

THE RASHBA SPIN-ORBIT COUPLING AND THE EXCHANGE ELECTRON-HOLE INTERACTION OF TWO-DIMENSIONAL MAGNETOEXCITONS

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(Received 24 December 2010)

Abstract

The Rashba spin-orbit coupling (RSOC) in the case of two-dimensional (2D) electrons and holes in a strong perpendicular magnetic field is studied. The spinor-type wave functions are characterized by different numbers of Landau levels in different spin projections. For electrons, they differ by 1 as was established earlier by Rashba [1], whereas for holes they differ by 3. Two lowest electron states and four lowest hole states of Landau quantization give rise to eight 2D magnetoexciton states. The exchange electron-hole interaction in the frame of these states is investigated.

1. Introduction

Since the mid-1980s, there has been an extensive interest in the effects of an applied electric field normal to the layers on the optical properties of semiconductor quantum wells (QWs) and superlattices (SLs) [2]. The electric field strength perpendicular to the layer surface gives rise to Rashba spin-orbit coupling (RSOC). The spin-orbit effects are discussed in a special monograph [3] and papers [2, 4-9]. In [10-12] the energy spectrum of 2D magnetoexcitons were studied supposing that the spin polarizations of electrons and holes take place and the spin-orbit coupling was neglected. In reality, as was shown in [13], the RSOC leads to breaking of the pure spin polarizations and the new spinor-type states are characterized by different numbers of Landau levels for different spin projections. These numbers for electrons differ by 1, whereas for holes differ by 3. Spin polarized states under the influence of the RSOC are transformed into mixed spinor components. The two lowest electron states and four lowest hole states were used to construct eight lowest 2D magnetoexciton states [13]. The direct Coulomb electron-hole interaction gives rise to the binding energies and ionization potentials of the magnetoexciton states. They were calculated in [10-12]. Below we will use these results to determine the exchange electron-hole interaction.

2. Exchange electron-hole interaction

The electron-hole Coulomb interaction is calculated below taking into account the influence of the RSOC in the frame of conduction and valence bands. The corresponding Bloch wave functions including their periodic parts are

$$\begin{aligned}
 |\Psi_c(R_1, p; x, y)\rangle &= \frac{e^{ipx}}{\sqrt{L_x}} U_{c,s,p}(\vec{r}) \begin{vmatrix} a_0 \varphi_{c,0}(y, p) \\ b_1 \varphi_{c,1}(y, p) \end{vmatrix}; \\
 |\Psi_c(R_2, p; x, y)\rangle &= \frac{e^{ipx}}{\sqrt{L_x}} U_{c,s,p}(\vec{r}) \begin{vmatrix} 0 \\ \varphi_{c,0}(y, p) \end{vmatrix}; \\
 |\Psi_v(R_1, q; x, y)\rangle &= \frac{e^{iqx}}{\sqrt{L_x}} \frac{1}{\sqrt{2}} (U_{v,P,X,q}(\vec{r}) - iU_{v,P,Y,q}(\vec{r})) \begin{vmatrix} c_3 \varphi_{v,3}(y, q) \\ d_0 \varphi_{v,0}(y, q) \end{vmatrix}; \\
 |\Psi_v(R_2, q; x, y)\rangle &= \frac{e^{iqx}}{\sqrt{L_x}} \frac{1}{\sqrt{2}} (U_{v,P,X,q}(\vec{r}) + iU_{v,P,Y,q}(\vec{r})) \begin{vmatrix} \varphi_{v,0}(y, q) \\ 0 \end{vmatrix}; \\
 |\Psi_v(R_3, q; x, y)\rangle &= \frac{e^{iqx}}{\sqrt{L_x}} \frac{1}{\sqrt{2}} (U_{v,P,X,q}(\vec{r}) - iU_{v,P,Y,q}(\vec{r})) \begin{vmatrix} c_4 \varphi_{v,4}(y, q) \\ d_1 \varphi_{v,1}(y, q) \end{vmatrix}; \\
 |\Psi_v(R_4, q; x, y)\rangle &= \frac{e^{iqx}}{\sqrt{L_x}} \frac{1}{\sqrt{2}} (U_{v,P,X,q}(\vec{r}) + iU_{v,P,Y,q}(\vec{r})) \begin{vmatrix} \varphi_{v,1}(y, q) \\ 0 \end{vmatrix}.
 \end{aligned} \tag{1}$$

The orthogonality each other of the conduction and valence electron Bloch wave functions is attained due to their orthogonal periodic parts, whereas the orthogonality of the wave functions belonging to the same bands and having the same periodic parts is reached due to different numbers of the Landau quantization wave functions $\varphi_{c,n}(y, p)$ and $\varphi_{v,m}(y, p)$. The conduction and valence electrons have the same electric charge — $|e|$ and their dimensionless variables have the same structure $\frac{y}{l} - pl$ and $\frac{y}{l} - ql$. The last variable looks as $\frac{y}{l} + ql$ in the case of the hole wave function $\varphi_{h,n}(y, q)$ due to the positive value of the hole charge $|e|$.

