Quantum-mechanical spin states and Zeeman-level diagrams of the positively charged exciton

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We consider the spin interaction in the Hamiltonian for the positively charged exciton X^+, determining the spin states and Zeeman-level diagrams for X^+ in which the heavy- and light-hole bands are degenerate and nondegenerate. The former case results in an X^+ with quintuplet and septet states in addition to the singlet and triplet states that are also observed for the negatively charged exciton X^-. When the heavy- and light-hole bands are split X^+ can comprise two heavy holes, two light holes, or a heavy and a light hole. The heavy-hole X^+ Zeeman-level diagram is found to be completely analogous to that of X^-, while the light-hole X^+ has more optical transitions and a different Zeeman splitting in photoluminescence. X^+ consisting of a heavy and a light hole has no coupled hole states, and is truly a heavy- (or light-) hole exciton plus a light (heavy) hole.

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I. INTRODUCTION

A neutral exciton X_0 is formed when a hole binds an electron due to their mutual Coulomb interaction. When more electrons are present than holes, the neutral exciton might be able to bind a second electron forming a three-particle system, the negatively charged exciton X^-. In a similar way, the positively charged exciton X^+ can be formed when X_0 binds a second hole. Due to the relatively small charged exciton (trion) binding energies with respect to X_0 in bulk semiconductors, the dimensionality of the host material has to be reduced to observe trions in experiments. X^- has been intensively studied both theoretically[1–5] and experimentally (see, for example Refs. 6–11) in quantum wells (QW's), usually in the presence of an external magnetic field. A consensus about the magneto-optical behavior of X^- in GaAs/AlGaAs QW's has now been obtained,[10] while for X^+ very few results have been reported, either experimentally[7,8,12,13] or theoretically.[14,15] In particular, the identification of the spin states of X^+ has not been considered in detail. In order to achieve a full description of X^+ in the presence of a magnetic field, it is clear that terms related to angular and spin momenta in the Hamiltonian must be considered.[3] A number of techniques have been used to calculate the trion eigenstates and eigenfunctions such as the stochastic variational method,[3,14] Monte Carlo simulations,[5] and the Haldane sphere technique[2], but these have been almost exclusively applied to the X^- problem. Since X^+ consists of two holes which are quantum-mechanically coupled, the determination of the X^+ spin states is much more complicated than for X^- because of the high total spin value of the holes and the complexity of the valence band.

In this work we focus on X^+, but no attempt will be made to solve the full trion Hamiltonian. Rather, we will restrict ourselves to the examination of the spin coupling of the trion particles in order to find all X^+ spin states and their Zeeman levels. Doing so, a full quantum-mechanical spin picture is obtained for X^+. The remainder of this paper is organized as follows. In Sec. II, we briefly review the X^- problem as a basis for discussing the more complex X^+. In Sec. III, we consider X^+ for the case where the heavy- and light-hole bands are degenerate at the top of the valence band, such that their states are strongly mixed and it is not possible to assign fully heavy- or light-hole character to either of the holes. In Sec. IV, we examine the three possible scenarios which arise when this is not the case, i.e. the holes are either (i) both heavy, (ii) both light, or (iii) one is heavy and another is light. In Sec. V, we present some discussion and compare our findings with the experimental data, whilst in Sec. IV we conclude.

II. ZEEMAN-LEVEL DIAGRAM OF X^-

In order to understand the spin states of X^+, we first briefly review the simpler X^- problem. X^- consists of two electrons and one hole, and is thus described by a total wave function Ψ_T, which has to be antisymmetric due to the Pauli exclusion principle. We start with the two electrons, which being the two identical particles in X^- are responsible for making Ψ_T antisymmetric. Let s_1^e (s_2^e) be the spin of electron 1 (2) with corresponding spin z component $m_{s_1}^e$ ($m_{s_2}^e$),[16] the four two-electron spin wave functions φ_i^{spin} then can be written as

$$\begin{aligned}\varphi_1^{spin}&=\alpha(1)\alpha(2),\\ \varphi_2^{spin}&=\alpha(1)\beta(2),\\ \varphi_3^{spin}&=\beta(1)\alpha(2),\\ \varphi_4^{spin}&=\beta(1)\beta(2).\end{aligned}\tag{1}$$

