Increase in the radiative decay rate of the indirect exciton due to application of the magnetic field

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Abstract. The indirect excitons in double quantum well structures can appear in the ground state under application of an external electric field along the growth axis. The relatively slow radiative decay rate of the indirect exciton can be enhanced by a magnetic field pointing in the same direction. In this report, we numerically calculate the exciton energy levels in the GaAs-based double quantum well structure as well as optimize parameters of the structure to allow a noticeable increase in the radiative decay rate of the indirect exciton there by application of the magnetic field.

1. Introduction
Excitons in semiconductor materials have been actively studied since their first experimental observation in bulk cuprous oxide by Gross and Karryev in 1952 [1]. Since then, many theoretical and experimental works have been devoted to description and measurements of spectra of the electron-hole pairs in various semiconductors and under different external conditions [2-7]. Interestingly enough, the cuprous oxide is still being under intensive investigation in spite of many recent works on graphene and TMDC structures [8-13].

Nowadays, the most studied material in the semiconductor optics is gallium arsenide (GaAs) [14, 15]. A relatively small binding energy of excitons in the bulk GaAs can be increased by growth of heterostructures with quantum wells (QWs) [16-19]. More recently, advances in the technology made it possible to grow high-quality heterostructures with coupled double and multiple QWs. The quantum confinement of carriers in these heterostructures as well as their radiative properties can be successfully described theoretically and verified experimentally [20-26]. An application of external fields allows one to study the exciton states in more detail and to control the radiative characteristics. As a very well-known example, the quantum cascade laser can be mentioned [27, 28]. Also, for instance, the strength of the applied tilted electric field can adjust the exciton-polariton interference and properties of the emitted light [29]. Another perspective application of the external electric field is a formation of the indirect exciton in the coupled double QW structure. The electron and hole in this exciton are spatially separated. As a result, the indirect exciton has low radiative characteristics and, thus, has a relatively long lifetime [30, 31]. This property of the indirect exciton makes it a good candidate for creating the Bose-Einstein condensation and excitonic devices [32].

In this report, we numerically calculate the energy levels of the exciton in a double QW structure under an external electric field applied along the growth direction. We simulate the
Al$_{0.2}$Ga$_{0.8}$As/GaAs/Al$_{0.2}$Ga$_{0.8}$As/GaAs/Al$_{0.2}$Ga$_{0.8}$As heterostructure with different widths of the left and right QWs. The width of the middle barrier is relatively small, so QWs are believed to be coupled due to tunneling of the carrier wave functions through the barrier.

For modeling, we use our method of the direct numerical solution of the three-dimensional Schrödinger equation for the exciton in a QW [33-41]. The method is based on the finite-difference discretization and allows one to obtain accurate exciton energies and wave functions for a wide range of the QW widths and potential profiles [42]. It is superior to the standard variational approach [16, 15, 43, 44] and makes it possible to calculate the excited states of excitons in external fields as well.

We obtain energies and wave functions of the ground and a few excited exciton states for different magnitudes of the electric and magnetic fields. The magnetic field is also applied in the growth direction [45, 46]. We study the dependence of the energy levels of the direct and indirect excitons on the magnitudes of the fields. Moreover, we calculate the radiative decay rates of the exciton states in the heterostructure [15] and show how one can increase the radiative decay rate of the indirect exciton there by increasing the magnitude of the magnetic field. We determine the optimal parameters of the structure that allow one to identify the indirect exciton in the reflectance spectra.

The obtained numerical results are important for experimental studies of indirect excitons as theoretical predictions of the parameters for brightening them [47-49].

2. Theoretical model

The energy states of the heavy-hole exciton in the double QW structure in an external electric field $F$ applied along the growth direction were modeled by solving the time-independent Schrödinger equation, described in references [38, 41]. Applying a co-directed magnetic field $B$ modifies this equation by the term proportional to $(B\rho)^2$ (where $\rho$ is the electron-hole distance in the QW plane), which introduces the diamagnetic shift [45, 35, 36, 50]. Then, the equation for $s$-like states of the heavy-hole exciton in a QW in both electric and magnetic fields directed along the growth axis is given by

$$K - \frac{\epsilon^2}{\epsilon \sqrt{\rho^2 + (z_e - z_h)^2}} + V_e(z_e) + V_h(z_h) + eF(z_e - z_h)\chi(z_e, z_h, \rho) = E\chi(z_e, z_h, \rho),$$  \hspace{1cm} (1)

where the kinetic term $K$ reads

$$K = -\frac{\hbar^2}{2} \frac{\partial}{\partial z_e} m_e(z_e) \frac{\partial}{\partial z_e} - \frac{\hbar^2}{2} \frac{\partial}{\partial z_h} m_h(z_h) \frac{\partial}{\partial z_h} - \hbar^2 \frac{1}{\mu_{xy}} \left( \frac{\partial^2}{\partial \rho^2} - \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \right) + \frac{e^2 (B\rho)^2}{8\mu_{xy} \epsilon^2}.$$

The wave function of the $s$-like state of the exciton is $\psi(z_e, z_h, \rho) = \chi(z_e, z_h, \rho)/\rho$. The terms $V_{e,h}(z_{e,h})$ denote the QW potentials of the heterostructure. The term $\mu_{xy} = m_{exy} m_{hxy}/[m_{exy} + m_{hxy}]$ is the reduced effective mass in the $xy$-plane (QW plane). The symbol $\epsilon$ denotes the dielectric permittivity and $c$ is the speed of light in vacuum.

