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Spin Effects in the Two-particle Equation of the Exciton

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Starting from a two-particle equation of the exciton which includes beside the Coulomb interaction a spin-dependent exchange term¹, the influence of the electron and hole spin on the exciton spectrum is studied by taking into account spin-orbit and spin-spin interaction. A rough estimate of the resulting splitting is given. In a second part the effect of the spin-dependent exchange term in a magnetic field is investigated. The result is that the usual spin splitting for s-states can not be observed.

The first effect of the spin which is important for the exciton spectrum is a splitting of the energy bands in a crystal because of the spin-orbit interaction of the electrons. New exciton series can appear as a result of it. A second effect arises in an external magnetic field which causes a Zeeman and a spin splitting of the exciton levels. These effects are well known². Further effects of spin are to be expected as a consequence of the spin-orbit and spin-spin interaction of the exciton's electron and hole. These effects will be studied in this paper in connection with the influence of the spin-dependent exchange term using an extended two-particle equation of the exciton.

1. The Influence of the Spin-Orbit and Spin-Spin Interaction

We treat the exciton on the basis of a two-particle model, m_1 , $e_1 = -e/\sqrt{\epsilon}$ and m_2 , $e_2 = e/\sqrt{\epsilon}$ being the effective masses and the screened charges of

electron and hole, respectively (ϵ is as usual the static dielectric constant). The Hamiltonian for this positronium-like system including spin-orbit (SO) and spin-spin (SS) interaction and furthermore a spin-dependent exchange term is given by

$$H = H_0 + H^{\text{SO}} + H^{\text{SS}} + H^{\text{e}}, \quad (1)$$

$$H_0 = -\frac{\hbar^2}{2\mu} \Delta - \frac{e^2}{\epsilon r} \quad \text{with} \quad \frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}. \quad (2)$$

The eigenvalues and eigenfunctions of the hydrogen-like Hamiltonian H_0 are well known. H^{SO} , the spin-orbit and H^{SS} , the spin-spin interaction terms can be derived from BREIT's relativistic two-particle equation^{3, 4}

$$H^{\text{SO}} = \frac{1}{2} \frac{e^2 \hbar^2}{\epsilon c^2} \frac{\mathbf{L}}{r^3} \cdot \left[\frac{\mathbf{S}_1}{m_1^2} + \frac{\mathbf{S}_2}{m_2^2} + \frac{2}{m_1 m_2} (\mathbf{S}_1 + \mathbf{S}_2) \right], \quad (3)$$

$$H^{\text{SS}} = -\frac{e^2 \hbar^2}{\epsilon m_1 m_2 c^2} \left[-\frac{8\pi}{3} \mathbf{S}_1 \cdot \mathbf{S}_2 \delta(\mathbf{r}) + \frac{1}{r^3} \left\{ \mathbf{S}_1 \cdot \mathbf{S}_2 - 3 \frac{(\mathbf{S}_1 \cdot \mathbf{r})(\mathbf{S}_2 \cdot \mathbf{r})}{r^2} \right\} \right]. \quad (4)$$



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The last term in (1) represents the exchange energy⁵

$$H^e = \delta(\mathbf{r}_1 - \mathbf{r}_2) \delta_{\sigma_1, -\sigma_2} \int \sum_{\sigma_1', \sigma_2'} \delta_{\sigma_1', -\sigma_2'} \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \delta(\mathbf{r}_1' - \mathbf{r}_2') \dots d^3\mathbf{r}_1' d^3\mathbf{r}_2'. \quad (5)$$

For the perturbation theory treatment of the additional terms (3), (4), (5) we use the following basis:

$$\Psi_{njl s}^m = \sum_{m_l = -l}^l \sum_{m_s = -s}^s (l s m_l m_s | j m) F_{nlm_l} \gamma_s^{m_s}. \quad (6)$$

The Ψ are constructed from hydrogen and spin eigenfunctions F_{nlm_l} and $\gamma_s^{m_s}$ by means of the Clebsch-Gordan coefficients⁶ in such a way as to be simultaneous eigenfunctions of the following operators: \mathbf{J}^2 , J_z , \mathbf{L}^2 , \mathbf{S}^2 . $\mathbf{J} = \mathbf{L} + \mathbf{S}$ is the total angular momentum, \mathbf{L} being the orbital angular momentum and \mathbf{S} the total spin angular momentum of the system. (Note that the spin-eigenfunctions are, of course, simultaneously eigenfunctions of \mathbf{S}_1^2 and \mathbf{S}_2^2 , the electron and hole spin operators.) Subsequently the symbol $\langle \dots \rangle$ stands for the expectation value of an operator calculated with the basis functions (6).