We use the notation $\alpha(i)\equiv|s_i^e=1/2;m_{s_i}^e=+1/2\rangle$, and $\beta(i)\equiv|s_i^e=1/2;m_{s_i}^e=-1/2\rangle$ for the single-particle electron spin wave functions where i ($i=1,2$) labels electron i. This means that, for example, φ_2^{spin} represents the two-electron spin wave function with electron 1 having spin up ($m_{s_1}^e=+1/2$) and electron 2 having spin down ($m_{s_2}^e=-1/2$). Note that $s_1^e=s_2^e=1/2$ since we deal with two electrons. The two-electron spin wave functions φ_i^{spin} ($i=1,2,3,4$) span a four-dimensional two-electron spin space which we refer to as the "uncoupled space." The two-electron spin wave functions of the four-dimensional "coupled space" are then given by three symmetrical spin wave functions $\psi_{S_i}^{spin}$ $(i=1,2,3)$ and one antisymmetrical spin wave function ψ_{AS}^{spin}, which are linear combinations of the uncoupled wave functions φ_i^{spin} as

$$\psi_{S_1}^{spin}=\alpha(1)\alpha(2),$$

$$\psi_{S_2}^{spin}=\frac{1}{\sqrt{2}}[\alpha(1)\beta(2)+\beta(1)\alpha(2)],$$

$$\psi_{S_3}^{spin}=\beta(1)\beta(2), \quad (2)$$

$$\psi_{AS}^{spin}=\frac{1}{\sqrt{2}}[\alpha(1)\beta(2)-\beta(1)\alpha(2)]$$

with $1/\sqrt{2}$ a normalization factor. The meaning of uncoupled and coupled spaces can be understood as follows. In the *uncoupled space*, both electron spins move independently, meaning that the spin z component and the magnitude of the spin momentum are specified for both electrons. In this case, s_1^e, s_2^e, $m_{s_1}^e$, and $m_{s_2}^e$ are good quantum numbers for the system. In the *coupled space*, the two particles combine to a composite system with a specified total spin z component m_s and magnitude of the total spin momentum s. Note that the spin wave functions $\psi_{S_i}^{spin}$ $(i=1,2,3)$ are symmetric with respect to particle exchange, while ψ_{AS}^{spin} is antisymmetric as required to make Ψ_T antisymmetric. The three symmetrical $s=1$ spin wave functions $\psi_{S_1}^{spin}$, $\psi_{S_2}^{spin}$, and $\psi_{S_3}^{spin}$ have a total spin z component of $m_s=+1$, $m_s=0$, and $m_s=-1$, respectively, and are therefore called the triplet spin states. On the other hand, ψ_{AS}^{spin} represents the singlet spin state with a total spin $s=0$ and spin z component $m_s=0$.

When a heavy hole with spin z component $m_s^{hh}=\pm 3/2$ is included, each level splits into two sublevels with a total spin z component of X^- being S_z.[9] The "singlet" level of X^- therefore has two spin states, and the "triplet" has six. Despite this, these states are still conventionally referred to as singlet and triplet in order to signify their origin in the coupling of the two electrons. The total spin S of X^- is half integer for both spin states making the X^- a fermion, whereas X_0 is a boson. On the application of a magnetic field, the degeneracy of the levels is lifted by the Zeeman interaction depending on the electron and hole g factors g_e and g_h, respectively, resulting in the X^- Zeeman-level diagram described in Ref. 9. A similar analysis can be applied to X^- with light holes, using $m_s^{lh}=\pm 1/2$, which results in the same number of spin states, but different optical transitions.

III. X^+ WITH DEGENERATE HEAVY- AND LIGHT-HOLE BANDS

We now turn our attention to X^+. As mentioned in Sec. I, the problem is considerably more complex for X^+ than for X^- due to the higher total spin of the holes, which allows spin z components of $\pm 3/2$ or $\pm 1/2$, and substantially increases the number of possible X^+ spin states compared with X^-. Furthermore, since two of these states ($m_s^{hh}=\pm 3/2$) are associated with the heavy-hole band, and two ($m_s^{lh}=\pm 1/2$) with the light-hole band, we can construct several alternative Zeeman-level diagrams, depending on whether we have entirely heavy or light holes, or a mixture of the two. In this section, we consider the most complex case, with two holes at wave vector $\mathbf{k}=0$ in a structure where the heavy- and light-hole bands are degenerate and mixed, i.e., where the holes are indistinguishable and cannot be clearly assigned fully heavy- or light-hole character. In such a situation, we must consider that either hole can have the full range of allowed values of z-component of the spin. The other possible scenarios are presented in Sec. IV.

