Metastable bound states of the two-dimensional bimagnetoexcitons with triplet-triplet spin structures in the lowest landau levels approximation

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***Abstract*—The possible existence of the bound states of the interacting two-dimensional (2D) magnetoexcitons with in-plane opposite wave vectors, as well as with antiparallel electric dipole moments oriented perpendicularly to the corresponding wave vectors was investigated in the lowest Landau levels approximation. Two definite spin structures of the two electrons and of the two holes forming the molecule were taken into account. One of them is the singlet-singlet structure in which the spins of two electrons and the effective spins of two holes separately form singlet states. Another one is the triplet-triplet structure. The variational wave functions describing the relative motion of two magnetoexcitons in the frame of the molecule depend on the modulus k in the forms of the ring and of the bell in momentum representation. It was shown that in four spin-orbital variants the bound states of the 2D bimagnetoexciton in the lowest Landau levels approximation do not exist. Instead of them in the ring configuration and triplet-triplet spin structure a metastable bound state with an activation barrier comparable with the double ionization potential of the magnetoexciton was revealed. The role of the dipole-dipole interaction in the formation of the bound states is discussed.**

Keywords—semiconductors; exciton; interaction; magnetic field

I. Introduction

As was underlined in [1,2] there is a similarity and even an exact mapping in some aspects between the two-spin and two-charge two-dimensional (2D) systems in a strong perpendicular magnetic field. One can talk about the 2D conduction electrons and about the holes in the valence band in such semiconductor structures as the single and double quantum wells (QW_s), where the interband magnetoexcitons can be formed being revealed experimentally, for example, by their luminescence properties.

From another hand there are such systems as the two dimensional electron gas (2DEG) injected in the monolayer or in bilayer structure in the conditions of the integer or fractional quantum Hall effects (FQHEs), when the holes appear in the same conduction band and in the same lowest Landau Levels (LLLs) filled by the electrons. For example, the spin waves (SWs) appear in the condition of the integer quantum Hall effects (IQHEs), when the spin polarized electrons occupy the lowest Landau level (LLL), as well as the lowest Zeeman splitted level with the spin oriented up $(\uparrow)$ with filling factor $\upsilon = 1$ forming the ground state of the ferromagnetic type. The spin wave (SW) is formed when one electron form the ground state is excited in a upper Zeeman splitted state with a reversed spin orientation down $(\downarrow)$ and with the Zeeman excitation energy $g\mu_B B$, where $g > 0$ is the electron *g*-factor Lande, *B* is the magnetic field strength and μ_B is the Bohr magneton. The spin waves are named also spin-excitons [1].

The case of bilayer interband magnetoexcitons with electrons in conduction band of one layer and with the holes in the valence band of another layer, in the empty LLLs was studied by Olivares-Robles and Ulloa [2]. The interlayer magnetoexcitons are characterized by the static constant dipole moments $\vec{p}_\perp$, oriented perpendicularly to the layers along the z axis and proportional to the distance δ between the layers: $\vec{p}_\perp = \vec{z}e\delta$. The interaction between such two dipoles separated by a radius vector $\vec{R}$ oriented in-plane and much greater than δ is repulsive, what favours to their BEC. Side by side with the perpendicular dipole moments the in-plane moving magnetoexcitons have also and the in-plane dipole moments. As was mentioned in [1], an important property of the 2D SWs and magnetoexcitons is the dynamical strong coupling induced by the Lorentz force, between the center-of-mass motion and the relative internal electron-hole (e-h) motion. As the result of this influence the radius vector $\vec{d}$ between the gyration points of the electron and hole Landau quantization orbits, can appear in the Landau gauge description. It gives rise to the in-plane dynamical electric dipole moment $\vec{p}_{\parallel}$. Its values is proportional to the center-of-mass wave vector k and is oriented perpendicularly to both vectors $\vec{k}$ and $\vec{z}$ as follows

$$\vec{p}_{\parallel}=e\vec{d},\ \vec{d}=\left[\vec{z}\times\vec{k}\right]l_0^2,\ d=kl_0^2,\ \vec{p}=\vec{p}_{\perp}+\vec{p}_{\parallel}. \quad (1)$$

Here l_0 is the magnetic length and $\vec{p}$ is the total electric dipole moment. The in-plane dipole moment exists only in the case when the center-of-mass magnetic momentum $\hbar\vec{k}$ is different from zero. The coplanar and bilayer magnetoexcitons have different dipole moments. There is only the dynamical in-plane component $\vec{p}_{\parallel}$ in the first case and two components $\vec{p}_{\perp}$ and $\vec{p}_{\parallel}$ in the second one.

