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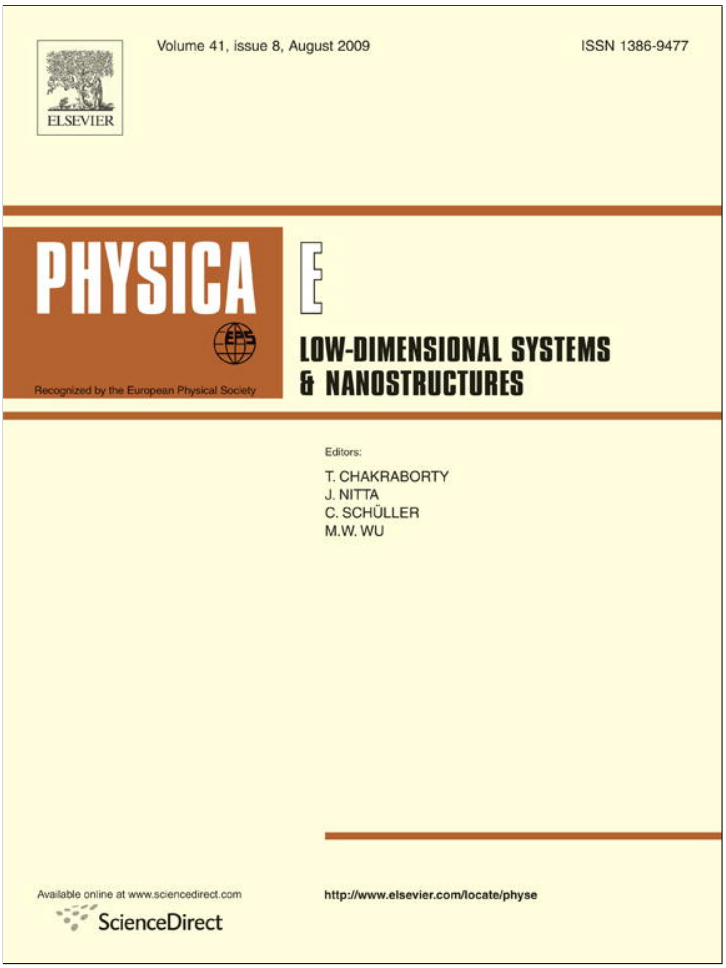

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Oscillator strengths of electron quantum transitions in spherical nano-systems with donor impurity in the center

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ABSTRACT

The exact solutions of Schrodinger equation for the electron in Coulomb field of donor impurity are obtained within the effective masses approximation and dielectric continuum model for the spherical quantum dot CdS/SiO_2 and anti-dot $ZnS/Cd_xZn_{1-x}S$. The dependences of electron energy spectrum and its probability density on nano-system radius are studied. The numeric calculations and analysis of oscillator strength of intersubband quantum transition from ground into first excited state at the varying radius are performed. It is shown that the oscillator strength for the big quantum dot is close to the respective value for the bulk semiconductor crystal.

1. Introduction

Quantum dots (QDs) stay one of the most intensively studied objects of low-dimensional systems. Their attracting peculiarity is that the quasi-particle (electron, hole) energy levels, determined by the shape, sizes and composition of nano-system, have the properties of real atoms. It influences on the quasi-particle energy of radiation transitions and allows create the semiconductor devices with demanded physical characteristics.

The presence of charged impurity in QD changes the potential of size quantization (Figs. 1 and 2), affecting both the quasi-particle energy spectra and oscillator strengths of radiation transitions. The theory of electron spectrum and wave functions in the field of donor impurity inside the semiconductor nano-system has been developed within the different methods [1–4]. In Ref. [1], the authors have established the general theory of quasi-particle energy spectra in multilayer spherical nano-systems with donor impurity. In Refs. [2,3] the exact energy spectrum and wave functions of electron in the field of donor impurity placed into the center of spherical QDs (HgS/CdS, CdS/H_2O, HgS/H_2O) have been obtained in the framework of the effective masses approximation. The evolution of energy spectrum and distribution of probability density of electron inside nano-system, depending on its sizes, have been investigated.

