Binding Energy of an Exciton Bound to a Charged

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ABSTRACT

Binding energies for an exciton (X) trapped in the two-dimensional quantum dot by a charged impurity located on the z axis at a distance from the dot plane are calculated by using the method of few-body physics. This configuration is called a barrier (D^+, X) center or a barrier (A^-, X) center. The dependences of the binding energy of the ground state of the barrier (D^+, X) and (A^-, X) centers on the electron-to-hole mass ratio σ and the dot radius R for a few values of the distance d between the fixed positive ion on the z axis and the dot plane are obtained.

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Exciton complexes have been the subject of intense studies in the last years, both experimentally and theoretically. The stability of exciton complexes in bulk semiconductors was proven theoretically in 1958 by Lampert[1]. After the first evaluation of binding energies for such systems performed by Thomas and Hopfield[2], based on a comparison with molecular analogues, several variational calculations have been presented in the literature[3−6]. The simplest exciton complex is formed when an electron and a hole of effective masses m_e^* and m_h^*, respectively, are trapped by a charged impurity. They can be used as a test for the theoretical description of exciton-impurity interaction. There are two kinds of exciton complexes: the (D^+, X) and (A^-, X) complexes. They result, respectively, from the binding of an exciton to an ionized hydrogenic donor or acceptor impurity. Their stability and binding energies in three-dimensional (3D) semiconductors have been the subject of several theoretical studies within the effective mass approximation as a function of the electron-to-hole effective mass ratio $\sigma = m_e^*/m_h^*$. As a result, it appears[6] that the (D^+, X) complex is stable if $\sigma \leq \sigma^c = 0.454$ and that the (A^-, X) complex is stable if $\sigma \geq \sigma^c$. However, only few theoretical studies have been devoted the exciton complex in low-dimensional structures[7−9]. Up to now, the study related to the quantum confinement effect on the (D^+, X) and $(A^-, X$) complexes in a quantum dot (QD) is still rare. So it is necessary to make theoretical study for the binding energy of (D^+, X) and (A^-, X) complexes in QDs.

A system in which an electron and a hole confined to a parabolic QD are bound by a charged impurity located on the z axis at a distance d from the dot plane is called a barrier (D^+, X) or (A^-, X) center QD. There has been interest in the subject lately. Rich electronic structures and optical properties, and a variety of structural phase transitions are predicted in such systems. In 3D semiconductors, the binding energies of (D^+, X) and (A^-, X) complexes are generally low, and their existence depends sometimes on specific stability conditions[10]. However, in quasi-zero-dimensional semiconductors (QDs), because the overlapping between the wave functions of the electron and the hole becomes more important, the (D^+, X) and (A^-, X) complex states are more bound than in the bulk. So it is expected that the observation of bound exciton complexes should be more easy in 0D semiconductors than in 3D semiconductors.

In this paper, we present a numerical diagonalization of Hamiltonian to determinate the binding energies of the (D^+, X) and the (A^-, X) complexes with a charged impurity placed on the z axis at a distance d from the dot plane. We also studied the stability and binding energy of the ground state of the barrier (D^+, X) and (A^-, X) centers in a parabolic quantum dot as a function of the electron-to-hole mass ratio and the dot radius.

The effective-mass Hamiltonian for the barrier (D^+, X) center in a parabolic QD can be written as follows:

$$H = -\frac{\hbar^2}{2m_e^*}\nabla_{r_e}^2 + \frac{1}{2}m_e^*\omega_0^2 r_e^2 - \frac{\hbar^2}{2m_h^*}\nabla_{r_h}^2 + \frac{1}{2}m_h^*\omega_0^2 r_h^2 + V_C \tag{1}$$

where

$$V_C = \frac{e^2}{\epsilon}\left[\frac{1}{\sqrt{r_h^2 + d^2}} - \frac{1}{\sqrt{r_e^2 + d^2}} - \frac{1}{|\vec{r}_e - \vec{r}_h|}\right], \tag{2}$$

ϵ is the effective dielectric constant, $\vec{r}_e$ and $\vec{r}_h$ are the position vectors of the electron and the hole with respect to the dot centre, d is the distance between the fixed positive ion on the z axis and the dot plane, and ω_0 is the strength of the confinement. We assume that the effective masses as well as the dielectric constants are the same in the well and barrier materials. The Hamiltonian for the barrier (A^-, X) centre in a parabolic QD can be obtained from V_C by changing the signs of the first term and the second term.