Starting with the computation of $\langle H^{S0} \rangle$ it can easily be shown that $\langle \mathbf{L} \cdot (\mathbf{S}_1 - \mathbf{S}_2) \rangle$ is zero⁷. Hence using the identity $\mathbf{S}_{1,2} = 1/2[\mathbf{S} \pm (\mathbf{S}_1 - \mathbf{S}_2)]$ we obtain

$$\langle H^{S0} \rangle = \frac{1}{2} \frac{e^2 \hbar^2}{\epsilon c^2} D \left\langle \mathbf{L} \cdot \mathbf{S} \frac{1}{r^3} \right\rangle \quad (7)$$

$$\text{with } D = \frac{1}{2m_1^2} + \frac{1}{2m_2^2} + \frac{2}{m_1 m_2}.$$

Since \mathbf{L} and \mathbf{S} commute we can write

$$\mathbf{L} \cdot \mathbf{S} = \frac{1}{2} [\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2] \quad (8)$$

and find

$$\langle \mathbf{L} \cdot \mathbf{S} \rangle = \frac{1}{2} [j(j+1) - l(l+1) - s(s+1)] \quad (9)$$

giving zero if either $l=0$ or $s=0$.

$$\text{With } \left\langle \frac{1}{r^3} \right\rangle = \frac{1}{a^3 n^3 (l+1)(l+\frac{1}{2})l}, \quad l \neq 0 \quad (10)$$

$$a = \epsilon \hbar^2 / \mu e^2 \quad (\text{exciton radius})$$

we finally obtain:

a) $s=0$ "Paraexciton",

$$\langle H^{S0} \rangle = 0; \quad (11)$$

b) $s=1$ "Orthoexciton",

$$\langle H^{S0} \rangle = \frac{1}{2} \frac{e^2 \hbar^2}{\epsilon c^2} D \frac{1}{a^3 n^3 (l+1)(l+\frac{1}{2})l} \begin{cases} l & \text{for } j=l+1 \\ -1 & \text{for } j=l \\ -(l+1) & \text{for } j=l-1 \end{cases} \quad \text{with } l \neq 0, \quad (12)$$

$$\langle H^{S0} \rangle = 0 \quad \text{for } l=0.$$

Next we study $\langle H^{SS} \rangle$. For convenience we split H^{SS} in two parts:

$$H^{SS} = K(\text{I} + \text{II}) \quad \text{with } K = -e^2 \hbar^2 / (m_1 m_2 c^2 \epsilon);$$

$$\text{I} = -\frac{8\pi}{3} \mathbf{S}_1 \cdot \mathbf{S}_2 \delta(\mathbf{r}); \quad (13)$$

$$\text{II} = \frac{1}{r^3} \left[\mathbf{S}_1 \cdot \mathbf{S}_2 - 3 \frac{(\mathbf{S}_1 \cdot \mathbf{r})(\mathbf{S}_2 \cdot \mathbf{r})}{r^2} \right].$$

Using $\mathbf{S}_1 \cdot \mathbf{S}_2 = \frac{1}{2} (\mathbf{S}^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2)$

we have immediately

$$\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = \frac{1}{2} s(s+1) - \frac{3}{4}. \quad (14)$$