TABLE I. Spin wave functions of the uncoupled space of the two-hole system with s_1^h (s_2^h) and z component $m_{s_1}^h$ ($m_{s_2}^h$) of hole 1 (2).

φ_i	$\lvert s_1^h,m_{s_1}^h\rangle\lvert s_2^h,m_{s_2}^h\rangle$	φ_i	$\lvert s_1^h,m_{s_1}^h\rangle\lvert s_2^h,m_{s_2}^h\rangle$
φ_1	$\lvert 3/2,+3/2\rangle\lvert 3/2,+1/2\rangle$	φ_9	$\lvert 3/2,-1/2\rangle\lvert 3/2,+1/2\rangle$
φ_2	$\lvert 3/2,+3/2\rangle\lvert 3/2,-1/2\rangle$	φ_{10}	$\lvert 3/2,-1/2\rangle\lvert 3/2,-1/2\rangle$
φ_3	$\lvert 3/2,+3/2\rangle\lvert 3/2,+3/2\rangle$	φ_{11}	$\lvert 3/2,-1/2\rangle\lvert 3/2,+3/2\rangle$
φ_4	$\lvert 3/2,+3/2\rangle\lvert 3/2,-3/2\rangle$	φ_{12}	$\lvert 3/2,-1/2\rangle\lvert 3/2,-3/2\rangle$
φ_5	$\lvert 3/2,+1/2\rangle\lvert 3/2,+1/2\rangle$	φ_{13}	$\lvert 3/2,-3/2\rangle\lvert 3/2,+1/2\rangle$
φ_6	$\lvert 3/2,+1/2\rangle\lvert 3/2,-1/2\rangle$	φ_{14}	$\lvert 3/2,-3/2\rangle\lvert 3/2,-1/2\rangle$
φ_7	$\lvert 3/2,+1/2\rangle\lvert 3/2,+3/2\rangle$	φ_{15}	$\lvert 3/2,-3/2\rangle\lvert 3/2,+3/2\rangle$
φ_8	$\lvert 3/2,+1/2\rangle\lvert 3/2,-3/2\rangle$	φ_{16}	$\lvert 3/2,-3/2\rangle\lvert 3/2,-3/2\rangle$

In a similar way to electrons in X^-, the holes in X^+ are fermions, and thus the total wave function Ψ_T should be anti-symmetric. Starting with the holes of X^+, we can use an analogous approach to that for X^- to construct the uncoupled and coupled two-hole spin wave functions. The hole spin s^h equals 3/2 with spin z components $m_s^{hh}=\pm 3/2$ and $m_s^{lh}=\pm 1/2$ for the heavy and light holes, respectively, thus there are in total 16 (4×4) uncoupled spin wave functions φ_i $(i=1,\ldots,16)$ spanning a 16- dimensional uncoupled space, rather than a four-dimensional one as for X^-. The uncoupled spin wave functions of the two-hole system are given in Table I with s_1^h and $m_{s_1}^h$ (s_2^h and $m_{s_2}^h$), the spin and spin z component of hole 1 (2). Note that $s_1^h=s_2^h=3/2$ since we deal with holes.

In the coupled space, the total spin s of two holes is defined and given by

$$s=|s_1^h-s_2^h|,|s_1^h-s_2^h|+1,\ldots,|s_1^h+s_2^h|. \quad (3)$$

Using $s_1^h=s_2^h=3/2$ for holes leads to $s=0$, 1, 2, or 3 with spin z components m_s shown in Table II. It is clear that Eq. (3) can also be used to determine the total spin of the X^- spin states with $s_1^e=s_2^e=1/2$ giving the same results as obtained previously. The third column of Table II indicates the spin states of the two-hole system related to s. As can be seen, in addition to a singlet and a triplet spin state corresponding to a total spin $s=0$ and $s=1$ respectively, there is a quintuplet and a septet spin state with total spins $s=2$ and $s=3$ respectively. Note that there are in total 16 m_s values

TABLE II. Total spin s and z component m_s of the two-hole system with corresponding spin states.

s	m_s	Spin state
0	0	Singlet
1	$-1,0,+1$	Triplet
2	$-2,-1,0,+1,+2$	Quintuplet
3	$-3,-2,-1,0,+1,+2,+3$	Septet

for the two-hole spin states which correspond with the dimensionality of the (un) coupled space as will be explained later.

