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Numerical modeling of indirect excitons in double quantum wells in an external electric field

P A Belov

Department of Computational Physics, St. Petersburg State University, Ulyanovskaya 1,
198504 St. Petersburg, Russia

E-mail: pavelbelov@gmail.com

Abstract. The ground state of an exciton in the GaAs-based double quantum well structure in an external electric field is calculated by the direct numerical solution of the three-dimensional Schrödinger equation. A formation of the indirect exciton is demonstrated by the study of the localization of the exciton wave function in the double quantum well structure for different electric field strengths. A relatively slow radiative decay rate of the indirect exciton is observed.

1. Introduction

Quantum states of excitons in semiconductors in external fields have been intensively studied since the discovery of the exciton in bulk cuprous oxide by Gross and Karryev [1]. Quite large binding energy of the exciton in this crystal as well as a relatively high purity of the structure made it possible to observe several lines of the Coulomb-like spectrum. An application of external fields allowed one to study the exciton states in more detail and to compare dependencies of energy levels on the field magnitudes with those for the hydrogen-like systems [2-11].

More recently, a development of the technology has allowed one to grow heterostructures with single, coupled double and multiple quantum wells (QWs). This triggered many experimental and theoretical studies of excitons in QWs [12-27]. The states of excitons in QWs in external electric and magnetic fields draw attention, in particular, due to the quantum-confined Stark effect [28] and ways to increase the exciton-light coupling by squeezing the exciton wave function [29], respectively. The coupled double QWs in electric fields are especially interesting due to a formation of long-lived indirect excitons and a search for the Bose-Einstein condensation in such systems [30, 31].

In the current paper, we present preliminary results of our modeling of the exciton states in double QWs in an external electric field. We simulate a heterostructure with $\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}/\text{GaAs}/\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}/\text{GaAs}/\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}$ QWs. The widths of the left and right QWs in the structure are 10 nm and 14 nm, respectively; the width of the middle barrier is 3 nm. The QWs are coupled due to tunneling of the carrier wave function through the barrier. The external electric field is applied in the growth direction in a such way that the electrons are forced to move from the left to the right. For modeling, we use our method of the direct numerical solution of the Schrödinger equation for the exciton in a QW [32-37]. The method is based on the finite-difference discretization and allows one to obtain accurate exciton energies for a wide range of the QW widths and potential profiles [38]. It is superior to the variational approach [14, 17] and makes it possible to calculate the excited states of excitons in external



fields. We obtain energies and wave functions of the ground and a few excited exciton states for different magnitudes of the electric field. A formation of the indirect exciton as a ground state of the studied quantum system is observed. We also calculate the radiative decay rate of the exciton in the heterostructure [17]. We compute the radiative decay rates of exciton transitions from different optically active states.

The obtained numerical results may be important for experimental studies of excitons, namely for identifying the exciton states in photoluminescence and reflectance spectra [24, 27, 39].

2. Theoretical model

In our model, the exciton states are defined by the Schrödinger equation derived assuming the parabolic conduction and valence bands. The latter one is defined by diagonal terms of the Luttinger Hamiltonian [40], since, for relatively narrow QWs, the nondiagonal terms contribute little to the energy states [41]. In other words, the heavy-hole–light-hole coupling and corrugation are small and, thus, ignored. The complete derivation of the Schrödinger equation without external fields is given in [32]. Following the same procedure, one can obtain that the equation for the s -like states of the exciton in a QW in the electric field applied in the growth direction is given by

$$\left(K - \frac{e^2}{\epsilon\sqrt{\rho^2 + (z_e - z_h)^2}} + V_e^{pot}(z_e) + V_h^{pot}(z_h) + eF(z_e - z_h) \right) \chi(z_e, z_h, \rho) = E_x \chi(z_e, z_h, \rho), \quad (1)$$

where the kinetic term K reads

$$K = -\frac{\hbar^2}{2} \frac{\partial}{\partial z_e} \frac{1}{m_{ez}(z_e)} \frac{\partial}{\partial z_e} - \frac{\hbar^2}{2} \frac{\partial}{\partial z_h} \frac{1}{m_{hz}(z_h)} \frac{\partial}{\partial z_h} - \frac{\hbar^2}{2} \frac{1}{\mu_{xy}} \left(\frac{\partial^2}{\partial \rho^2} - \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \right)$$

and the wave function of the s -like state of the exciton is $\psi(z_e, z_h, \rho) = \chi(z_e, z_h, \rho)/\rho$. In equation (1), indices e and h denote the electron and the hole, respectively. The potentials $V_{e,h}^{pot}(z_{e,h})$ are the finite double QW potentials. We neglect here the self-interaction potentials as well as screening of the Coulomb potential by the image charges [42, 14]. Our calculations show that these effects are small in comparison to the impact of the electric field of the strength $F = 2$ kV/cm. The term $\mu_{xy} = m_{exy}m_{hxy}/[m_{exy} + m_{hxy}]$ is the reduced effective mass in the (x, y) -plane. We assume that the center-of-mass motion in the (x, y) -plane is separated. Other mass terms depend on the coordinate z along the growth direction.