Introducing the coordinates

$$\vec{r} = \vec{r}_e - \vec{r}_h, \vec{R} = \frac{m_e^*\vec{r}_e + m_h^*\vec{r}_h}{m_e^* + m_h^*}, \quad (3)$$

then Eq. (1) can be rewritten as

$$H = H_0 + V_C, \quad (4)$$

with

$$H_0 = -\frac{\hbar^2}{2M}\nabla_R^2 + \frac{1}{2}M\omega_0^2 R^2 - \frac{\hbar^2}{2\mu}\nabla_r^2 + \frac{1}{2}\mu\omega_0^2 r^2, \quad (5)$$

where $M = m_e^* + m_h^*$; and $\mu = m_e^* m_h^*/M$.

The eigenstates of the barrier (D^+, X) center QD can be classified according to the total orbital angular momentum of the electrons along the z direction. To obtain the eigenfunctions and eigenenergies associated with the system motion, we diagonalized H in a model space spanned by the translationally invariant harmonic product bases $\Phi_{[K]} = [\phi^{\omega}_{n_1\ell_1}(\vec{R})\phi^{\omega}_{n_2\ell_2}(\vec{r})]_L$, where $[K]$ denotes the whole set of quantum numbers $(n_1, \ell_1, n_2, \ell_2)$ in brevity, $\ell_1 + \ell_2 = L$ is the total orbital angular momentum, $\phi^{\omega}_{n\ell}$ is a two-dimensional harmonic oscillator state with a frequency ω, an energy $(2n + |\ell| + 1)\hbar\omega$[11]. When $\omega = \omega_0$, the basic function is an exact solution of H if the Coulomb interaction is removed. In practice, ω serves as a variational parameter around ω_0 to minimize the eigenenergies. The matrix elements of H are then given by the following expressions

$$\langle \Phi_{[K]} | H_0 | \Phi_{[K']} \rangle = [2(n_1+n_2)+|\ell_1|+|\ell_2|+2]\hbar\omega\delta_{[K][K']} \quad (6)$$

$$\langle \Phi_{[K]} | V_C | \Phi_{[K']} \rangle = -U^I_{n_1 n_1'}\delta_{\ell_1\ell_1'}\delta_{n_2 n_2'}\delta_{\ell_2\ell_2'} + \sum_{[K''][K''']} B_{[K][K'']}B_{[K'][K''']}\sqrt{\frac{M}{m_h^*}} \times(1 - \sqrt{\frac{m_h^*}{m_e^*}})U^{II}_{n_1'' n_1'''}\delta_{\ell_1''\ell_1'''}\delta_{n_2'' n_2'''}\delta_{\ell_2''\ell_2'''}, \quad (7)$$

with

$$U^I_{n,n'} = \int_0^\infty R_{n\ell}(r)\frac{e^2}{\epsilon r}R_{n'\ell}(r)rdr, \quad (8)$$

$$U^{II}_{n,n'} = \int_0^\infty R_{n\ell}(r)\frac{e^2}{\epsilon\sqrt{r^2+d^2}}R_{n'\ell}(r)rdr, \quad (9)$$

$$B_{[K][K']} = \int \Phi_{[K]}(\vec{R},\vec{r})\Phi_{[K']}(\vec{R}',\vec{r}')d\vec{R}d\vec{r}, \quad (10)$$

where $R_{n\ell}$ is the radial part of two-dimensional harmonic oscillator function, $B_{[K][K']}$ is the transformation bracket of two-dimensional harmonic product states with two different sets of relative coordinates for the systems, which allows us to reduce the otherwise multi-integral into single-integral. Nonvanishing $B_{[K][K']}$ occurs only when both the states $\Phi_{[K]}(\vec{R},\vec{r})$ and $\Phi_{[K']}(\vec{R}',\vec{r}')$ have exactly the same eigenenergy and eigenangular momentum. Analytical expression for $B_{[K][K']}$ has already been derived in Ref. 12.