We will consider eight combinations of the electron-hole pairs taking into account two spin-splitted electron Landau levels $|e, R_1\rangle$ and $|e, R_2\rangle$ and four spin-splitted hole Landau levels $|h, R_j\rangle$ with $j = 1, 2, 3, 4$. These combinations will be denoted by

$$f_s = (e, R_i; h, R_j); s = 1, \dots, 8; i = 1, 2; j = 1, 2, 3, 4. \tag{2}$$

The wave functions of eight magnetoexciton states with electron states R_1 and R_2 and with four hole states R_1, R_2, R_3 , and R_4 can be expressed through the corresponding creation and annihilation operators. For example, in the compositions f_s represented by formulas (2), we have

$$\Psi_{ex}(\vec{k}, f_s) = \frac{1}{\sqrt{N}} \sum_t e^{-ik_y t l^2} a_{R_i, \frac{k_x}{2} + t}^\dagger b_{R_j, \frac{k_x}{2} - t}^\dagger; s = 1, 2, \dots, 8; i = 1, 2; j = 1, 2, 3, 4. \tag{3}$$

Side by side with the direct Coulomb interaction, it is necessary to study the exchange Coulomb e-h interaction. In the case of Wannier-Mott excitons in the absence of external magnetic field and RSOC, it gives rise to the singlet-triplet splitting of the exciton levels. It is due to the contact or short-range part of the exchange e-h interaction and is revealed very well experimentally in the case of ortho- and para-excitons in Cu_2O crystal. The long-range part of this interaction determines the longitudinal-transverse splitting of the three-fold degenerated dipole-active exciton levels in cubic crystals as well as the polariton gap [14]. These questions

were not studied at all in the case of 2D magnetoexcitons and more so in the presence of the RSOC. They will be discussed below. The exchange e-h interaction has its origin in the exchange Coulomb interaction between the conduction electron and valence electron. At first we will consider the conduction electron in the state R_1 and the valence electron in the state R_1 in the frame of Landau quantization and RSOC.

The corresponding Hamiltonian is

$$H_{exch}^{c-v} = \sum_{p,q,s} F_{c-v}(c, R_1, p; v, R_1, q; v, R_1, p-s; c, R_1, q+s) a_{c,R_1,p}^\dagger a_{v,R_1,q}^\dagger a_{c,R_1,q+s} a_{v,R_1,p-s}, \quad (4)$$

where

$$\begin{aligned} & F_{c-v}(c, R_1, p; v, R_1, q; v, R_1, p-s; c, R_1, q+s) \\ &= \int d\bar{1} \int d\bar{2} \langle c, R_1, p, (\bar{1}) | \langle v, R_1, q, (\bar{2}) | V(\bar{1}-\bar{2}) | v, R_1, p-s, (\bar{1}) \rangle | c, R_1, q+s, (\bar{2}) \rangle \\ &= \int d\bar{1} \int d\bar{2} \frac{e^{is(x_2-x_1)}}{L_x^2} W(\bar{1}; c, p; v, p-s) \\ &\times \left[a_0^* c_3 \varphi_{c,0}^*(y_1, p) \varphi_{v,3}(y_1, p-s) + b_1^* d_0 \varphi_{c,1}^*(y_1, p) \varphi_{v,0}(y_1, p-s) \right] V(\bar{1}-\bar{2}) \\ &\times W^*(\bar{2}; c, q+s; v, q) \left[c_3^* a_0 \varphi_{v,3}^*(y_2, q) \varphi_{c,0}(y_2, q+s) + d_0^* b_1 \varphi_{v,0}^*(y_2, q) \varphi_{c,1}(y_2, q+s) \right] \end{aligned} \quad (5)$$

and

$$\begin{aligned} b_1 &= \frac{-i\alpha\sqrt{2}a_0}{\frac{1}{2} + \sqrt{\frac{1}{4} + 2\alpha^2}}; |a_0|^2 + |b_1|^2 = 1; \\ c_3 &= \frac{-i\beta 4\sqrt{3}d_0}{\frac{3}{2} + \sqrt{\frac{9}{4} + 48\beta^2}}; |d_0|^2 + |c_3|^2 = 1. \end{aligned} \quad (6)$$

with electron and hole SOC parameters $\alpha = \frac{\alpha_e E_z}{\hbar\omega_{ce}}$, $\beta = \frac{\beta_h E_z}{\hbar\omega_{ch}}$ correspondingly.

