

Electron-hole interaction in spherical quantum dots of nanoheterostructures

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The main states of electron and hole in spherically semiconductor quantum-dot are studied. The wave function of the system is optimized by variation of effective radii of electron and hole orbits. The main state and Coulomb energy as function of quantum-dot radius are calculated.

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1. Introduction

In recent years physical properties of Quantum Dots (QD) in nanoheterostructures are intensively studied both experimentally [1-4] and theoretically [5-8]. It is connected not only with the purpose of their application in nanoelectronic devices, but also to the fundamental understanding of the quantum phenomena. QD is possible to present as a particle of the semiconductor (the size $\sim 5-100$ Å and with energy gap E_{g1}) which plunged into semiconductor-matrix or insulator (with energy gap $E_{g2} > E_{g1}$). The wells (W) with depth $-V$ (ΔE_C for electrons and ΔE_V for holes, See fig.1) might be formed depending on the values of band discontinuity.

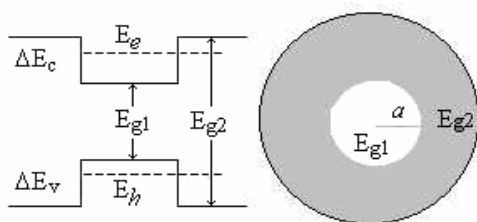


Fig. 1. The formation of W and QD in the nanoheterostructures.

With sufficient small sizes of a W, QD can have one or several levels. Optical characteristics of similar systems are appreciably defined by an energy spectrum of electrons and holes. If the depth of the well, V is large enough it is possible to apply a spherical W approach with infinite depth [5-6,9]. On the other hand, at a small size of V , it is important to consider the penetration of particles into a crystal-matrix [7,8]. The problem of an exciton in QD with

a well of an infinite depth is considered for the first time in this study [8]. The certain interest also represents the application of a variational method to calculate the low energy levels of an exciton.

2. The variational method to calculate the lower energy levels of an exciton

The Hamiltonian of an exciton in QD with spherical form is

$$H = -\frac{\hbar^2}{2m_1}\Delta_1 - \frac{\hbar^2}{2m_2}\Delta_2 + V(r_1) + V(r_2) - \frac{e^2}{\epsilon|r_1 - r_2|} \quad (1)$$

$$V(r_i) = \begin{cases} -V_i & r_i < a \\ 0 & r_i > a \end{cases} \quad i = 1, 2 \quad (2)$$

where, a is the radius of a spherical QD; r_1, r_2 - coordinates electrons and holes respectively; m_1, m_2 are their effective masses and ϵ is the dielectric constant. m_1, m_2 and ϵ for are simply considered identical in all areas. Wave function of the basic level ($l=0$) is $\Psi(r_1, r_2) = \phi(r_1)\phi(r_2)$ in the form. In concrete calculations applied functions are as follows: hydrogen as $\phi(r_i) \sim \exp(-\delta_i r_i)$ and Gaussian $\phi(r_i) \sim \exp(-\delta_i^2 r_i^2)$ in all areas of space $0 < r < \infty$ (δ_i is the varied parameter, $i = 1, 2$). Pre-computations have shown that the energy of system is better estimated by Gaussian function $\phi(r_i) \sim \exp(-\delta_i^2 r_i^2)$ as used below.

If QD is filled only by one electron (the hole is absent), the problem is solved precisely [9], i.e. energy of the basic level is from the transcendental equation $\alpha \text{ctd}(\alpha a) = -\beta$, where $\hbar^2 \alpha^2 / 2m = V_0 + E$ and

$\hbar^2\beta^2/2m = -E\langle 0$. For comparison the exact and variational energy are shown in the table below.

Its accuracy allows for using trial functions $\sim \exp(-\delta_i^2 r_i^2)$ as a basis for a problem of an exciton in QD. It is possible to find the energy function of an exciton averaging the Hamiltonian (1) trial functions. The following functions are alike Gaussian;

$$E[\mu_1, \mu_2] = \langle K_1 \rangle + \langle K_2 \rangle + \langle V_1 \rangle + \langle V_2 \rangle - \langle C \rangle \quad (3)$$

where

$$\langle K_i \rangle = 3 \frac{\hbar^2 \mu_i^2}{2m_i a^2} \quad (4)$$

$$\langle C \rangle = 2\sqrt{\frac{2}{\pi}} \frac{e^2}{\varepsilon a} \frac{\mu_1 \mu_2}{\sqrt{\mu_1^2 + \mu_2^2}}, \quad \mu_i = \delta_i a, \quad i = 1, 2 \quad (5)$$

$$\langle V_i \rangle = -\mu_i V_i \cdot 2\sqrt{\frac{2}{\pi}} \left[\int_0^1 dt \exp(-2\mu_i^2 t^2) - \exp(-2\mu_i^2) \right] \quad (6)$$

In motionless excitons localized in QD the kinetic energy is equal to zero and the total energy measured from edge of a zone of a crystal-matrix is equal to $E = E_{g2} + E_{ex}$. For concrete calculations it is believed: for electron $V_1 = 0.0675$ eV, $m_1 = 0.2 m_0$, for holes $V_2 = 0.1575$ eV, $m_2 = m_0$, $\varepsilon = 9$ which is typical for QD on the basis of nitrides InGaN [8].