Remembering that the hydrogenfunctions contain a factor r^l we realize that $\langle \text{I} \rangle$ can be different from zero only if $l=0$ (because of the delta-function):

$$\langle \text{I} \rangle = -\frac{8\pi}{3} |F_{n00}(0)|^2 \left\{ \frac{1}{2} s(s+1) - \frac{3}{4} \right\} \delta_{l0},$$

$$|F_{n00}(0)|^2 = \frac{1}{a^3 n^3 \pi}. \quad (15)$$

To calculate $\langle \text{II} \rangle$ we use the following relation⁴ which is valid for any two vector operators \mathbf{a} and \mathbf{b} commuting with each other and with \mathbf{r} and \mathbf{L} :

$$\langle (\mathbf{a} \cdot \mathbf{b}) r^2 - 3(\mathbf{a} \cdot \mathbf{r})(\mathbf{b} \cdot \mathbf{r}) \rangle = -\frac{\langle r^2 \rangle}{(2l+3)(2l-1)} \cdot \langle \{2\mathbf{L}^2(\mathbf{a} \cdot \mathbf{b}) - 3(\mathbf{a} \cdot \mathbf{L})(\mathbf{b} \cdot \mathbf{L}) - 3(\mathbf{b} \cdot \mathbf{L})(\mathbf{a} \cdot \mathbf{L})\} \rangle. \quad (16)$$

Substituting \mathbf{S}_1 and \mathbf{S}_2 for \mathbf{a} and \mathbf{b} , respectively, and using^{4,7}

$$(\mathbf{S}_1 \cdot \mathbf{L})(\mathbf{S}_2 \cdot \mathbf{L}) + (\mathbf{S}_2 \cdot \mathbf{L})(\mathbf{S}_1 \cdot \mathbf{L}) = (\mathbf{S} \cdot \mathbf{L})^2 - (\mathbf{S}_1 \cdot \mathbf{L})^2 - (\mathbf{S}_2 \cdot \mathbf{L})^2$$

$$\text{and } (\mathbf{S}_1 \cdot \mathbf{L})^2 = \frac{1}{4} \mathbf{L}^2 - \frac{1}{2} \mathbf{S}_1 \cdot \mathbf{L} \quad (17)$$

we obtain with (9) and (10)

$$\langle \text{II} \rangle = -\frac{s(s+1)l(l+1) - \frac{3}{4}\eta - \frac{3}{4}\eta^2}{a^3 n^3 (2l+3)(2l-1)(l+1)(l+\frac{1}{2})l} \quad \text{if } l \neq 0, \quad (18)$$

$$\eta = j(j+1) - l(l+1) - s(s+1);$$

$$\langle \text{II} \rangle = 0 \quad \text{if } l=0.$$

The last term we have to study is the exchange interaction (5). Since we are mainly interested in

the spin dependence we factorize H^e in a space- and a spin-dependent part, the space-dependent part having been evaluated elsewhere⁸:

$$H^e = A(\mathbf{r}) \delta_{\sigma_1, -\sigma_2} \sum_{\sigma_1, \sigma_2} \delta_{\sigma_1', -\sigma_2'} =: A(\mathbf{r}) B. \quad (19)$$

Calculating the matrixelements of B with the spinfunctions of (6) we find⁷

$$\langle s m_s | B | s' m_s' \rangle = 2 \delta_{s1} \delta_{m_s0} \delta_{s'1} \delta_{m_s'0}. \quad (20)$$

Collecting all terms we obtain as the first order energy corrections to the hydrogen-like energy eigenvalues of H_0

$$\Delta E := \langle H^{SO} \rangle + \langle H^{SS} \rangle + \langle H^e \rangle. \quad (21)$$

Paraexciton: $s=0$

$$\Delta E = C(-2/n^3) \quad \text{for } l=0, \quad (22)$$

$$\Delta E = 0 \quad \text{for } l \neq 0.$$

Orthoexciton: $s=1$

$$\Delta E = C \cdot 2/(3n^3) + 2\langle A \rangle \quad \text{for } l=0, \quad (23)$$

$$\Delta E = \frac{1}{2} m_1 m_2 C D \frac{1}{n^3(l+1)(l+\frac{1}{2})l} \begin{Bmatrix} l \\ -1 \\ -(l+1) \end{Bmatrix} + C \frac{1}{2n^3(2l+3)(2l-1)(l+1)(l+\frac{1}{2})l} \begin{Bmatrix} l(1-2l) \\ (2l+3)(2l-1) \\ -(2l+3)(l+1) \end{Bmatrix} \begin{matrix} j=l+1, \\ j=l, \\ j=l-1 \end{matrix} \quad (24)$$

for $l \neq 0$

with
$$C = \frac{e^2 \hbar^2}{\varepsilon m_1 m_2 c^2 a^3}$$

and a from (10), D from (7) and $\langle A \rangle$ from⁸.

