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Impurity states of two-dimensional magnetic electron–hole complexes on a spatially separated donor center

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Abstract

The barrier impurity states of two-dimensional electron–hole complexes are considered in the strong magnetic field limit. The energies of the lowest impurity states of the exciton, the 2e–h complex and the biexciton are calculated for the different projections of the total angular momentum M with arbitrary spin orientations. The stable impurity bound states of the exciton and the biexciton exist for the case of an impurity located near the barrier edge. The magnetic evaporation of such states is expected. The magnetic induced binding of the 2e–h complex by impurities in the barrier is predicted as the magnetic field increases. The energy of the exciton separation for the $S_e = 0, M = 0$ barrier impurity bound state of the 2e–h complex can be 2 times larger than that of the delocalized trion.

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Interest in two-dimensional (2D) electron–hole (e–h) systems in a strong perpendicular magnetic field with a low carrier density has increased substantially recent years. In such systems the formation of excitonic complexes can occur. Although a great part of the works are devoted to the free e–h complexes (excitons, trions, biexcitons) in quantum wells [1–13], very little attention is paid to the impurity states of such complexes [14–18]. However these complexes can be easily trapped by the impurities which are invariably present in the wells and barriers. As was shown in recent experiments [9–12], for example, trions in quantum wells are strongly localized, and the lines previously attributed to the free trion correspond to the recombination of localized complexes on an impurity in a barrier next to a well. Recent theoretical [19–22] and experimental [23] studies of spatially separated D^- centers revealed that quite unusual phenomena like angular momentum transitions and magnetic evaporation can take place for such systems. This stimulates a detailed investigation of impurity states of 2D e–h complexes, not only in-well impurity states, but also the barrier impurity states. This is the subject of the present paper.

In the present paper we will use the model of Fox and Larsen for a spatially separated D^- system [20], suggesting that the quantum well is infinitesimally

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thin and the positive Coulomb impurity is located at a distance d from the well. Tunneling will be neglected. The spectrum of the e–h system is assumed to be a simple two-band spectrum and the electron (hole) wave functions correspond to the motion of free 2D particles in a magnetic field. It was confirmed by the numerical simulations for the real structures [21,22] that this model is a reasonably good approximation for spatially separated D^- system, and the predicted magnetic evaporation in this model was recently observed by Jang et al. [23]. We expect also that the main features of impurity states of the 2D e–h system will be kept within this model.

The magnetic field direction is perpendicular to the layers and the value of the magnetic field H is assumed to be strong enough so that the following inequality for the the magnetic length $r_H = (\hbar c/eH)^{1/2}$ holds:

$$r_H \ll a_{\mathrm{e,h}}, \tag{1}$$

where $a_{\mathrm{e,h}} = \hbar^2\varepsilon/m_{\mathrm{e,h}}e^2$ are the effective Bohr radii of an electron and a hole, $m_{\mathrm{e,h}}$ and ε are the effective masses at $H = 0$ and the dielectric constant, respectively. For simplicity, it will be assumed below that electrons and holes occupy only the zeroth Landau levels.

The barrier impurity states of the exciton, the 2e–h complex and the biexciton are considered for different d and different values of electron and hole spin. It is clear that as d increases from zero, the attractive interaction responsible for the binding of e–h complexes decreases. However, the stability of impurity bound e–h complexes in such a system depends on the possibility of the separation of a e–h pair to infinity, leaving bound the exciton and the electron, for the case of the biexciton and the 2e–h complex, respectively. The difference between the binding energy of initial complex and the sum of the binding energies of the e–h complex left (after separation of the e–h pair) and the free exciton with zero momentum will determine whether such states will be impurity-bound or not. Both of these parts decrease as d increases. The question is which decreases faster. Therefore one cannot rule out without examination whether barrier states will exist or not. Similar studies of spatially separated D^- centers [20] revealed that the number of barrier bound states even more than in-well impurity bound states.

The impurity states of 2D e–h complexes in a magnetic field can be described by the exact quantum number – the projection of the total angular momentum M on the magnetic field direction. In the symmetric gauge $\boldsymbol{A} = [\boldsymbol{Hr}]/2$ the wave function of the 2D exciton bound to the positive Coulomb impurity with $M \geq 0$ can be represented in the form [15,17]:

$$\Psi_M(\boldsymbol{r}_1,\boldsymbol{r}_2) = \sum_{m=0}^{\infty} A_m(m)\,\Phi_{-m}^{(\mathrm{e})}(\boldsymbol{r}_1)\,\Phi_{M+m}^{(\mathrm{h})}(\boldsymbol{r}_2), \tag{2}$$

