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Optical Transitions in Infinitely High Cylindrical Quantum Dot

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Direct optical absorption of light in cylindrical quantum dot is theoretically investigated. Analytical expressions for light absorption coefficients at strong and weak size quantization regimes are found. The corresponding selection rules for optical transitions are defined. The expressions for absorption threshold frequencies are found.

Introduction

Quantum dots (QD) belong to the most intensively investigated objects of nanophysics. The unique feature of such systems consists in the fact, that the motion of particles inside them is quantized in all three directions. Therefore it is not occasionally that these systems are called as "artificial atoms". An outstanding property of QD is the possibility to rule their energy spectrum during the growth of particular patterns. Up-to-date growth methods of nanostructures allow to obtain QD's of different shapes and sizes [1]. Till now spherical, pyramidal and cylindrical QD's are grown up.

Physical properties of QD's are studies both theoretically and experimentally. In particular, electronic and impurity states in QD's are investigated in details (see, e.g., [2-8]). As a result of these investigations the strong coupling between the character of QD energy spectrum and its geometrical parameters (size, shape) is revealed. At this physical chemical properties of both QD and surrounding medium form the character of potential well. On the other hand QD shape and sizes define the height and symmetry of this potential.

Thus it is natural to suppose that optical, kinetic, etc. properties of QD depend on abovementioned characteristics as well. In particular, it is well-known that the spectrum of direct optical absorption in semiconductors is conditioned by wave functions and energy spectrum of charge carriers inside them [9]. One of the first articles, investigating optical absorption in QD belong to Efros' [10]. The authors of it theoretically investigated the pecularities of direct optical absorption in spherical QD with confinement potential, described within the frameworks of spherically symmetrical infinitely high potential well. Later on the authors of [11] considered light absorption in spherical QD and took into account the anysotropy of band structure. It was shown, that the account of anysotropy results in appearance of optical transitions, forbidden in isotropic approximation. That is why it is reasonable to expect, that changing QD geometrical shape may result in the appearance of new transitions between levels as well. Therefore the interest towards the investigation of QD nonsphericity influence onto direct optical absorption appears in quite natural way.

In given article direct optical absorption in cylindrical QD is theoretically investigated. At this strong and weak regimes of size quantization are discussed.

Theory

Let's consider a particle inside cylindrical QD with confinement potential of the form

$$V_{conf}(\rho,\varphi,z) = V_{conf\,\rho}(\rho) + V_{conf\,z}(z)\,, \tag{1}$$

where $V_{conf\,z}(z)$ is QD confinement potential in the oZ direction (cylinder axis direction), $V_{conf\,\rho}(\rho)$ is QD confinement potential in xoy plane:

$$V_{conf\,z}(\rho)=\begin{cases}0, & |\rho|\le a,\\ \infty, & |\rho|>a.\end{cases}, \tag{2}$$

$$V_{conf}\left(z\right)=\frac{\mu\omega_z^2 z^2}{2};\ \left(\omega_z=\frac{\gamma\hbar}{\mu L^2}\right). \tag{3}$$

Here a is the radius of crossection of cylindrical QD, L is the height of cylinder, γ is dimensionless fitting parameter.

Sroedinger equation looks like

$$-\frac{\hbar^2}{2\mu}\Delta\psi+V_{conf\,\rho}(\rho)\psi+V_{conf\,z}(z)\psi=E\psi\ . \tag{4}$$

The corresponding solution of this equation can be written as [12]

$$\psi_{n_\rho,m,n}=CJ_m\left(\kappa_{n_\rho,|m|}\rho\right)e^{im\varphi}\chi\left(z\right), \tag{5}$$

where

$$\chi(z)=\left(\frac{\mu\omega_z}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}e^{-\frac{\mu\omega_z}{2\hbar}z^2}H_n\left[\sqrt{\frac{\mu\omega_z}{\hbar}}z\right],$$