The investigations of the interaction energy between two spin waves (SWs) (or magnetoexcitons) were effectuated in [1] in the case of the spin polarized 2DEG injected in the monolayer structure occupying the LLL with the filling factor $\upsilon=1$ and with the ferromagnetic type ground state. In difference from the case discussed in our paper as well as in [2], where two magnetoexciton do exist in the empty LLLs, the case of the filled by electrons LLL must be calculated in more sophisticated description. Such calculations were a problem of the theoretical physics. It was solved by Haldane [3], who introduced the spherical geometry instead of the planar one, with discrete orbital quantum number l instead of the continuous wave vector $\vec{k}$. On the sphere with the radius R and with the surface area $4\pi R^2$ N electrons with the density n_e are placed. The density n_e corresponds to the partially filled LLLs: $n_e=\upsilon/(2\pi l_0^2)$.

In the center of the sphere a Dirac magnetic monopole is introduced. The magnetic field perpendicular to the surface of the sphere has the strength B such as the magnetic flux through the sphere surface would be in the case of $\upsilon=1$ equal to N flux quanta $\phi_0=2\pi\hbar c/e$.

The single-particle states in this geometry are the eigenstates of the angular momentum l and form the $(2l+1)$ fold angular momentum shells. The values $l/R=k_l$ plays the role of the wave vector. When the curvature of the sphere decreases the discrete values of k_l quickly converge to the continuous values. In [1] the numerical diagonalization was used to calculate in Haldane geometry the interaction between two spin waves or excitons. It was shown that because of the complicated statistics of the composite particles their interaction is completely different from the dipole-dipole interaction predicted in the model of independent bosonic waves. It was understand that the spin waves moving in-plane in the same direction attract one another, which leads to their dynamical binding. Two spin waves moving in opposite directions undergo the repulsion. Olivares-Robles and Ulloa [2] considered a more simple case of two magnetoexcitons in the empty LLLs but with spatially separated electrons and holes confined in different layer with distance δ between them. As was mentioned above in this case the perpendicular components $\vec{p}_{\perp,1},\vec{p}_{\perp,2}$ of the resultant electric dipoles do exist, which leads to the preponderant repulsion between the two-layer magnetoexcitons. But even in these conditions it was shown that the total interaction between excitons will be more repulsive for the antiparallel in-plane wave vectors $\vec{k}_1$ and $\vec{k}_2$ $\left(\vec{k}_1=-\vec{k}_2\right)$ and it will be less repulsive in the case $\vec{k}_1=\vec{k}_2$, in a full accordance with [1].

II. The Hamiltonian of the Electron-Hole System and the Wave Functions of the Bimagnetoexcitons in the LLL_S Approximation

In [4,5] the spinless 2D electrons and holes were considered paying the main attention to the Landau quantization of their orbital motion on the surface of the layer subjected to the action of the external perpendicular magnetic field. In the Landau gauge the charged particles have a free motion in one in-plane direction described by the plane waves with one-dimensional wave numbers p and q and undergo the quantized oscillations around the gyration points in another in-plane direction perpendicular to the previous one.

The quantum numbers of the Landau quantized levels for electrons and holes are n_e and n_h correspondingly. In our case they were choosen as the lowest levels $n_e=n_h=0$. The excited Landau levels ELL_S were neglected and this approach is named as the LLL_S approximation. The spin of the electrons and the effective spin of the holes were taken into account by introducing a supplementary label $\sigma=\pm 1/2$. The creation and annihilation operators of the 2D electrons and holes are denoted as $a^+_{p,\sigma},a_{p,\sigma}$ and $b^+_{q,\sigma},b_{q,\sigma}$, correspondingly. In these denotations the Hamiltonian of the Coulomb interaction in the system of the electrons and holes lying on the LLL_S, following [5,6], looks as

$$H^{LLL}_{Coul}=H^{LLL}_{e-e}+H^{LLL}_{h-h}+H^{LLL}_{e-h}, \quad (2)$$

$$H^{LLL}_{e-e}=\frac{1}{2}\sum_{\vec{Q}}\sum_{p,q}\sum_{\sigma_1,\sigma_2}W(\vec{Q})e^{-iQ_xQ_yl_0^2}e^{iQ_y(p-q)l_0^2}a^+_{p,\sigma_1}a^+_{q,\sigma_2}a_{q+Q_x,\sigma_2}a_{p-Q_x,\sigma_1},$$

