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The role of hydrostatic pressure and temperature on bound polaron in semiconductor quantum dot

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ABSTRACT

We studied theoretically the effects of hydrostatic pressure and temperature on the binding energy of shallow hydrogenic impurity in a cylindrical quantum dot (QD) using a variational approach within the effective mass approximation. The hydrostatic stress was applied along the QD growth axis. The interactions between the charge carriers and confined longitudinal optical (LO) phonon modes are taken into account. The numerical computation for $GaAs/Ga_{1-x}Al_xAs$ QD has shown that the binding energy with and without the polaronic correction depends on the location of the impurity and the pressure effect and it is more pronounced for impurities in the QD center. Both the binding energy and the polaronic contribution increase linearly with increasing stress. For each pressure value, these energies are also found to decrease as the temperature increases. The results obtained show that in experimental studies of optical and electronic properties of QDs, the effects of pressure, temperature and polaronic correction on donor impurity binding energy should be taken into consideration.

1. Introduction

The advances in semiconductor nanofabrication technology make it possible to produce semiconductor nanostructures whose characteristic dimensions are similar to the electronic de Broglie wavelength. Because of their reduction of dimensionality, the nanostructures exhibit many new physical effects [1–13] which are extremely interesting from the point of view of fundamental physics and also for their potential applications in microelectronic device technology. Thus, much theoretical and experimental studies have recently been devoted to understand and explore the physical properties of these systems. Optical measurements of semiconductors are of great value for the understanding of the physical nature of confined electron, hole, and coulomb-bound states such as impurities and excitons. Impurities and excitons in semiconductor heterostructures are known to promote a number of qualitative changes in electronic and optical properties which may be properly controlled by adequate choice of the sample geometry and external fields [14–27].

Theoretical studies related to the effects of hydrostatic pressure and temperature on shallow-donor impurity and exciton states in the considered low-dimensional structures have been reported [28–40]. The results found by Oyoko et al. [28] and Lopez et al. [29] have shown that the donor binding energy of a shallow impurity increases with increasing stress and decreasing QD sizes. The same behavior was found by Elabsy [30] in the case of QW heterostructures. Gerardin et al. [31] have investigated the effects of electric field and hydrostatic pressure on the donor binding energies in a spherical QD. They have found that the hydrostatic pressure increases the donor ionization energy and that the effect is larger for a smaller dot. Oyoko et al. [32] have calculated the effects of hydrostatic pressure and temperature on shallow-impurity related optical absorption spectra in quantum wells. Kasapoglu [33] has studied the hydrostatic pressure and temperature effects on donor impurities in $GaAs/Ga_{1-x}Al_xAs$ double quantum well under the external fields. John Peter et al. [34] have calculated the binding energies of hydrogenic donors in $GaAs/Ga_{1-x}Al_xAs$ single quantum well as a function of the pressure and the temperature.

Taking into account the optical phonons, several works have studied the pressure dependence of the optical phonon in low dimensional semiconductors [35–40]. The presence of applied hydrostatic stress introduces an extra confinement which is added to the geometrical one, and modifies the carrier motion and the nature of corresponding wave function. We have studied in our previous works the hydrostatic stress [13] and the temperature [41] dependence of exciton–phonon coupled states in a cylindrical QD. To our knowledge, a theoretical study for the donor binding energy of shallow impurity in QD systems with consideration of

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confined LO phonon modes contribution and simultaneous effects of hydrostatic pressure and temperature has not been given.

GaAs/AlGaAs QD is an interesting system because of its several advantages compared to others. Recently, a new experimental method permits us to obtain GaAs/$Ga_{1-x}Al_xAs$ QD via multistep self-assembly [42]. These structures are characterized by some new properties which allow us to calculate the electronic ones without the complication of uncertain composition and strain profiles [42].

In the present paper we report a variational calculation in the effective mass approximation of the binding energy of shallow donor impurity in a cylindrical QD under simultaneous effects of hydrostatic pressure and temperature. The pressure is applied along the z-direction. In the present calculation, the coupling of the confined LO phonon modes with the charge carriers (electron and ion) is considered. According to the properties of QD structures and the on-center impurity position [43,44], the effect of confined LO phonon modes to the binding energies is much more important than that due to the surface optical phonon modes. Therefore these surface phonons are not included in this work. This approximation is valid in the case of the present study in which the cylindrical QD has a radius $R \simeq a^*$ and height H greater than $\sim a^*$ (Bohr radius). Furthermore, the position of the impurity has a strong influence. The binding energy is much larger for on-center than on-edge impurity positions in such structures [27,45–47]. For these reasons, in our investigation, we focus our attention on the on-center impurity position. The quantum confinement is described by a finite deep potential well. The paper is organized as follows. After a brief introduction, we describe in Section 2 the Hamiltonian and the model of calculation. The numerical results and discussions are presented in Section 3, and we give our conclusions in Section 4.

2. Formalism

Let us consider an electron which is confined perfectly in a cylindrical QD of radius R and height $H=2d$ embedded in barrier material semiconductor. Within the framework of the effective mass and non-degenerated-band approximations, the Hamiltonian of a shallow hydrogenic impurity versus pressure and temperature can be written as

$$H(P,T)=H_e(P,T)+H_{LO}(P,T)+H_{e-LO}(P,T)+H_{ion-LO}(P,T), \tag{1}$$

where H_e is the electronic Hamiltonian which is given by

$$H_e(r,P,T)=-\frac{\hbar^2}{2m^*(P,T)}\nabla^2-\frac{e^2}{\varepsilon(P,T)r}+V_b(r,P,T), \tag{2}$$

where $m^*(P,T)$ is the electronic effective mass and $r=[\rho^2+(z-z_i)^2]^{1/2}$. z_i is the impurity position along the z-axis. The dielectric constant $\varepsilon(P,T)$ at pressure P and temperature T is taken as the static constant $\varepsilon_0(P,T)$, in the absence of the confined LO phonon modes, and the high frequency dielectric constant $\varepsilon_\infty(P,T)$, in the presence of the confined LO phonon modes. $V_b(r,P,T)$ is the electron confining potential in the QD at pressure P and temperature T, given by

$$V_b(r,P,T)=\begin{cases}0 & \text{if } \rho\le R \text{ and } |z|\le d\\ V_0(P,T) & \text{otherwise}\end{cases}. \tag{3}$$