Having determined the spin states of the two-hole system, we now go on to construct the band-degenerate X^+ Zeeman-level diagram. To do so we have to include an electron with spin z component $m_s^e = \pm 1/2$. This results in $16\times 2 = 32$ energy levels with total X^+ spin z components S_z (see Fig. 1). Throughout this work we draw our Zeeman-level diagrams under the assumption that $g_e < 0 < g_h$ and $|g_e| < |g_h|$, which is consistent with experimental data on all but the narrowest GaAs QW's.[17] A very similar approach may be used in other cases. Although there are in total 32 Zeeman levels for X^+, we label the spin states as singlet, triplet, quintuplet, and septet according to the convention consistent with X^-. The total spin of X^+ is half integer for all spin states making the positively charged exciton a fermion, as was the case for X^-. The large quantity of energy levels is a direct result of the hole spin being 3/2. In fact, since $m_s^{hh} = \pm 3/2$ and $m_s^{lh} = \pm 1/2$ corresponding to the heavy and light holes, respectively, the construction of the coupled space includes both type of holes. Note that different X^+ Zeeman levels can have the same S_z value since all levels have different spin wave functions. When applying a magnetic field B, the degeneracy is lifted by the Zeeman interaction giving the complete X^+ Zeeman-level diagram shown in Fig. 1. The optical selection rules $\Delta S_z = +1$ and $\Delta S_z = -1$ are applicable here and correspond to recombination emitting right- (σ^+) and left-handed (σ^-) circularly polarized lights respectively. In total there are 44 optical transitions leaving an excess hole with spin z component $m_s^{hh} = \pm 3/2$ or $m_s^{lh} = \pm 1/2$. Note that although the total spin of X^+ exceeds 1 for the quintuplet and septet spin states, an optical transition can occur as long as $\Delta S_z = \pm 1$ is fulfilled. This means that, depending on the X^+ spin state, an optical transition leaves an unbound heavy or light hole in the final state. For brevity we will restrict the discussion of the optical transitions here to the singlet and triplet spin states. It should be mentioned that our approach does not allow us to determine which spin state has the lowest energy, however, comparison with X^- leads us to conclude that a low total spin value corresponds to low energy, at least in low magnetic fields. Transitions 1 and 3 in Fig. 1 refer to the σ^- polarized optical transitions of the singlet, while 2 and 4 have σ^+ polarization. The singlet splitting is only determined by g_e, while the final level is always a hole with spin z component $\pm 1/2$ or $\pm 3/2$, and therefore four distinguishable optical transitions from the singlet are expected. This is very different from X^- where only two different singlet transitions are allowed.[9] For the triplet, there are five transitions having σ^- polarization (transitions 5, 6, 8, 10, and 12) and five with σ^+ (transitions 7, 9, 11, 13, and 14). Thus, the triplet state has in total ten different optically-allowed transitions, but only four of them are distinguishable in photoluminescence (PL) experiments. For example, transitions 5, 8, and 12 have the same transition energy even though they originate from different energy levels. The same is true for transitions 7, 11, and 13. As a result, the numbers