To estimate the order of magnitude of the corrections due to SO and SS interaction we calculate C for ZnS. With $m_1=0.28$, $m_2=0.49$ (in units of the electron mass), $\varepsilon=8.1$ and the exciton Rydberg $R=e^2/(2\varepsilon a)=115 \text{ (cm}^{-1}\text{)}$ we find $C \approx 0.5 \cdot 10^{-4} \text{ (cm}^{-1}\text{)}$.

This leads to a splitting which is small compared with the other effects of spin and is below the nowadays attainable resolve power.

2. The Effect of the Exchange Term in the Presence of a Magnetic Field

The spin splitting of exciton levels due to a magnetic field is well known². However there is no spin-dependent exchange term included so far. Hence it should be interesting to find out the consequences of this term in a magnetic field \mathcal{H} .

As we have shown the effect of SO and SS interactions is very small and we can neglect both in what follows. Therefore we have the Hamiltonian (cf. ²):

$$\begin{aligned} H &= H_0 + H^m + H^e, \\ H^m &= \mathcal{H} \mu_0 (g^l L_z + g_1^s S_{1z} - g_2^s S_{2z}) \\ &= c L_z + d \sigma_{1z} - b \sigma_{2z} \end{aligned} \quad (25)$$

(μ_0 : Bohr magneton; σ : Pauli matrices; g : gyro-magnetic factor).

The first term represents the interaction of the orbital magnetic momentum with the external field, whereas the last two terms take into account the magnetic momentum resulting from electron and hole spins.

Since the total angular momentum is no longer a constant of motion, we choose as basis for the computation of the matrix elements of H^m and H^e the simple product functions [cf. (6)]:

$$\chi_{nlsm_l m_s} = F_{nlm_l} \gamma_s^{m_s}. \quad (26)$$

Again we are only interested in the spin-dependent part of the problem. If we calculate the matrix of (25) with the functions (26) and diagonalize it with respect to spin, we obtain the following eigenvalues λ and spin eigenfunctions $\bar{\gamma}$ for $l=0$ (cf. ^{7,9}):

$$\begin{aligned} \lambda_1 &= E_n^0 + (d-b), \quad \lambda_2 = E_n^0 - (d-b), \\ \lambda_3 &= E_n^0 + \langle A \rangle (1 + \sqrt{1+x^2}), \\ \lambda_4 &= E_n^0 + \langle A \rangle (1 - \sqrt{1+x^2}); \end{aligned} \quad (27)$$

$$\begin{aligned} \bar{\gamma}_1 &= \gamma_1^1 = \zeta_+ (\sigma_1) \zeta_+ (\sigma_2), \\ \bar{\gamma}_2 &= \gamma_1^{-1} = \zeta_- (\sigma_1) \zeta_- (\sigma_2), \\ \bar{\gamma}_3 &= \frac{1}{\sqrt{2}} (\alpha \gamma_1^0 + \beta \gamma_0^0) \\ &= \frac{1}{2} \{ (\alpha + \beta) \zeta_+ (\sigma_1) \zeta_- (\sigma_2) \\ &\quad + (\alpha - \beta) \zeta_- (\sigma_1) \zeta_+ (\sigma_2) \}, \\ \bar{\gamma}_4 &= \frac{1}{\sqrt{2}} (\beta \gamma_1^0 - \alpha \gamma_0^0) \\ &= \frac{1}{2} \{ (\beta - \alpha) \zeta_+ (\sigma_1) \zeta_- (\sigma_2) \\ &\quad + (\alpha + \beta) \zeta_- (\sigma_1) \zeta_+ (\sigma_2) \}, \end{aligned} \quad (28)$$

$$\begin{aligned} x &= \frac{d+b}{\langle A \rangle}, \quad \alpha = \left(1 + \frac{1}{\sqrt{1+x^2}} \right)^{1/2}, \\ \beta &= \left(1 - \frac{1}{\sqrt{1+x^2}} \right)^{1/2}. \end{aligned} \quad (29)$$

E_n^0 are the hydrogen-like eigenvalues of the exciton, $\langle A \rangle$ is the contribution of the exchange term⁸ and ζ are the spin functions of the electron and hole, respectively; the magnetic field is contained in d and b according to (25). The corresponding expressions for $l \neq 0$ are independent of the exchange

energy; the spinfunctions for this case are obtained from (28) by setting $\alpha = \beta = 1$.