$$\kappa_{n_\rho,|m|}=\sqrt{\frac{2\mu E_{n_\rho,|m|}}{\hbar^2}}, \tag{6}$$

$$E_{n_\rho,|m|}=\frac{\hbar^2\alpha^2_{n_\rho+1,|m|}}{2\mu a^2}, \tag{7}$$

$E_{n_\rho,|m|}$ defines the energy of flat motion, μ is the effective mass of charge carriers, C is normalizing constant of flat motion, $J_m\left(\kappa_{n_\rho,|m|}\rho\right)$ is Bessel cylindrical function, m is magnetic quantum number, n_ρ is radial quantum number, equal to the number of zeroes of $J_m\left(\kappa_{n_\rho,|m|}\rho\right)$ function (excluding zeroes at $\rho=a$ and $\rho=0$ (for $m\neq 0$ case)), $H_n(x)$ is Hermit polynomial,

n is the quantum number, describing the motion in oZ direction, $\alpha_{n_\rho+1,|m|}$ is ($n_\rho+1$)-th root of $J_m\left(\alpha_{n_\rho+1,|m|}\right)=0$ Bessel function (in ascending order of $\alpha_{n_\rho+1,|m|}$); particularly, $\alpha_{10}\approx 2.40$, $\alpha_{11}\approx 3.83$ and, correspondingly, $E_{00}\approx 2.88\frac{\hbar^2}{\mu a^2}$, $E_{01}\approx 7.33\frac{\hbar^2}{\mu a^2}$, (for details see [12]).

For energy levels, in its turn, we have

$$E=\frac{\hbar^2\alpha^2_{n_\rho+1,m}}{2\mu a^2}+\hbar\omega_z\left(n+\frac{1}{2}\right). \tag{8}$$

Thus considered QD model is analytically exact solvable. This fact allows to calculate the coefficients of interband direct light absorption in this system. The calculation of absorption coefficient (AC) of light will be performed for two cases of size quantization:

a. The regime of strong size quantization, when excitonic effects can be neglected.

b. The regime of weak size quantization, when the main input into the energy of system is conditioned by excitonic interactions.

a. The regime of strong size quantization.

According to Ref. [10] AC is determined using the formulae

$$K=A\sum_{\substack{n_\rho,n_\rho'\\ mm'\\ nn'}}\left|\int\psi^e_{n_\rho mn}\psi^h_{n_\rho' m'n'}d\vec{r}\right|^2\delta\left(\Delta-E^e_{n_\rho mn}-E^h_{n_\rho' m'n'}\right), \tag{9}$$

where $\Delta=\hbar\omega-E_g$ (E_g is the width of forbidden band), ω is the frequency of incident light, e subscript denotes electron, h denotes the hole, A is the quantity, proportional to the square of modulus of dipole moment matrix element, taken on Bloch functions. Let's also mention, that we suppose, that $\mu_e<<\mu_h$.

At strong size quantization regime, when $\{\rho_0, L\} << \{a_B^e, a_B^h\}$ ($a_B^{e(h)}$ is Bohr radius of electron (hole)), the influence of QD walls is so strong, that we can use one-particle approximation and neglect Coulumb interactions between electron and hole. Then we can use Eqs. (5)-(9) and for AC write

$$K_1 = A\sum_{\substack{n_\rho m\\ nn'}}\left|I_{nn'}D\pi a^2\left\{J_{m+1}\left(\alpha_{n_\rho+1,|m|}\right)\right\}^2\right|^2 \delta\left(\hbar\omega - E_g - \left(\frac{\hbar^2\alpha^2_{n_\rho+1,m}}{2a^2}\right)\left(\frac{1}{\mu_e}+\frac{1}{\mu_h}\right) - \hbar\omega_z^e\left(n+\frac{1}{2}\right) - \hbar\omega_z^h\left(n'+\frac{1}{2}\right)\right) \tag{10}$$

where

$$I_{nn'} = \int_{-\infty}^{+\infty} H_n\left(\sqrt{\lambda_{ze}}\,z\right)H_{n'}\left(\sqrt{\lambda_{zh}}\,z\right)\exp[-\tfrac{1}{2}(\lambda_{ze}+\lambda_{zh})z^2]dz\,,$$

$$\lambda_{ze} = \frac{\mu_e\,\omega_z^e}{\hbar},\ \lambda_{zh} = \frac{\mu_h\,\omega_z^h}{\hbar}\ ,$$

D is the constant, which can be expressed through normalizing constants of wave functions.

b. The regime of weak size quantization.