where $\Phi_m^{\mathrm{e(h)}}$ is a wave function of a noninteracting electron (hole) with the definite projection of the angular momentum m on the magnetic field direction. The wave function of the three-particle 2e–h complex $\Psi_{M,S_\mathrm{e}}^{2\mathrm{e}-\mathrm{h}}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3)$ with angular momentum M includes the superposition of orthonormal states [16,17],

$$|n;m;l\rangle = (a_n a_m a_l)^{-1}\left(\frac{\bar z_1 - \bar z_2}{\sqrt{2}}\right)^n\left(\frac{\bar z_1 + \bar z_2}{\sqrt{2}}\right)^m z_3^l, \tag{3}$$

where $z = x + iy$ and $a_m = \left(2\pi r_H^2\, 2^m m!\right)^{1/2} r_H^m$. The integers n, m, l satisfy the condition $l - n - m = M$ and the bar denotes the complex conjugate. For electrons in the triplet state, $S_\mathrm{e} = 1$, the numbers n should be odd, whereas in the singlet state, $S_\mathrm{e} = 0$, the quantum numbers n are even. In what follows the variables $\boldsymbol{r}_1,\boldsymbol{r}_2$ for 2D coordinates of electrons and $\boldsymbol{r}_3,\boldsymbol{r}_4$ for coordinates of holes are used. Similar to the case of the 2e–h complex the wave function of the biexciton $\Psi_{M,S_\mathrm{e},S_\mathrm{h}}^{2\mathrm{e}-2\mathrm{h}}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3,\boldsymbol{r}_4)$ with angular momentum M includes the superposition of the orthonormal four-particle states [16,17]

$$\begin{aligned}|n_1;m_1;n_2;m_2\rangle = {} & (a_{n_1}a_{m_1}a_{n_2}a_{m_2})^{-1} \\ & \times\left(\frac{\bar z_1 - \bar z_2}{\sqrt{2}}\right)^{n_1}\left(\frac{\bar z_1 + \bar z_2}{\sqrt{2}}\right)^{m_1} \\ & \times\left(\frac{z_3 - z_4}{\sqrt{2}}\right)^{n_2}\left(\frac{z_3 + z_4}{\sqrt{2}}\right)^{m_2}\end{aligned} \tag{4}$$

with the condition $n_2 + m_2 - n_1 - m_1 = M$. The quantum numbers n_1 (n_2) should be odd for $S_\mathrm{e} = 1$ ($S_\mathrm{h} = 1$) and even for $S_\mathrm{e} = 0$ ($S_\mathrm{h} = 0$). Also, for

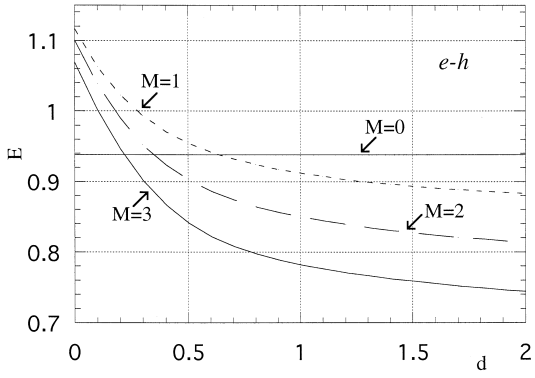

Fig. 1. The dependence of the binding energies of the lowest impurity states of the exciton on the impurity separation d. The binding energy and the impurity separation are expressed in units of E_0 and r_H, respectively.

simplicity, the common exponential part of the wave function $\exp\left(-\sum_i |z_i|^2/4r_H^2\right)$ in the expressions (3), (4) is omitted.

The coefficients with which the functions (4) and (3) enter, respectively, in $\Psi_{M,S_e,S_h}^{2e-2h}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3,\boldsymbol{r}_4)$ and $\Psi_{M,S_e}^{2e-h}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3)$ and the coefficients A_m are determined by solving the secular equation involving the Hamiltonian of the Coulomb interactions. The decreasing behavior of the matrix elements allow us to consider only N first terms in each sum for sufficiently large N [14–17]. The energies of the impurity states are obtained by the numerical diagonalization of 50×50 matrices corresponding to the secular equation where 50 orbitals are taken into account. The matrix elements and details of the calculations have already been published [15–17] for the case of spatially separated 2D e–h systems. In what follows the energy of free 2D exciton with zero momentum E_0 (depending on H) as a unit of energy and r_H as a unit of length are used. The achieved accuracy in determining the binding energies to be of the order $5 \times 10^{-3} E_0$ for the lowest levels of the magnetic biexciton and $10^{-4} E_0$ for the the 2e–h complex and the exciton. The values of the binding energies of the exciton, the 2e–h complex and the biexciton for $d = 0$ coincide with the results obtained by Dzyubenko [14]. Throughout the paper we will neglect the Zeeman energy associated with the spin of electrons and holes. However, the corresponding energy can be easily incorporated in the calculated binding energies.

