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Excitonic states in a quantum well.

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Abstract

New approach to calculate both bound and continuum excitonic states in a quantum well are presented. Green functions technique for appropriate Schrödinger equation allowed transforms it to system of linear algebraic equations and to obtain a general numerical solution for excitonic wave function in a matrix form. The exciton binding energy was determined as poles of the wave function. Calculated quantum-mechanical transverse average size of an exciton correlates with binding energy. The results for different well widths and excitonic states are presented and analyzed.

Key words: Exciton, binding energy, wave function, quantum well.

Introduction.

Bound state of an electron and hole called an exciton, is being studied for last several decades. A new impact to the study of excitonic states and related effects has been stimulated by the development of the technology and physics of low-dimensional structures. In particular, the

binding energy of an exciton in a quantum well is increased by 2 and more times compared to the bulk materials, and that is favorable for creating a laser based on the condensation of polaritons [1] – bound states of an exciton and light. In addition, in bulk semiconductors the exciton states manifest itself only at low temperatures, that don't allow its practical use. In contrast, in low-dimensional structures the exciton states are well defined at room temperature. Changing, for example, the size of nanostructures, it is possible to change the binding energy and other parameters of excitons and thus to control excitons in low-dimensional structures and to create new devices operating due physical processes with excitons [1-3]. The most publications related to the calculation of excitonic states were done in the 80-90 years of the last century. This amount of papers contain a way from from the simple models with a parabolic bands [4] to the more complex models taking into account nonparabolicity factor, mixing of light and heavy holes states in the valence band [5], etc. At that, variational [1, 6] as well as numerical methods [7] has been used. Non-trivial approach to the calculation of the exciton states was used in [8,9] where the Green's function method was applied to solve the appropriate Schrödinger equation. A similar approach is developed in presented paper. The difference is in construction of Green's function and in the method used to solve final equations. While 3 stages are necessary to calculate the Green's function in Ref. [8], it is determined by the specific expressions in the present work. The effectiveness of our approach are demonstrated on the example of excitonic states in a heterostructure $Ga_{1-x}Al_xAs/GaAs/ Ga_{1-x}Al_xAs$

Solution of Shredinger equation for excitonic states in a quantum well.

We consider the so-called Wannier-Mott exciton, when the electron and hole are separated by a distance a much more than material lattice constant. Then to calculate the exciton energy levels and wave functions we use Hamiltonian in the effective mass approximation:

$$H=H_{ze}+H_{zh}+H_{eh} \tag{1}$$

where H_{ze} (H_{zh}) - describe the quantized electron (hole) states:

$$H_{ze,zh} = -\frac{\hbar^2}{2m_{ze,zh}}\frac{d^2}{dz^2} + V_{e,h}(z)$$

where $m_{ze,zh}$ – electron (e) or hole (h) mass along z direction, $V_{e,h}(z)$ – square-well confinement potential, and H_{eh} is responsible for electron-hole in-plane relative motion

$$H_{eh} = -\frac{\hbar^2}{2m_{\perp e,h}}\left[\frac{d^2}{d\rho^2} + \frac{1}{\rho}\frac{d}{d\rho} + \frac{1}{\rho^2}\frac{d^2}{d\theta^2}\right] - U(\rho, z_e, z_h) \tag{2}$$

where (ρ,θ) are the distance and angle describing the e-h relative motion in the QW plane, $m_{\perp e,h}$ – mass corresponding to electron (e) or hole (h) bands in the QW plane. $U(\rho, z_e, z_h) = \frac{q^2}{4\pi\kappa\kappa_0}\frac{2}{\sqrt{\rho^2 + (z_e - z_h)^2}}$ - electron - hole Coulomb interaction, q – unit charge, κ - permittivity, κ_0 - dielectric constant.

To solve the Schredinger equation with the full Hamiltonian (1) we construct a basis of single-particle states which satisfy the following one-dimensional equations:

$$H_{ze,zh}\varphi^i_{e,h}(z_{e,h}) = \varepsilon^i_{e,h}\varphi^i_{e,h}(z_{e,h})$$

Next, we do expand excitonic wave function $\psi(ze,zh,\ \rho\ ,\ \theta\ )$ into a basis of functions $\varphi^i_e(z_e)$, $\varphi^j_h(z_h)$:

$$\psi(z_e, z_h, \rho, \theta) = \sum_{i=1}^{Ne}\sum_{j=1}^{Nh} F_{ij}(\rho,\theta)\varphi^i_e(z_e)\varphi^j_h(z_h) \tag{3}$$

Because of the axial symmetry of the system, angular momentum projection onto the z axis is conserved $L_z = \hbar m$ (m=0, ±1, ±2, … - magnetic quantum number), and their eigenfunctions $exp(-im\theta)$ determine the dependence of the unknown exciton wave function versus an angle θ. Thus we can rewrite (3) as:

$$\psi(z_e, z_h, \rho, \theta) = \sum_{i=1}^{Ne}\sum_{j=1}^{Nh}\sum_{m} f^m_{ij}(\rho)\exp(im\theta)\varphi^i_e(z_e)\varphi^j_h(z_h) \tag{4}$$