In Fig. 2 below the dependence of a total exciton energy E_{ex} and Coulomb energy of the electron and holes on the radius of QD are shown. By reducing the size of a QD (the width of a W) their electron levels and holes are pushed out from a W. Therefore the energy E_{ex} is decreased, and the energy of corresponding photon $E = E_{g2} + E_{ex}$ increases.

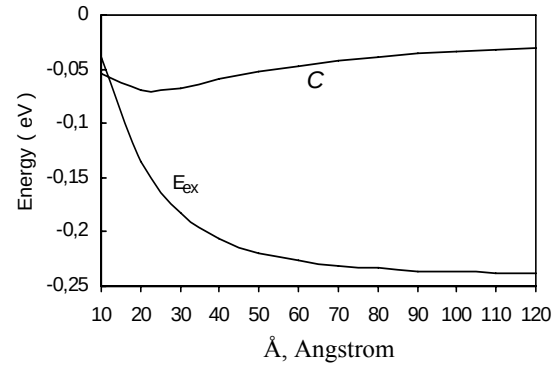


Fig. 2. The dependence of a total exciton energy - E_{ex} and Coulomb energy of the electron and holes- C on the radius of QD.

Reducing the process the Coulomb energy of the electron and holes firstly increases in a QD size and it has a maximum at $a_c \sim 30$ Å and then begins to reduce. An origin of this maximum as explained in [8] is according to which the particles at the greater sizes of QD are strongly localized and the energy of their interaction is inversely proportional to the size of QD. At the small sizes of QD, the levels of particles are pushed out from a W and have an appreciable penetration into the forbidden zone of a crystal-matrix (especially easy particle - electron), owing to the decrease of their interaction.

It is distinctly observed in the dependence of the sizes of an electron and hole “cloud” on the radius of QD. In figure 3 below the dependence of the size of an electron and hole orbits on the radius of QD is shown. It is seen that the hole clouds (a heavy particle - a hole which is localized more strongly than electron) continue to decrease monotonously in the process of QD narrowing while the easy particle-electron begins to penetrate deep into W leaving from the centre.

Table 1. Comparison of the exact and variational energy.

$a, \text{Å}$	E_{ex}, eV				E_{var}, eV			
	$V_0=0.2 \text{ eV}$		$V_0=2 \text{ eV}$		$V_0=0.2 \text{ eV}$		$V_0=2 \text{ eV}$	
	$m/m_0=0.2$	$m/m_0=5$	$m/m_0=0.2$	$m/m_0=5$	$m/m_0=0.2$	$m/m_0=5$	$m/m_0=0.2$	$m/m_0=5$
10	0.0000	-0.1481	-0.9602	-1.9333	0.0000	-0.1457	-0.9421	-1.9169
50	-0.1481	-0.1972	-1.9333	-1.9970	-0.1457	-0.1962	-1.9169	-1.9951
90	-0.1811	-0.1991	-1.9783	-1.9990	-0.1787	-0.1987	-1.9699	-1.9983

Except the Coulomb interactions, amendments to the total energy still give the distinctive account of masses and dielectric constants of carriers in QD and crystal-matrix.

The account of these amendments allows a correctly estimated length of a wave of the radiated laser in QD on the basis of nitrides InGaN.

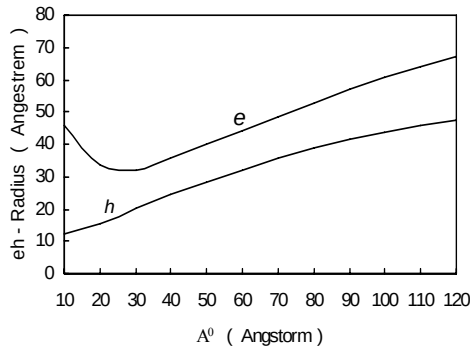


Fig. 3. Dependence of the size of an electron and hole orbits on the radius of QD.

3. Conclusions

The results were obtained from the variational analysis of the behaviour of the bottom energy levels and the structure of an exciton in spherical QD, comparatively with the results got from Hartree equation.

The results are basically related to an exciton in QD with a simple W. Nevertheless, it is easy to generalize for other problems such as the D-centers where biexcitons and polarons are localized in simple or multilayered QD.

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