We can write the expression of $V_0(x,P,T)$ as follows [33] $V_0(x,P,T)=0.6\Delta E_g(x,P,T)$, where

$$\Delta E_g(x,P,T)=\Delta E_g(x,0,0)-P(1.3\times10^{-3})x-T(1.11\times10^{-4})x, \tag{4}$$

$\Delta E_g(x,0,0)$ can be expressed as

$$\Delta E_g(x,0,0)=Eg_{Ga(1-x)Al(x)As}(x)-Eg_{GaAs}(x)=1.155x+0.37x^2. \tag{5}$$

In the case in which the dimensions of the QD are greater than a^* our approximation is good $m_w^*(P,T)=m_b^*(P,T)$ and $\varepsilon_w(P,T)=\varepsilon_b(P,T)$.

In Eq. (1), H_{LO}, H_{e-LO} and H_{ion-LO} are, respectively, the Hamiltonian operator for the confined LO phonon modes, the electron–LO phonon interaction and the ion–LO phonon coupling:

$$H_{LO}(P,T)=\sum_{l,n1}\hbar\omega_{LO}a_{ln1}^+a_{ln1}, \tag{6}$$

$a_{ln1}^+(a_{ln1})$ are creation (annihilation) operators for the confined LO phonon modes of the $(l,n1)$ th mode, with frequency ω_{LO} and wave vector $(K_{\|}=\chi_{n1}/R, K_z=l\pi/2d)$ where χ_{n1} is the $n1$-th root of the Bessel function of the zero order:

$$H_{e-LO}(P,T)=-e\phi_{LO}(r,P,T), \tag{7}$$

where

$$\phi_{LO}(r,P,T)=\sum_{l,n1}\left(\frac{\hbar}{8\pi\omega_{LO}}\right)^{1/2}(a_{ln1}+a_{ln1}^+)\phi_{\pm}(r), \tag{8}$$

after obtaining the expression of $\phi_{\pm}(r)$ from Ref. [48], we express $H_{e-LO}(P,T)$ and $H_{ion-LO}(P,T)$ as

$$H_{e-LO}(P,T)=-\sum_{n1}J_0\left(\frac{\chi_{n1}}{R}\rho\right)\times\left[\begin{array}{l}\sum_{l=1,3..}V_{ln1}(P,T)\cos\left(\frac{l\pi}{2d}z\right)(a_{ln1}+a_{ln1}^+)\\ +\sum_{l=2,4..}V_{ln1}(P,T)\sin\left(\frac{l\pi}{2d}z\right)(a_{ln1}+a_{ln1}^+)\end{array}\right], \tag{9}$$

and

$$H_{ion-LO}(P,T)=\sum_{n1}\sum_{l=1,3..}V_{ln1}(P,T)(a_{ln1}+a_{ln1}^+), \tag{10}$$

where

$$V_{ln1}^2(P,T)=\frac{1}{V}\frac{4\pi e^2\hbar\omega_{LO}}{\left(\frac{\chi_{n1}}{R}\right)^2J_1^2(\chi_{n1})\left[1+\left(\frac{l\pi R}{2d\chi_{n1}}\right)^2\right]}\left(\frac{1}{\varepsilon_\infty(P,T)}-\frac{1}{\varepsilon_0(P,T)}\right), \tag{11}$$

$V=2\pi R^2d$ being the volume of the cylindrical dot.

To deal with the Hamiltonian of this system, we shall adopt the variational treatment developed by Lee et al. [49], for quasi-zero-dimensional systems. To facilitate the calculation, we use the following unitary transformation:

$$U=\exp\left(\sum_{l,n1}(f_{ln1}a_{ln1}^+)-cc\right), \tag{12}$$

where f_{ln1} is the variational parameter to be selected by minimizing the energy of the system. The wave function of the system can be written as

$$|\psi(\rho,z,k)\rangle=|\phi(\rho,z)\rangle|N_{l,n1}\rangle, \tag{13}$$

where $\phi(\rho,z)$ is the particle wave function confined in a finite cylindrical potential well and $|N_{l,n1}>$ is the wave function of the phonon field in the particle number representation.

We have

$$a_{l,n1}^+|N_{l,n1}\rangle=A_+|N_{l,n1}+1\rangle, \tag{14}$$

$$a_{l,n1}|N_{l,n1}\rangle=A_-|N_{l,n1}-1\rangle, \tag{15}$$

where A_+ and A_- are the normalization coefficients. For the normalization condition we have

$$\langle N_{l,n1}\pm1|N_{l,n1}\pm1\rangle=1,$$

$$|A_-|^2=\langle N_{l,n1}|a_{l,n1}^+a_{l,n1}|N_{l,n1}\rangle=\eta_{LO}, \tag{16}$$

$$|A_+|^2=\langle N_{l,n1}|a_{l,n1}a_{l,n1}^+|N_{l,n1}\rangle=1+\eta_{LO}, \tag{17}$$

where η_{LO} is the average number of the phonon with frequency ω_{LO}:

$$\eta_{LO}=\frac{1}{\exp\left(\frac{\hbar\omega_{LO}}{KT}\right)-1}. \tag{18}$$