The three-dimensional equation (1) cannot be solved analytically even for zero electric field. In our study, equation (1) is solved numerically and energies as well as wave functions of different exciton states are obtained. Having a wave function, we can calculate the exciton-light coupling characteristics of the exciton, the radiative decay rate, by the formula [17]

$$\Gamma_0 = \frac{2\pi q}{\hbar\epsilon} \left(\frac{e|p_{cv}|}{m_0\omega_0} \right)^2 \left| \int_{-\infty}^{\infty} \psi(z_e = z_h = z, \rho = 0) \exp(iqz) dz \right|^2, \quad (2)$$

where $q = \sqrt{\epsilon}\omega/c$ is the light wave vector, ω_0 is the exciton frequency, $|p_{cv}|$ is the matrix element of the momentum operator between the single-electron conduction- and valence-band states.

3. Numerical method

According to our method (see references [32-34]), one numerically solves the boundary value problem for equation (1) and accurately obtains energies and wave functions of the exciton states. For the current study, we consider the exciton states with energies which are much

smaller than the heights of QW barriers. The wave functions of such states almost totally vanish under the external QW barriers. So, these states are localized in the double QW. Then, the exponential decrease in the exciton wave function at large values of ρ , $\pm z_e$, $\pm z_h$ as well as its finiteness at $\rho = 0$ allow us to impose zero boundary conditions for the function $\chi(z_e, z_h, \rho)$ at the boundary of some rectangular domain.

For discretization, we employ the second-order finite-difference (FD) approximation [43, 44] of the partial derivatives in equation (1) on the equidistant grids over three variables. We use the central second-order FD formula for approximation of the second partial derivative over z with the discontinuity at the interface [45, 35]:

$$\frac{1}{\Delta_z^2} \left(\frac{2}{m^{i-1} + m^i} \chi(z^{i-1}) - \left[\frac{2}{m^{i-1} + m^i} + \frac{2}{m^i + m^{i+1}} \right] \chi(z^i) + \frac{2}{m^i + m^{i+1}} \chi(z^{i+1}) \right), \quad (3)$$

where m^i is a value of the mass parameter at the grid point z^i . A simplified form of formula (3) is used for the second partial derivative over ρ . The FD formula for the first partial derivative over ρ can be easily found in the cited literature. The grid steps over each variable have been taken to be the same, $\Delta = \Delta_{z_e} = \Delta_{z_h} = \Delta_\rho$. Equation (3) defines the theoretical uncertainty of the numerical solution of order of Δ^2 as $\Delta \rightarrow 0$. A discretization of equation (1) leads to a large, block-tridiagonal matrix with sparse blocks [46]. A small part of the matrix spectrum is obtained by the Arnoldi algorithm [47]. As a result, we calculate several lowest eigenvalues of the matrix and the corresponding eigenvectors. After the extrapolation to the limit $\Delta = 0$ [32], the accurate results are obtained.

The calculations were performed for the $\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}/\text{GaAs}/\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}/\text{GaAs}/\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}$ heterostructure. The widths of the left and right QWs are 10 nm and 14 nm, respectively; the barrier width is 3 nm. The external electric field, F , is applied along the growth direction in such a way that the electrons are forced to move from the left to the right. The material and energy gap parameters in equation (1) are taken from [32, 48]. In particular, the difference of the gap energies, as a function of x , is modeled by the formula $\Delta E_g = 1087x + 438x^2$ meV. The ratio of potential barriers is taken to be $V_e/V_h = 65/35$. The Luttinger parameters used in the calculations are $\gamma_1 = 6.85$, $\gamma_2 = 2.10$ for GaAs and $\gamma_1 = 3.76$, $\gamma_2 = 0.82$ for AlAs; the dielectric constants are 12.53 and 10.06, respectively. Masses and dielectric constants for ternary alloys are obtained by a linear interpolation on x .

4. Results of calculations

The electric field applied along the growth direction significantly changes properties of the quantum system. It makes the carrier bound states in QWs to be quasi-bound due to the inclination of the QW potential and penetration of the wave function beyond the outer barriers [49, 10]. Moreover, the external electric field forms the so-called indirect excitons with much lower optical activity [31].

