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Edge of intrinsic absorption of light in a quantized semiconductor wire

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Abstract: The Coulomb interaction of an electron and a hole in the plane of the cross section of a cylindrical wire into exciton states is considered. The energy spectrum of the Wannier-Mott exciton in a semiconductor wire in the presence of dimensional quantization is calculated. An expression is obtained and analyzed for the interband light absorption coefficient taking into account exciton effects. It is shown that the interaction of an electron and a hole leads to the appearance of new lines in the absorption spectrum.

Key Words: Coulomb interaction, exciton, electron, hole, absorption, lower-dimensional heterosystems.

I. Related Work

In the last decade in the physics of semiconductors, there has been a sharp turn of interests towards lower-dimensional heterosystems. These include the so-called quantum wells, quantum wires and quantum dots, as well as transition states between them [1]. Advances in low-dimensional heterosystems led to the start of research work on the study of light absorption in a quantized semiconductor wire.

II. Introduction

By changing the dimension and adjusting the quantum confinement, one can radically change the energy spectrum of the system, which contributes not only to the solution of fundamental problems of quantum mechanics and physics of semiconductor crystals, but also to the creation of completely new semiconductor devices (by the way, also optimization of the known ones). There was appearance of lasers, photodetectors and optical transistors, built on the properties of an exciton gas [2,3].

For the first time, a one-dimensional (1D) hydrogen-like impurity atom was considered in [4].

Theoretically [5–8] and experimentally [9–13], the behavior of excitons in dimensionally quantized semiconductor wires was studied. The features of the energy spectrum of electrons and holes and their density of states, the formation of exciton states, an increase in the oscillator strength, binding energy, and stabilization of excitons with a decrease in the dimension of the system are studied.

In this work, we determine the energy spectrum and wave functions of a one-dimensional (1D) exciton and study the effect of excitons on the intrinsic absorption edge of a cylindrical-shaped quantized semiconductor wire (QSW).
Semiconductors with a parabolic dispersion law are considered, the bands are considered non-degenerate, the temperature is quite low, so that the valence band is completely filled, and the conduction band is empty. The dielectric constant of the semiconductor is assumed to be large, and the effective masses of current carriers are small, which is necessary for the existence of a large radius exciton. The potential barrier at the interface between the semiconductor wire and the environment is assumed to be infinitely large. It is also neglected by the influence of the forces of the electrostatic image of electrons and holes.

III. The Wave Function And Exciton Energy

Suppose that
$r_0 \ll a_B^*$, (1)
holds
where $a_B^* = \varepsilon\hbar^2/\mu e^2$ - Bohr radius of the exciton, ε- semiconductor dielectric constant, e - electron charge, μ - given effective mass of an electron and a hole, r_0 - QSW radius. If in (1) we replace r_0 with the radius of the cyclotron orbit in a magnetic field, then criterion (1) will correspond to the condition of applicability of the adiabatic approximation when considering the Coulomb coupled pair, when the particle motion in a magnetic field is considered to be fast compared to the motion in the Coulomb field [14]. In accordance with this condition, for a hydrogen-like system in a strong magnetic field, the method of separation of variables was used in [15]. When relation (1) is fulfilled, the movement normal to the wire cross section (along the z axis) can be considered fast compared to the movement in the wire cross section plane (in the oxy plane). Then, separating the variables of the fast and slow subsystems, we obtain, similarly to [7–8], for the wave function Ψ and the energy of the one-dimensional (1D) exciton E

$$\Psi(\vec{r}_e, \vec{r}_h, z, Z) = \psi(\vec{r}_e)\psi(\vec{r}_h)\phi_n(z, Z), \quad (2)$$

$$E = E_g + E_e + E_h + E_z, \quad (3)$$

where

$$\psi(\vec{r}_{e(h)}) = \left[1/\sqrt{\pi}\, r_0 J_{l_{e(h)}+1}(\lambda_{n_{e(h)},l_{e(h)}})\right] e^{il_{e(h)}\varphi} J_{l_{e(h)}}[\lambda_{n_{e(h)},l_{e(h)}}(r_{e(h)}/r_0)] \quad (4)$$

$$E_{e(h)} = \hbar^2\lambda^2_{n_{e(h)},l_{e(h)}}/2m_{e(h)}r_0^2, \quad (5)$$

E_g - semiconductor band gap; $m_{e(h)}$- effective mass of an electron (hole); $\lambda_{n_{e(h)},l_{e(h)}}$- zeros of the Bessel function, i.e.

$$J_{l_{e(h)}}\left(\lambda_{n_{e(h)},l_{e(h)}}\right)=0, \tag{6}$$

$n_{e(h)}$- the ordinal number of the root of the Bessel function for a given $l_{e(h)}$.

