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**ABSORPTION AND SCATTERING OF LIGHT  
IN SEMICONDUCTOR QUANTUM DOTS****S.I. POKUTNYI**UDC 535.34  
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A theory of the interaction of an electromagnetic field with single-particle states of the charge carriers arising in the bulk of a semiconductor quantum dot is developed in the framework of the dipole approximation. It is shown that the oscillator strength of the transition, the transition dipole moments for single-particle states, and the light absorption cross-section in quantum dots have large values greater than the typical corresponding values for semiconductor materials.

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**1. Introduction**

At the present time, the intense studies are carried out on the optical [1–5] and electrooptical [6–8] properties of quasi-zero-dimensional structures consisting of spherical quantum dots (QD) with a radius  $a \simeq 1 \div 10^2$  nm grown in transparent semiconductor (dielectric) matrices.

Such investigations are caused by the fact that such heterophase systems are new promising materials for producing the new components for nonlinear optoelectronics (specifically, the components that control optical signals in optical computers [9–12] and as an active range of injection semiconductor lasers [5, 13–17]).

Optical and electrooptical properties of such quasi-zero-dimensional structures are governed by the energy spectrum of space-limited electron-hole pairs (excitons) [1–8]. The effect of size quantization of the energy spectrum of electrons [1, 2] and excitons [3, 4] in heterophase structures of this kind was found with the methods of optical spectroscopy.

In [18], the conditions for the charge-carrier localization near a spherical interface between two dielectric media have been analyzed. As a result,

the obtained polarization interaction  $U(\mathbf{r}, a)$  (where  $\mathbf{r}$  is the distance of a charge carrier to the center of a dielectric, and  $a$  is the radius of a particle) between the charge carriers and a surface charge induced at the spherical interface depending upon the relative permittivity  $\varepsilon = (\varepsilon_1/\varepsilon_2)$  (where  $\varepsilon_1$  and  $\varepsilon_2$  are the dielectric permittivities of the dielectric and a dielectric particle immersed in it, respectively.)

For charge carriers moving near a dielectric particle, there are two possibilities:

1) the polarization interaction  $U(\mathbf{r}, a)$  results in the attraction of charge carriers by the particle surface (for  $\varepsilon < 1$  and  $\varepsilon > 1$ , they attract, respectively, to the outer and inner surfaces of the particle) and in the formation of exterior surface states [19, 20] and interior surface states [21];

2) for  $\varepsilon < 1$ , the polarization interaction  $U(\mathbf{r}, a)$  causes the repulsion of charge carriers from the inner surface of a dielectric particle and gives rise to local bulk states in the volume [22, 23]. Here, the spectrum of the low-lying bulk states has an oscillatory form.

In [18–23], it was shown that the formation of the above-indicated local states is of threshold nature and is feasible provided the radius of a dielectric particle  $a$  is greater than some critical dimension  $a_c$ :

$$a \geq a_c = 6|\beta|^{-1}a_{B_i}, \quad \beta = (\varepsilon_1 - \varepsilon_2)/(\varepsilon_1 + \varepsilon_2),$$

$$a_{B_i} = \frac{\varepsilon_i \hbar^2}{m_i e^2}. \quad (1)$$

Here,  $a_{B_i}$  is the Bohr radius of a charge carrier with effective mass  $m_i$  in a medium with dielectric constant  $\varepsilon_i$  ( $i = 1, 2$ ).

In [24, 25], the interaction of an electromagnetic field with above-indicated single-particle local states of charge carriers in the neighborhood of a dielectric particle was theoretically studied. The size and frequency dependences of the resonance absorption and scattering cross sections in such states were obtained.

In the experimental papers [7, 8], the optical properties of massive QDs of GaAs in the GaAs and GaSb matrices and the relevant instrument characteristics of an injection laser with the active range on the levels of massive QDs were studied, and a strong short-wave length shift of the line of the laser generation was observed.

In such massive QD, the energy spectrum of charge carriers will be absolutely discrete above the QD dimensions  $a \simeq 1 \div 7$  nm [15, 18]. In the first approximation, the spectrum of size-quantization states of this kind can be described by the spectrum of a charge carrier moving in a spherical symmetric well with infinite walls [26–28].

As the theory of the absorption and scattering of light by discrete states of this kind has not been studied so far, we develop a theory of the interaction of an electromagnetic field with single-particle size-quantization states of the charge carriers arising in the bulk of a semiconductor QD to fill this gap.

