rangle = \langle\Phi(r)|H_e|\Phi(r)\rangle - \sum_{nl}\frac{V_{nl}^2}{\hbar\omega_{LO}}\left|\langle\Phi(r)|J_0\left(\frac{\chi_n}{d}\rho\right)\cos\left(\frac{n\pi}{2D}z\right)|\Phi(r)\rangle\right|^2 - \sum_{n}\frac{\Gamma_n^2}{\hbar\omega_{sp}}\left|\langle\Phi(r)|I_0(k_n\rho)\cos\left(\frac{n\pi}{2D}z\right)|\Phi(r)\rangle\right|^2. \quad (19)$$

The axis of the wire is assumed to be along the z direction. To solve the electronic part, one can employ the perturbative-variational approach. Two variational parameters α and β are introduced by adding and subtracting two terms $\alpha e^2/\varepsilon\rho$ and $(\beta^2\hbar^2/2\mu)z^2$ into the original Hamiltonian H_e and then regroup H_e into three groups

$$H_e = H_{01}(\beta) + H_{02}(\alpha) + H'(\alpha,\beta), \quad (20)$$

where

$$H_{01}(\beta) = \frac{-\hbar^2}{2\mu}\frac{\partial^2}{\partial z^2} + \frac{\beta^2\hbar^2}{2\mu}z^2, \quad (21)$$

$$H_{02}(\alpha) = \frac{-\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) - \frac{\alpha e^2}{\varepsilon\rho} + V(\rho) \quad (22)$$

$$H'(\alpha,\beta) = \frac{\alpha e^2}{\varepsilon\rho} - \frac{\beta^2\hbar^2}{2\mu}z^2 - \frac{e^2}{\varepsilon r}. \quad (23)$$

In the above equations, $H'(\alpha,\beta)$ is treated as a perturbation, and α and β are treated as variational parameters which can be determined by requiring the perturbation term to be as small as possible. Decomposing H_e into two terms H_{01} and H_{02} is equivalent to dividing the space into a two-dimensional (in xy plane) and a one-dimensional (in z-axis) subspace. The unperturbed part of the Hamiltonian H_e contains two terms, i.e. H_{01} and H_{02}, where H_{01} represents the one-dimensional harmonic oscillator, and H_{02} represents a two-dimensional hydrogen atom located inside a quantum disk [16]. Both can be solved exactly. For illustration, the ground-state energy and wave function of the unperturbed part can be expressed as

$$E_g^{(01)}(\alpha,\beta) = E_g^{(01)}(\beta) + E_g^{(02)}(\alpha), \quad (24)$$

$$\Psi_g^{(0)}(r,\alpha,\beta) = \varphi_g^{(01)}(z;\beta)\varphi_g^{(02)}(x,y;\alpha), \quad (25)$$

respectively, where $\varphi_g^{(01)}(z;\beta)$ is the ground-state wave function of the 1D harmonic oscillator, and $\varphi_g^{(02)}(x,y;\alpha)$ is the ground-state wave function of the 2D hydrogen atom located at the center of an infinite circular well. The ground-state eigenvalue and eigenfunction of the 1D harmonic oscillator can be expressed as

$$E_g^{(01)}(\beta) = \frac{\beta\hbar^2}{2\mu}, \quad (26)$$

$$\varphi_g^{(01)}(z;\beta) = \left(\frac{\beta}{\pi}\right)^{1/4} e^{-(\beta/2)z^2}. \quad (27)$$

The ground-state eigenvalue and eigenfunction of the 2D hydrogenic impurity located at the center of an infinite circular well can be obtained as [16]

(1) For $E<0$,

$$\varphi_g^{(02)}(x,y;\alpha) = N_1 e^{-\xi_1/2}\xi_1^{|m|+1}\Phi(|m| + 1/2 - \lambda_1, 2|m| + 1, \xi_1), \quad (28)$$

where $\xi_1 = \alpha_1\rho$, $\alpha_1 = -8\mu E/\hbar^2$, $\lambda_1 = 2\mu\alpha e^2/\varepsilon\hbar^2\alpha_1$, $\Phi(a,b,x)$ is the confluent hypergeometric function, and N_1 is the normalization constant.