We see from (27) that there is a fourfold spin splitting in the general case ($d \neq b$); this holds with the exchange term and without it and also for the case $l \neq 0$. However, the corresponding lines are not all observable because of selection rules for the transitions. To get these selection rules we need the transition matrix elements and therefore a function which describes the ground state of the two-particle system. Such a function has been constructed in coordinate space as a special linear combination of two-particle functions^{8, 10}. Generalizing this procedure by including the spinfunctions we can write:

$$\Phi_0 = \Psi_0(\mathbf{r}) \varphi_0(\sigma), \quad (30)$$

$$\varphi_0(\sigma) = \frac{1}{\sqrt{2}} \sum_s \zeta_s(\sigma_1) \zeta_{-s}(\sigma_2) = \frac{1}{\sqrt{2}} \delta_{\sigma_1, -\sigma_2}. \quad (31)$$

Calculating the transition matrix elements between this ground state and the excited states we obtain integrals over the space coordinates and sums over the spin variables of the spinfunctions (28) and (31), only the latter being of interest here:

$$\langle \bar{\gamma}_f | \varphi_0 \rangle = \frac{1}{\sqrt{2}} \sum_{\sigma_1 \sigma_2} \bar{\gamma}_f \delta_{\sigma_1, -\sigma_2}. \quad (32)$$

Introducing the expressions (28) we see immediately that the matrix elements vanish for $f=1, 2$;

this holds for $l=0$ and $l \neq 0$ because the spinfunctions are the same in these cases. For $f=3, 4$ we find:

$$\langle \bar{\gamma}_3 | \varphi_0 \rangle = \frac{1}{\sqrt{2}} \alpha, \quad \langle \bar{\gamma}_4 | \varphi_0 \rangle = \frac{1}{\sqrt{2}} \beta \quad \text{for } l=0, \quad (33)$$

$$\langle \bar{\gamma}_3 | \varphi_0 \rangle = \langle \bar{\gamma}_4 | \varphi_0 \rangle = \frac{1}{\sqrt{2}} \quad \text{for } l \neq 0. \quad (34)$$

It follows that only a twofold spin splitting is observable. As the transition probabilities are proportional to $|\alpha|^2$ and $|\beta|^2$ for $l=0$ (s-states) we have the interesting result that they depend on the magnetic field as a consequence of the exchange energy $\langle A \rangle$ — cf. (29), (25). The ratio of these probabilities is:

$$\frac{|\beta|^2}{|\alpha|^2} = \frac{\sqrt{1+x^2}-1}{\sqrt{1+x^2}+1}. \quad (35)$$

This ratio becomes very small for small values of x , i. e. for small magnetic fields. The transition probability for the state $\bar{\gamma}_4$ is then negligible as compared with that for the state $\bar{\gamma}_3$. Thus the spin-dependent exchange term H^e has the effect that no spin splitting of s-states should be observed in not too large magnetic fields.

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⁵ For the derivation of the exchange interaction operator from the many-electron problem see ¹. The difference between H^e in (5) and the expression derived in ¹ is the minus sign in the spin-deltas resulting from a different two-particle-space basis we have chosen:

$$\varphi_{cv} = \psi_c(r_1) \zeta_{sc}(\sigma_1) \psi_v^*(r_2) \zeta_{-sv}(\sigma_2)$$

where the transition from the electron to the hole standpoint is characterized by the substitutions of the Fock-operators $h \rightarrow -h^*$ and $\psi_v(r) \zeta_{sv}(\sigma) \rightarrow \psi_v^*(r) \zeta_{-sv}(\sigma)$,

ψ_v being the one-particle function determined by h . — The exact value of the exchange-screening-factor ε is still unknown. SHAM and RICE (Phys. Rev. **144**, 708 [1966]) have shown that it does not contain any electronic contribution.

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