In Ref. [4], the authors have calculated the oscillator strengths of inter sub-band quantum transitions for the electron in CdS/SiO_2 QD with donor impurity, placed into its center. The energies and wave functions of ground and first excited electron states were obtained within the effective masses approximation using the variation method. From the dependence of quantum transition oscillator strength on QD sizes (in dipole approximation), it was clear that it was almost vanishing at the increasing QD radius. According to physical considerations, it must correspond to the quantum transition oscillator strength of electron interacting with charged impurity in bulk crystal. Thus, the variation method gave the oscillator strength hundreds times bigger than the respective magnitude for bulk crystal. This result is to be checked up by other methods.

The localized states of quasi-particles are absent in quantum anti-dots (QADs), creating the potential barrier in semiconductor matrix. The stationary, quasi-stationary and pre-surface localized electron states can exist due to the Coulomb interaction with donor impurity, placed into the center of QAD (inset in Fig. 2). It is also clear that the height of the potential barrier and QAD radius would influence on the energies. As far as we know, the theoretical investigation of quasi-particle energy spectra and

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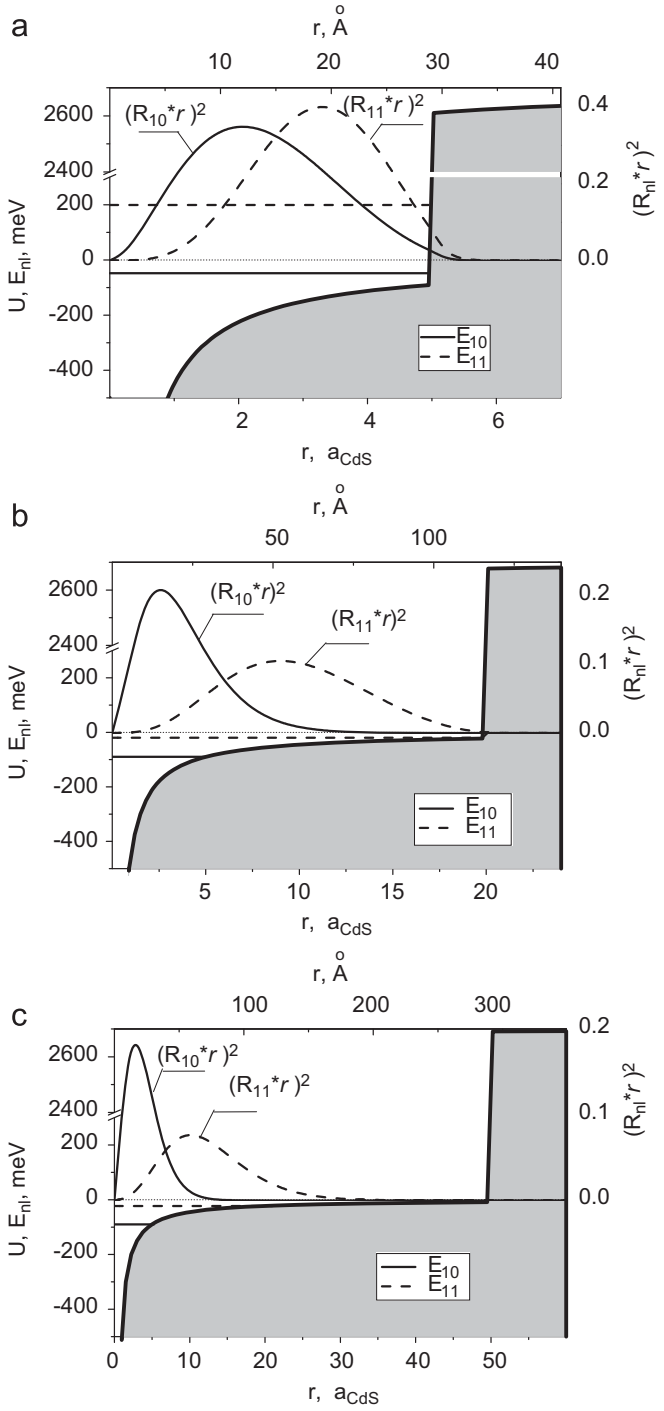

Fig. 1. Scheme of potential energy, electron energy spectrum (E_{10}, E_{11}) and distribution of probability density in CdS/SiO_2 QD with donor impurity at $r_0 = 5a_{CdS}$ (a), $r_0 = 20a_{CdS}$ (b) and $r_0 = 50a_{CdS}$ (c).

wave functions in QAD with donor impurity inside was not performed yet.

