On two-dimensional exciton bound by distant ionized-donor in a narrow quantum well

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Abstract

The ground state energy of exciton bound by distant ionized donor impurity in two-dimensional semiconductor quantum well (QW) is studied theoretically within the Hartree approach in the effective mass approximation. The influence of the distance between QW plane and ionized donor, as well as of the electron-hole mass ratio, the magnetic field and dielectric constant of the barrier material on the stability of exciton bound by ionized donor impurity is analyzed and discussed.

1. Introduction

One of the simplest possible three-particle bound-exciton complex \((D^+, X)\) consist of an exciton \(X\) (electron hole pair) bound to an ionized donor impurity \(D^+\). Its possible existence was first predicted by Lampert [1] in 1958. Since then its stability and binding energy as a function of the electron to hole effective mass ratio \(\sigma = m_e/m_h\) has been the subject of few theoretical studies in bulk (3D) semiconductor [2, 3] and in two-dimensional QW structures [4, 5]. As a result in 3D case Stauffer and Stébé using a 55-term Hylleraas-type wave function obtained [3] that the complex \((D^+, X)\) is stable until \(\sigma < \sigma_{c}^{3D} \approx 0.365\). Skettrup et al. using more elaborated wave functions obtained [5] critical value of this ratio \(\sigma_{c}^{3D} \approx 0.426\). In 2D case the overlapping between the wave functions of the constituents of the \((D^+, X)\) complex become more important (due to the quantum confinement), binding energy of the complex is increased and so the stability in 2D structures is increased compared to their 3D counterparts. Therefore it is expected that the observation of bound excitons should be easier in 2D structures than in the bulk. In the case of two-dimensional QW, Stauffer and Stébé using the same method as in 3D case obtained [5] critical value \(\sigma_{c}^{2D} \approx 0.88\). However more recently, Ruan and Chang using the hyperspherical adiabatic expansion approach found that the complex \((D^+, X)\) is stable in 2D case with any value of the electron to hole effective mass ratio in the range \(0 \leq \sigma \leq 1\) whereas for \(1 \leq \sigma \leq \infty\) negatively charged acceptor ion \(A^-\) can bound exciton and the complex \((A^+, X)\) is stable [6].

For finite well width Liu and co-workers [5], using a two-parameter wave function, calculated variationally the binding energy of an exciton bound to an ionized donor impurity \((D^+, X)\) in GaAs/Al,Ga\(_{1-x}\)As QW for the values of the well width from 1 to 30 nm, when the dopant is located in the center of the well and at the edge of the well. da Cunha Lima et al. [6] performed a variational calculation of the binding energy of the \((D^+, X)\) complex for all values of well widths, and impurity position inside the well, including \(\Gamma-X\) mixing in GaAs/AlAs QWs. Stébé and co-workers [7] studied variationally the influence of the magnetic field on the binding energy of \((D^+, X)\) in GaAs/Al\(_{1-x}\)As QWs.

Nevertheless no one has yet analyzed the impact of ionized donor shifted from the QW plane. The lateral crosssection of singular potential of ionized donor, as acting on charge carriers in distant 2D well, resembles a nonsingular potential of type-II quantum dot (defined by the electrostatic field) — thus recognition of exciton evolution with respect to the donor separation is of crucial importance in order to differentiate both confinements.

In this paper the ground state energy of exciton bound by ionized donor shifted from two-dimensional QW is studied theoretically within the Hartree approach in the effective mass approximation. The influence of the donor distance, the electron-hole mass ratio, varying dielectric constant of barrier material and of the external uniform magnetic field (aligned across the QW plane) on the stability of two-dimensional exciton bound by ionized donor is analyzed and discussed.

2. Model and method

For the model analysis, we assume that the QW is quasi-two-dimensional and lies in the x-y plane, while the magnetic field is aligned across this plane, i.e., along the z axis. Moreover, we restrict our model only to the spatial coordinates — spin degrees of freedom and the associated Zeeman splitting (linear in B) were not included in our description (for GaAs this splitting is very small ~ 0.03 meV/T.)