(2) For $E>0$,

$$\varphi_g^{(02)}(x,y;\alpha) = N_2\xi_2^m\Phi_{m-1/2}(\eta_2,\xi_2), \quad (29)$$

where $\xi_2 = \alpha_2\rho$, $\alpha_2 = -8\mu E/\hbar^2$, $\eta_2 = -\mu\alpha e^2/\varepsilon\hbar^2\alpha^2$, $\Phi_{m-1/2}(\eta_2,\xi_2)$ is the irregular Coulomb wave function, and N_2 is the normalization constant.

(3) The turning point for energy changing from $E>0$ to $E<0$ in the quantum circle system may be determined by setting

$$d^{-1/2}J_0\left[\left(\frac{8\mu e^2}{\varepsilon\hbar^2}\right)^{1/2}d^{1/2}\right] = 0 \quad \text{for } m=0 \quad (30)$$

and

$$d^{-1/2}J_2\left[\left(\frac{8\mu e^2}{\varepsilon\hbar^2}\right)^{1/2}d^{1/2}\right] \subset 0 \quad \text{for } m=1. \quad (31)$$

The requirement of the continuity of the wave functions and its first derivative at boundary yields

(1) For $E<0$:

$$\phi(|m| + \tfrac{1}{2} - \lambda_1, 2|m| + 1, \alpha, d) = 0. \quad (32)$$

(2) For $E > 0$:

$$\Phi_{m-1/2}(\eta_2, \alpha_2 d) = 0. \tag{33}$$

The eigenvalues are then given as

$$E_g^{(02)}(\alpha) = \begin{cases} -\dfrac{\mu\alpha^2 e^4}{2\varepsilon^2\hbar^2\lambda_1^2} & \text{for } E < 0, \\ \dfrac{\mu\alpha^2 e^4}{2\varepsilon^2\hbar^2\eta_2^2} & \text{for } E > 0. \end{cases} \tag{34}$$

The first-order energy correction can thus be obtained as

$$\begin{aligned} \Delta E_g^{(1)}(\alpha,\beta) &= \langle \Phi_g^{(0)}(r;\alpha,\beta)|H'(\alpha,\beta)|\Phi_g^{(0)}(r;\alpha,\beta)\rangle \\ &= \langle \varphi_g^{(02)}(x,y{:}\,\alpha)|\frac{\alpha e^2}{\varepsilon\rho}|\varphi_g^{(02)}(x,y;\alpha)\rangle \\ &\quad - \langle \varphi_g^{(01)}(z;\beta)|\frac{\beta^2\hbar^2 z^2}{2\mu}|\varphi_g^{(01)}(z;\beta)\rangle \\ &\quad - \langle \Phi_g^{(0)}(r;\alpha,\beta)|\frac{e^2}{\varepsilon r}|\Phi_g^{(0)}(r;\alpha,\beta)\rangle. \end{aligned}$$

The second term of the above equation can be integrated analytically and the result is

$$\langle \varphi_g^{(01)}(z;\beta)|\frac{\beta^2\hbar^2 z^2}{2\mu}|\varphi_g^{(01)}(z;\beta) > \varphi_g^{(02)}(x,y;\alpha)\rangle = \frac{\beta\hbar^2}{\mu}. \tag{35}$$

Then, the total energy up to the first-order perturbation correction can then be obtained as

$$E_g(\alpha,\beta) = E_g^{(01)}(\beta) + E_g^{(02)}(\beta) + \Delta E_g^{(1)}(\alpha,\beta). \tag{36}$$

The variational parameters are then chosen by requiring the total energy $E_g(\alpha,\beta)$ to be minimized with respect to the variation of α and β. This is equivalent to requiring

$$\frac{\partial E}{\partial \alpha} = 0, \tag{37}$$

$$\frac{\partial E}{\partial \beta} = 0. \tag{38}$$

For the excited states, the eigenvalues and eigenfunctions can be treated in the same way.

3. Results and discussions

We have calculated the effect of the confined longitudinal-optical phonon and surface phonon interactions on the hydrogenic impurity located in a quantum wire. And the well potential is considered as infinite. Fig. 1 shows the ground-state energy as a function of the wire radius. The binding energy E_b of the hydrogenic impurity is defined as the energy difference between the ground-state energy of the cylindrical wire system with and without the impurity, i.e.