Table 1. Zeros of the Bessel Function

$\lambda_{n^*,l}$				
n^*	l =0, s	$l=1,p$	$l=2,d$	$l=3,f$
1	2,405	3,832	5,136	6,380
2	5,520	7,016	8,417	9,761
3	8,654	10,173	11.620	13,015
4	11,792	13,324		

We represent the function $\phi_n(z,Z)$ in the form

$$\phi_n(z,Z)=e^{i\mathcal{K}Z}\chi_n(z), \tag{7}$$

where $\mathcal{K}$ - the wave vector characterizing the translational motion of the center-mass of the exciton, Z - coordinate of the center-mass of the exciton.
$\chi_N(z)$ is a solution to the following equation

$$\left[-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial z^2}+V_{eff}^{n_e,l_e;n_h,l_h}(z)\right]\chi_n(z)=E_z'\chi_n(z), \tag{8}$$

where
$E_z'=E_z-\hbar^2\mathcal{K}^2/2M$, $M=m_e+m_h$ - effective mass of the exciton. (9)

$$V_{eff}^{n_e,l_e;n_h,l_h}(z)=-(e^2/\varepsilon\pi^2r_0^4)\left[J_{l_e+1}^2\left(\lambda_{n_e,l_e}\right)J_{l_h+1}^2\left(\lambda_{n_h,l_h}\right)\right]^{-1}\times$$
$$\int_0^{2\pi}d\varphi_e\int_0^{2\pi}d\varphi_h\int_0^{r_0}r_e dr_e\int_0^{r_0}r_h d\,r_h\frac{\left|J_{l_e}\left[\lambda_{n_e,l_e}(r_e/r_0)\right]\right|^2\left|J_{l_h}\left[\lambda_{n_h,l_h}(r_h/r_0)\right]\right|^2}{\sqrt{r_e^2+r_h^2+z^2-2r_e r_h\cos(\varphi_e-\varphi_h)}}, \tag{10}$$

The numerical solution of equation (8) was performed in [8]. To obtain an analytical solution to equation (8), the effective
potential can be approximated by the following expression [4,7]

$$V_{eff}(z)=-\frac{e^2}{\varepsilon(|z|+z_0)}. \tag{11}$$

Substituting (11) into (8), after certain mathematical transformations, we obtain

$$\frac{\partial^2\chi_n}{\partial u^2}+\left(\frac{\varkappa_n}{u}-\frac{1}{4}\right)\chi_n=0. \tag{12}$$

where
$u = 2(|z| + z_0)/a_B^* \varkappa_n$;

For the self-energies of the bound state (discrete) exciton, we obtain

$$E_z = \hbar^2 \mathcal{K}^2/2M - Ry/\varkappa_n^2, \quad (13)$$

where $Ry = \mu e^4/2\varepsilon^2\hbar^2$ - Rydberg effective constant.
The solution of the one-dimensional equation (12) is well known and is given by the Whittaker functions:

$$\chi_n(z) = C_n W_{\varkappa_n, 1/2}[2(|z| + z_0)/a_B^* \varkappa_n]. \quad (14)$$

where C_n - normalization multiplier, $W_{\varkappa_n, 1/2}(z)$ – Whittaker function.
Due to the invariance of the potential $V_{\text{eff}}(z)$ with respect to the transformation $z \to -z$, the eigenfunctions are divided into even odd ones, and the eigenvalues of the energy ($\varkappa_N$) are determined from the equations [4]

$$W_{\varkappa_n, 1/2}(2z_0/a_B^* \varkappa_n) = 0 \quad \text{for odd states,} \quad (15)$$

$$W'_{\varkappa_n, 1/2}(2z_0/a_B^* \varkappa_n) = 0. \quad \text{for even states.} \quad (16)$$