In the QW plane potential of ionized donor shifted by the distance \(d\) in the axial direction has the form

\[
V_i(\rho_i) = \mp \frac{q^2}{4\pi\epsilon\epsilon_0} \frac{1}{\sqrt{\rho_i^2 + d^2}}
\]

where minus sign corresponds to the electron \((i = e)\), plus to the hole \((i = h)\), \(\rho_e\) and \(\rho_h\) are the radial distances of electron and hole in the QW plane, \(q\) is the elementary positive charge and \(\epsilon_1\) is the relative dielectric constant of the barrier material.
Despite the fact that the potential (1) is attractive only for one type of charge carrier it is however possible for the distant donor to captured the electron-hole pair (exciton) due to Coulomb interaction between charge carriers.

It should be noted here, that in more realistic model, for very small $d$ and shallow QWs, electron tunneling through the potential barrier has to be taken into account. Nevertheless, the probability of this process rapidly decreases as the donor is shifted away from QW plane.

Within the Hartree method exact exciton wave function can be approximated by

$$\Psi(r_x, r_h) = \psi_e(r_x) \psi_h(r_h) \text{ where } r_x = (r_e, \varphi_e) \text{ and } r_h = (r_h, \varphi_h).$$

Using axial symmetry we assume one particle wave functions in the form

$$\psi_i(r_i) = \frac{1}{\sqrt{2\pi}} \exp(il_i \varphi_i) \phi_i(\rho_i),$$

where $l_x = 0, \pm 1, \pm 2, \ldots$ and $s = e,h$. Then the single-particle Hartree energies and wave functions are found in the effective mass approximation by iterative solving of self-consistent Hartree equations

$$-\frac{\hbar^2}{2m_e} \frac{\partial}{\partial \rho_e} \left( \frac{\partial \phi_e(\rho_e)}{\partial \rho_e} \right) + \frac{\hbar^2}{2m_h} \frac{\partial^2 \phi_h(\rho_h)}{\partial \rho_h^2} + U_e(\rho_e) \phi_e(\rho_e) = \epsilon_e \phi_e(\rho_e),$$

$$-\frac{\hbar^2}{2m_h} \frac{\partial}{\partial \rho_h} \left( \frac{\partial \phi_h(\rho_h)}{\partial \rho_h} \right) + \frac{\hbar^2}{2m_e} \frac{\partial^2 \phi_e(\rho_e)}{\partial \rho_e^2} + U_h(\rho_h) \phi_h(\rho_h) = \epsilon_h \phi_h(\rho_h),$$

with the effective Hartree potentials

$$U_e(\rho_e) = V_e(\rho_e) + \frac{1}{8m_e \omega_e^2 \sigma^2} \int |\psi_e(r_x)|^2 |r_x - r_h|^2 dr_h,$$

$$U_h(\rho_h) = V_h(\rho_h) + \frac{1}{8m_h \omega_h^2 \sigma^2} \int |\psi_h(r_h)|^2 |r_h - r_x|^2 dr_x,$$

where $m_e$ and $m_h$ are effective electron and hole masses respectively, $\omega_e = qB/m_e$, and $\omega_h = qB/m_h$ are electron and hole cyclotron frequencies and $\sigma$ is the relative dielectric constant of the QW material.

The exciton energy in Hartree approximation is given by

$$E = \epsilon_e + \epsilon_h - V_C,$$

where

$$V_C = -\frac{q^2}{4\pi \epsilon_0} \int |\psi_e(r_x)|^2 |\psi_h(r_h)|^2 |r_x - r_h|^2 dr_x dr_h.$$ (6)

As we deal with single electron-hole pair there is no exchange energy term (related to Pauli exclusion principle) and only correlation energy is omitted. Moreover, as it was shown for quantum dots (whose potential is similar to the potential of shifted donor in QW plane), the contribution of the correlation to the total energy for single electron-hole pair is expected to be less than 2% \[8\].

Hartree equations (2) were solved numerically with finite difference scheme on nonuniform grid (more details about the implementation of this finite difference scheme can be found in work of Peeters et al. \[9\]). Using this scheme we obtained symmetric tridiagonal matrix. Its eigen values were calculated with Martin-Dean algorithm \[10\], whereas eigen vectors were found using DWSZ method \[11\]. Hartree integrals in (3), (4) and (6) were calculated with use of logarithmically weighted method after Janssens et al. \[12\]. The convergence in the self-consistent Hartree procedure is obtained in a few rounds.