In this paper, the theory of electron stationary states spectrum and wave functions is developed for the spherical QD and QAD with hydrogen-like donor impurity placed into the center. The dependences of oscillator strengths of electron inter sub-band quantum transitions on nano-system radius are obtained using the exact solutions of Schrodinger equation.

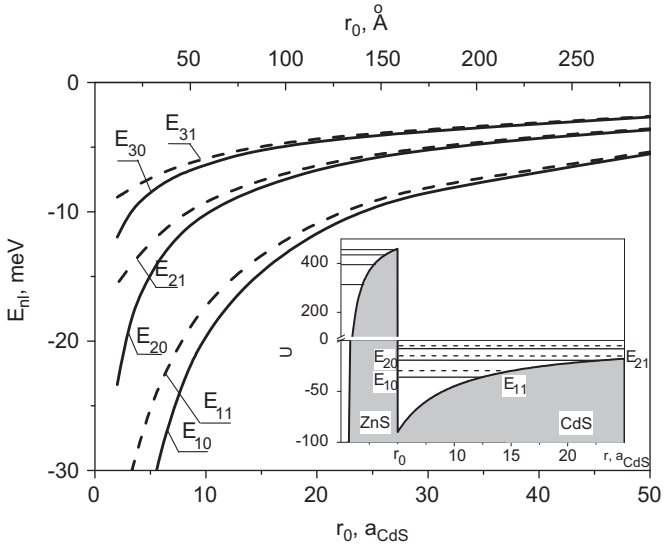

Fig. 2. Dependence of electron energy spectrum on nano-system radius (r_0) for ZnS/CdS QAD with donor impurity in the center. The inset presents the scheme of the potential energy.

2. Hamiltonian of the system and solution of Schrodinger equation

The spherical semiconductor nano-system ("0", QD or QAD) with radius (r_0), embedded into the massive semiconductor matrix ("1") is under study. The donor impurity, placed in its center, creates Coulomb potential for the electron. The electron spectrum is obtained within the effective mass approximation with its

$$m(r) = \begin{cases} m_0, r < r_0, \\ m_1, r \geqslant r_0. \end{cases} \tag{1}$$

The Hamiltonian of the system is written as

$$H = -\nabla \frac{\hbar^2}{2m(r)} \nabla + U(r), \tag{2}$$

where $U(r) = V(r) - (Ze^2/\varepsilon r)$ with $V(r) = \begin{cases} 0, & r < r_0, \\ V_0, & r \geqslant r_0. \end{cases}$ for the QD and $V(r) = \begin{cases} V_0, & r < r_0, \\ 0, & r \geqslant r_0. \end{cases}$ for the QAD and ε-dielectric constant of QD or QAD because it most of all provides the screening of Coulomb interaction.

Solving the Schrodinger equation for the QD in spherical coordinate system, it is clear that the radial one has the form

$$\frac{\hbar^2}{2m_0}\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{\ell(\ell+1)}{r^2}\right] R_{nl}(r) + \left(E_{nl} + \frac{e^2}{\varepsilon r}\right) R_{nl}(r) = 0, \quad r < r_0 \tag{3}$$

$$\frac{\hbar^2}{2m_1}\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{\ell(\ell+1)}{r^2}\right] R_{nl}(r) + \left(E_{nl} - V_0 + \frac{e^2}{\varepsilon r}\right) R_{nl}(r) = 0, \quad r > r_0 \tag{4}$$