Substituting (4) in (1), we obtain a system of differential equations.

$$\left[\frac{d^2}{d\rho^2} + \frac{1}{\rho}\frac{d}{d\rho} + E - \varepsilon^i_e - \varepsilon^j_h - \frac{m^2}{\rho^2}\right] f^m_{ij}(\rho) = \sum_{s,p} U_{ij,sp}(\rho) f^m_{sp}(\rho) \tag{5}$$

where

$$U_{ij,sp}(\rho) = \int \varphi_e^i(z_e)^* \varphi_h^j(z_h)^* U(\rho, z_e, z_h) \varphi_e^s(z_e) \varphi_h^p(z_h) dz_e dz_h \qquad (6)$$

In (5) we use dimensionless variables, introducing Bohr radius a_b as unit of distance and Rydberg R_y as energy respectively

$$a_b = \frac{4\pi\varepsilon\varepsilon_0\hbar^2}{\mu_\perp e^2}, \quad Ry = \frac{\hbar^2}{2\mu_\perp a_b^{\,2}}$$

where $1/\mu_\perp = 1/m_{\perp,e} + 1/m_{\perp,h}$. The solution of equations (4) is written in the form analogous to the [10, 11]:

$$f_{Nm}(R) = \int_0^\infty R' dR' G(R, R', E) \sum_n U_{Nn}(R') f_{nm}(R') \qquad (7)$$

where the Green's function $G_N(R,R',E)$ corresponds to homogenous equation (4) (without right side). The procedure of getting solutions for binding energy and wave function have been described in [11].

Binding energy and average transverse size of exciton.

As usually we classified excitons in QW according to the pairs of subband involved, eg. *e1-hh1*, *e1-hl2* etc. We have calculated the binding energies of the ls state of the heavy-hole exciton (*e1-hh1*, *e1-hh2*) and the light-hole exciton (*e1-hl1, e1-hl2*) as a function of QW width for values of Al concentration x=0.15. We used next values for electron, heavy hole and light hole masses (in the unit of free electron mass m_0): 0.067, 0.45, 0.08 in barrier and in the well. The reduced mass in QW plane is 0.04 and 0.051 for the heavy-hole exciton and light-hole exciton respectively. Also the same values for the static dielectric constant in the well and barrier were assumed. All data are the same as in Ref. [4].

First we compare results of numerical solution of Eq. (4) to analogous obtained in Ref. [4] (close lying solid and dotted curves on Fig.1). As can be seen from Fig. 1 both curves are almost same.

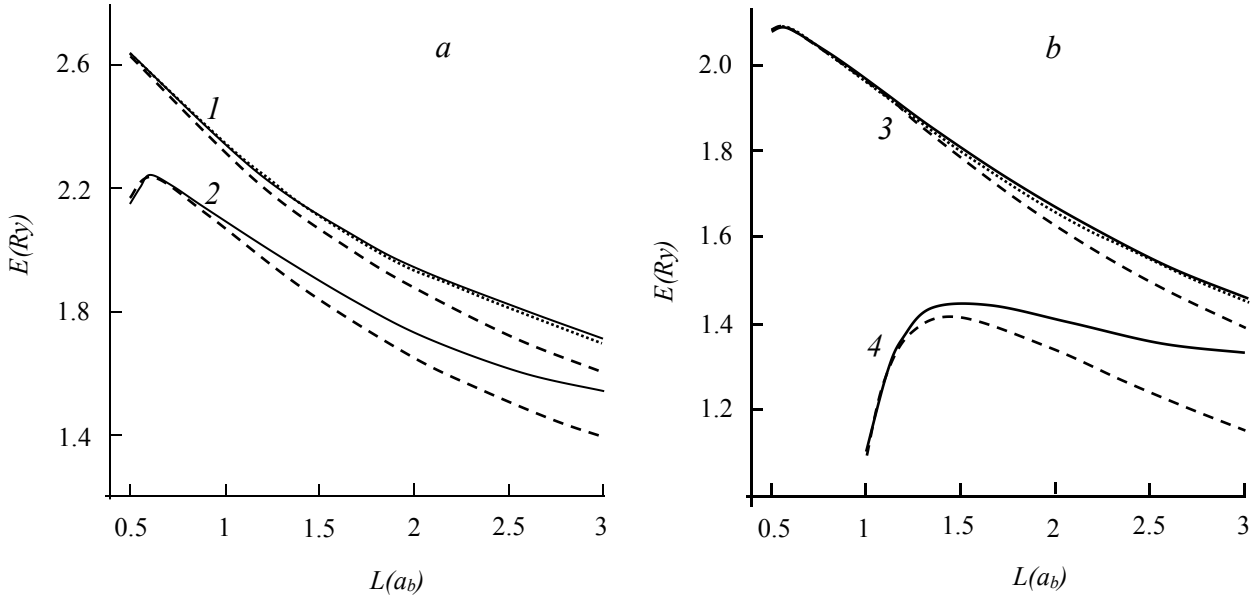

Fig.1. Binding energy of heavy-hole (*a*) and light-hole (*b*) excitons as function of quantum well width *L*: *1 – e1-hh1*, *2 – e1-hh2, 3 – e1-hl1*, *4 – e1-hl2*.
The dashed curves correspond to the case of only two subband contribution, while dotted lines are results from Ref. [4] and are compared to our curves *1*.