## 2. Hamiltonian of an Electron-Hole Pair in a Quantum Dot

We consider the simple model quasi-zero-dimensional system including a neutral spherical semiconductor QD of radius  $a$  with the permittivity  $\varepsilon_2$  surrounded by the medium, whose permittivity is  $\varepsilon_1$ . An electron  $e$  and a hole  $h$  with the effective masses  $m_e$  and  $m_h$ , respectively, are moving in this QD ( $\mathbf{r}_e$  and  $\mathbf{r}_h$  are the distances of the electron and the hole from the center of the QD). It is also assumed that the electron and hole energy bands are parabolic.

The characteristic dimensions of the problem are  $a$ ,  $a_e$ ,  $a_h$ , and  $a_{ex}$ , where

$$a_e = \frac{\varepsilon_2 \hbar^2}{m_e e^2}, \quad a_h = \frac{\varepsilon_2 \hbar^2}{m_h e^2}, \quad a_{ex} = \frac{\varepsilon_2 \hbar^2}{\mu e^2} \quad (2)$$

are the Bohr radii of an electron, a hole, and an exciton in a semiconductor, whose permittivity is  $\varepsilon_2$  ( $e$  is the electron charge, and  $\mu = m_e m_h / (m_e + m_h)$  is the

effective mass of an exciton). All the characteristic dimensions of the problem obey the inequality

$$a, \quad a_e, \quad a_h, \quad a_{ex} \gg a_0, \quad (3)$$

where  $a_0^1$  is the interatomic distance. This fact allows us to consider the motion of an electron and a hole in QD in the effective mass approximation.

Using the above-mentioned approximations of the adopted model of a quasi-zero-dimensional system, we can write the Hamiltonian of an electron-hole pair as

$$H = -\frac{\hbar^2}{2m_e} \Delta_e - \frac{\hbar^2}{2m_h} \Delta_h + V_{eh}(\mathbf{r}_e, \mathbf{r}_h) + U(\mathbf{r}_e, \mathbf{r}_h, a) + E_g, \quad (4)$$

where the first two terms describe the kinetic energy of an electron and a hole,  $E_g$  is the band gap in an infinite semiconductor with dielectric permittivity  $\varepsilon_2$ , the energy of the Coulomb interaction of an electron with a hole

$$V_{eh}(\mathbf{r}_e, \mathbf{r}_h) = -\frac{e^2}{2\varepsilon_2 a} \frac{2a}{(r_e^2 - 2r_e r_h \cos \theta + r_h^2)^{1/2}}, \quad \theta = \widehat{\mathbf{r}_e \mathbf{r}_h}, \quad (5)$$

$U(\mathbf{r}_e, \mathbf{r}_h, a)$  is the interaction energy of an electron and a hole with the induced field of polarization on the spherical interface between the two media. For arbitrary  $\varepsilon_1$  and  $\varepsilon_2$ , we can write the interaction energy  $U(\mathbf{r}_e, \mathbf{r}_h, a)$  in an analytic way [18, 22]:

$$U(\mathbf{r}_e, \mathbf{r}_h, a) = -\frac{e^2 \beta}{\varepsilon_2 a} \times \frac{1}{[(r_e r_h / a^2)^2 - 2(r_e r_h / a^2) \cos \theta + 1]^{1/2}} - \frac{e^2 \beta}{2(\varepsilon_2 + \varepsilon_1) a} \int_0^\infty \frac{dy (a^2 / r_h y)^\alpha \Theta(y - (a^2 / r_h))}{|\mathbf{r}_e - y(\mathbf{r}_h / r_h)|} - \frac{e^2 \beta}{2(\varepsilon_2 + \varepsilon_1) a} \int_0^\infty \frac{dy (a^2 / r_e y)^\alpha \Theta(y - (a^2 / r_e))}{|\mathbf{r}_h - y(\mathbf{r}_e / r_e)|}. \quad (6)$$

Here,  $\Theta(x)$  is the conventional step function, and

$$\alpha = \frac{\varepsilon_1}{\varepsilon_1 + \varepsilon_2}. \quad (7)$$

<sup>1</sup>Generally speaking,  $a_0$  should be understood as a characteristic size of surface or bulk states which make the main contribution to the medium polarization. If such states have low frequencies,  $a_0$  can considerably exceed the interatomic distances. In this case, it is necessary to take into account corrections to the electrostatic potential of images (see [27] and references therein). But we assume that such low-frequency excitations do not make the main contribution to  $\varepsilon_1, 2$ .