Here the exchange charge density of electron was introduced.

$$W(\vec{r}; c, p; v, p-s) = U_{c,S,p}^*(\vec{r}) \frac{1}{\sqrt{2}} \left(U_{v,P,X,p-s}(\vec{r}) - i U_{v,P,Y,p-s}(\vec{r}) \right). \quad (7)$$

It depends on the product of two periodic parts of the Bloch functions of electron in conduction and valence bands. We have introduced the variables $\vec{\rho}_1$ and $\vec{\rho}_2$, changing inside the lattice cell with the volume $v_0 = a_l^3$, where a_l is the lattice period, as well as two continuous variables $\vec{R}_1$ and $\vec{R}_2 = \vec{R}_1 + \vec{R}$ enumerating the lattice nodes. Four integrations are effectuated separately, two on the volume v_0 of the lattice cell and two integrations on $\vec{R}_1$ and $\vec{R}$ on the surface of the 2D layer. In difference on the case of the direct Coulomb interaction, the integration on the lattice cell volume v_0 of the exchange charge densities without participation of the functions describing the Coulomb interaction vanish due to the orthogonality of the periodic parts of the Bloch functions belonging to different bands

$$\frac{1}{v_0} \int d\vec{\rho}_1 W(\vec{\rho}_1; c, p; v, p-s) = 0; \quad \frac{1}{v_0} \int d\vec{\rho}_2 W^*(\vec{\rho}_2; c, q+s; v, q) = 0. \quad (8)$$

It means that, in the frame of the exchange Coulomb interaction, two electrons do not behave as point charges, but rather as two inter-band dipoles situated on different nodes ($R \neq 0$) of the lattice. To demonstrate this picture, the Coulomb interaction potential will be represented in the form

$$\frac{1}{|\vec{r}_2 - \vec{r}_1|} = \frac{1}{|\vec{R} + \vec{\rho}_2 - \vec{\rho}_1|} = \begin{cases} \frac{1}{|\vec{\rho}_2 - \vec{\rho}_1|}, & R = 0 \\ \frac{1}{R} + \frac{(\vec{\rho}_1 \cdot \vec{\rho}_2)}{R^3} - \frac{3(\vec{\rho}_1 \cdot \vec{R})(\vec{\rho}_2 \cdot \vec{R})}{R^5}, & R \neq 0. \end{cases} \quad (9)$$

This representation permits separating the contact or short-range interaction, when both electrons are in the same unit lattice cell ($R = 0$), and the long-range part, where $\vec{R}$ differs from zero ($\vec{R} \neq 0$).

The inter-band dipole moments appear as follows

$$\begin{aligned} \vec{d}_{cv}(p, p-s) &= \frac{e}{v_0} \int d\vec{\rho}_1 W(\vec{\rho}_1; c, p; v, p-s) \vec{\rho}_1 e^{-is\rho_{1x}}, \\ \vec{d}_{cv}^*(q+s, q) &= \frac{e}{v_0} \int d\vec{\rho}_2 W^*(\vec{\rho}_2; c, q+s; v, q) \vec{\rho}_2 e^{-is\rho_{2x}}. \end{aligned} \quad (10)$$

The integrations on the large-scale variable $\vec{R}_1$ involve different combinations of the Landau quantization functions $\varphi_n(R_{1y}, p)$ and $\varphi_n(R_{1y} + R_y, p)$ in the following combinations