At this regime of size quantization the highest energy is exciton binding energy. Therefore wave function of the system by analogy with Ref. [10] can be presented as

$$\psi(\vec{r}_e, \vec{r}_h) = \varphi(\vec{r})f(\vec{R})\,, \tag{11}$$

where $\vec{r} = \vec{r}_e - \vec{r}_h$, $\vec{R} = \dfrac{\mu_e\vec{r}_e + \mu_h\vec{r}_h}{\mu_e + \mu_h}$, $\varphi(\vec{r})$ is the wave function of relative motion of electron and hole, $f(\vec{R})$ is the wave function, describing the motion of exciton center of mass. Thus for considered model the expression for $f(\vec{R})$ will coincide with (5). The only difference is that instead of μ_e or μ_h will be the $M = \mu_e + \mu_h$ quantity. Correspondingly, energy values will look like:

$$E_{ex}^1 = \frac{\hbar^2 \alpha_{n_\rho+1,m}^2}{2Ma^2} + \hbar\Omega_z\left(n + \frac{1}{2}\right) - E_{ex}, \tag{12}$$

where $\Omega_z \sim \frac{\hbar}{ML^2}$, E_{ex} is exciton binding energy. As to $\varphi(\vec{r})$ function, it can be expressed through the well-known wave functions of hydrogen-like atom.

Supposing, that exciton is mainly localized near QD center and the influence of QD walls onto the binding energy E_{ex} is weak, at the same time, taking into account inequalities $\{a_B^e, a_B^h\} << \{\rho_0, L\}$ for the AC we have [10]

$$K_2 = A\sum_{n_\rho mn} |\varphi(0)|^2 \left|\int f_{n_\rho mn}(\vec{R})d\vec{R}\right|^2 \delta\left(\hbar\omega - E_g - E_{ex}^1\right). \tag{13}$$

By the relative motion, the only non trivial value of $\varphi(0)$ corresponds to the state $l = m = 0$ and is equal to

$$\varphi(0) = \frac{1}{\sqrt{\pi a_{ex}^3}}, \tag{14}$$

where a_{ex} is exciton radius.

For AC after the integration we correspondingly have:

$$K_2 = A\sum_{n_\rho n}\left|\frac{C_{n_\rho 0n}^1 n!}{\left(\pi a_{ex}^3\right)^{1/2}\left(\frac{n}{2}\right)!} \cdot \frac{1-\alpha_{n_\rho+1,0}^2 J_{-1}\left(\alpha_{n_\rho+1,0}\right)}{\alpha_{n_\rho+1,0}^3}\right|^2 \delta\left(\hbar\omega - E_g + E_{ex} - \left(\frac{\hbar^2\alpha_{n_\rho+1,m}^2}{2Ma^2} + \hbar\Omega_z\left(n+\frac{1}{2}\right)\right)\right). \tag{15}$$

Discussion

Let's mention at once that in the first case in z direction the transitions takes place, satisfying the selection rule $|n-n'|=2t$, where t is integer, as it straightforwardly follows from the properties of Hermite polynomials. Thus the transitions in oz direction take place between the levels with same parity. As to the transitions in xoy plane, the selection rule $m=-m'$, $n_\rho = n_\rho{}'$ takes place for them. Let's mention, that in the case of spherical impermeable well [10] due to the orthogonality of Bessel functions at the analogous quantization regime the transitions took place between levels with equal orbital and radial quantum numbers. As to the magnetic quantum numbers, they again satisfy the relation $m=-m'$. With the help of Eq. (10) for absorption threshold frequencies we can write

$$\hbar\omega_{001} = E_g + \left(\frac{2.88\hbar^2}{a^2} + \frac{\gamma\hbar^2}{2L^2}\right)\left(\frac{1}{\mu_e} + \frac{1}{\mu_h}\right). \tag{16}$$

In Eq. (15) the summation is performed over odd values of n. It means, that the transitions on oZ direction take place between odd levels. In this case threshold frequencies will be determined according to the relations

$$\hbar\omega_{001} = E_g + \frac{2.88\hbar^2}{Ma^2} + \frac{\gamma\hbar^2}{2ML^2} - E_{ex}. \tag{17}$$

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