### 3. Spectrum of Charge Carriers in a Quantum Dot

In the bulk of QD, the energy levels

$$E_{n,l}(a) = \frac{\hbar^2}{2m_{e(h)}a^2}\varphi_{n,l}^2 \quad (8)$$

of an electron (hole) can arise [28] due to the purely spatial limitation of the region of quantization. Here,  $n$  and  $l$  are the principal and orbital quantum numbers of an electron (hole), and  $\varphi_{n,l}$  are the roots of the Bessel functions  $J_{l+1/2}(\varphi_{n,l}) = 0$ . For the size quantization levels of this kind to appear, it is necessary that the kinetic energy of an electron (hole)  $E_{n,l}(a)$  (8) in Hamiltonian (4) be much greater than the interaction energy  $U(a)$  (6) of an electron (hole) with the polarization field arising on the spherical interface “QD – dielectric (semiconductor) matrix”:

$$E_{n,l}(a) = \frac{\hbar^2}{2m_{e(h)}a^2}\varphi_{n,l}^2 \gg U(a) \sim \frac{e^2\beta}{2\varepsilon_2\alpha}. \quad (9)$$

Condition (9) holds for QDs with radii

$$a \ll a_s^{e(h)} = \frac{\varphi_{n,l}^2}{\beta}a_{e(h)}. \quad (10)$$

It should be noted that the local volume states arise in QD with the dimension  $a$  satisfying, except (1), such inequalities [23]:

for  $l = 0$ ,

$$(a/a_{e(h)})^{1/2} \gg ((1 + \alpha)/2\beta)^{1/2}2^{-1}\left(t + \frac{3}{2}\right), \quad (11)$$

for  $l \neq 0$ ,

$$(a/a_{e(h)})^{1/4} \gg 2^{-1}(2\beta/(1 + \alpha))^{-1/4}(l(l + 1))^{1/4} \times \\ \times [1 - (1 - 2^{-1}B)^{1/2}]^{-1}B, \quad (12)$$

$$B = 2[(3/8)((7 + 5\alpha)/(2 + \alpha)) + 1] -$$

$$-(t + (3/2))(l(l + 1))^{-1/2}.$$

Here,  $t = 2n_r + l = 0, 1, 2, \dots$  is the principal charge carrier quantum number ( $n_r = 0, 1, 2, \dots$  is the radial quantum number).

Thus, according to conditions (10)–(12) for the arising quasi-zero-dimensional states, QDs must be of much smaller dimensions than those for the arising local volume states.

The discrete levels of an electron (hole)  $E_{n,l}(a)$  (8) in QD will be slightly broadened at room temperature  $T_0$  if the distance between them

$$\Delta E_{n,l}(a) = E_{n',l'}(a) - E_{n,l}(a) \ll kT_0 \quad (13)$$

is much smaller than  $kT_0$  (where  $k$  is Boltzmann constant [20, 22]).

Using (8), inequality (13) can be expressed in the following form:

$$\frac{\hbar^2}{2m_{e(h)}a^2} \frac{(\varphi_{n',l'}^2 - \varphi_{n,l}^2)}{kT_0} = \eta(a) \ll 1. \quad (14)$$

The spectrum of charge carriers in QD, which follows from Eq. (8), is valid only for the lowest states  $(n, l)$ , for which the inequality

$$\Delta E_{n,l}(a) \ll \Delta V_0(a) \quad (15)$$

is satisfied. Here,  $\Delta V_0(a)$  is the depth of the potential well for holes in QD (e.g., in a CdS QD with the dimension  $a$  satisfying inequality (10),  $\Delta V_0(a) = 2.3 \div 2.5$  eV [29]).

The realization of condition (10) affords a possibility to use the electron wave function in a spherical symmetric well with infinite walls as the electron wave function in QD [30]:

$$\Psi_{n,l,m}(r, \theta, \varphi) = Y_{l,m}(\theta, \varphi) \frac{J_{l+1/2}(\varphi_{l,n}(r/a))}{J_{l+3/2}(\varphi_{l,n})} \frac{\sqrt{2}}{a\sqrt{r}}, \quad (16)$$

where  $r$  is the distance between the electron and the center of QD;  $\theta, \varphi$  are the azimuthal and polar angles of the electron (hole);  $Y_{l,m}$  are the normal spherical functions ( $m$  is the magnetic quantum number of an electron (hole));  $J_\nu(x)$  are the Bessel functions which can be expressed in terms of the spherical Bessel functions  $j_\nu(x)$  [30]:

$$J_{l+1/2}(\varphi_{l,n}(r/a)) = \sqrt{2/\pi}\varphi_{l,n}(r/a)j_l(\varphi_{l,n}(r/a)),$$

$$J_{l+3/2}(\varphi_{l,n}) = \sqrt{2/\pi}\varphi_{l,n}j_{l+1}(\varphi_{l,n}). \quad (17)$$

Let us consider  $m = 0$ . Then the spherical functions can be expressed as  $Y_{l,m}(\theta, \varphi) = Y_{l,0}(\theta)$ .

