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22 November 1999

PHYSICS LETTERS A

Physics Letters A 263 (1999) 127–130

www.elsevier.nl/locate/physleta

Negative donor centers in a GaAs parabolic quantum dot

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Received 13 August 1999; accepted 11 October 1999
Communicated by J. Flouquet

Abstract

Using the method of few-body physics, the solutions of low-lying states of negative donor centers in a GaAs parabolic quantum dot have been obtained. The dependence of the binding energy of the D^- center on the quantum dot radius is also studied.

PACS: 73.20.Dx; 71.35.Gg

Neutral donors in semiconductors can trap an extra electron to form negative donor centers (D^- centers), which are the solid-state analog of H^- ions [1]. D^- centers are one of the simplest 'many-body' electronic systems, which cannot be solved exactly. They can be used as a test for the theoretical description of electron-electron interaction [2] and have already been observed in both elemental semiconductors [3] III-V compounds [4]. Recent advances in material-growth techniques allow one to study such a system in lower dimensions. A number of experimental [5–8] and theoretical papers [9–13] have been devoted to the investigation of the energy levels of quasi-two-dimensional D^- states. The fundamental study is important in its own right as reducing the dimensionality often introduces unexpected physical phenomena.

A quantum dot (QD) is semiconductor nanostructure with a three-dimensional confinement of electrons [14]. Recently the QD's have been fabricated in different shapes, for example, disk-like (cylindrical) shape [15] and spherical shape [14,16]. In contrast to the various studies on a D^- center in a spherical quantum dot, experimental and theoretical results related to the quantum confinement effect on D^- states in a disk-like quantum dot are still rare. In experimentally realized quantum dots, the motion in the z direction is always frozen out into the lowest subband. Since the corresponding extent of the wave function is much less than the one in the xy-plane, we can treat the QD's in a disk-like two-dimensional limit. For most QD's, the harmonic oscillator is a very good approximation to describe the lateral confinement. Therefore it is interesting to study electronic properties of D^- centers in a disk-like QD for understanding the dimensionality dependence of the energies of D^- low-lying states and the possibility of some future device applications.

In this paper, we will propose a procedure to calculate energy spectrum of D^- centers in disk-like QDs with a parabolic lateral confining potential by

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0375-9601/99/$ - see front matter
PII: S0375-9601(99)00723-9

using the method of few-body physics. We will investigate the energies of the low-lying states and the ground-state binding energy of the D^- centres as a function of the QD size.

The D^- center in a disk-like QD can be described as a system composed of two electrons and a positively charged donor impurity located the centre of the disk potential-well region. We consider a single QD embedded in a matrix material. We assume the validity of the effective-mass approximation and neglect the difference of the electron band masses and dielectric constant between the QD region and the surrounding medium. It is reasonable for the case of the strong confinement and small dielectric-constant difference. However, we should point out that if there is significant penetration into the barrier, the effect of the electronic effective masses can be important, and that the effect of the discontinuity of the dielectric constants on the D^- states should be considered for large differences. With the effective-mass approximation, the Hamiltonian of two electrons bound to an ionized donor located in the center of a GaAs parabolic disk-like QD can be written as

$$H = \sum_{i=1,2}\left[\frac{p_i^2}{2m_e^*} + \tfrac{1}{2}m_e^*\omega^2 r_i^2\right] + V, \tag{1}$$

$$V = -\frac{e^2}{\epsilon}\sum_{i=1,2}\frac{1}{r_i} + \frac{e^2}{\epsilon r_{12}}, \tag{2}$$

where $\boldsymbol{r}_i$ ($\boldsymbol{p}_i$) is the position vector (the momentum vector) of the ith electron originating from the center of the dot; m_e^* is the effective mass of an electron; $r_{12} = |\boldsymbol{r}_1 - \boldsymbol{r}_2|$ is the electron-electron separation; ω is the strength of the confinement. In this work we have used the natural units of the material: the effective Bohr radius $a_B^* = \hbar^2\epsilon/m_e^* e^2$ as the length unit and the effective Rydberg $Ry^* = m_e^* e^4/\hbar^2\epsilon^2$ as the energy unit.

Introducing the coordinates

$$\boldsymbol{r} = \boldsymbol{r}_{12} = \boldsymbol{r}_1 - \boldsymbol{r}_2, \quad \boldsymbol{R} = (\boldsymbol{r}_1 + \boldsymbol{r}_2)/2, \tag{3}$$

then Eq. (1) can be rewritten as

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

with

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

where $M = 2m_e^*$; and $\mu = m_e^*/2$.

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

$$\Phi_{[K]} = \tilde{A}\left\{\left[\phi_{n_1\ell_1}(\boldsymbol{R})\,\phi_{n_2\ell_2}(\boldsymbol{r})\right]_L \chi_S\right\}, \tag{6}$$

where $\chi_S = [\xi(1)\xi(2)]_S$, $\xi(i)$ is the spin state of the ith electron and the spins of two electrons are coupled to S, $\phi_{n\ell}(\boldsymbol{r})$ is a two-dimensional harmonic oscillator state with frequencies ω (ω is considered as an adjustable variational parameter), an energy $(2n + |\ell| + 1)\hbar\omega$, and $\tilde{A}$ is the antisymmetrizer. $[K]$ denotes the whole set of quantum numbers (n_1,ℓ_1,n_2,ℓ_2) in brevity, $\ell_1 + \ell_2 = L$ is the total orbital angular momentum. The angular momentum L = odd if the spin $S = 1$, and L = even if $S = 0$ such that the wave function is antisymmetried. The matrix elements of H are then given by the following expressions:

$$\langle \Phi_{[K]}|H_0|\Phi_{[K']}\rangle = \left[2(n_1 + n_2) + |\ell_1| + |\ell_2| + 2\right] \times \hbar\omega\delta_{[K][K']}, \tag{7}$$

$$\langle \Phi_{[K]}|V|\Phi_{[K']}\rangle = U_{n_2n_2'}\delta_{n_1n_1'}\delta_{\ell_1\ell_1'}\delta_{\ell_2\ell_2'} - 2\sum_{[K''],[K''']} B_{[K][K'']}B_{[K'][K''']} \times U_{n_2''n_2'''}\delta_{n_1''n_1'''}\delta_{\ell_1''\ell_1'''}\delta_{\ell_2''\ell_2'''}, \tag{8}$$

with

$$U_{nn'} = \int_0^\infty R_{n\ell}(r)\frac{e^2}{\epsilon r}R_{n'\ell}(r)\,r\,dr, \tag{9}$$

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

where $R_{n\ell}(\boldsymbol{r})$ 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 coordinates, which allows us to reduce the otherwise multi-integral into single-integral. Nonvanishing $B_{[K][K']}$ occurs only when both the states $\Phi_{[K]}(\boldsymbol{R},\boldsymbol{r})$ and $\Phi_{[K']}(\boldsymbol{R}',\boldsymbol{r}')$ have exactly the same eigen-energy and eigen-angu-

lar momentum. Analytical expression for $B_{[K][K']}$ has already been derived in Ref. [17]. The set of canonical coordinates $(\boldsymbol{R}', \boldsymbol{r}')$ are defined by $\boldsymbol{r}' = \boldsymbol{r}_1$, $\boldsymbol{R} = \boldsymbol{r}_2$. The dimension of the model space is constrained by $0 \le N = 2(n_1 + n_2) + |\ell_1| + |\ell_2| \le 28$. If N is increased by 2, the ratio of the difference in energy is less than 0.001%.

In this paper, effective atomic units are used so that all energies are measured in units of the effective Rydberg Ry^* and all distances are measured in units of the effective Bohr radius a_B^*. Using $m_e^* = 0.067 m_e$ (m_e is the free-electron mass) and $\epsilon = 12.4$ for GaAs QD's, we calculated the energy spectrum of the four lowest states, i.e., ^1S, ^3P, ^1P, and ^3S states, of a D^- center as a function of the dot radius R (Fig. 1). As the radius of the dot increases, the energies decrease, i.e., the stronger the confinement, the higher the energy. Compared with the case in two-electron dots [18], the crossover of two levels do not appear as the dot radius changes. It is obvious that the electronic properties of two-electron systems with and without a positive charge centre are different. We define the binding energy of the D^- centres as

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

where $E(D^-)$ is the D^- ground-state energy in the QD's, E_0 and $E(D^0)$ are, respectively, the lowest levels of an electron in the QD's without and with the Coulomb potential. The dependence of $E_B(D^-)$ on the dot radius R is plotted in Fig. 2. The binding energy reduces as the dot radius is increased. However, as the dot size is increased further, the binding energy begins to becomes negative, i.e., there exists a critical radius R^c, such that if $R < R^c$ ($R > R^c$) the D^- configuration is stable (unstable). From $E_B(D^-) = 0$ we obtain $R^c \simeq 0.4\, a_B^*$.

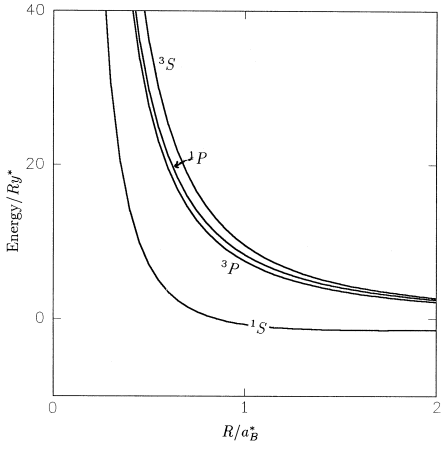

Fig. 1. Dependence of the energy spectrum of the four lowest states of the D^- centres in a QD on the QD radius R normalized by the effective Bohr radius a_B^* is plotted.

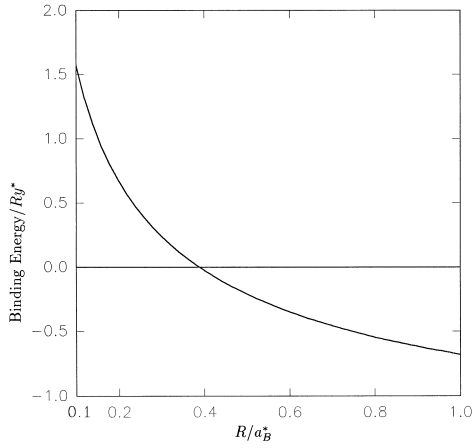

Fig. 2. Dependence of the binding energy $E_B(D^-)$ on the QD radius R normalized by the effective Bohr radius a_B^* is plotted.

Acknowledgements

This work is financially supported by the National Natural Science Foundation of China under Grant No. 19975013.

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