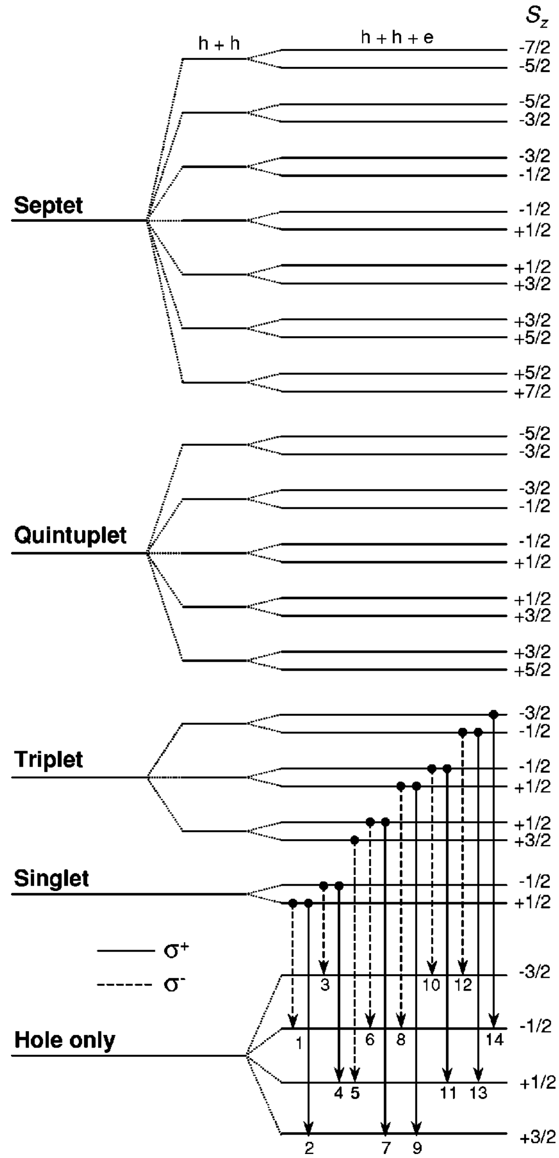

FIG. 1. Zeeman-level diagram of the band degenerate X^+, with total exciton spin z component S_z. σ^+ and σ^- indicate right- and left-handed circularly polarized photoluminescence, while e and h denote electron and hole, respectively (see text for more details). The X^+ levels labeled "singlet" through to "septet" represent the initial state, whilest the levels labeled "hole only" correspond to the final state after recombination. Note that only the optically allowed transitions (arrows) for the singlet and triplet are shown, and the size of the Zeeman splitting of the hole only state is exaggerated compared to the other states for clarity. Transitions 5, 8, and 12 are indistinguishable in photoluminescence, as are 7, 11, and 14.

of optically distinguishable singlet and triplet spin state PL transitions for the band degenerate X^+ are four and four, respectively, which is twice that of X^- in each case.

The experimental X^+ Zeeman-splitting energy, i.e., observed in a PL experiment, ΔE_Z, is not so straightforward to determine as for X^-. For example, for the singlet, the difference in PL energy between transitions 2 and 3, which leave a heavy hole, is the same as for X^- and given by $\Delta E_Z=(g_e+3g_h)\mu_B B$ (see Fig. 1), where μ_B is the Bohr magneton. For transitions 1 and 4, which leave behind a light hole, $\Delta E_Z=(-g_e+g_h)\mu_B B$. A similar approach can be used for the triplet and all other high-energy spin states to obtain ΔE_Z in each case, though the selection of which PL lines should be used to determine ΔE_Z becomes somewhat arbitrary as the number of optically distinguishable transitions increases. It is clear from Fig. 1 that for all transitions, the final state is either a light or a heavy hole in the valence band. However, since the spin z component of the hole is $\pm 3/2$ or $\pm 1/2$, it is not *a priori* clear to what extent the spin wave functions of the band degenerate X^+ are composed of heavy and light holes. Indeed, the spin states of X^+ are determined using Eq. (3), giving no information at all about the relation between the coupled and the uncoupled spin spaces. In order to know the influence of the heavy and light holes on the spin states of X^+, it is necessary to investigate the spin wave functions of the two-particle system in the coupled space. As we shall see, for degenerate heavy- and light-hole bands, it is impossible to construct almost all of the band-degenerate X^+ spin states without a mixture of heavy and light holes.

The spin z components of the two-hole states of the band degenerate X^+, i.e., singlet, triplet, quintuplet, and septet, correspond with spin wave functions ψ_i $(i=1,\ldots,16)$ of the coupled space in a similar way to X^-, but the quantum-mechanical construction of ψ_i is not as straightforward. The wave functions are linear combinations of the uncoupled wave functions φ_i $(i=1,\ldots,16)$ given in Table I, and the coefficients can be found using

$$|s,m_s;s_1^h,s_2^h\rangle=\sum\sum_{m_{s_1}^h+m_{s_2}^h=m_s} C_{m_{s_1}^h m_{s_2}^h}|s_1^h,m_{s_1}^h\rangle|s_2^h,m_{s_2}^h\rangle, \quad (4)$$