We numerically solve the boundary value problem for equation (1) and obtain energies and wave functions of the exciton states. We use our well-established finite-difference method [33, 35, 37]: for discretization, we employ the second-order finite-difference approximation [51, 52] of the partial derivatives in equation (1) on the equidistant grids over three variables. Such a discretization leads to a large, sparse block-tridiagonal matrix [53]. Several lowest eigenvalues of the matrix and the corresponding eigenvectors are calculated by the Arnoldi algorithm [54]. As a result, the energies as well as the wave functions of the lowest exciton states are obtained.

Having a wave function, we can calculate the exciton-light coupling characteristics of the
Figure 1. Energies of the exciton states (the lowest state of the direct exciton is the solid line; the lowest indirect exciton state is the dashed line) as a function of the applied electric and magnetic fields for a heterostructure with the double 10-3-14 nm QW. The size of the lines denotes the relative radiative decay rate. The values in italics are the magnitudes of the radiative decay rate in $\mu$eV for given values of the fields.

The exciton, the radiative decay rate, by the formula [15]

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

where $q = \sqrt{\varepsilon \omega/c}$ is the light wave vector, $\omega_0$ is the exciton frequency, $|p_{cv}|$ is the matrix element of the momentum operator between the single-electron conduction- and valence-band states.

The calculations were performed for the Al$_{0.2}$Ga$_{0.8}$As/GaAs/Al$_{0.2}$Ga$_{0.8}$As/GaAs/Al$_{0.2}$Ga$_{0.8}$As heterostructure. The widths of the left and right QWs are 10 nm and 14 nm, respectively, and 5 nm and 7 nm, respectively; the widths of the central barrier are 3 nm and 2 nm. The external electric and magnetic fields, $F$ and $B$, are applied along the growth direction. In particular, the electric one is applied in such a way that the electron is forced to move from the left QW to the right one. The heavy-hole exciton states were calculated. The light-hole exciton states in narrow QWs are well enough separated by energy and, thus, they are disregarded. The material and energy gap parameters in equation (1) are taken from [33, 55]. 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 $x$.

3. Results of calculations

It has already been shown in [40] that, for 10-3-14 nm heterostructure, the indirect exciton in the ground state appears at an electric field of the magnitude $F > 5$ kV/cm. It was also shown that the indirect exciton has a very slow radiative decay rate and can hardly be seen in the reflectance spectra. Nevertheless, it is well known that the magnetic field in the growth direction, due to the parabolic structure of the corresponding term in the Hamiltonian, introduces an additional radial confinement of the electron and the hole [56, 45, 15]. As a result, the radiative decay rate of the exciton substantially increases. Such an increase has already been seen for the direct excitons in a single QW [36]. However, for the indirect exciton, such a calculation is important, since several heterostructures are expected to be grown in the St. Petersburg State University, and the optimized parameters of the structure would be helpful.

We calculated the energy levels and corresponding radiative decay rates for several heterostructures and applied electric and magnetic fields of various magnitudes. First, we reproduced the results of [40] for electric fields up to $F = 15$ kV/cm as well as applied an external magnetic field up to 15 Tesla. The results are shown in Figure 1. Despite many calculated energy levels, hereinafter, for simplicity, we will show only the relevant ones. For relatively low and high electric fields, the shown states are well separated in energy from other calculated states. They can also be distinguished by the radiative characteristics. The general pattern of energy levels is the same for different magnetic fields. One can see almost horizontal solid lines which represent the lowest direct exciton state as well as tilted dashed curves which show how the indirect exciton in the ground state appears. For zero electric field, the indirect exciton is realized as an excited state of the system. As the electric field increases, the energy levels of the indirect excitons go down and then become the ground states of the system. It should be noted that the shown energy levels of the direct and indirect exciton states (corresponding to the same magnetic field) exhibit the avoided crossings. They are relatively small, however still can be observed in results of our calculations. The radiative decay rates ($\hbar \Gamma_0$ in $\mu$eV) of the shown states for $F = 15$ kV/cm are also denoted in the figure. They grow with an increase in the magnetic field. However, the values of $\hbar \Gamma_0$ for the indirect exciton are relatively small even for a magnetic field of 15 Tesla. It means that this structure seems to be inappropriate for studying indirect excitons by reflectance experiments.