$$H^{LLL}_{h-h}=\frac{1}{2}\sum_{\vec{Q}}\sum_{p,q}\sum_{\sigma_1,\sigma_2}W(\vec{Q})e^{iQ_xQ_yl_0^2}e^{-iQ_y(p-q)l_0^2}b^+_{p,\sigma_1}b^+_{q,\sigma_2}b_{q+Q_x,\sigma_2}b_{p-Q_x,\sigma_1},$$

$$H^{LLL}_{e-h}=-\sum_{\vec{Q}}\sum_{p,q}\sum_{\sigma_1,\sigma_2}W(\vec{Q})e^{iQ_y(p+q)l_0^2}a^+_{p,\sigma_1}b^+_{q,\sigma_2}b_{q+Q_x,\sigma_2}a_{p-Q_x,\sigma_1}.$$

The interaction coefficients depend only on the difference ($p-q$) in the case of the electron-electron and of the hole-hole terms, and on the sum ($p+q$) in the case of the electron-hole term. The magnetoexciton creation operator introduced in [5,6] with the spin labels looks as $\hat{\psi}^{+}_{ex}(\vec{k},\Sigma_e,\Sigma_h)=\frac{1}{\sqrt{N}}\sum_t e^{ik_y t l_0^2} a^{+}_{t+\frac{k_x}{2},\Sigma_e} b^{+}_{-t+\frac{k_x}{2},\Sigma_h}$; $N=\frac{S}{2\pi l_0^2}$. (3)

Here $\vec{k}(k_x,k_y)$ is the vector of the center of mass in-plane motion, t is the unidimensional vector of the relative $e-h$ motion. The function of the relative motion $e^{ik_y t l_0^2}$ in the momentum representation leads to the $\delta(y-k_y l_0^2)$ function of the relative motion in the real space representation. l_0 is the magnetic length, B is the magnetic field strength and S is the layer surface area.

Now the wave functions of the bound, molecule-type states with resultant wave vector $\vec{k}=0$, formed by two 2D magnetoexcitons with wave vectors $\vec{k}$ and $-\vec{k}$ and with different spin structures will be introduced. The spins of two electrons and the effective spins of two holes forming the bound states were combined separately in the symmetric or in the antisymmetric forms $(\uparrow\downarrow+\eta\downarrow\uparrow)$ with the same parameter $\eta=\pm1$ for electrons and holes. Two types of wave functions one with singlet electron and with singlet hole structures and another one with triplet electron and triplet hole structures were constructed. The variational wave functions of the relative motion $\varphi_n(k)$ of two magnetoexcitons in the frame of the bound states were introduced. The wave functions of the bimagnetoexciton bound states in these conditions have the forms

$$\left|\psi_{bimex}(0,\eta,\varphi_n)\right\rangle=\frac{1}{2N^{3/2}}\sum_{\Sigma_e,\Sigma_h}(\eta)^{\Sigma_e+\Sigma_h+1}\sum_{\vec{k}}\varphi_n(\vec{k})\sum_{s,t}e^{ik_y(t-s)l_0^2}\cdot$$

$$\cdot\, a^{+}_{t+\frac{k_x}{2},\Sigma_e} a^{+}_{s-\frac{k_x}{2},-\Sigma_e} b^{+}_{-s-\frac{k_x}{2},-\Sigma_h} b^{+}_{-t+\frac{k_x}{2},\Sigma_h}\left|0\right\rangle. \quad (4)$$

The normalization conditions of these wave functions are

$$\left\langle\phi_{bimex}(0,\eta,\varphi_n)\middle|\phi_{bimex}(0,\eta,\varphi_n)\right\rangle=2(1-\eta L_n(\alpha)), \quad (5)$$

$$L_n(\alpha)=\int_0^\infty xdx\int_0^\infty ydy\varphi_n^*(x)\varphi_n(y)J_0(xy),$$

where $J_0(xy)$ is the Bessel function of the zeroth order. The average values of the Coulomb interaction Hamiltonian (2) calculated with the wave functions (4) equals to

$$E_{bimex}(0,\eta,\varphi_n)=\frac{\left\langle\phi_{bimex}(0,\eta,\varphi_n)\middle|H^{LLL}_{Coul}\middle|\phi_{bimex}(0,\eta,\varphi_n)\right\rangle}{\left\langle\phi_{bimex}(0,\eta,\varphi_n)\middle|\phi_{bimex}(0,\eta,\varphi_n)\right\rangle}. \quad (6)$$