where $|s,m_s;s_1^h,s_2^h\rangle$ denotes the spin wave functions ψ_i $(i=1,\ldots,16)$ of the coupled space with s and m_s given in Table III and $s_1^h=s_2^h=3/2$ for holes. The expansion coefficients $C_{m_{s_1}^h m_{s_2}^h}$ are the Clebsch-Gordan (CG) coefficients[18] and $|s_1^h,m_{s_1}^h\rangle|s_2^h,m_{s_2}^h\rangle$ are the uncoupled spin wave functions φ_i given in Table I. The summation runs over the quantum numbers $m_{s_1}^h$ and $m_{s_2}^h$ with the constraint $m_{s_1}^h+m_{s_2}^h=m_s$. As an example, the singlet spin state $(s=0,m_s=0)$ originates from $\psi_1=|0,0;3/2,3/2\rangle$ given by the expansion

$$\psi_1=C_{+3/2-3/2}\cdot\varphi_4+C_{+1/2-1/2}\cdot\varphi_6+C_{-1/2+1/2}\cdot\varphi_9 +C_{-3/2+3/2}\cdot\varphi_{15}, \quad (5)$$

with $C_{+3/2-3/2}=C_{-1/2+1/2}=1/2$ and $C_{+1/2-1/2}=C_{-3/2+3/2}=-1/2$, and all other coefficients zero. All expansion coefficients $C_{m_{s_1}^h m_{s_2}^h}$ for a two-hole system are given in Table III where blank cells represent zero coefficients. The fourth column of Table III denotes the X^+ spin states using the notation S, T, Q, and SP for singlet, triplet, quintuplet, and septet, respectively. Note that these states correspond with those given in Table II. The last column of Table III reflects the symmetry of the spin states with SYM = symmetric and ASYM = antisymmetric. This symmetry follows directly from the sign of the CG coefficients where $C_{xy}=C_{yx}$ signifies a symmetric and $C_{xy}=-C_{yx}$ an anti-symmetric spin wave function ψ_i for all valid x and y. Note that the symmetry of the singlet and triplet states of X^+ is exactly the same as for X^-. The significance of a CG coefficient, for example, $C_{+3/2-1/2}$, is such that $|C_{+3/2-1/2}|^2$ represents the probability to find a heavy (3/2) and a light (1/2) hole with spin up (+) and down (−), respectively, in the corresponding X^+ spin state with fixed s and m_s values. (Note that $\Sigma_{m_1^h}\Sigma_{m_2^h}|C_{m_{s_1}^h m_{s_2}^h}|^2=1$ in Table III for all states as necessary.) Therefore, since only $C_{-3/2-3/2}=1$ and $C_{+3/2+3/2}=1$ for the septet state with $m_s=-3$ and $m_s=+3$, respectively, this is the only state in which both holes in the band degenerate X^+ can be heavy holes. This means that no septet PL transition originating from $m_s=\pm 3$ leaving a light hole (final level $m_s^{lh}=\pm 1/2$) is allowed in Fig. 1. However, all other states involve the presence of the heavy *and* light holes as can be seen in Table III, and therefore all optically allowed transitions for the singlet and triplet of Fig. 1 are confirmed by the CG coefficients. We note that for X^-, the CG coefficients can be found using the same expansion of Eq. (4) with the corresponding spin wave functions φ_i^{spin} of Eq. (1). This results in six nonzero CG coefficients equal to the coefficients in Eq. (2).

IV. X^+ WITH NON-DEGENERATE HEAVY- AND LIGHT-HOLE BANDS

In the preceding section, we examined the situation in which the heavy- and light-hole bands are degenerate, and analyzed the Zeeman interaction making no assumptions about the contribution of heavy and light holes, but only considering the spin. However, in some structures, such as narrow or strained quantum wells, it is likely that the heavy-light hole valence-band degeneracy will be lifted, such that each hole can be clearly assigned as either heavy or light. For this reason, and for the sake of completeness, we now turn to the three other possible situations, which are (i) two heavy holes, (ii) two light holes, and (iii) one heavy and one light hole.

As was already realized by Shields *et al.*[13] the restriction of the problem to one type of hole, be it either heavy or light, reduces the X^+ problem to one which is essentially analogous to X^-, and results in the formation of singlet and triplet states, as discussed in detail in Sec. II. It is not necessary to repeat the derivation here, rather we can simply exchange the relevant electron and hole spin-states to arrive at the Zeeman-level diagrams for the heavy- and light-hole X^+ shown in Figs. 2(a) and 2(b), respectively. Several remarks should be made about these diagrams. First, because of the

TABLE III. Clebsch-Gordan coefficients for a two-hole system with total spin s and spin z component m_s in the coupled space. The spin states are singlet (S), triplet (T), quintuplet (Q), and septet (SP) having a symmetric (SYM) or antisymmetric (ASYM) spin wave functions ψ_i. The blank cells represent coefficients being zero.