$$\begin{aligned} G_{0,0;3,3}(R_y) &= G(0, p; 0, q+s; 3, p-s; 3, q | R_y) \\ &= \int dR_{1y} \varphi_{c,0}^*(R_{1y}, p) \varphi_{c,0}(R_{1y} + R_y, q+s) \varphi_{v,3}(R_{1y}, p-s) \varphi_{v,3}^*(R_{1y} + R_y, q); \\ G_{1,1;0,0}(R_y) &= G(1, p; 1, q+s; 0, p-s; 0, q | R_y) \\ &= \int dR_{1y} \varphi_{c,1}^*(R_{1y}, p) \varphi_{c,1}(R_{1y} + R_y, q+s) \varphi_{v,0}(R_{1y}, p-s) \varphi_{v,0}^*(R_{1y} + R_y, q); \\ G_{0,1;3,0}(R_y) &= G(0, p; 1, q+s; 3, p-s; 0, q | R_y) \\ &= \int dR_{1y} \varphi_{c,0}^*(R_{1y}, p) \varphi_{c,1}(R_{1y} + R_y, q+s) \varphi_{v,3}(R_{1y}, p-s) \varphi_{v,0}^*(R_{1y} + R_y, q); \\ G_{1,0;0,3}(R_y) &= G(1, p; 0, q+s; 0, p-s; 3, q | R_y) \\ &= \int dR_{1y} \varphi_{c,1}^*(R_{1y}, p) \varphi_{c,0}(R_{1y} + R_y, q+s) \varphi_{v,0}(R_{1y}, p-s) \varphi_{v,3}^*(R_{1y} + R_y, q). \end{aligned} \quad (11)$$

The exchange e-h interaction is represented below as a sum of contact and long-range parts

$$F_{c-v}(c, R_1, p; v, R_1, q; v, R_1, p-s; c, R_1, q+s) = A_{cont}(R_1, R_1; p, q, s) + V_{l-r}(R_1, R_1; p, q, s). \quad (12)$$

The contact part equals to

$$\begin{aligned}
 & A_{\text{cont}}(R_1, R_1; p, q, s) \\
 &= \frac{a_l^2}{L_x} \frac{1}{v_0} \int_{v_0} d\vec{\rho}_1 \frac{1}{v_0} \int_{v_0} d\vec{\rho}_1 W(\vec{\rho}_1; c, p; v, p-s) W^*(\vec{\rho}_2; c, q+s; v, q) \frac{e^2}{\varepsilon_0 |\vec{\rho}_2 - \vec{\rho}_1|} e^{-s(\rho_{2x} - \rho_{1x})} \\
 & \times \left[|a_0|^2 |c_3|^2 G_{0,0;3,3}(0) + |d_0|^2 |b_1|^2 G_{1,1;0,0}(0) + a_0^* d_0^* c_3 b_1 G_{0,1;3,0}(0) + b_1^* c_3^* d_0 a_0 G_{1,0;0,3}(0) \right],
 \end{aligned} \tag{13}$$

whereas the long-range part contains a supplementary summation on the large scale variable $\vec{R}$

$$\begin{aligned}
 & V_{l-r}(R_1, R_1; p, q, s) = \frac{a_l^2}{L_x} \sum_{\vec{R} \neq 0} e^{isR_x} \\
 & \times \left[\frac{(\vec{d}_{cv}(p, p-s) \cdot \vec{d}_{cv}^*(q+s, q))}{R^3} - \frac{3(\vec{d}_{cv}(p, p-s) \cdot \vec{R})(\vec{d}_{cv}^*(q+s, q) \cdot \vec{R})}{R^5} \right] \\
 & \times \left[|a_0|^2 |c_3|^2 G_{0,0;3,3}(R_y) + |d_0|^2 |b_1|^2 G_{1,1;0,0}(R_y) + a_0^* d_0^* c_3 b_1 G_{0,1;3,0}(R_y) + b_1^* c_3^* d_0 a_0 G_{1,0;0,3}(R_y) \right].
 \end{aligned} \tag{14}$$

Here the summation on the variable $\vec{R}$ can be substituted by integration as follows $a_l^2 \sum_{\vec{R} \neq 0} = \int dR_x \int dR_y$.

The Hamiltonian (4) with the operators

$$\begin{aligned}
 & b_{R_j, q}^\dagger = a_{v, R_j, -q}; \quad b_{R_j, q} = a_{v, R_j, -q}^\dagger; \quad a_{c, R_i, p} = a_{R_i, p}; \\
 & a_{v, R_j, q}^\dagger a_{v, R_j, q+s} = b_{R_j, -q}^\dagger b_{R_j, -q-s}^\dagger = -b_{R_j, -q-s}^\dagger b_{R_j, -q}^\dagger + \delta_{kr}(s, 0).
 \end{aligned} \tag{15}$$

after the normal ordering of the hole operators will give rise to the Hamiltonian of the exchange e-h interaction concerning the states c, R_1 and v, R_1 . It is

$$H_{\text{exch}}^{e-h} = \sum_{p, q, s} [A_{\text{cont}}(R_1, R_1; p, q, s) + V_{l-r}(R_1, R_1; p, q, s)] a_{R_1, p}^\dagger b_{R_1, -p+s}^\dagger b_{R_1, -q} a_{R_1, q+s}. \tag{16}$$