Our numerical computation is carried out for one of the typical semiconducting materials, GaAs, as an example with the material parameters shown in the following: $\epsilon = 12.4$, and $m_e^* = 0.067m_e$ (where m_e is the single electron bare mass). In this work we have used the energy unit is meV and the length unit is nm.

We define the binding energy of the barrier (D^+, X) centers as

$$E_B(D^+, X) = E(D^0) + E_0 - E(D^+, X) \quad (11)$$

where $E(D^+, X)$ is the ground-state energy of the barrier (D^+, X) center in the QDs, E_0 is the lowest levels of a hole in the QDs without the Coulomb potential, and $E(D^0)$ is the ground state energy for the barrier donor impurity.

We have calculated the binding energy of the ground-state of the complex as a function of the effective mass ratio σ and the dot radius R. The dependences of $E_B(D^+, X)$ and $E_B(A^-, X)$ on the electron-to-hole effective mass ratio σ with a fixed value of $\hbar\omega_0 = 1.0meV$ for a few different values of distances are plotted in Figs. 1. Fig. 1a shows the variations of $E_B(D^+, X)$ as a function of the electron-to-hole effective mass ratio $\sigma$and Fig. 1b shows that of $E_B(A^-, X)$. Obviously the binding energy of the barrier (D^+, X) center is larger than that of the barrier (A^-, X) center in the same conditions. From Fig. 1a, it is seen that, at the beginning, the binding energy $E_B(D^+, X)$ increases with decreasing the electron-to-hole effective mass ratio σ, then the binding energy reaches a maximum at some σ which is d-dependent, after that, as the σ is reduced further, the binding energy begins to decrease and eventually becomes negative, i.e., there exists a critical mass ratio σ^c, such that if $\sigma < \sigma^c$ the barrier (D^+, X) center configuration is unstable. It is obviously different from the 3D case because the (D^+, X) complex is stable if $\sigma < \sigma^c = 0.454$[6] and the spherical QDs with an infinite potential well case[7] because the (D^+, X) complex remains always stable. Both the maximum position and the critical mass ratio are dependent of the distance d. Compared with the binding energies for different distances d between the charged impurity located on the z axis and the dot plane, we find that the larger the distance d, the higher the binding energy. It is clear that as d increases from zero, the attractive interaction responsible for binding increases. However, the barrier (A^-, X) center configuration does not exist a critical mass ratio σ^c, i.e., when $d > 0.1nm$, the barrier (A^-, X) center configuration is always stable. This point is obviously different from the (A^-, X) complex in 3D semiconductors[6] which is stable if $\sigma \geq \sigma^c = 0.454$. From Fig. 1b, we can see that the binding energy increases with decreasing the electron-to-hole effective mass ratio σ, i.e., the heavy hole gives rise to larger binding energies than the light hole.

It is interesting to study the results when $d \to 0$. In this case, the (D^+, X) and (A^-, X) complexes do not

exist any bound state. This physical origin is that the increase in the repulsion energy becomes predominant and cannot be compensated for by the increase of attraction energy when $d \to 0$.

In order to understand the bound state feature , it is useful to study the change of the binding energy of the barrier (D^+, X) and (A^-, X) center QDs as a function of the dot radius R. In Figs. 2, we plot the binding energies of the barrier (D^+, X) (Fig. 2a) and (A^-, X) (Fig. 2b) center QDs with the dot radius R from 10 to $50nm$ for a fixed value of mass ratio $\sigma = 0.68$. It is readily seen that the binding energies increase with increasing the dot radius except the case of the binding energy of the (D^+, X) complex at $d = 0.2nm$. In this case, we find there exists a critical radius R^c, such that if $R < R^c$ the barrier (D^+, X) center configuration is unstable. It is obviously seen that these results are in good agreement with those in Figs. 1.

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Figure Captions:

Figs. 1 Dependences of the binding energy of the ground-state on electron-to-hole effective mass ratio σ for a few different values of d with $\hbar\omega_0 = 1.0meV$ are plotted: (a) the barrier (D^+, X) center; (b) the barrier (A^-, X) center..

Figs. 2 Dependences of the binding energy of the ground-state on the dot radius R for a few different values of d with $\sigma = 0.68$ are plotted: (a) the barrier (D^+, X) center; (b) the barrier (A^-, X) center.