ψ_i	s	m_s	State	$C_{+3/2+1/2}$ φ_1	$C_{+3/2-1/2}$ φ_2	$C_{+3/2+3/2}$ φ_3	$C_{+3/2-3/2}$ φ_4	$C_{+1/2+1/2}$ φ_5	$C_{+1/2-1/2}$ φ_6	$C_{+1/2+3/2}$ φ_7	$C_{+1/2-3/2}$ φ_8	$C_{-1/2+1/2}$ φ_9	$C_{-1/2-1/2}$ φ_{10}	$C_{-1/2+3/2}$ φ_{11}	$C_{-1/2-3/2}$ φ_{12}	$C_{-3/2+1/2}$ φ_{13}	$C_{-3/2-1/2}$ φ_{14}	$C_{-3/2+3/2}$ φ_{15}	$C_{-3/2-3/2}$ φ_{16}	Symmetry
ψ_1	0	0	S				1/2		$-1/2$			1/2						$-1/2$		ASYM
ψ_2	1	-1	T								$\sqrt{3/10}$		$-\sqrt{2/5}$			$\sqrt{3/10}$				SYM
ψ_3	1	0	T				$\sqrt{9/20}$		$-\sqrt{1/20}$			$-\sqrt{1/20}$						$\sqrt{9/20}$		SYM
ψ_4	1	+1	T		$\sqrt{3/10}$			$-\sqrt{2/5}$						$\sqrt{3/10}$						SYM
ψ_5	2	-2	Q												$\sqrt{1/2}$		$-\sqrt{1/2}$			ASYM
ψ_6	2	-1	Q								$\sqrt{1/2}$					$-\sqrt{1/2}$				ASYM
ψ_7	2	0	Q				1/2		1/2			$-1/2$						$-1/2$		ASYM
ψ_8	2	+1	Q		$\sqrt{1/2}$									$-\sqrt{1/2}$						ASYM
ψ_9	2	+2	Q	$\sqrt{1/2}$						$-\sqrt{1/2}$										ASYM
ψ_{10}	3	-3	SP																1	SYM
ψ_{11}	3	-2	SP												$\sqrt{1/2}$		$\sqrt{1/2}$			SYM
ψ_{12}	3	-1	SP								$\sqrt{1/5}$		$\sqrt{3/5}$			$\sqrt{1/5}$				SYM
ψ_{13}	3	0	SP				$\sqrt{1/20}$		$\sqrt{9/20}$			$\sqrt{9/20}$						$\sqrt{1/20}$		SYM
ψ_{14}	3	+1	SP		$\sqrt{1/5}$			$\sqrt{3/5}$						$\sqrt{1/5}$						SYM
ψ_{15}	3	+2	SP	$\sqrt{1/2}$						$\sqrt{1/2}$										SYM
ψ_{16}	3	+3	SP			1														SYM

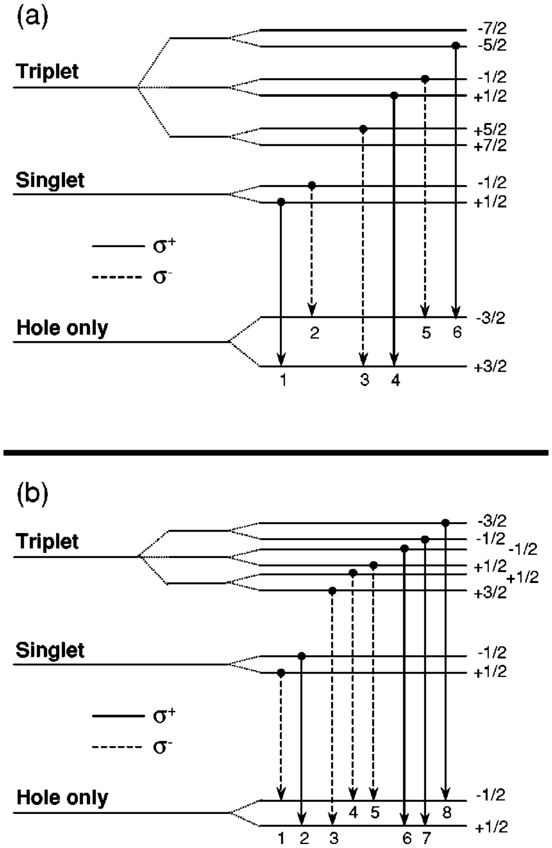

FIG. 2. Zeeman-level diagram of (a) the heavy hole X^+ and (b) the light hole X^+. For the heavy hole X^+, transitions 3 and 4 have the same PL energy, as do 4 and 6. For the light hole X^+ transitions 3 and 5 have the same PL energy, as do 6 and 8.