3. Results and discussion

As an example we consider the case of GaAs semiconductor QW and choose material parameters $\epsilon_2 = 12.4$, $m_e = 0.0665$, $m_h = 0.3774$ so that $\sigma = 0.176$. For such choice Fig. 2 shows dependence of effective Hartree hole potential (a) and corresponding hole wave function (b) on the donor distance $d$ from the plane for listed parameters. For the barrier material, at this point, we choose $\epsilon_1 = \epsilon_2$. When $d$ is small Hartree hole potential is repulsive in the center of the QW and has minimum at certain distance. As $d$ increases donor repulsion become weaker and for $d \sim 5$ nm hole moves to the center.

Electron Hartree potential does not change qualitatively as the donor is moved away from the plane — first becomes shallower with increasing $d$, next it deepens when the hole moves...
to the center (due to the increase of electron-hole coulomb interaction), and then becomes shallower again.

Fig. 2(a) illustrates electron (dashed line) and hole (dash-dot) Hartree energies as a function of the donor distance $d$ from the QW plane for $\epsilon_1 = \epsilon_2 = 12.4$ (a) and $\epsilon_1 = 10.1$, $\epsilon_2 = 12.4$ (b).

For distance greater than about 15 nm exciton energy almost stop changing despite further change of electron and hole one-particle Hartree energies. (It should be noted here that in the system of interacting particles unambiguous qualification of one-particle energies is not possible. The energy of the whole system is the only direct contact with the experiment, therefore, further change of one-particle energies may be irrelevant from a physical point of view.) So for large distances $d$ energy should correspond to the energy of free two-dimensional exciton.

On the other hand, as can be shown by extrapolating for small $d$ the Hartree hole energy (it never reaches zero) ionized donor should bound exciton even for $d = 0$.

The other situation is for $\epsilon_1 < \epsilon_2$. As an example we will consider GaAs/AlAs for which $\epsilon_1 = 10.1$ and $\epsilon_2 = 12.4$. In contrast to the previous situation, as we can see in Fig. 2(b), the hole is not bound until the distance of donor reaches the critical value $d_{\text{min}}$. Thus the lower dielectric constant of the barrier prevents the exciton binding for small $d$ — hole is more strongly repelled and the electron Coulomb attraction is insufficient to bound a hole until we move the donor at an appropriate distance. The question arises how far to move the donor from the plane of the well for a given dielectric constant of the barrier in order to obtain a bound state.

Fig. 3 shows the dependence of this critical distance on the $\epsilon_1$ (solid line) for GaAs/AlGa$_{1-x}$As, for which we can assume that

$$\epsilon_1(x) = 12.4 - 2.3x. \quad (7)$$

As one might expect the critical distance $d_{\text{min}}$ decreases with increasing $\epsilon_1$ and reaches zero before $\epsilon_1$ equals $\epsilon_2$. It follows that the exciton bound state could exists for $\epsilon_1 = \epsilon_2$.

The situation is different for mass ratio $\sigma = 1$ (dashed line in Fig. 4), for which $d_{\text{min}}$ tends to zero when $\epsilon_1$ tends to $\epsilon_2$. Although we can not show that $d_{\text{min}}$ is exactly equal to zero for $\epsilon_1 = \epsilon_2$, however, by our calculation we can show that it is smaller than the desired numerical accuracy.

So far our approach was limited to the analysis of the Hartree hole energy — if it was less than zero we assumed that exciton is bound by ionized donor impurity. Nevertheless, even in this situation, created complex may be unstable due to the following dissociation processes

$$(D^+, X) \rightarrow D^0 + h, \quad (8)$$

$$(D^+, X) \rightarrow D^0 + X. \quad (9)$$

In these equations $(D^+, X)$ and $D^0$ denote respectively exciton or electron bound by ionized donor in the QW, while $h$ and $X$ denote free hole and free exciton in the QW plane. Therefore, we need to consider the binding energies $E_{D^0}^B = E_{D^0}^B + E_{h}^B$, $E_{X}^B = E_{X}^B - E_{D^0}^B$, $E_{D^0}^B = E_{D^0}^B - E_{D^0}^B$, whose physical meaning is that the $E_{D^0}^B$ is the minimum energy required to liberate the hole from the bound exciton and $E_{D^0}^B$ is the minimum energy required to liberate the exciton from the influence of ionized donor. So the complex remains stable if $E_{D^0}^B > 0$ and $E_{D^0}^B > 0$.