Using the expansion of the Whittaker function at $z_0 \ll a_0$ [16], from conditions (14) and (15) we obtain the following expressions [8]:

$$\varkappa_n^- = n + 2z_0/a_B^* \quad \text{for odd states,} \quad (17)$$

$$\varkappa_n^+ = n - 1/\ln(2z_0/na_B^*) \quad \text{for even states.} \quad (18)$$

where $n = 1, 2, 3, \ldots$ correspond to the excited states of the exciton. The ground state ($n = 0$) of the 1D exciton has a special character. For this state, $\varkappa_0$ satisfies the equation

$$ln(2z_0/a_B^* \varkappa_0) + (1/2\varkappa_0) = 0. \quad (19)$$

As $z_0 \to 0$ and $\varkappa_0 \to 0$. In this case, the binding energy of the ground state in the 1D case is infinite and corresponds to the incidence of the particle on the center. But at finite z_0, the ground state energy becomes finite, and double degeneracy is removed so that the excited levels of a one-dimensional exciton with $n = 1, 2, 3, \ldots$ turn out to be doublets, and transitions are allowed only to even components of these doublets.
When $z_0 \to 0$ (except the ground state) for coupled even and odd states, respectively, with $\varkappa_N^+ = \varkappa_N^- = n = 1, 2, 3, \ldots$ the wave functions have the form:

$$\chi_n^+(z) = [2/(a_B^*)^2 n^5 (n!)^2]^{1/2} |z| exp(-|z|/na_B^*) \mathcal{L}_n^1(2|z|/na_B^*), \quad (20)$$

$$\chi_n^-(z) = [2/(a_B^*)^2 n^5 (n!)^2]^{1/2} z exp(-|z|/na_B^*) \mathcal{L}_n^1(2|z|/na_B^*), \quad (21)$$

where $\mathcal{L}_n^1(x)$ is the Lagger polynomial.

For the base bound state of the 1D exciton, the wave function and self-energy are respectively written in the form

$$\chi_0(z) = lim_{\varkappa_0 \to 0} \frac{exp(-|z|/\varkappa_0 a_B^*)}{\sqrt{\varkappa_0 a_B^*}} = \sqrt{\delta(z)}, \quad (22)$$

$$E_0 = -\infty. \quad (23)$$

IV. Exciton Absorption

Let us consider the process of electron transfer from the valence band to discrete energy levels in the quantized semiconductor wire in the conduction band and the formation of an exciton as a result of absorption of the incident light photon. Since the radius of the quantized semiconductor wire is small compared to the wavelength of light, the absorption in such a quantized semiconductor wire is not described by the law $exp(-\alpha r_0)$, where α is the volume absorption coefficient, but should be determined from the solution of Maxwell's equations. As applied to the surface layer in a metal-dielectric-semiconductor system, this question considered in [17] for interband magneto-optical absorption. According to [17], the frequency dependence of absorption is completely determined by the dimensionless function $\alpha(\omega, 0)$, which, up to a multiplier determined by the geometry of the experiment, is proportional to the fraction of the energy of the light beam absorbed by the quantized semiconductor wire. In the case of exciton absorption, the function $\alpha(\omega, 0)$ has the form

1) For allowed transitions

$$\alpha(\omega, 0) = \alpha(0) \sum_{n^* ln} |\chi_n^+(0)|^2 \delta(\tau_{n^* ln}), \quad (24)$$

2) For prohibited transitions

$$\alpha(\omega, 0) = \alpha(0) \sum_{n^* ln} \left| \frac{d\chi_n^+(0)}{dz} \right|^2 \delta(\tau_{n^* ln}), \quad (25)$$

where

$$\alpha(0) = \left(8/\pi\sqrt{\varepsilon_0}\right)(e^2/\hbar c) \left(\left|P_{cv}^y\right|^2 / m_0 E_g \right) (\mu/m_0), \quad (26)$$

$$\tau_{n^* ln} = \Gamma_{n^* l} - (Ry/E_0) n^{-2}, \; n = 1,2, \ldots \quad (27)$$

$$\Gamma_{n^* l} = \left(E - E_g - \hbar^2 \lambda_{n^* l}^2 / 2\mu r_0^2\right)/E_0, \quad E_0 = \pi\hbar^2/\mu \, . \quad (28)$$