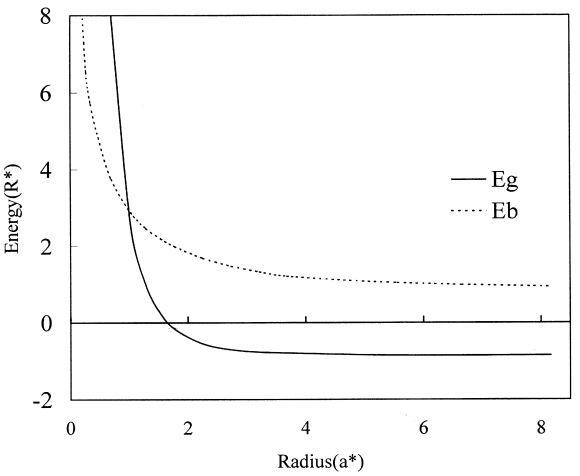

Fig. 1. The ground-state energy (solid line) and the binding energy (dotted line) of a hydrogenic impurity located at the axis of a cylindrical wire as a function of the radius of the wire. (Ry* and a^* are the effective Rydberg and the effective Bohr radius.)

$$E_b = E_0 - E_g, \tag{39}$$

where E_0 is the ground-state energy of the quantum wire system without the impurity, while E_g is the ground-state energy of the quantum wire system with the impurity located on the axis of the cylindrical wire. One can see from Fig. 1 that the energy of the 1s state becomes negative when the wire radius is larger than $1.65a^*$. It means that the confining energy is larger than the Coulomb energy as the wire radius is smaller than $1.65a^*$. And one can also note that as the radius of the quantum wire is decreased, the ground-state energy increases. As the wire radius d becomes smaller, the electron is pushed toward the axis of the cylindrical wire. This makes the electron get close to the nucleus. As the electron gets close to the nucleus, both the ground-state energy and the binding energy increase rapidly. This is because the Coulomb

potential, which varies with $\sim 1/d$ (d is the wire radius), becomes more negative, while the kinetic energy of the electron, which varies with $\sim 1/d^2$ (by the uncertainty relation), increases more rapidly. As a result, the ground state energy is increased as the electron gets close to the nucleus. The binding energy defined in Eq. (39) is effectively the negative sign of the Coulomb interaction energy between the electron and the nucleus, i.e. $\sim 1/d$, therefore, the binding energy of the electron is also increased as the electron gets near to the nucleus. Our results show that for small wire radius, the binding energies are in good agreement with the previous results [12,16]. As the radius becomes very large, our result approaches the correct limit $1R^*$ while the previous work [14] can only yield a value of $0.22R^*$. The large discrepancy of the previous work may be due to the artificial dividing of the variational trial wave function into a one-dimensional hydrogen atom and a two-dimensional hydrogen atom and thus forces the creation of an additional node of the wave function at $z = 0$. In this work, the trial wave function is adopted to be in the form of 1D harmonic oscillator wave function instead of the one-dimensional hydrogen atom. This prevents our wave function from introducing any additional node at $z = 0$. Fig. 2 presents the 2s excited state binding energies as the functions of wire radius. One can note from the figure that as the wire radius increases, the binding energy approaches $0.25R^*$ which gives correctly the limiting value of 3D hydrogen atom.

Fig. 3 presents the confined BO phonon and SO phonon effects as functions of wire radius. With increasing the wire radius, the magnitude of the confined BO phonon effect decreases from large value and then approaches to the bulk value. When the wire radius is less than $1.5a^*$, the polaron effect increases rapidly. One might think as the radius becomes very small, the confined BO phonon effect should approach zero, like the case in quantum well [33]. In fact, similar results were obtained by Oshiro in a spherical quantum dot [34]. They found that the polaron energy shift is enhanced as the dot radius becomes small. This is due to the fact that the electron becomes completely localized (E_b approaches infinity) in small wire (or dot) radius while the binding energy approaches $4R^*$ in small