To study these issues, we first considered the ground single-particle states of the electron and the hole in a one-dimensional double QW structure. The wave functions of these states for different magnitudes of the applied electric field are shown in figure 1. The wave functions are localized in the QWs, so a propagation of the wave functions beyond the barriers is negligible. We also estimate the size of the domain where the wave function can be treated as nonzero by 50 nm. It is seen that the ground state wave function of the electron in the double QW is mainly localized in the right QW for all studied strengths of the external electric field. However, the ground state wave function of the hole changes its main localization from right QW to the left one with an increase in the electric field strength. These pictures of single-particle states shed light to a nature of the indirect exciton: the electron and the hole, mainly localized in different QWs (the electron in the right one and the hole in the left one), are coupled by the Coulomb interaction.

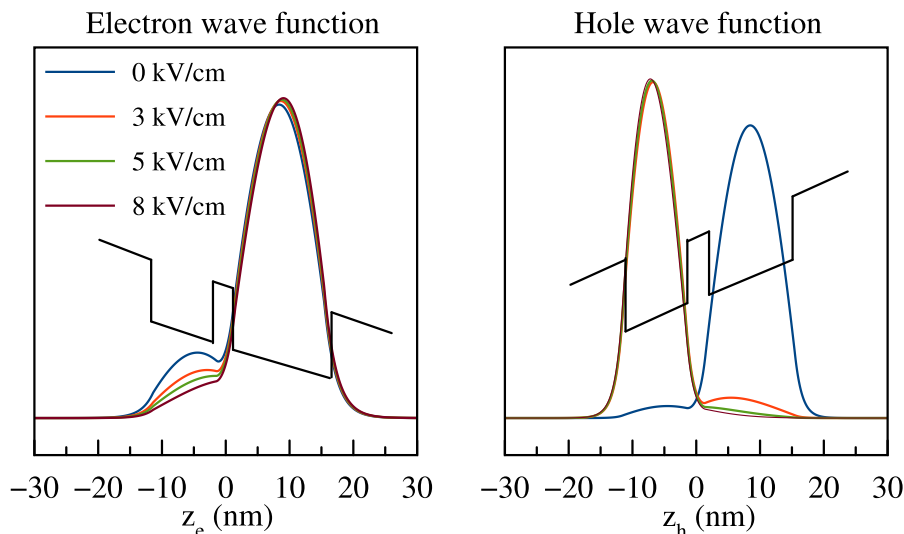


Figure 1. The ground single-particle states of the electron and the hole in the corresponding double QW structures for different strengths of the external electric field.

For zero external electric field, the energies of bound states of the electron-hole pairs in QWs are smaller than the lower boundary of the continuous spectrum of the in-plane relative electron-hole motion. This boundary is defined by a sum of the lowest quantum-confined energies of the uncoupled electron and hole in a QW [37]. This is also valid for a relatively small external electric field in the growth direction, namely, if the propagation of the wave function beyond the decreasing barrier is negligible. The states with energies above the boundary are the quasi-bound states or so-called resonant states [49]. These states are characterized by a complex energy. The imaginary part of the energy corresponds to the linewidth of the energy level. In our calculations, we obtain only the real part of the energy.

We calculated the exciton states in the double QW structure for different electric field strengths: $F = 0 - 13$ kV/cm. Energies of the ground and the first excited electron-hole bound states as functions of the electric field strength are shown in figure 2. In addition to the calculated energies, we show the energy of the lower boundary of the continuous spectrum of the in-plane relative electron-hole motion. For electric field strengths $F < 6$ kV/cm, there are two calculated electron-hole bound states below the continuum and for larger strengths, $F > 6$ kV/cm, there is only one such state. For small electric fields, the ground state corresponds to the direct exciton, which has a moderate radiative decay rate in energy units $\hbar\Gamma_0 = 36 \mu\text{eV}$. It is shown in the right panel of figure 2 by yellow color. For larger fields, the ground state changes to the indirect exciton. Such an exciton is optically inactive, and its $\hbar\Gamma_0$ is below $1 \mu\text{eV}$. It is seen that the first excited exciton state transits from the discrete part of the spectrum to the continuum, i.e. it becomes a quasi-bound state with the energy above the lower boundary of the continuous spectrum. According to our calculations, with increase in the electric field strength this state exhibits anticrossing with the ground state and becomes optically active. Then, it anticrosses with an upper resonant state and becomes optically inactive. Its energy gradually decreases. As a result, for $F > 6$ kV/cm there is a series of anticrossings of the optically active quasi-bound direct exciton state with other resonant states in the continuum at the energy of about 12 meV. Another calculated optically active quasi-bound exciton state at the energy of about 26 meV, far above the lower boundary of the continuum, is also shown in figure 2. The quasi-bound

