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EXCITONS IN NANOSTRUCTURES

Modeling of Exciton Exchange Interaction in GaAs/AlGaAs Quantum Wells

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Abstract—In this work, we study the exchange interactions between two excitons in the GaAs/AlGaAs quantum wells of various widths. We numerically solved the Schrödinger equation for an exciton in a quantum well to find the two-exciton wave functions and to calculate the exchange integral. The results suggest that the strongest interactions between excitons occur in the quantum wells of widths of about 40–50 nm, with the exchange energy being of about of 9 μeV for an exciton density of $1/\mu m^2$.

Keywords: quantum wells, exciton, exchange interaction

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INTRODUCTION

Optical nonlinearities in semiconductor nanostructures are the hot topic nowadays in view of various proposals of optical and quantum computing [1]. Although the realization of quantum computer is a questionable problem [2], the underlying physics of the nonlinear optical processes is rich and interesting. Many phenomena such as photon blockade, "liquid light", and photon crystallization related to the nonlinearities are described in literature, see, e.g., [3, 4]. These nonlinearities allow the photons to interact in the nanostructures, thus making the concept of optical computations, in principle, possible. The nonlinearity can be drastically magnified at the resonant excitation of the exciton transitions in semiconductor nanostructures. It arises at the sufficiently high exciton densities due to the exciton-exciton interactions. However, the magnitude of the interactions must be known with reasonable precision in order to estimate the required exciton densities.

Two main exciton-exciton interactions exist in an exciton system: the Coulomb interaction and different variants of the exchange interaction. In quantum wells (QWs), the exchange interaction is expected to be considerably stronger than the Coulomb one [5, 6]. In the present work, we study the exchange interaction between two excitons in the GaAs QWs of various widths. Although there are nanostructures with much stronger exciton-light coupling and, correspondingly, possible optical nonlinearity, e.g., the GaN-based nanostructures [7] and the 2D materials [8], the GaAs-based nanostructures are the most model objects for experimental study and for quantitative comparison with the theoretical results. For simplicity, we assume the interacting excitons to be in the same spin states. This is a typically realized in experiments when the excitons are resonantly created by circularly polarized light. These results can be easily generalized with no complex calculations using spin-related factors published in a paper by Ciuti et al. [5]. We compare our QW data with the results of [5] for the 2D excitons and to the case of excitons in the bulk GaAs. The results suggest that the strongest interactions between excitons occur in QWs of widths of about 40 nm.

1. BASIC EQUATIONS

The quantities under study are the energy contributions to the exchange interaction, $J^{xx}_{e-e}n$ and $J^{xx}_{h-h}n$, caused by the electron–electron (e–e) or hole–hole (h–h) exchange between two excitons in a QW. Here, n is the exciton areal density in the QW. The simultaneous exchange of electrons and holes results in a much smaller contribution [5], therefore it is not considered here. As shown by Ciuti et al. [5], the exchange of electrons and of holes gives rise to the same exchange energy, so the total energy of the exchange interaction is: $J^{xx}n = 2J^{xx}_{e-e}n$, where the exchange constant J^{xx} is determined by the expression:

$$J^{xx} = -2S_n \int \ldots \int \Psi^*(r_e, r_h)\Psi^*(r_e', r_h') \times V_I(r_e', r_h, r_e, r_h')\Psi(r_e', r_h) \times \Psi(r_e, r_h')d^3r_e d^3r_h d^3r_e' d^3r_h'. \quad (1)$$

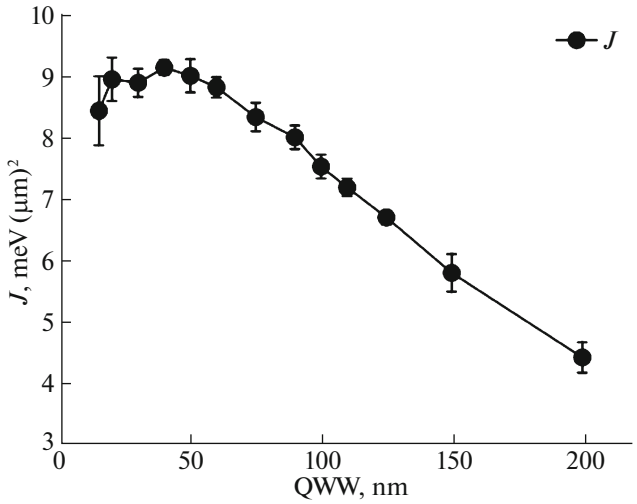

Fig. 1. Dependence of the exchange constant on the QW width.