Using the convenient parameters

$$\xi_0 = \frac{\sqrt{8m_0 E_{nl}}}{\hbar}, \quad \xi_1 = \frac{\sqrt{8m_1(E_{nl} - V_0)}}{\hbar}, \quad \eta_{0,1} = \frac{2m_{0,1}e^2}{\varepsilon \xi_{0,1}\hbar^2} \tag{5}$$

and radial wave function

$$R_{nl}(r)=\begin{cases}\dfrac{\chi_0(\xi_0 r)}{r}, & r<r_0,\\ \dfrac{\chi_1(\xi_1 r)}{r}, & r>r_0\end{cases} \tag{6}$$

there are obtained the differential equations

$$\frac{1}{\xi_0^2}\frac{\partial^2\chi_0(\xi_0 r)}{\partial^2 r}-\left(\frac{1}{4}+\frac{\eta_0}{\xi_0 r}-\frac{1/4-(\ell+1/2)^2}{\xi_0^2 r^2}\right)\chi_0(\xi_0 r)=0,\quad r<r_0 \tag{7}$$

$$\frac{1}{\xi_1^2}\frac{\partial^2\chi_1(\xi_1 r)}{\partial^2 r}-\left(\frac{1}{4}+\frac{\eta_1}{\xi_1 r}-\frac{1/4-(\ell+1/2)^2}{\xi_1^2 r^2}\right)\chi_1(\xi_1 r)=0,\quad r>r_0. \tag{8}$$

Their general solution can be written within Whittaker functions [5]

$$\chi_0(\xi_0 r)=A_0 M(\eta_0,\ell+\tfrac{1}{2},\xi_0 r),\quad \chi_1(\xi_1 r)=A_1 W(\eta_1,\ell+\tfrac{1}{2},\xi_1 r) \tag{9}$$

Whittaker functions are expressed through the hyper geometrical functions of the first and second kind $F(\alpha,\gamma,z)$, $G(\alpha,\gamma,z)$. Finally, the radial wave function is written as

$$R_{nl}(r)=\begin{cases}A_0\exp[-\xi_0 r/2]r^{\ell}F(\ell+1+\eta_0,2\ell+2,\xi_0 r), & r<r_0,\\ A_1\exp[-\xi_1 r/2]r^{\ell}G(\ell+1+\eta_1,2\ell+2,\xi_1 r), & r>r_0.\end{cases} \tag{10}$$

From the condition of the radial wave function and its density of current continuity at the interface

$$R_{n\ell}^{(0)}(r)\Big|_{r=r_0}=R_{n\ell}^{(1)}(r)\Big|_{r=r_0}, \tag{11}$$

$$\frac{1}{m_0}\frac{\partial R_{n\ell}^{(0)}(r)}{\partial r}\bigg|_{r=r_0}=\frac{1}{m_1}\frac{\partial R_{n\ell}^{(1)}(r)}{\partial r}\bigg|_{r=r_0}, \tag{12}$$

the discrete energy spectrum (E_{n1}) of electron in QD with donor impurity in the center is obtained.

The stationary electron states in QAD or near its surface ($E_{n1}<0$) are obtained in analogy. The quasi-stationary states ($E_{n1}>0$) of electron with finite lifetimes in the Coulomb well would be studied in future within the modified S-matrix method [6,7].

Using the obtained electron energy spectrum and wave functions, the oscillator strengths of inter sub-band radiation transitions between the states ψ_{nlm} and $\psi_{n'l'm'}$ in dipole approximation with radiation (absorption) of linearly polarized light are found from the expression

$$F_{nlm-n'l'm'}=\frac{2m_0}{\hbar^2}(E_{n'l'}-E_{nl})\int R_{nl}^{*}(r)Y_{lm}^{*}(\theta,\varphi)r\cos\theta R_{n'l'}(r)Y_{l'm'}(\theta,\varphi)d\vec{r}, \tag{13}$$

where E_{nl} and $E_{n'l'}$ are the energies of the initial and final states, respectively. The selection rules for such transitions are determined by integral over angular variables. The probability of quantum transition is unequal to zero at $l-l'=\pm 1$.

3. Discussion of results

Computer calculations of the energies, wave functions and oscillator strengths of quantum transitions have been performed for CdS/SiO_2, ZnS/CdS and ZnS/$Cd_xZn_{1-x}S$ nano-systems with physical parameters presented in Table 1 (m_e, pure electron mass; a, lattice constant; V_e, electron affinity).