#### 4. Transition Dipole Moments of Charge Carriers in QD

In the frequency region corresponding to the type of charge-carrier states under consideration ( $n, l$ ) in the bulk of QD, the wavelength is much greater than the dimensions of these states ( $\simeq a_e, a_h$ ). Thus, their behavior ( $n, l$ ) in the electromagnetic field is described well by the dipole approximation. Here, the dipole moment operator for an electron (hole) in the bulk of QD has the following form [31]:

$$\mathbf{D}(\mathbf{r}) = L\mathbf{D}^0(\mathbf{r}); \quad \mathbf{D}^0(\mathbf{r}) = e\mathbf{r}; \quad L = \frac{3\varepsilon_1}{2\varepsilon_1 + \varepsilon_2}. \quad (18)$$

To estimate the dipole moments, it is sufficient to examine the transition between the lowest discrete states (8) (e.g., between the principal  $|1s\rangle = (n = 1, l = 0, m = 0)$  and  $|1p\rangle = (n = 1, l = 1, m = 0)$  states). For calculating the matrix element of the transition dipole moment  $\mathbf{D}_{1,0}(a)$  of a charge carrier between the  $1s$  and  $1p$  states, we assume that the uniform field of a light wave  $\mathbf{E}(\omega, t)$  is directed only along the  $Z$  axis ( $\omega$  is the frequency of the wave). Then, as the perturbation causing the dipole transitions, we take the dipole moments  $\mathbf{D}(\mathbf{r})$  induced by the field  $\mathbf{E}(\omega, t)$  (18).

We write the expression for the transition dipole moment  $\mathbf{D}_{1,0}(a)$  in the following form:

$$\mathbf{D}_{1,0}(\mathbf{r}) = L\mathbf{D}_{1,0}^0(a), \quad (19)$$

where

$$\mathbf{D}_{1,0}^0(a) = \langle 1s | \mathbf{D}^0(\mathbf{r}) | 1p \rangle = e \langle 1s | \mathbf{r} | 1p \rangle \quad (20)$$

is the transition dipole moment in vacuum. In view of (16) and (17), the state wave functions  $|1s\rangle$  and  $|1p\rangle$  have the following form:

$$\begin{aligned} \langle 1s | &= \Psi_{1,0,0}(r, \theta) = Y_{0,0}(\theta) \frac{2}{a^{3/2}} \frac{j_0(\varphi_{0,1}(r/a))}{j_1(\varphi_{0,1})}, \\ |1p\rangle &= \Psi_{1,1,0}(r, \theta) = Y_{1,0}(\theta) \frac{2}{a^{3/2}} \frac{j_1(\varphi_{1,1}(r/a))}{j_2(\varphi_{1,1})}. \end{aligned} \quad (21)$$

Here, the spherical functions  $Y_{0,0}(\theta) = (4\pi)^{-1/2}$  and  $Y_{1,0}(\theta) = (3/4\pi)^{1/2} \cos \theta$ .

After the introduction of (21) into (20) and its integration, we obtain the expression for the transition dipole moment:

$$\left| \mathbf{D}_{1,0}^0(a) \right| = \frac{\sqrt{6}2\pi}{3\varphi_{1,1}j_2(\varphi_{1,1})(\varphi_{1,1}^2 - \pi^2)} \times$$

$$\times \left[ \cos \varphi_{1,1} - \frac{3\varphi_{1,1}^2 - \pi^2}{\varphi_{1,1}(\varphi_{1,1}^2 - \pi^2)} \sin \varphi_{1,1} \right] ea = 0.433ea. \quad (22)$$

With regard for (22) and (19), the transition dipole moment in QD with dielectric constant  $\varepsilon_2$  surrounded by the matrix with  $\varepsilon_1$  has the form

$$\left| \mathbf{D}_{1,0}(a) \right| = L \left| \mathbf{D}_{1,0}^0(a) \right| = L \cdot 0.433ea. \quad (23)$$