Here, $S_n = 1/n$ is the area occupied by a single exciton, $\Psi^*(r_e, r_h)$ is the wave function of the exciton in the QW, and V_I is the interaction potential given by

$$V_I(r_e', r_h, r_e, r_h') = V(|r_e - r_e'|) + V(|r_h - r_h'|) - V(|r_e - r_h'|) - V(|r_h - r_e'|), \quad (2)$$

where $V(r) = e^2/(\varepsilon r)$, vectors r_e, r_h determine coordinates of the electron and the hole in the exciton, and ε is the dielectric constant of the medium.

The method of the numerical solution of the Schrödinger equation for a heavy-hole exciton in a GaAs QWs described in [9–12]. The cylindrical symmetry of the problem is considered and the degeneration of the valence band in the GaAs crystal is neglected. These approximations are well justified for relatively narrow QWs in which the degeneracy is removed because of different quantum confinement energies for the heavy-hole and light-hole excitons. In wide QWs, the degeneracy can be removed by a built-in or external stress of the structure. Material parameters of GaAs and $Al_xGa_{1-x}As$ are taken from [14]. The aluminum concentration in the barrier layers, $x = 0.3$, is chosen as heterostructures with such concentration are frequently used in experimental studies.

The 12-dimensional exchange integral (1) is calculated using a simple Monte Carlo method as it is described in Supplementary materials of [13]. A pseudorandom number generator was used to generate coordinates of electrons and holes in a large enough three-dimensional region where the exciton wave functions are noticeably nonzero. Then the expression under the integral was calculated and accumulated. Typically 10^{10} random coordinates have been used to obtain the integral with reasonable accuracy for each QW width.

2. NUMERICAL RESULTS

Figure 1 shows the QW width dependence of the exchange constant obtained in the calculations. As seen the exchange constant has a maximum for the QW width range 20–60 nm, and then it slowly decreases with the QW width increase. The decrease can be qualitatively explained by the fact that the average distance between the interacting excitons increases when the QW width becomes larger than the effective diameter ($2a_B$ with $a_B = 14$ nm for GaAs) of the excitons [11].

For the narrow QWs we have compared our results with those obtained by Ciuti et al. in [5] in the limit of the ultranarrow QW (the 2D limit). For this purpose, we used Eq. (22) from this paper:

$$H^e_{exch}(\Delta Q, q, \Theta) = \frac{-1}{S_n}\frac{e^2}{\varepsilon}\lambda_{2D}\left(\frac{2}{\pi}\right)^2 I_{exch}(\Delta Q, q, \Theta), \quad (3)$$

where $\varepsilon = 12.53$ is the static dielectric constant of GaAs, λ_{2D} is the exciton Bohr radius in the narrow QW. We have numerically calculated the exciton wave function for the 5-nm $GaAs/Al_{0.3}Ga_{0.7}As$ QW and determined the value $\lambda_{2D} \approx 10.3$ nm in the QW middle [11]. Using the value of $I_{exch}(\Delta Q, q, \Theta, \beta_e) \approx -15$ from [5] (see Fig. 3 in this paper), we obtain: $J_{exch} = S_n H_{exch} = -7.2$ μeV(μm)^2. This value is close to that obtained in our numerical calculations of the exchange integral for the narrow QWs (see Fig. 1).

It is also important to compare our results in the other limit of the wide QWs to the bulk case of hydrogen-like excitons, where the wave functions can be computed analytically. The expression for J^{xx} in the bulk case is similar to (1):

$$J^{xx}_{3d} = -2V_n \int \ldots \int \Psi^*(r_e, r_h)\Psi^*(r_e', r_h') \times V_I(r_e', r_h, r_e, r_h')\Psi(r_e', r_h) \times \Psi(r_e, r_h')d^3r_e d^3r_h d^3r_e' d^3r_h'.$$

However, the dimension of this quantity differs from that of J^{xx} because of the V_n multiplier. Thus, we cannot compare the values J^{xx}_{3d} and J^{xx} directly. To make the comparison possible, we multiply the integral in Eq. (1) by $L \cdot S_n$ instead of S_n. The resulting quantity $J^{xx} \cdot L$ should approach the bulk case in the limit of very large QW width L. The QW data for the largest width studied in our work ($L = 200$ nm) gives the value of the integral, $J^{xx} \cdot L \approx 0.9$ μeV(μm)^3. A separate calculation using the hydrogen-like wave function for the exciton in the bulk GaAs gives the value of the exchange integral, $J^{xx}_{3d} \approx 0.4$ μeV(μm)^3. The agreement should be considered as acceptable taking into account large extrapolation from the QW width $L = 200$ nm to the bulk case.

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CONFLICT OF INTEREST

The authors declare no conflict of interest.

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