On the ways from the initial expression (4) to the final form (16) correspondingly we have separated the quadratic free electron Hamiltonian

$$\begin{aligned}
 & \sum_p [F_{c-v}(c, R_1, p; v, R_1, q; c, R_1, p-s; v, R_1, q+s) \\
 & - F_{c-v}(c, R_1, p; v, R_1, q; v, R_1, p-s; c, R_1, q+s)] a_{R_1, p}^\dagger a_{R_1, p}.
 \end{aligned} \tag{17}$$

It describes the influence on the conduction electron of the valence electrons, which together with the electrons of the inner atomic shells create the effective periodic potential of the lattice. Terms (17) compensate the difference between the periodic potential created by the inner atomic shells and the real effective periodic potential created by all electrons including the valence electrons [14]. The effective periodic potential determines the electron wave functions (1) used in our calculations and, at the same time, depends in a self-conjugated way on their forms, i.e., on the presence of a strong perpendicular magnetic field as well as on the RSOC. Above we have calculated the exchange interaction matrix element for the first combination f_1 of the electron wave functions $|c, R_i, p\rangle$ and $|v, R_j, q\rangle$ with $i=1, 2$ and $j=1, 2$. For other three combinations, we have obtained the formulas similar to expressions (13) and (14). The only differences concern the square brackets, where must be written, respectively:

$$\begin{aligned} & |a_0|^2 G_{0,0,0,0}(R_y) \text{ for } f_2 = (c, R_1; v, R_2), \\ & |d_0|^2 G_{1,1,0,0}(R_y) \text{ for } f_3 = (c, R_2; v, R_1), \\ & 0 \text{ for } f_4 = (c, R_2; v, R_2). \end{aligned} \quad (18)$$

The Hamiltonian describing the exchange electron-hole interaction has the form

$$H_{exch}^{e-h} = \sum_{p,q,s} \sum_{i=1,2} \sum_{j=1,2,3,4} F_{c-v}(c, R_i, p; v, R_j, q; v, R_j, p-s; c, R_i, q+s) a_{R_i,p}^\dagger b_{R_j,-p+s}^\dagger b_{R_j,-q} a_{R_i,q+s}. \quad (19)$$

The average values of this Hamiltonian were calculated with the exciton wave functions (3). They determine the shifts of the magnetoexciton energy levels due to the exchange e-h interactions. They are equal to

$$\frac{1}{N} \sum_{p,q} F_{c-v}(c, R_i, p; v, R_j, q; v, R_j, p-k_x; c, R_i, q+k_x) e^{ik_y(p-q-k_x)l^2}, \quad i=1,2; \quad j=1,2,3,4. \quad (20)$$

3. Conclusions

The spinor-type wave functions of the 2D electrons and holes in the presence of the RSOC were used to calculate the exchange electron-hole interaction in the frame of 2D magnetoexcitons. Two lowest Landau levels for electrons $|e, R_1\rangle$, $|e, R_2\rangle$ and four lowest Landau levels for holes $|h, R_1\rangle$, $|h, R_2\rangle$, $|h, R_3\rangle$, and $|h, R_4\rangle$ were combined in such a way so as to form eight electron-hole states corresponding to the combinations: $f_1 = (e, R_1; h, R_1)$; $f_2 = (e, R_1; h, R_2)$; $f_3 = (e, R_2; h, R_1)$; $f_4 = (e, R_2; h, R_2)$; $f_5 = (e, R_1; h, R_3)$; $f_6 = (e, R_1; h, R_4)$; $f_7 = (e, R_2; h, R_3)$; $f_8 = (e, R_2; h, R_4)$. The exchange e-h interaction consists of the contact and long-range terms. The contact interaction depends only on the integration on the elementary lattice cell, whereas the long-range part contains a supplementary summation on the large scale variable representing the distance between two lattice nodes in the neighborhood of which the electron and hole are localized. In the frame of exchange Coulomb interaction, conduction electron and valence electron do not behave as point charges, but rather as two inter-band dipoles situated on different nodes of the lattice.

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