V. Discussion Of The Results

As can be seen from (27), in the considered model, the system of exciton subbands characterized by the quantum number n is "suspended" under the bottom of each size-quantized subband with the quantum numbers n^* and l (a similar situation occurs in the problem of the volume exciton in a magnetic field [14,15], in a dimensionally quantized semiconductor film [18] and in the surface layer in a metal-dielectric-semiconductor system [19]). Thus, in the case of interband absorption in quantized semiconductor wire, a series of δ-shaped discrete lines should be observed (see (24) and (25)). The absorption threshold is

$$\hbar\omega = E_g + \hbar^2\lambda_{n^*l}^2/2\mu r_0^2. \quad (29)$$

From here one can see the law, the displacements of the lines in the short-wavelength direction with a decrease in the radius of the wire and an increase in the numbers of dimensionally quantized subbands n^* and l.

In conclusion, we note that the series of exciton absorption, as in the case of diamagnetic excitons [14, 15], have a number of specific features. Due to the invariance of 1D, the Coulomb potential $e^2/\varepsilon|z|$ with respect to the transformation $z \to -z$, the eigenfunctions must be divided into even and odd. These even and odd states in the case $z_0 \to 0$, when the interaction between the electron and the hole increasingly tends to the 1D Coulomb state, turn out to be pairwise degenerate, with the exception of the ground state, which is described by function (22), which has no nodes, and is always even [4]. Such a twofold degeneracy of the "1D Coulomb series" states is analogous to the degeneracy in the azimuthal quantum number in the case of three-dimensional (3D) Coulomb interaction. The energy of the Coulomb motion along z with respect to the boundaries of the continuous spectrum has the form

$$E_z' = -Ry/n^2, \quad n = 0, 1, 2, \ldots \quad (30)$$

It follows from (23) and (30) that the binding energy of the ground state with $n = 0$ in the 1D case is infinite and corresponds to the particle incident on the center. At $z_0 \to const$, the base state energy becomes finite, and double degeneracy is removed so that the excited exciton levels with $n = 1, 2, \ldots$ turn out to be doublets (Fig. 1), and transitions are allowed only into the even components of these doublets.

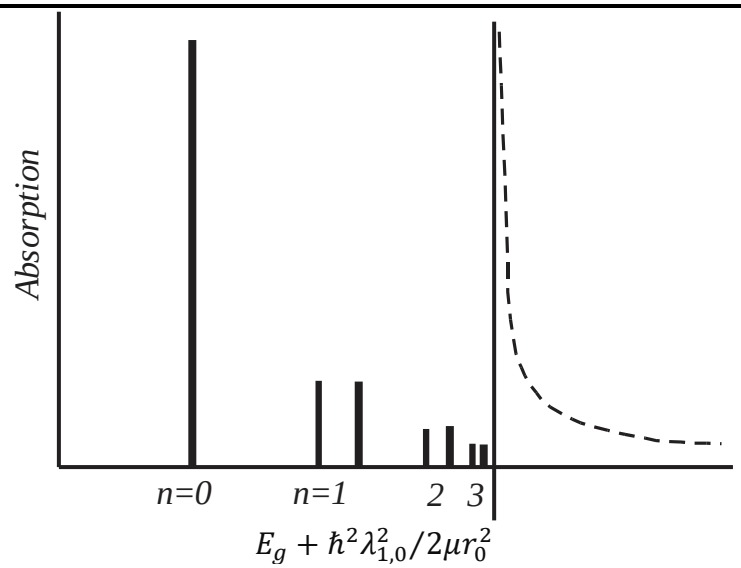

Fig. 1. Schematic representation of the 1D series exciton adjacent to the size-quantized QSW subband with $n^* = 1$ and $l = 0$. (The dotted line shows the absorption in a bulk semiconductor without excitons. The doublet structure of the excited states of the 1D exciton with $n \neq 0$ is presented. Narrow vertical lines are components corresponding to odd states: they should not appear in the spectrum).

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