Table 1
Physical parameters.

Crystal	m (m_e)	ε	a (Å)	V_e(eV)
CdS	0.2	5.5	5.818	3.65
SiO_2	0.42	3.9	–	0.95
ZnS	0.28	5.07	5.41	3.1

The energies of ground (E_{10}) and excited (E_{11}) states, potential energy and distribution of probability density of electron location in the states ψ_{100} and ψ_{100} are presented in Fig. 1 for the QDs with different radii and hydrogen-like donor impurity in the center. It is clear that size quantization weakly influence at the energies E_{10}, E_{11} and distribution of probability density for the QD of big radius. The electron is localized by Coulomb potential ($E_{10}<0$, $E_{11}<0$) and its energy spectrum is like the respective one for the electron in the field of hydrogen-like impurity in bulk semiconductor crystal. When the QD radius becomes smaller, the influence of size quantization increases and, consequently, the electron energy levels shift into the region of higher energies. The energy of ground state is still negative, even for the small QD radius ($r_0=5\,a_{CdS}$), while the energy of the first excited state is positive ($E_{11}>0$). The dependence of electron energy spectrum on radius is qualitatively similar to the one obtained in Ref. [2], where it is shown the degeneration of electron energy spectrum over the orbital quantum number (λ) at increasing radius for HgS/CdS QD with donor impurity.

In Fig. 2, it is shown as the dependence of electron energy spectrum on radius for ZnS/CdS QAD with hydrogen-like impurity in the center. From the scheme of potential energy, in the inset of the figure, it is clear that the attracting Coulomb potential forms two potential wells: deep one inside QAD and shallow—outside it. Herein, the electron quasi-stationary states with positive energy can exist in the deep well. The numeric calculations of electron energies and wave functions of stationary states, performed for ZnS/CdS QAD prove that the electron is localized in outer shallow well at arbitrary radius. The increase in the radius decreases quantum well depth, thus resulting in decreased electron-impurity binding energy.

In Fig. 3, the evolution of oscillator strength ($F_{100-110}(r_0)$) is presented for the different spherical nano-systems: CdS/SiO_2 QD with donor impurity (solid curve), CdS/SiO_2 QD without the impurity (dashed curve), ZnS/CdS QAD with donor impurity (dash–dot curve) and massive semiconductor CdS crystal (dotted line). For CdS/SiO_2 QD with donor impurity, the oscillator strength of inter sub-band transition is maximal when $r_0<10a_{CdS}$. It happens due to the big magnitude of the respective wave functions overlapping (Fig. 1a) and big difference between E_{11} and E_{10}. The further decrease in QD radius causes the repulses of electron energy level (E_{11}) out of the potential well, where the maximum of excited state wave function shifts out of the QD due to the tunnel effect and the tail of Coulomb potential at $r>r_0$. As a result, the wave functions overlapping decrease and oscillator strength also decreases. The increase in QD radius (Fig. 1b) decreases the energy difference, as well as wave functions overlapping. Thus, the oscillator strength becomes more than two times smaller, tending in the limit case to the respective magnitudes for the massive CdS crystal.

The oscillator strength ($F_{100-110}$) almost does not depend on QD radius when the charged impurity is absent. It is because the smaller energy difference ($E_{11}-E_{10}$) is compensated by the increased wave functions overlapping. The oscillator strength ($F_{100-110}$) first rapidly decreases and then saturates for ZnS/CdS QAD with donor impurity in the center.