#### 5. Absorption and Scattering of Light by the Single-Particle States of Charge Carriers in QD

The obtained results for the transition dipole moments  $\mathbf{D}_{1,0}(a)$  [formulas (22), (23)] can explain the behavior of the quasi-zero-dimensional systems in question in respect to the absorption of the energy from the electromagnetic field in the frequency region corresponding to the energies of size-quantization states  $E_{n,l}$  (8) in QD. The absorption cross section for a spherical QD of radius  $a$  can be expressed in terms of the polarizability  $A''(\omega, a)$  [31]:

$$\sigma_{\text{abs}}(\omega, a) = 4\pi(\omega/c)A''(\omega, a). \quad (24)$$

Here,  $c$  is the speed of light in vacuum, and  $\omega$  is the frequency of the external electromagnetic field.

Consider QD with radius  $a$  satisfying condition (10). In it, the size-quantization states of charge carriers ( $n, l$ ) (8) arise, and they are slightly broadened at room temperature (for which inequality (14) should be satisfied). The polarizability  $A''(\omega, a)$  can be easily found, by treating QD as one giant ion, in terms of the matrix elements of the dipole moments  $\mathbf{D}_{1,0}(a)$  (23) between the lowest states  $1s$  and  $1p$  [25]:

$$A''(\omega, a) = \frac{e^2}{m_{e(h)}\omega_1^2(a) - \omega^2 - i\omega\Gamma_1(a)} f_{0,1}. \quad (25)$$

Here,

$$f_{0,1} = \frac{2m_{e(h)}}{\hbar e^2} [\omega_1(a) - \omega_0(a)] |\mathbf{D}_{1,0}(a)|^2 \quad (26)$$

is the oscillator strength of the transition of a charge carrier with effective mass  $m_e$  (or  $m_h$ ) from the ground state  $1s$  to the  $1p$  state,  $\hbar\omega_1(a) = E_{1,1}(a)$  and  $\hbar\omega_0(a) = E_{1,0}(a)$  are, respectively, the energies of discrete levels  $1p$  and  $1s$  which are determined by formula (8), and  $\Gamma_1(a)$  is the width of the  $1p$  level [20, 22].

Using Eqs. (8) and (23), the oscillator strength of transition (26) can be expressed as

$$f_{0,1} = (\varphi_{1,1}^2 - \pi^2) \frac{L^2 \left( \left| \mathbf{D}_{1,0}^0(a) \right| \right)^2}{e^2 a^2}. \quad (27)$$

Let us assume that the frequency  $\omega$  of a light wave is far from the resonance frequency  $\omega_1$  of the discrete state  $1p$  of the charge carrier in QD and that the broadening  $\Gamma_l$  of the level  $1p$  is small (i.e.  $(\Gamma_l/\omega_1) \ll 1$  [20, 22]). Using (8), we obtain the polarizability of QD

$$A''(a) = \frac{4f_{0,1}}{\varphi_{1,1}^4} \left( \frac{m_{e(h)}}{m_0} \right) \left( \frac{a}{a_B} \right)^4 a_B^3, \quad (28)$$

where  $a_B = (\hbar^2/m_0e^2)$  is the Bohr radius of an electron in vacuum.

We can write the cross section of the elastic scattering of an electromagnetic wave  $\omega$  on QD of radius  $a$  [31] as

$$\sigma_{sc}(\omega, a) = 2^7 3^{-3} \pi^3 (\omega/c)^4 |A''(a)|^2. \quad (29)$$

The comparison of expressions (24), (28), and (29) shows that the frequency and size dependences of the cross section for the resonance absorption are different:

$$\sigma_{abs}(\omega, a) \sim \omega a^4. \quad (30)$$

We can also estimate the cross section of the scattering of the electromagnetic field on QD with size quantization single-particle states  $(n, l)$  (8) as

$$\sigma_{sc}(\omega, a) \sim \omega^4 a^8. \quad (31)$$

It should be noted that the frequency and size dependences of the cross sections of the absorption and scattering of light [24,25] on the volume local states [22, 23] arising in QD with radii  $a$  satisfying inequalities (11), (12), namely

$$\sigma_{abs}(\omega, a) \sim \omega a^{3/2}, \quad (32)$$

$$\sigma_{sc}(\omega, a) \sim \omega^4 a^3, \quad (33)$$

differ greatly from dependences (30) and (31) in the case of the absorption and scattering of light on the size-quantization states (8).