Next, we calculated the binding energy for the *1s* state of *e1-hh1*, *e1-hh2*, *e1-hl1*, *e1-hl2* excitons as function of QW width *L* in the range of 50-300 Å. The obtained dependencies confirm the well-known results: after initial maximum as the QW widths increase the binding energy decreases. The initial maximum is a consequence of a limiting case: as QW width reduces to zero the binding energy also tends to zero. For exciton *e1-hh1* the maximum is located at smaller values of the QW width. In equation (4) we took into account only the contribution of electron and hole subbands such that $\varepsilon_e^i + \varepsilon_h^j - E < 25Ry$. The contribution of subbands beyond the last inequality led to change in the binding energy of an exciton less than 0.1 %. We also present the results when the contribution of only two subband involved in exciton have been taken into account. It is easy to see that this approximation is adequate for cases of narrow QWs and low-lying exciton levels. Let's note that the increase of the contribution of the other subbands leads to an increase in the binding energy, in contrast to the case of impurity states [10] when increase of the contribution of additional subband can led both to increase and to decrease of the binding

energy. The reason is that the modified 2D potential (5) has the same sign for any of the considered states.

For further analysis we introduce the quantum-mechanical average distance between the electron and hole forming an exciton as:

$$d_{eh}^{ij} = \int\int \varphi_e^i(z_e)^* \varphi_h^j(z_h)^* \mid z_e - z_h \mid \varphi_e^i(z_e)\varphi_h^j(z_h)\, dz_e dz_h \tag{8}$$

In fact, it is an integral characteristic for the structure of wave functions of different electronic and hole states. It should be noted that the similar expression has been used in [12] as a parameter for analytical solutions for the impurity states. The use of such quantity follows from next arguments. The binding energy of the exciton is determined by the Coulomb interaction between electrons and holes, which depends on the distance between them. We examine the binding energy as function of the QW width, which is measured along the *z* axis. That is the reason why *z* component of the distance we are interested in. In fact, it turned out that its values are completely correlated with the calculated dependencies of binding energy versus QW widths. This can be

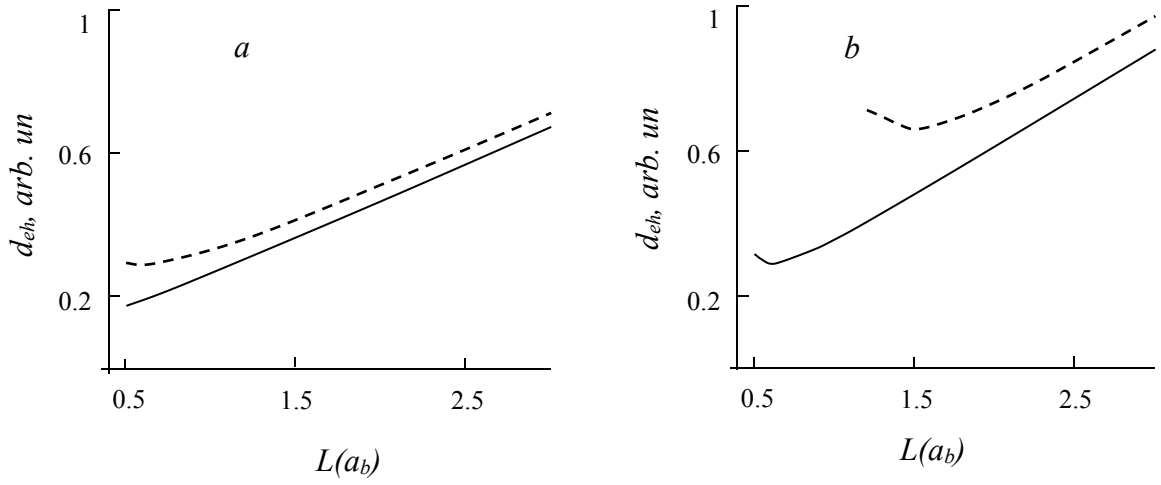

Fig.2. The average size of heavy-hole (*a*) and light-hole (*b*) excitons as function of quantum well width *L*: solid line – *e1-hh1, e1-hl2*, dashed – *e1-hl1, e1-h12*.

seen from Fig.2. Moreover, this value is extremely sensitive to the slightest changes in the dependencies of binding energy versus QW widths. For example, it repeats a barely noticeable extremums for the states of *e1-hl1*, *e1-hl2*.

Conclusion.

The method of Green's function is used to construct solutions of the Schrödinger equation describing the excitonic states in a quantum well. The method allows calculating the binding energy and building the wave functions of the different series of the excitonic states. The results of the calculations show qualitative and quantitative agreement with known data. The calculated quantum-mechanical average distance between the electron and hole forming an exciton qualitatively and quantitatively follows the dependence of the binding energy of an exciton versus QW width.

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