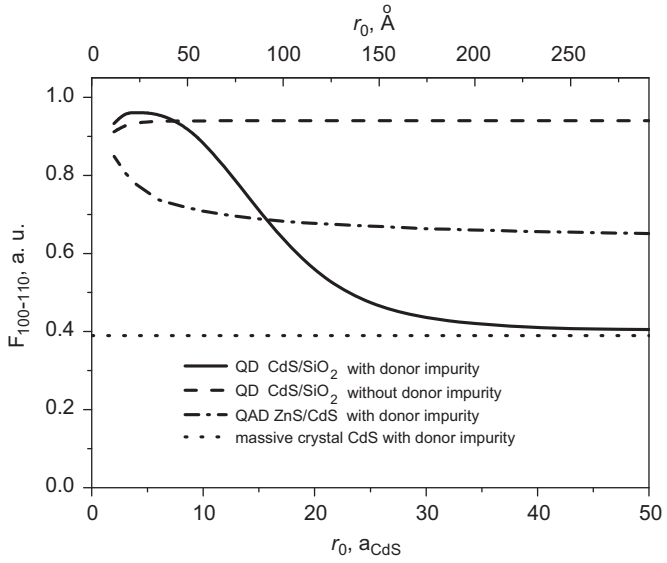

Fig. 3. Dependences of quantum transition oscillator strength ($F_{100-110}$) on radius (r_0) for different nano-systems.

The investigation of barrier height influence at electron energy spectrum and its localization in nano-system has been performed for $ZnS/Cd_xZn_{1-x}S$ QAD, Fig. 4(a–d). Herein, the potential barrier height linearly depends on Cd concentration (x). The numeric calculations prove that the electron can be localized in the inner deep potential well at small concentration (x). The energy of these states, on the contrary to the states of electron localized in the outer well, almost does not depend on QAD radius, Fig. 4(a and b). When the barrier height becomes bigger, the energy of electron localized in inner well becomes bigger too. When the energies reach the bottom of the outer well, the localization of electron changes, Fig. 4(c and d)––it is inside the outer well with bigger probability.

In Fig. 5, the energies of ground (E_{10}) and first excited (E_{11}) states as functions of concentration (x) are shown by dashed curves and oscillator strength $F_{100-110}$—by solid curve. The linear increasing part of dashed curve corresponds to the electron localization in inner well and horizontal one in the outer well. Consequently, it is easy to explain the non-monotonous dependence $F_{100-110}(r_0)$. The oscillator strength of electron quantum transition from the ground to the first excited state, when it does not change its localization in the well, is much bigger than if it is tunneling from one well into another during the quantum transition.