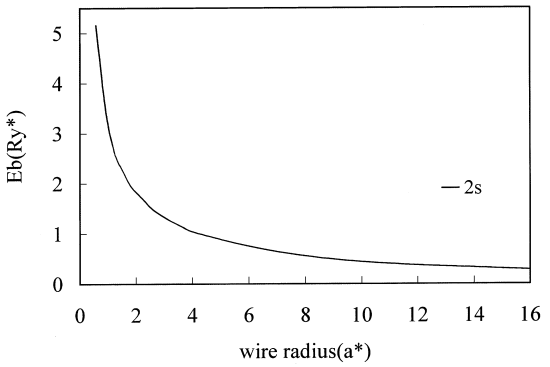

Fig. 2. The binding energy of the 2s excited state as a function of the wire radius. (Ry* and a^* are the effective Rydberg and the effective Bohr radius.)

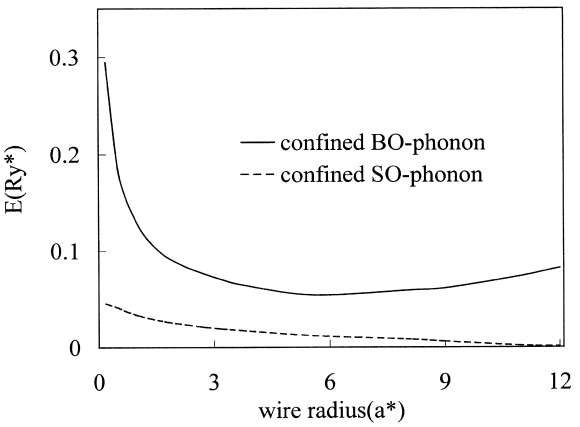

Fig. 3. The energies of the wire radius modified by the confined BO and SO phonon. The solid line stands for the BO phonon effect, and the dashed line for the SO phonon effect. (Ry* and a^* are the effective Rydberg and the effective Bohr radius.)

well width. In the case of quantum well, the confined SO phonon effect plays the dominant role for small well width [33]. But in quantum wire, the confined SO phonon is less important, just like that in quantum dot system [34]. This is because the surface area of a quantum wire (or quantum dot) decreases with the radius. Thus, the number of vibration modes of confined SO phonon becomes fewer.

In Fig. 4, three curves are presented. The dotted curve represents the binding energy of the impurity

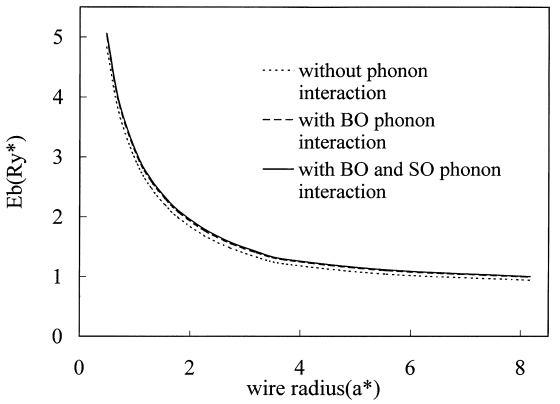

Fig. 4. The binding energy with/without phonon effect. The dotted line stands for the binding energy without the phonon effect. The dashed line stands for that only BO phonon effect on the binding energy, and the solid line for both the BO and SO phonons effects on the binding energy. (Ry* and a^* are the effective Rydberg and the effective Bohr radius.)

without considering the interactions between the electron and phonon. The dashed curve represents the binding energy of the impurity with only the confined BO phonon effect being taken into account. While the solid curve is the binding energy of the impurity including both confined BO phonon and SO phonon effects in the calculation. Compared with the impurity binding energy, the confined SO phonon is negligible in quantum wire. We then conclude that because of the similarity in geometry, the behavior of the polaron effect on the quantum wire system is like that on the quantum dot system.

4. Conclusion

In this work, analytical solutions for the effects of the electron–phonon interaction on the binding energies of an impurity located inside a quantum wire are obtained by a simple but efficient perturbation-variation method. As the radius becomes very large, the correct limiting value can be obtained. We have also discussed both the confined BO and SO phonon effects. We found that the confined BO phonon effect is prominently for a quantum wire with a small radius. We have also found that the energy corrections of the polaron effects on the impurity binding energies increase rapidly when the wire radius is less than $1.5a^*$.

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