To obtain the optimized heterostructure, we firstly varied the barrier width to increase the overlap of the electron and hole wave functions. However, it was not enough to get $\hbar \Gamma_0 > 10 \mu$eV. Secondly, we varied widths of the left and right QWs. It led us to a decrease in the total size of the double QW structure. The point is that the left and right QWs should be narrow to enhance penetration of the wave functions under the barriers. This additionally increases the overlap of the electron and hole wave functions. It was obtained that the total size of the double QW structure should be not larger than the Bohr radius of the exciton, that is of about 15 nm.

As a result, the optimized structure with appropriate energy and radiative characteristics is the 5-2-7 nm QW heterostructure. The calculated direct and indirect exciton energy levels for this heterostructure for various external electric and magnetic fields are shown in Figure 2. One can see the similar behavior of the energy levels with a variation of the magnitudes of the fields as it was for the 10-3-14 nm heterostructure. Each energy curve shows the direct exciton as well as the indirect one. The solid parts of curves conventionally correspond to direct excitons and the dashed ones to the indirect ones.

However, there are several important features. Since the QWs became narrower, the energies of states, originating from quantization energies, became larger. The magnitudes of the avoided
crossings also became larger due to a narrower barrier between QWs and, in turn, a more significant overlap of the one-particle wave functions. It is worth noting that this magnitude is obtained to be of about 3 meV. This may open up good opportunities for studying the terahertz radiation [57-59], since the frequency of the transition between states with such energy separation is about 0.73 THz. The magnitude of the avoided crossings depends strongly on the width of the barrier between QWs. Our calculations show that if the barrier is increased up to 3 nm, then the magnitude of the avoided crossings reduces to 1 meV.

The radiative decay rates of the indirect exciton states are increased in the optimized structure. One can see that for a magnetic field of 10 Tesla, $\hbar \Gamma_0$ of indirect exciton is of about 10 $\mu$eV for $F = 0$ kV/cm as well as for $F = 30$ kV/cm. Since the energies of the indirect exciton are well separated from the ones of the direct exciton, this value of the radiative decay rate is believed to be enough to observe the corresponding indirect exciton states in the contemporary reflectance spectra [33, 25, 36, 41]. For larger magnetic fields, $\hbar \Gamma_0$ of the indirect exciton (as well as of the direct one) further increases due to a stronger radial confinement of the carriers.

In Figure 3, we show the dependence of the radiative decay rates of the calculated states as a function of the electric field strength for different magnetic fields. The behavior of $\hbar \Gamma_0$ is rather

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**Figure 2.** Energy levels of the calculated direct and indirect exciton states as a function of the applied electric and magnetic fields for the heterostructure with the double 5-2-7 nm QW. Each energy curve consists of two parts: the solid part conventionally denotes the direct exciton and the dashed part corresponds to the indirect one. The size of the lines denotes the relative radiative decay rate. The values in italics are the magnitudes of the radiative decay rate in $\mu$eV for given values of the fields.
complicated. We describe here only the main features related to a change in $\hbar \Gamma_0$ during the crossover of the energy level from the direct exciton to the indirect one. As in Figure 2, the solid parts of curves correspond to the direct excitons and the dashed parts of curves correspond to the indirect ones. One can see that for small electric fields, the direct exciton has a relatively large $\hbar \Gamma_0$, while the indirect one has a small one. Then, for the strengths of the electric fields close to the values of the crossover from the direct exciton to the indirect one, respectively, the radiative decay rates in Figure 3 change vice versa with the increase in an electric field. One can also see from the curves for a magnetic field of 10 Tesla that $\hbar \Gamma_0$ of about 20 $\mu$eV can be achieved for $F = 25$ kV/cm. However, the energy separation between the direct and indirect exciton states for such an electric field is not as large as for $F = 32$ kV/cm, that is only of about 5 meV.

![Figure 3](image-url)  
**Figure 3.** The radiative decay rates of the calculated states of the direct and indirect excitons as a function of the applied electric and magnetic fields for the heterostructure with a double 5-2-7 nm QW. As in Figure 2, each curve consists of two parts: the solid part conventionally denotes the direct exciton and the dashed part corresponds to the indirect one. The size of the lines denotes the relative radiative decay rate.

4. Conclusions
In summary, we have calculated the lowest states of the exciton in GaAs-based double quantum well structures in external co-directed electric and magnetic fields by the direct numerical solution of the three-dimensional Schrödinger equation. It was found that the radiative decay rate of the indirect exciton can be increased up to a few tens of $\mu$eV which are enough to have
the indirect exciton observed in the reflectance spectra by application of 10 Tesla magnetic field. The optimized parameters of the structure were determined: 1) the width of the double QW structure should not be larger than the Bohr radius of the exciton; 2) the width of the middle barrier is of about 2 nm. The energy and radiative characteristics of the optimized heterostructure were calculated.

Acknowledgments

Financial support from RFBR (grants No. 19-02-00576, 20-32-70131) and from the conjoint SPbU/DAAD Dmitrij-Mendeleev-Programme 2020/2021 (grant No. 57516244) is acknowledged. The author also acknowledges the Saint-Petersburg State University for the laboratory research grant No. 73031758. The calculations were carried out using the facilities of the SPbU Resource Center “Computational Center of SPbU”.

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