The evolution of the lowest levels of the barrier impurity states of the 2D exciton is shown in Fig. 1 for different values of M. The ground state of the impurity bound 2D magnetoexciton corresponds to $M = 1$ at $d = 0$. With increasing d this state remains the lowest impurity state of the exciton if $d < 0.66$. However, the $M = 1$ state is unstable at $d > 0.28$, when its binding energy is less than that of the free exciton with zero momentum. At $d > 0.66$ the lowest level corresponds to $M = 0$. The binding energy of the $M = 0$ state does not depend on d. The interaction of the 2D magnetoexciton with any axially symmetric external field is absent for the $M = 0$ state in the lowest Landau level approximation. This is due to the fact that the electron- and hole-impurity interactions are canceled in the expansion (2): $V_{1m} = -V_{2m}$ [15], because the wave function of e and h are identical. The difference between the wave functions of the motion of electrons and holes perpendicular to a well, and the admixture of higher Landau levels will cause a weak interaction of the $M = 0$ 2D exciton with impurity [24].

The evolution of the lowest $S_e = 0$ and $S_e = 1$ impurity states of the 2e–h complex is shown in Fig. 2. The energy of the electron bound to the spatially separated positive impurity plus the energy of the free exciton with zero momentum is also shown. One

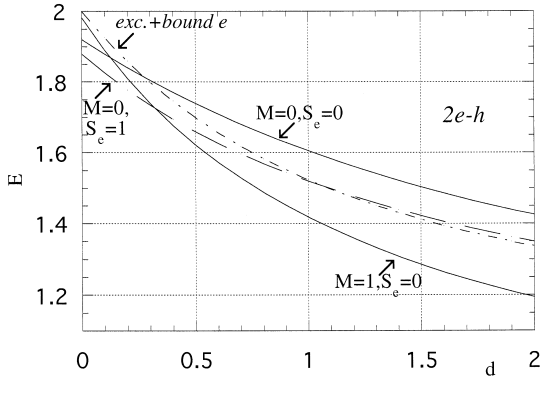

Fig. 2. The dependence of the binding energies of the lowest impurity states of the 2e–h complex on the impurity separation d. The energy of impurity bound electron + the energy of delocalized exciton with zero momentum is also shown. The binding energy and the impurity separation are expressed in units of E_0 and r_H, respectively.

can see that the $S_e = 0, M = 1$ state is the lowest state only at $d < 0.13$. At $d > 0.13$ the lowest state is $S_e = 0, M = 0$, and this state become stable and bound against separation of the e–h pair to infinity at $d > 0.28$. However, due to the decreasing behavior of binding energy with the further increase of d the system will be eventually evaporated at sufficiently large d.

The evolution of the lowest levels of the $S_h = 0$ and $S_h = 1$ impurity states of the biexciton is shown in Figs. 3 and 4. The energy of the exciton bound to the spatially separated positive impurity plus the energy of the free exciton with zero momentum is also shown. The only stable impurity bound states of the biexciton (with fixed values of S_e, S_h) at $d = 0$ are $(M = 2; S_e = 0; S_h = 0)$ and $(M = 3; S_e = 0; S_h = 1)$. However, these states become unbound at $d > 0.08$ and $d > 0.05$, respectively, as one can see from Figs. 3 and 4. The general feature of the impurity states of e–h complexes in such a system is that with the increase of d the states with smaller momentum become more favorable, contrary to impurity states in the spatially separated e–h system [15–17] and the spatially separated D^- centers [19–23]. Finally, the lowest level becomes the $M = 0$ state. The energy of this state depends very weakly on the impurity location in the lowest Landau level approximation. This is similar to the case of the exciton, considered above. The reason is that matrix elements which

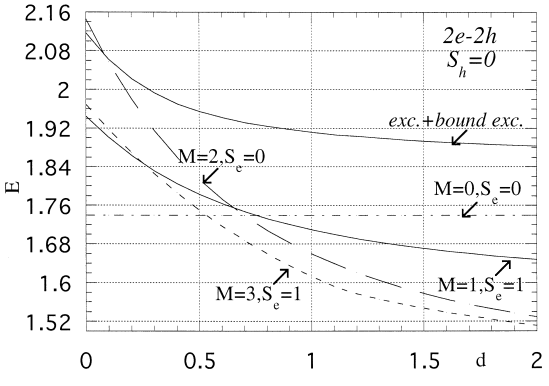

Fig. 3. The dependence of the binding energies of lowest levels for $S_h = 0$ impurity states of the biexciton on the impurity separation d. The energy of impurity bound exciton + the energy of delocalized exciton with zero momentum is also shown. The binding energy and the impurity separation are expressed in units of E_0 and r_H, respectively.