In our calculations for $E_{D^0}^B$ we take the value to which the energy of bound exciton tends, when $d$ tends to infinity, and we put $E_{D^0}^B$ equal $\hbar \omega_{k_{\text{b}}} / 2$ (lowest landau level in magnetic field).

Fig. 4 represents the dependence of the energies $E_{D^0}^B$ and $E_{D^0}^B$, both in meV, on the donor distance from the QW and on the dielectric constant of the barrier material in the range
10 < \epsilon_1 < 12.4 \text{ (as for Al}_{0.1}\text{Ga}_{0.9}\text{As). Additional dotted lines indicate the limit distance for donor.}

\text{As can be seen by comparing parts (a) and (b) the complex is stable when 11.4 \leq \epsilon_1 \leq 12.4 (which incidentally corresponds to the interval in which our heterostructure has a direct energy gap) and only for } d_{\text{min}} < d \lesssim 4 \text{ nm (for } \epsilon_1 \text{ close to } \epsilon_2 \text{ we should be especially careful with the interpretation of our results because the difference between energy gaps of GaAs/Al}_{0.1}\text{Ga}_{0.9}\text{As becomes small so the electron can tunnel through the potential barrier). For } d \text{ greater than } \sim 4 \text{ nm, in the whole range of } \epsilon_1, \text{ complex may dissociate into } X \text{ and } D^+ \text{ or, if in addition } d \text{ is not much larger than the } d_{\text{min}}, \text{ into hole and } D^0.\n
\text{It is also interesting to check what impact on the stability of discussed complex has the magnetic field perpendicular to the QW plane. Fig. 5 shows the dependence of the binding energies } E_{bp}^D \text{ and } E_{bp}^X \text{ on the donor distance from the QW and magnetic field for } \sigma = 0.176, \epsilon_2 = 12.4 \text{ and } \epsilon_1 = 11.71, \text{ (which according to } 7 \text{ corresponds to } x = 0.3). \text{ As can be seen from Fig. 5(a) } E_{bp}^D \text{ is less than zero only for small } d \text{ and sufficiently high magnetic field. In this range of parameters the complex } (D^+, X) \text{ is unstable due to dissociation process } 5. \text{ In turn, Fig. 5(b) shows that it is unstable due to dissociation process } 9 \text{ if } d \text{ is sufficiently large. This critical distance decreases with increasing field — it may be due to the fact that in a magnetic field the Coulomb interaction energy in } X \text{ is growing relatively quickly while the ionized donor (because of repulsive potential for hole) prevents such rapid growth of this energy in bound exciton.}\n
\text{Summarizing, in the magnetic field for } x = 0.3 \text{ the complex is stable only for respectively small } d \text{ (the smaller the greater is the field) excluding the range (small } d \text{ and big } B \text{) in which complex can dissociate into } D^0 \text{ and } h.\n
4. Conclusions

\text{In the present work we have calculated, using Hartree approximation, the energy of exciton bound by distant ionized donor in 2D QW for dielectric constant of QW material equal and greater than the dielectric constant of a barrier, where the donor was located. In the latter case it turned out that in order to bound exciton the donor has to be shifted from the QW on certain distance. Dependence of this distance on the dielectric constants has been calculated. Moreover, we have also studied stability of created complex depending on the value of dielectric constant of the barrier material and on the magnetic field.}\n
\text{Despite the fact that the potential of shifted donor resembles (in the QW plane) the potential of type II quantum dot it should be however possible to distinguish between the two due to the mentioned lack of stability of donor bound exciton in the growing magnetic field.}\n
\text{References}\n
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