Exciton bound by distant ionized donor in two-dimensional GaAs/AlGaAs quantum well

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The ground state energy of exciton bound by distant ionized donor impurity in quasi-two-dimensional GaAs/Al$_x$Ga$_{1-x}$As 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 magnetic field aligned across the QW plane and varying dielectric constant of the barrier material on the stability of exciton bound by ionized donor impurity is analyzed and discussed.

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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 in 1958. Since then its stability and binding energy has been the subject of few theoretical studies in bulk (3D) semiconductor and in two-dimensional QW structures. In 2D case the overlappings 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.

The binding energy of an exciton bound to an ionized donor in GaAs/Al\(_x\)Ga\(_{1-x}\)As QW has been calculated for finite well widths and different impurity position by Liu and co-workers and da Cunha Lima et al. Stébé and co-workers studied variationally the influence of the magnetic field on the stability of created complex. 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 letter the ground state energy of exciton bound by ionized donor shifted from 2D well is studied theoretically within the Hartree approach in the effective mass approximation. The influence of the donor distance, varying dielectric constant of barrier material and of the external uniform magnetic field on the stability of 2D exciton bound by ionized donor is analyzed and discussed.

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. 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 \(\sim 0.03\) meV/T.)

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

\[
V_i (\rho_i) = \mp \frac{q^2}{4\pi\epsilon_1 \epsilon_0} \frac{1}{\sqrt{\rho_i^2 + d^2}},
\]  

(1)
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 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 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 \(\Psi (r_e, r_h) = \psi_e (r_e) \psi_h (r_h)\). Using axial symmetry we assume

\[
\psi_s (r_s) = \frac{1}{\sqrt{2\pi}} \exp (il_s \varphi_s) \phi_s (\rho_s),
\]

where \(l_s = 0, \pm 1, \pm 2, \ldots\) 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

\[
\begin{align*}
- \frac{\hbar^2}{2m_i} \frac{1}{\rho_i} \frac{\partial}{\partial \rho_i} \left( \rho_i \frac{\partial}{\partial \rho_i} \right) + \frac{\hbar^2 l_i^2}{2m_i \rho_i^2} + U_i (\rho_i) + \frac{1}{8} m_i \omega_c^2 \rho_i^2 \pm \frac{l_i}{2} \hbar \omega_c \right) \phi_i (\rho_i) = \epsilon_i \phi_i (\rho_i)
\end{align*}
\]

with the Hartree potentials

\[
U_i (\rho_i) = V_i (\rho_i) - \frac{q^2}{4\pi \epsilon_2 \epsilon_0} \int \frac{|\psi_j (r_j)|^2}{|r_i - r_j|} dr_j
\]

where \(i = e\) and \(j = h\) (or opposite), the upper sign corresponds to the electron and the lower sign to the hole, \(m_e\) and \(m_h\) are effective electron and hole masses respectively, \(\omega_{ce} = qB/m_e\) and \(\omega_{ch} = qB/m_h\) are electron and hole cyclotron frequencies and \(\epsilon_2\) 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

\[
V_C = - \frac{q^2}{4\pi \epsilon_2} \int \int \frac{|\psi_e (r_e)|^2 |\psi_h (r_h)|^2}{|r_e - r_h|} dr_e dr_h.
\]

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%.

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 algorithm10, whereas eigen vectors were found using DWSZ method. Hartree integrals in (3) and (4) were calculated with use of logarithmically weighted method after Janssens et al.12.

For GaAs semiconductor QW we choose as material parameters $\epsilon_2 = 12.4$, $m_e = 0.0665$, $m_h = 0.3774$. Fig. 1(a) shows electron (dashed line) and hole (dash-dot) Hartree energies as well as coulomb (dot) and exciton (solid) 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).