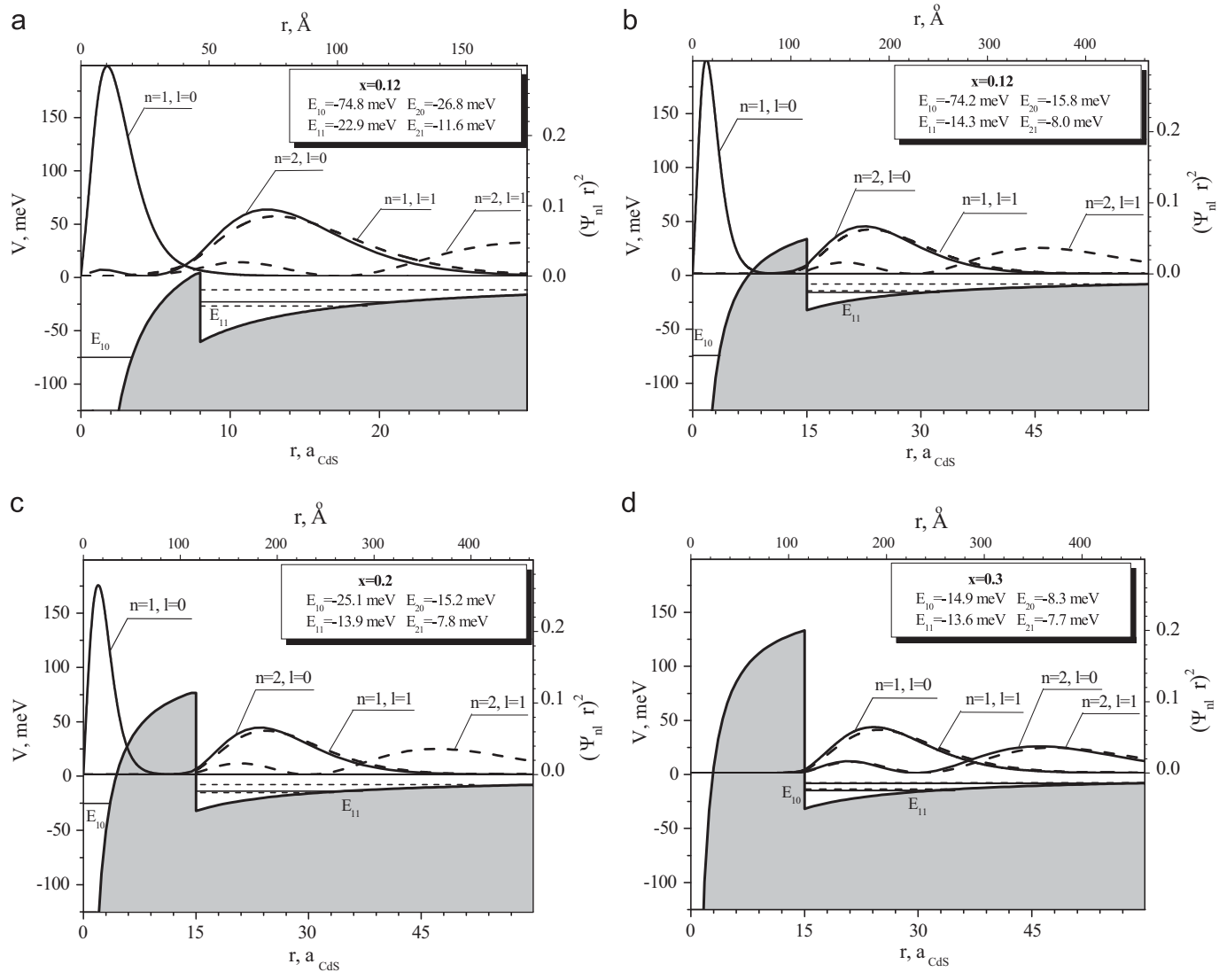

Fig. 4. Scheme of potential energy, electron spectrum (E_{nl}) and distribution of probability density in $ZnS/Cd_xZn_{1-x}S$ QAD with donor impurity at $x = 0.12$, $r_0 = 8a_{CdS}$ (a) $x = 0.12$, $r_0 = 15a_{CdS}$ (b), $x = 0.2$, $r_0 = 15a_{CdS}$ (c) and $x = 0.3$, $r_0 = 15a_{CdS}$ (d).

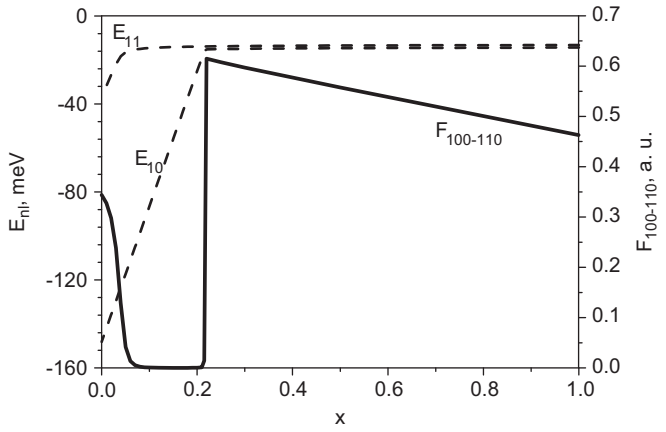

Fig. 5. Dependences of quantum transition oscillator strength ($F_{100-110}$, solid curve) and electron energies (E_{10} and E_{11}, dashed curves) on concentration (x) for $ZnS/Cd_xZn_{1-x}S$ QAD with donor impurity.

4. Conclusions

The exact solutions of Schrodinger equation within the effective mass approximation are obtained for the electron in different spherical nano-systems with charged impurity in the center (CdS/SiO_2 QD and $ZnS/Cd_xZn_{1-x}S$ QAD). The numeric calculations and analysis of oscillator strengths of inter sub-band transitions from ground into first excited state of electron evolution on nano-system radius are performed using the obtained energy spectrum and wave functions. It is shown that the oscillator strength for the big quantum dot ($r > 200$ Å) is close to the respective value for the bulk semiconductor crystal. The localization of an electron bounded by a central donor impurity in QAD and the oscillator strength depend on a QAD potential barrier height.

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