Thus, the localization of charge carriers in the bulk of QD is manifested differently in the size and frequency dependence of the absorption  $\sigma_{abs}(\omega, a)$  (30), (32) and scattering  $\sigma_{sc}(\omega, a)$  (31), (33) of an electromagnetic field. This circumstance affords an additional possibility for the spectroscopic detection and investigation of these size-quantization states.

The developed theory only deals with interband transitions of an electron (hole) in QD. The spectrum of an electron (hole)  $E_{nl}^{e(h)}(a)$  is defined by formula (8). In the case of interband transitions in QD, the spectrum of an electron (hole) is given by

$$E_{nl}^e(a) = \hbar\omega_{nl}^e(a) = E_g + \frac{\hbar^2}{2m_e a^2} (\varphi_{nl}^e)^2, \quad (34)$$

$$E_{nl}^h(a) = -\hbar\omega_{nl}^h(a) = -\frac{\hbar^2}{2m_h a^2} (\varphi_{nl}^h)^2, \quad (35)$$

where the energy states of electron levels are marked from the top of the valence zone  $E_\nu$  of QD. According to the selection rules, electron (hole) transitions are possible when the quantum numbers  $n$  and  $l$  are preserved [28]. Then the formulas for the polarization  $A''(\omega, a)$  (25), (28), oscillator strength transition  $f$  (26), light absorption cross-section  $\sigma_{abs}(\omega, a)$  (24), and scattering cross-section  $\sigma_{sc}(\omega, a)$  (29) include the frequencies  $\omega_{nl}^e(a)$  and  $\omega_{nl}^h(a)$  which are defined by formulas (34) and (35).

The optical extinction coefficient including both the absorption and scattering of light on the single-particle size-quantization states arising in QD of radius  $a$  with the number density  $N$  has the form [32]

$$\gamma(\omega, a) = N [\sigma_{abs}(\omega, a) + \sigma_{sc}(\omega, a)]. \quad (36)$$

Formula (36) pertains to an ensemble of noninteracting QD. The condition, under which QDs of radius  $a$  with the number density  $N$  do not interact with one another reduces to the statement that the distance between QDs ( $\sim N^{-1/3}$ ) must be much larger than the dimension of the above-indicated single-particle states ( $\sim a$ ):

$$aN^{1/3} \ll 1. \quad (37)$$

For  $a \simeq 5$  nm, criterion (37) is met for the densities of QDs of some semiconductors  $A_3B_5$  at most  $10^{15}$  cm $^{-3}$  which are attained under the experimental conditions [13–17].

## 6. Comparison of Theory and Experiment

Let us conclude with a brief discussion of the possible physical situations, for which the results obtained are pertinent. We can assume that, as in [29], the heat ejection of a low-weight electron occurs under the conditions of the experiments [13–17] during the firing of massive QDs of GaAs and InAs in the matrix of GaAs and GaSb at  $T = 973$  K, and the bulk of QD contains only a hole. Here, the electron can be localized at a deep trap in the matrix. We neglect the energy of the Coulomb interaction  $V_{eh}(\mathbf{r}_e, \mathbf{r}_h)$  (5) of the hole with the electron provided the distance  $d$  between the trap and the center of QD is large as compared with the radius  $a$

**Parameters of size-quantization states of a hole moving in the bulk of QD of radius  $a$  with dielectric constant  $\varepsilon_2$  dispersed in semiconductor matrices with dielectric constant  $\varepsilon_1$** 