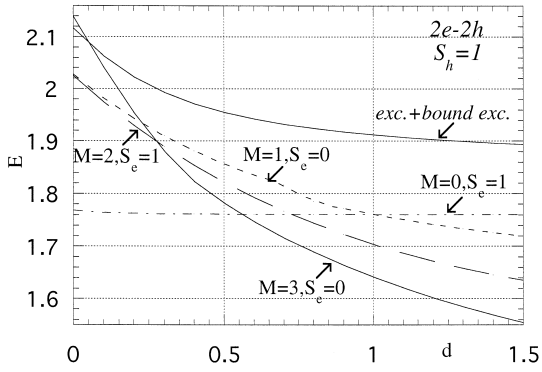

Fig. 4. The dependence of the binding energies of lowest levels for $S_h = 1$ impurity states of the biexciton on the impurity separation d. The energy of impurity bound exciton + the energy of delocalized exciton with zero momentum is also shown. The binding energy and the impurity separation are expressed in units of E_0 and r_H, respectively.

depend on an impurity location are extremely small [14] for the neutral complexes, and they do not change the value of an energy at $d = 0$ and at larger values of d. The physical origin of the lack of interaction with impurity is that in our consideration the electron and hole wave functions are identical. The $M = 0$ 2D e–h complex (with equal number of e and h) is almost a perfectly neutral object. Therefore the interaction with charged impurity is very weak. It is expected that the inclusion of quasi-2D effects and the admixture of higher Landau levels is of qualitative importance for $M = 0$ states of neutral e–h complexes.

We should note that the properties of a barrier impurity states of the 2D e–h system in a magnetic field with e and h moving in one plane (coplanar geometry) are completely different from those of the spatially separated e–h system (biplanar geometry) in a magnetic field [15–18]. The main reason is the absence of asymmetry between the e–h and e–e (h–h) interactions in the case of a coplanar geometry considered in the present paper. Such an asymmetry leads to strong angular correlations between particles of the same sign [20] and gives rise to ground state transitions with increasing total angular momentum value when the distance from the impurity is increased [15–18]. We did not find strong correlations in the present case of coplanar geometry. Moreover, with the increase of d the ground states with smaller

angular momentum become more favorable, in which strong angular correlations cannot occur. Another consequence of the symmetric case is the absence of impurity bound states of the neutral e–h complexes already at small d. Although for both geometries the magnetic induced binding of the 2e–h complexes is predicted, the structure of the ground state wave function is completely different in these cases, because of the strong angular correlations in the asymmetric case.

In conclusion, we have calculated the binding energies of the barrier impurity states of 2D e–h complexes in a strong magnetic field. It is shown that with the increase of the impurity separation from the well, the states with smaller angular momentum become more favorable, contrary to the impurity states in spatially separated 2D e–h systems [15–18] and off-well D^- centers [19–23]. This progression leads to the $M = 0$ lowest level. We have found that the exciton and the biexciton can be trapped by impurities located near the barrier edge. For the biexciton the only impurity bound states are ($M = 2; S_e = 0; S_h = 0$) and ($M = 3; S_e = 0; S_h = 1$). For the exciton, the lowest impurity bound level corresponds to $M = 1$. However, such states can be easily destroyed by the increasing value of the magnetic field – the magnetic evaporation should occur in such a system, similar to spatially separated D^- centers [19–23]. The increasing value of H first of all will course evaporation of impurity bound biexcitons by the process: impurity bound biexciton $\rightarrow$ impurity bound exciton + delocalized exciton with zero momentum. The further increase of H will course evaporation of impurity bound excitons. For barrier impurity states of the 2e–h complex the situation is completely different. The increasing value of H will give rise to a magnetic induced binding of the 2e–h complex by the impurities in the barrier. The energy of the separation of the e–h pair to infinity in the $M = 0$ state is quite big, for example, it is about $0.1E_0$, if $d/r_H = 1$. This energy is approximately 2 times more than the corresponding energy of the free trion [5]. The barrier impurity states of the trion can be responsible for the strong qualitative disagreement between experiment [12] and theory [7] which describes the evolution of the singlet state of the delocalized trion in a high magnetic field. At sufficiently large values of the H 2e–h complex will be eventually evaporated. Such transitions, like magnetic induced binding and unbinding of 2D e–h complexes can be observed in the optical spectra and by low-temperature magnetotransport measurements [23]. For a quantitative description of the experimental situation the mixing between the Landau levels, finite size of the well and the motion perpendicular to the quantum well are to be included in the present consideration. The corresponding calculations are in progress now.

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