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# Binding energy of an exciton bound to ionized donors in quantum dots

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**Abstract**

Binding energies for an exciton $(X)$ trapped in the two-dimensional quantum dot by a positive ion located on the $z$ axis at a distance $d$ from the dot plane are calculated by using the method of few-body physics. This configuration is called a barrier $(D^+, X)$ center. The dependence of the binding energy of the ground state of the barrier $(D^+, X)$ center on the dot radius for a few values of the distance $d$ between the fixed positive ion on the $z$ axis and the dot plane is obtained. We find that when $d < 0.2$ nm the barrier $(D^+, X)$ center does not form a bound state. 

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A charged donor center in semiconductors consists of a single positive ion and two electrons $(D^-)$ or an electron and a hole (i.e., an exciton) which are bound to the positive ion. Recently, the $D^-$ donor centers in semiconductor nanostructures have been investigated from both the experimental [1–5] and theoretical [6–9] points of view. However, up to now, only few theoretical studies have been devoted to the exciton bound to an ionized donor $(D^+, X)$ complex in low-dimensional structures [10–13]. A $(D^+, X)$ center is the simplest exciton complex which is formed when an electron and a hole are trapped by a charged impurity. They can be used as a test for the theoretical description of exciton-impurity interaction.

A system in which an electron and a hole confined to a parabolic quantum dot (QD) are bound by a positive ion located on the $z$ axis at a distance $d$ from the dot plane is called a barrier $(D^+, X)$ center QD. There has been interest in the subject later [14,15]. Rich electronic structures and optical properties, and a variety of structural phase transitions are predicted in such systems.

In this paper, we concentrate our study on the barrier $(D^+, X)$ complex. It results from the binding of an exciton to an ionized hydrogenic donor. Its possible existence was predicted in 1958 by Lampert [16]. We will propose a procedure to diagonalize the Hamiltonian of the barrier $(D^+, X)$ center in QD's with a parabolic lateral confining potential by using the method of few-body physics. The dependence of the binding energy of the ground state of the barrier $(D^+, X)$ center on the dot radius for a few values of

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the distance $d$ between the fixed positive ion on the $z$ axis and the dot plane is obtained. We find that when $d < 0.2\,\mathrm{nm}$, the barrier $(D^+, X)$ center does not form a bound state.

The Hamiltonian for the barrier $(D^+, X)$ center QD in the effective-mass approximation is given by

$$H = \frac{p_e^2}{2m_e^*} + \frac{1}{2}m_e^*\omega_0^2 r_e^2 + \frac{p_h^2}{2m_h^*} + \frac{1}{2}m_h^*\omega_0^2 r_h^2 + V_c, \tag{1}$$

$$V_c = \frac{e^2}{4\pi\epsilon\epsilon_0}\left[\frac{1}{\sqrt{r_h^2 + d^2}} - \frac{1}{\sqrt{r_e^2 + d^2}} - \frac{1}{|r_e - r_h|}\right], \tag{2}$$

where $\boldsymbol{r}_e$ ($\boldsymbol{r}_h$) is the position vector of the electron (the hole) originating from the center of the dot and $p_e$ ($p_h$) is the moment vector; $m_e^*$ ($m_h^*$) is the effective mass of an electron (a hole); $\epsilon$ is the static dielectric constant; $\omega_0$ is the strength of the confinement, and $d$ is the distance between the fixed positive ion on the $z$ axis and the dot plane.

Introducing the coordinates

$$\boldsymbol{r} = \boldsymbol{r}_e - \boldsymbol{r}_h, \quad \boldsymbol{R} = (\boldsymbol{r}_e + \boldsymbol{r}_h)/2, \tag{3}$$

then Eq. (1) can be rewritten as

$$H = H_0 + V_c, \tag{4}$$

with

$$H_0 = \frac{P^2}{2M} + \frac{1}{2}M\omega_0^2 R^2 + \frac{p^2}{2\mu} + \frac{1}{2}\mu\omega_0^2 r^2, \tag{5}$$

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 eigen-function and eigen-energies, we diagonalized $H$ in a model space spanned by the translationally invariant harmonic product bases

$$\Phi_{[K]} = \left[\phi^{\omega}_{n_1\ell_1}(\boldsymbol{R})\,\phi^{\omega}_{n_2\ell_2}(\boldsymbol{r})\right]_L, \tag{6}$$

where $\phi^{\omega}_{n\ell}(\boldsymbol{r})$ is a two-dimensional harmonic oscillator state with frequencies $\omega$ [17], an energy $(2n + |\ell| + 1)\hbar\omega$. $[K]$ 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. When $\omega = \omega_0$, the basis function is an exact solution of $H$ if the Coulomb interaction is removed. In practice, $\omega$ serves as a variational parameter around $\omega_0$ to minimize the eigenenergies. The accuracy of solutions depends on how large the model space is. The dimension of the model space is constrained by $0 \le N = 2(n_1 + n_2) + |\ell_1| + |\ell_2| \le 24$. If $N$ is increased by 2, the ratio of the difference in energy is less than 0.01%. In what follows the energies are in meV and the lengths are in nm; $m_e^* = 0.067 m_e$ ($m_e$ is the free-electron mass), and $\epsilon = 12.4$ for GaAs QD's are adopted in the calculation.