FIG. 1. Electron (dashed line) and hole (dash-dot) Hartree energies, coulomb (dot) and exciton (solid) 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).
The different situation is for $\epsilon_1 < \epsilon_2$. As we can see in Fig. 1(b) ($\epsilon_1 = 10.1$ as for AlAs), the hole is not bound until the distance of donor reaches the critical value $d_{\text{min}}$. It turns out that the lower dielectric constant of the barrier material, 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. 2 shows the dependence of this critical distance on the $\epsilon_1$ for GaAs/Al$_x$Ga$_{1-x}$As, for which we assume $\epsilon_1(x) = 12.4 - 2.3x$. As one might expect $d_{\text{min}}$ decreases with increasing $\epsilon_1$ and reaches zero before $\epsilon_1$ equals $\epsilon_2$.

Even if exciton is bound by ionized donor impurity ($\varepsilon_h < 0$) created complex may be unstable due to the following dissociation processes

\begin{align*}
(D^+, X) &\rightarrow D^0 + h, \\
(D^+, X) &\rightarrow D^+ + X.
\end{align*}

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 $E_{D^0}^B = E_{D^0} + E_h^f - E_{(D^+,X)}$ and $E_X^B = E_X^f - E_{(D^+,X)}$ whose physical meaning is that the $E_{D^0}^B$ is the minimum energy required to liberate the hole from the bound exciton and $E_X^B$ 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 $E_X^B > 0$.

In our calculations for $E_X^f$ we take the value of bound exciton energy for very large $d$ (for
Fig. 3. Contour plots of energies $E^{B \, 0}_{D}$ (a) and $E^{B}_{X}$ (b), both in meV, depending on the dielectric constant of barrier material $\epsilon_1$ and the donor distance $d$ from the QW plane. Dotted lines indicate the limit distance for donor.

which it stabilizes), and we put $E^{f}_{X}$ equal $\hbar \omega_{ch}/2$ (lowest landau level in magnetic field).

Fig. 3 represents the dependence of the energies $E^{B \, 0}_{D}$ and $E^{B}_{X}$, both in meV, on the donor distance from the QW and on the dielectric constant of the barrier material in the range $10 < \epsilon_1 < 12.4$ (as for Al$_x$Ga$_{1-x}$As). Additional dotted lines indicate the limit distance for donor (cf. Fig. 2). As can be seen by comparing parts (a) and (b) the complex is stable when $11.4 \leq \epsilon_1 \leq 12.4$ and only for $d_{\min} < d \leq 4$ nm. For $d$ greater than $\sim 4$ nm, in the whole range of $\epsilon_1$, complex may dissociate into $X$ and $D^+$ or, if in addition $d$ is not much larger than the $d_{\min}$, into hole and $D^0$.

Fig. 4 shows the dependence of the binding energies $E^{B \, 0}_{D}$ and $E^{B}_{X}$ on the donor distance from the QW and magnetic field for $\epsilon_1 = \epsilon_2 = 12.4$. As can be seen $E^{B \, 0}_{D}$ is less than zero only for high magnetic field and respectively small $d$. In this range of parameters the complex $(D^+, X)$ is unstable due to dissociation process (5). Moreover, in the absence of magnetic field $E^{B}_{X}$ is less than zero for $d$ greater than about 3.9 nm, which means that the complex is unstable due to dissociation process (6). This critical distance decreases with increasing field which may reflect the fact that in a magnetic field the Coulomb interaction energy in $X$ is growing relatively quickly while the ionized donor (because of repulsive potential for hole) prevents such rapid growth of this energy in bound exciton.
FIG. 4. The dependence of energies $E_{D_0}^B$ (a) and $E_X^B$ (b), both in meV, on the donor distance $d$ from the plane of QW and magnetic field $B$ for $\epsilon_1 = \epsilon_2 = 12.4$.

In summary, we have found critical distance at which the donor has to be moved from GaAs/Al$_x$Ga$_{1-x}$As QW plane in order to bound exciton. We have also studied stability of created complex — it turned out that it is stable only if $11.4 \lesssim \epsilon_1 < 12.4$, the distance of the donor $d_{\text{min}} < d \lesssim 4$ nm and the amplitude of magnetic field is sufficiently small.

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