III. The Obtained Results and the Electron Structure of the Bound States

The 2D magnetoexcitons with $\vec{k}\neq0$ look as the electric dipoles with the in-plane arms having the length $d=kl_0^2$, where l_0 is the magnetic length. The arms are oriented perpendicularly to the direction of the wave vectors $\vec{k}$. The molecule and its bound states can be formed by two magnetoexcitons with antiparallel wave vectors $\vec{k}$ and $-\vec{k}$. They have the structure of two antiparallel dipoles bound together. The possibility of their orientation as a whole in any direction of the layer plane with equal probability was supposed. Such possibility is achieved introducing the variational wave function of the relative motion of two magnetoexcitons in the frame of the bound state $\varphi_n(\vec{k})$, which depends on the modulus k.

The numerical calculations made in the case of the function $\varphi_2(\vec{k})=(8\alpha^3)^{1/2}(kl_0)^2 e^{-\alpha(kl_0)^2}$ permitted to obtain the full energies of the bound states in dependences on the

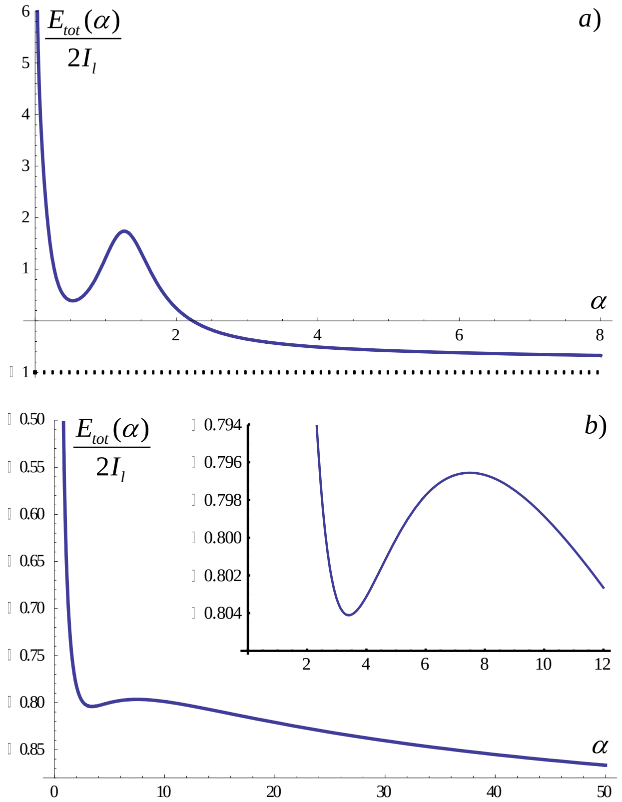

Fig. 1. The total energies of two bound 2D magnetoexcitons with wave vectors $\vec{k}$ and $-\vec{k}$, with different spin structures $\eta=\pm1$ and with the variational wave function $\varphi_2(k)$, in dependence on the parameter α. a) the case $\eta=1$, b) the case $\eta=-1$. The total energies are related to the value $2I_l$, where I_l is the ionization potential of a free magnetoexciton with wave vector $\vec{k}=0$.

parameter α of the variational wave function in two cases with $\eta=\pm1$, corresponding to two electron and hole spin structures. In both spin configurations the full energies of the bound states are greater than the value $-2I_l$ in all range of the values α.

All these states are unstable as regards the dissociation in the form of two free magnetoexcitons with $\vec{k} = 0$.

In spite of it, a deep metastable bound state with the activation barrier comparable with two magnetoexciton ionization potentials $2I_l$ in the case $\eta = 1$ and $\alpha = 0.5$, as well as a shallow state in the case $\eta = -1$ and $\alpha = 3.4$ were revealed. All these details are reflected in the Fig. 1.