QD				Matrix		$a_h$ (Å)	$L$	$a$ (Å)	$f_{0,1}$	$D_{1,0}^0$ (e Å)	$D_{1,0}$ (e Å)	$\eta$ (%)	$A''$ ( $10^{-24}$ cm $^3$ )	$\sigma_{\text{abs}}$ ( $10^{-24}$ cm $^2$ )
Compound	$\varepsilon_2$	$\frac{m_e}{m_0}$	$\frac{m_h}{m_0}$	Compound	$\varepsilon_1$									
GaSb	15	0.045	0.39	GaN	5.8	20.4	0.65	20	0.41	6.12	4	10	$4.9 \times 10^2$	$4 \times 10^6$
								30		9.2	6	23	$2.5 \times 10^3$	$2 \times 10^7$
GaAs	12	0.07	0.5	GaN	5.8	12.7	0.74	20	0.52	6.12	4.5	13	$7.7 \times 10^2$	$6.3 \times 10^6$
								30		9.2	6.75	29.3	$3.9 \times 10^3$	$3.2 \times 10^7$
InSb	18	0.013	0.18	AlSb	11	53	0.83	20	0.658	6.12	5.05	4.7	$3.5 \times 10^2$	$2.9 \times 10^6$
								30		9.2	7.6	10.6	$1.8 \times 10^3$	$1.5 \times 10^7$
								40		12.2	10.1	19	$5.6 \times 10^3$	$4.7 \times 10^7$
								50		15.3	12.63	29.4	$1.4 \times 10^4$	$1.2 \times 10^8$
GaSb	15	0.045	0.39	AlSb	11	20.4	0.89	20	0.77	6.12	5.46	10	$9.1 \times 10^2$	$7.4 \times 10^6$
								30		9.2	8.19	23	$4.6 \times 10^3$	$3.8 \times 10^7$
InAs	12.5	0.028	0.33	GaAs	12	20	0.99	20	0.95	6.12	6.04	8.7	$9.2 \times 10^2$	$7.5 \times 10^6$
								30		9.2	9.06	19.6	$4.7 \times 10^3$	$3.8 \times 10^7$
InSb	18	0.013	0.18	GaAs	12	53	0.86	20	0.715	6.12	5.26	4.7	$3.9 \times 10^2$	$3.2 \times 10^6$
								30		9.2	7.9	10.6	$1.96 \times 10^3$	$1.6 \times 10^7$
								40		12.2	10.5	19	$6.2 \times 10^3$	$5.1 \times 10^7$
								50		15.3	13.15	29.4	$1.52 \times 10^4$	$1.3 \times 10^8$
InSb	18	0.013	0.18	GaAb	12	53	0.94	20	0.85	6.12	5.74	4.7	$4.6 \times 10^2$	$3.7 \times 10^6$
								30		9.2	8.61	10.6	$2.3 \times 10^3$	$1.9 \times 10^7$
								40		12.2	11.5	19	$7.4 \times 10^3$	$6.1 \times 10^7$
								50		15.3	14.4	29.4	$1.8 \times 10^4$	$1.6 \times 10^8$

\*Here,  $m_e$  and  $m_h$  are the effective masses of an electron and a hole in QD,  $a_h$  is the Bohr radius of the hole in QD,  $L = (3\varepsilon_1/(2\varepsilon_1 + \varepsilon_2))$ ,  $f_{0,1}(a)$  (27) is the oscillator strength of the transition,  $|\mathbf{D}_{1,0}^0|$  (22) and  $|\mathbf{D}_{1,0}|$  (23) are, respectively, the transition dipole moments in vacuum and in QD,  $\eta$  is the parameter of broadening of size-quantization states at room temperature,  $A''(a)$  (28) is the polarizability of QD, and  $\sigma_{\text{abs}}$  is the light absorption cross section.

of QD (i.e.  $d \gg a$ ). As a result, the single-particle size-quantization states of the hole ( $n, l$ ) arise in the bulk of QD, whose spectrum  $E_{n,l}(a)$  is described by formula (8).

Let us give a qualitative estimate of the cross-sections  $\sigma_{\text{abs}}(\omega, a)$  (24), (28) and  $\sigma_{\text{sc}}(\omega, a)$  (29) of the absorption and scattering of light, respectively, by the above-indicated size-quantization states of a hole in QD in the case of the preferred transition ( $1s \rightarrow 1p$ ) under the experimental conditions [13–17]. Assume that the frequency  $\omega$  of the light wave is far from the resonance frequency  $\omega_1$  of a discrete state of the hole in QD and that the broadening  $\Gamma_1$  of the level with the energy  $E_{1,1} = \hbar\omega_1$  (8) is small [20,22] (i.e.  $\Gamma_1/\omega_1 \ll 1$ ). Using expressions (24), (28), and (29), we get

$$\sigma_{\text{abs}}(\omega, a) = \frac{16\pi f_{0,1}}{\varphi_{1,1}^4} \left(\frac{\omega}{c}\right) \left(\frac{m_h}{m_0}\right) \left(\frac{a}{a_B}\right)^4 a_B^3, \quad (38)$$

$$\sigma_{\text{sc}}(\omega, a) = \frac{2^{11}\pi^3 f_{0,1}^2}{3^3 \varphi_{1,1}^8} \left(\frac{\omega}{c}\right)^4 \left(\frac{m_h}{m_0}\right)^2 \left(\frac{a}{a_B}\right)^8 a_B^6. \quad (39)$$