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

$$E_B(D^+, X) = E(D^0) + E_0 - E(D^+, X) \tag{7}$$

where $E(D^+, X)$ is the barrier $(D^+, X)$ center ground-state energy in the QD's, $E_0$ is the lowest levels of a hole in the QD's without the Coulomb potential, and $E(D^0)$ is the ground state energy for the barrier donor. $E(D^0)$ is determined by solving the appropriate Schrödinger equations in which the ground state for the barrier donor Hamiltonian is given by linear combinations of the eigenstates with zero angular momentum for the electron which is

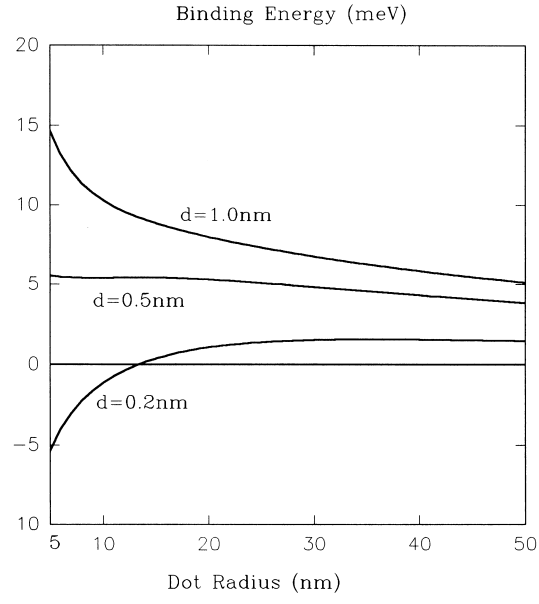


Fig. 1. Dependences of the binding energy $E_B(D^+, X)$ on the QD radius $R$ for a few different values of $d$ with $\sigma = 0.707$ are plotted.

bound by a positive ion located on the $z$ axis at a distance $d$ from the dot plane. The binding energy defined by (7) possesses the following physical interpretation: this is the minimum energy, which is required to liberate one hole from the bound state of the barrier $(D^+,X)$ center QD. After this dissociation process, the hole is bound in the ground state of the barrier $(D^+,X)$ center. The considered the ground state of the barrier $(D^+,X)$ center is bound if $E_B(D^+,X)>0$.

The dependences of $E_B(D^+,X)$ on the dot radius $R$ with the ratio of the effective masses of the electron and the hole $\sigma = m_e^*/m_h^* = 0.707$ for a few different values of distances are plotted in Fig. 1. The calculation shows that when $d < 0.2$ nm there does not exist the bound state in the barrier $(D^+,X)$ center QD's. From Fig. 1, we see that the binding energy reduces as the dot radius is increased for large values of $d$. However, when $d$ is small, the binding energy reduces as the dot radius is reduced for small dot radius $R$ but as the dot radius is increased for larger dot radius $R$. For $d = 0.2$ nm, as the dot size is increased further, the binding energy becomes negative, i.e., there exists a critical radius $R^c$, such that if $R < R^c$ the barrier $(D^+,X)$ center configuration is unstable. From $E_B(D^+,X)=0$ we obtain $R^c \simeq 14$ nm, this critical position depends on the distance $d$. It is clear that the critical radius $R^c$ increases as $d$ increases. When $d > 0.3$ nm, the barrier $(D^+,X)$ center configuration is always stable. It is clear that as $d$ increases from zero, the attractive interaction responsible for binding increases.

In order to understand the bound state feature, it is useful to study the mass effect of the barrier $(D^+,X)$ center QD's. In Fig. 2, we plot the binding energy of the barrier $(D^+,X)$ center QD's for $\hbar\omega_0 = 3.6$ meV with the mass ratio $\sigma$ from 0 to 1.0. It is readily seen that, at the beginning, the binding energy increases as the mass ratio $\sigma$ decreases, then the binding energy reaches a maximum at some $\sigma$ which is $d$-dependent, after that, as the $\sigma$ is reduced further, the binding energy begins to decrease and eventually becomes negative, i.e., there exists a critical mass ratio $\sigma^c$, such that if $\sigma < \sigma^c$ the barrier $(D^+,X)$ center configuration is unstable. Both the maximum position and the critical mass ratio are dependent of the distance $d$. This point is obviously different from the case of the exciton without a positive ion in QD's because at where, the heavier hole (i.e., the litter $\sigma$) gives rise to the larger binding energy. When $d$ becomes larger, the result will be in agreement with the exciton in QD's.

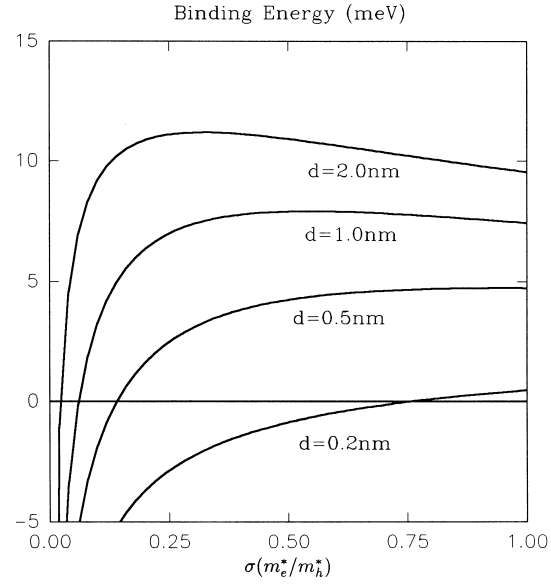


Fig. 2. Dependences of the binding energy $E_B(D^+,X)$ on the mass ratio $\sigma$ with $\hbar\omega_0 = 3.6$ meV are plotted.

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