To better understand the obtained results it is necessary to remember the important results concerning the dipole-dipole interactions published in [1,2]. Wójs, Gładysiewicz, Wodziński, and Quinn [1] arrived to the conclusion that two spin waves (magnetoexcitons) moving in-plane in the same direction with parallel dipole moments attract each other, what leads to their dynamical binding. Two spin waves (magnetoexcitons) moving in opposite directions with antiparallel dipole moments undergo repulsion. To similar conclusions arrived also Olivares-Robles and Ulloa [2] considering the two-layer 2D magnetoexcitons with spatially separated electrons and holes in two layers of the double quantum well. In this case there are static inter-layer dipole moment perpendicularly oriented to the layers with the repulsion between them, as well as dynamical in-plane dipole moments due to the motion of the two-layer magnetoexcitons. But even in these conditions the total interaction between excitons became more repulsive in the case of their antiparallel in-plane motion and less repulsive in the case of their parallel motion. These trends can be demonstrated with the formula of the dipole-dipole interaction

$$V(\vec{R}) = \frac{e^2}{\varepsilon}\left[\frac{\vec{d}_1 \cdot \vec{d}_2}{R^3} - \frac{(\vec{d}_1 \cdot \vec{R})(\vec{d}_2 \cdot \vec{R})}{R^5}\right];\; R >> d_i,\; i = 1, 2, \quad (7)$$
$$\vec{d}_i = \left[\vec{z} \times \vec{k}_i\right] l_0^2,$$

where ε is the dielectric constant and $\vec{R}$ is the distance between the electric dipoles $e\vec{d}_i$.

In the case of equal and parallel $(\uparrow\uparrow)$ or antiparallel $(\uparrow\downarrow)$ dipoles the expression (7) takes the form

$$V_{\substack{(\uparrow\uparrow)\\(\uparrow\downarrow)}}(R) = \pm\frac{e^2 d^2}{\varepsilon R^3}\left(1 - 3\cos^2\varphi\right) \approx \mp\frac{e^2 d^2}{2\varepsilon R^3};\; \overline{\cos^2\varphi} = \frac{1}{2}. \quad (8)$$

Here φ is the angle between two in-plane vectors $\vec{R}$ and $\vec{d}$. This rough estimation shows that two parallel in-plane dipole moments attract each other, whereas two antiparallel dipoles do repeal in concordance with [1,2]. Let us apply this formula in the case of variational wave functions $\varphi_2(k)$. The average distance $\langle R\rangle$ between the magnetoexcitons can be estimated as $2\sqrt{\alpha} l_0$, whereas the average values of $\langle k\rangle$ and $\langle d\rangle$ can be written as $1/(\sqrt{\alpha} l_0)$ and $l_0/\sqrt{\alpha}$ correspondingly. The condition $R >> d$ can be satisfied only in the case $2\alpha >> 1$.

The interaction between two magnetoexcitons reflected in the Fig. 1 can be described by the formula (8) in the region $\alpha >> 1/2$, where the repulsion of two in-plane, antiparallel dipoles prevents the formation of the stable bound state of the 2D magnetoexciton.

Side by side with the results demonstrated in the Fig. 1, the similar calculations were effectuated with the variational wave function $\varphi_0(x) = (4\alpha)^{1/2} e^{-\alpha x^2}$. In this case the stable and metastable bound states at any values of α were not obtained.

IV. Conclusions

The magnetoexcitons with wave vectors $\vec{k} \neq 0$ acquire the electric dipole moments and their interaction is different from zero. Their Bose-Einstein condensation (BEC) with considerable values of wave vectors $kl_0 \sim 3-4$ was studied in [6]. In these conditions the existence of the metastable dielectric liquid phase was revealed. This result suggests the possibility to find out another metastable collective states including the case of the bimagnetoexcitons. In our model two 2D magnetoexcitons with opposite in-plane wave vectors are forming a bound state of molecule type with resultant wave vector equal to zero. In spite of the absence of the stable bound states however the metastable bound state with considerable activation energy was revealed. The wave function describing the bound molecule-type states were constructed as the products of the wave functions of two magnetoexcitons with opposite oriented wave vectors multiplied by the variational wave function describing the relative motion of two magnetoexcitons inside the molecule. In our calculations the variational wave functions $\varphi_n(k)$ were chosen in the forms $(kl_0)^n \exp(-\alpha(kl_0)^2)$, with $n = 0, 2$. The Coulomb interaction energy was averaged using the constructed wave functions and was compared with the energy of two free 2D magnetoexcitons with wave vectors $\vec{k} = 0$ [7].

Taking into account that the magnetoexcitons forming the bound state have equal but opposite oriented wave vectors and antiparallel dipole moments, they do repeal each other. The stable bound state cannot be formed, what is demonstrated in the Fig. 1. The metastable bound state revealed at the parameter $\eta = 1$ and $\alpha = 0,5$ cannot be described by the dipole-dipole interaction and is due to more short-range magnetoexciton-magnetoexciton interactions. In the case of the variational wave function $\varphi_0(x)$ the both stable and metastable bound states do not exist.

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