The Table gives estimates of the oscillator strength of the transitions  $f_{0,1}(a)$  (27), transition dipole moments  $|\mathbf{D}_{1,0}^0|$  (22) and  $|\mathbf{D}_{1,0}|$  (23), the polarizability  $A''(a)$  (28), the light absorption cross-sections  $\sigma_{\text{abs}}(\omega, a)$  (38) of a

light wave with frequency  $\omega$  and with the quantum energy  $\hbar\omega = 12.2$  meV (here,  $(\omega/\omega_1) = 10^{-3}$ , and the wave frequency  $\omega$  is in the infrared region) for the above-indicated size-quantization states of a hole arising in the bulk of QD in the quasi-zero-dimensional structures consisting of semiconductor  $A_3B_5$  matrices and semiconductor  $A_3B_5$  QDs dispersed in them. Here, the size-quantization states of the hole are slightly broadened at room temperature (the parameter is at most 30%).

It is seen from the table that the oscillator strength of the transition  $f_{1,0} \simeq (0.4 \div 0.9)$  and the transition dipole moments  $D_{1,0} \simeq 10$  D (where D = e Å stands for 1 Debye) in QDs of radii  $a \simeq 2 \div 5$  nm have large values many times greater than the typical values of the transition dipole moments for unbounded semiconductor materials  $A_3B_5$ , where they have values  $\simeq 10^{-1}$  D [33]. Moreover, the selection rules allow the dipole transitions in an electromagnetic field between adjacent levels  $E_{n,l}(a)$  (8) in QD with a change of the orbital quantum number  $l$  by 1 [30]. Therefore, it is clear that the quasi-zero-dimensional systems under discussion are highly nonlinear media for the electromagnetic radiation.

It follows from these estimates that the value of the absorption cross section for light in QDs of radii

$a \simeq 2 \div 5$  nm is  $\simeq 10^{-16}$  cm<sup>2</sup>. That is, it is six orders of magnitude higher than the typical values of atomic absorption cross sections [34]. Since the cross sections for the scattering of light  $\sigma_{sc}(\omega, a)$  (39) in comparison with the cross sections for absorption of light by the same states  $\sigma_{abs}(\omega, a)$  (38) are negligible ( $\sigma_{sc}/\sigma_{abs} \simeq 10^{-12}$ ) under the experimental conditions [13–17], we omit the values of  $\sigma_{sc}$  in the Table.

With regard for the latter circumstance, the optical extinction coefficient  $\gamma(\omega, a)$  (36) in QDs is mainly determined by the absorption of light by single-particle local states on size-quantization states  $(n, l)$  (8) of charge carriers. For QDs with radii  $a$  satisfying condition (37) and at the particle densities  $N \simeq 10^{-15}$  cm<sup>-3</sup>, the quantity  $\gamma(\omega, a)$  (36) for the absorption of light in QDs takes the values  $\simeq 10^{-1}$  cm<sup>-1</sup> (see Table).

Thus, the larger values of the absorption cross section and the optical extinction coefficient in the quasi-zero-dimensional structures under study present a possibility to use heterophase structures of this kind as new materials which strongly absorb over a wide range of wavelengths which can be varied by varying the nature of the materials in contact.

I express my sincere gratitude to Prof. V.M. Agranovich for his support and discussion of the work. I am also thankful to Prof. B.P. Antonyuk, Dr. N.A. Efremov, Dr. Yu.E. Lozovik, Prof. A.G. Malshukov, Prof. V.I. Rupasov, and the whole staff of the Theoretical Department of the Institute of Spectroscopy of the Academy of Sciences of Russia for fruitful discussions and critical remarks.

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Received 03.06.05

#### ПОГЛИНАННЯ ТА РОЗСІЮВАННЯ СВІТЛА В НАПІВПРОВІДНИКОВИХ КВАНТОВИХ ТОЧКАХ

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#### Резюме

У рамках дипольного наближення розвинуто теорію взаємодії електромагнітного поля з одностинковими квантоворозмірними станами носіїв заряду, які виникали в об'ємі напівпровідникової квантової точки. Показано, що сили осциляторів переходів, дипольні моменти переходів для одностинкових станів, а також значення перерізів поглинання світла на одностинкових квантоворозмірних станах у квантовій точці набувають великих значень, що перевищують типові значення для напівпровідникових матеріалів.