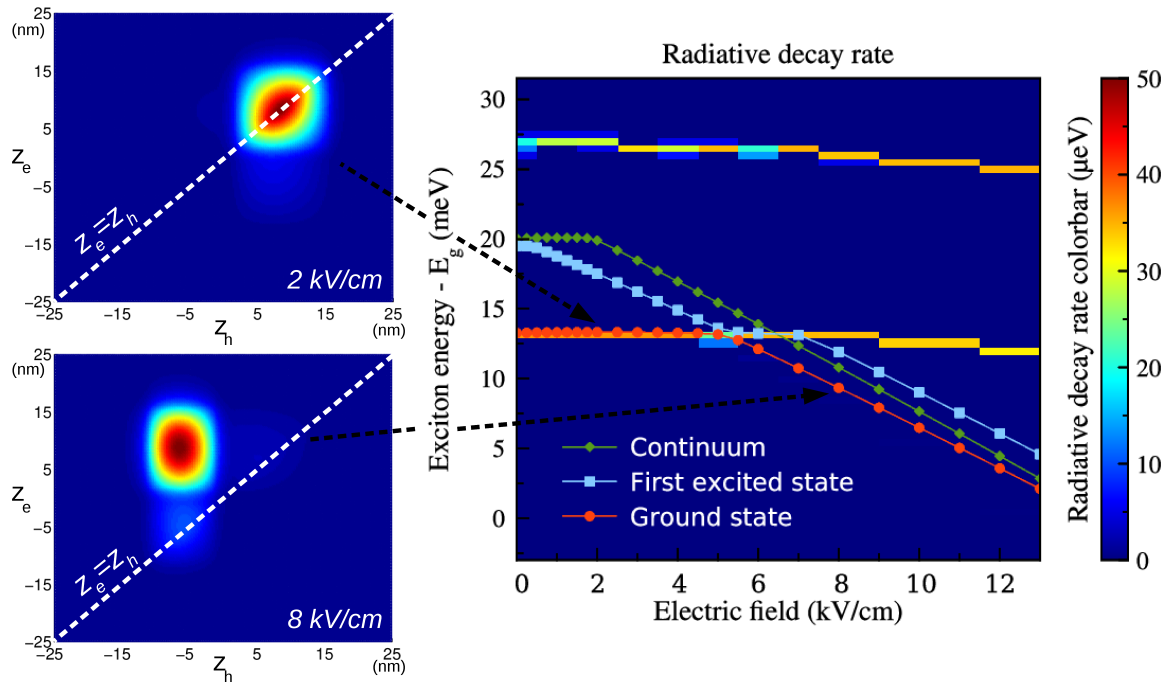


Figure 2. *Left colormaps:* slices of the ground state wave function of the exciton in the double QW as $\rho = 0$ for the electric field strengths $F = 2$ kV/cm (top panel) and $F = 8$ kV/cm (bottom panel). The line $z_e = z_h$ is indicated by the white dashed line. *Right colormap:* The calculated radiative decay rates of bound and quasi-bound exciton states as well as the energies of exciton states of weak optical activity (thin red and blue curves). The lower boundary of the continuous spectrum is shown by the green curve.

states should be studied in more detail by more advanced methods [37, 50, 51] in future because of their numerous anticrossings with other resonant states. In the current paper, we are mainly concerned with the ground exciton state (below the continuum).

A formation of the indirect exciton as a ground state of the quantum system is confirmed by the slices of the exciton wave function $\psi(z_e, z_h, \rho = 0 \text{ nm})$ for electric field strengths $F = 2$ kV/cm and $F = 8$ kV/cm. These slices are shown in the two left colormaps of figure 2. It is seen that the localization of the wave function over z_e is not changed. However, over z_h the wave function shifts from the right to the left. This shift corresponds to a change of the localization of the hole single-particle state from the right QW to the left QW (see figure 1). As a result, the indirect exciton is formed. According to equation (2), the radiative decay rate is related to the value of the exciton wave function at the line $z_e = z_h$. From the top left colormap, we see that the exciton wave function for $F = 2$ kV/cm is localized at the line $z_e = z_h$. So, the direct exciton has a noticeable radiative decay rate. The bottom left plot shows that for $F = 8$ kV/cm the main localization of the exciton does not belong to the line $z_e = z_h$. The exciton wave function is almost negligible at this line. This explains a relatively slow radiative decay rate of the indirect exciton and, thus, its long-lived nature.

5. Conclusions

In summary, we have calculated the states of the exciton in a GaAs-based double quantum well structure in an external electric field by the direct numerical solution of the three-dimensional Schrödinger equation. The direct and indirect excitons as the ground states of the studied quantum system for different strengths of the electric field were observed. A formation of

the indirect exciton was demonstrated by a change of the localization of the exciton wave function in (z_e, z_h) coordinate plane. The radiative decay rates of direct and indirect excitons were calculated. A relatively small value of the obtained rate for the indirect exciton was demonstrated.

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