restriction to one type of hole in each case, we have only two rather than four final states. Combining this with the restriction of the values of the z component of the hole spin in the initial (X^+) state reduces the number of allowed optical transitions to a manageable number, six for the heavy hole X^+ and eight for the light hole X^+. Indeed, it can be seen that the Zeeman-level diagram for the heavy hole X^+ is completely analogous to that of X^-, with two singlet transitions and four triplet transitions. The two σ^- triplet transitions are indistinguishable in PL, as are the two σ^+ transitions, giving only two distinguishable PL transitions for the heavy-hole X^+ triplet, exactly as was the case for X^-.[9] Note that our assumption $g_e<0<g_h$ and $|g_e|<|g_h|$ results in a different order of heavy-hole X^+ spin states to that published previously,[13] and changes the order and number of observable PL transitions, as was also found the case for X^-.[9] Finally, the experimental Zeeman splitting for the PL transitions of the heavy hole X^+ is also the same as it is for the X^- and the neutral exciton, and is given by $\Delta E_Z=(g_e+3g_h)\mu_B B$.

Although the spin states of the light hole X^+ may be constructed in analogy with that of X^-, the similarity of the two cases ceases once the optical transitions are considered. The light hole X^+ has two singlet transitions, but six triplet transitions rather than four. Four of these are experimentally distinguishable in PL; transitions 3 and 5 have the same PL energy, as do 6 and 8. Notably, and in contrast to all other charged excitons considered so far, the light hole X^+ has no optically forbidden transitions, at least according to spin selection rules. This is a direct result of the restriction of the z component of the spin of the holes to $\pm 1/2$. There are further differences between the light hole X^+ and its heavy hole or X^- counterparts. The experimental Zeeman splitting for the singlet recombination is given by $\Delta E_Z=(-g_e+g_h)\mu_B B$, which is the same value as was found for the splitting between transitions 1 and 4 of band degenerate X^+. This follows from the restriction of the z components of the spin in the final states to m_s^{lh} to $\pm 1/2$, since the initial state of the singlet is constructed from a two-particle state that has total spin $s=0$, and is therefore insensitive to the presence of heavy or light holes. Moving onto the triplet state, we have four optically distinguishable transitions, and therefore cannot define a unique value for the experimental Zeeman splitting, as was also the case for the band degenerate X^+. Taking the two lowest initial states which have optically allowed σ^- and σ^+ transitions (3 and 6 in Fig. 2(b), respectively, or equivalently 5 and 8), we find $\Delta E_Z=(-g_e+g_h)\mu_B B$, the same value as for the singlet, whilst for the other two transitions (4 and 7) we obtain $\Delta E_Z=(g_e+3g_h)\mu_B B$.

We now turn to the final case, that of X^+ consisting of one light hole, one heavy hole, and one electron, which we denote as the heavy-light hole X^+. It should be remarked at the outset that the heavy-light hole X^+ is fundamentally different from all the other charged excitons considered up to now, in that all the particles are distinguishable. For this reason, there are no coupled hole (singlet or triplet) states, but instead a series of single-particle states which arise from summing the spin contributions of the individual particles, i.e, there is no coupled spin space, but only uncoupled spin space. The heavy-light hole X^+ is thus a heavy- (or light-) hole exciton plus an extra light (heavy) hole. The possible states are shown in Fig. 3, again assuming that $g_e<0<g_h$ and $|g_e|<|g_h|$. In order to find the optically allowed transitions, we can simply look for states which contain states of the neutral exciton that are optically active according to spin selection rules, i.e., $m_s^{hh}=+3/2$, $m_s^e=-1/2$, and $m_s^{hh}=-3/2$, $m_s^e=+1/2$ for σ^- and σ^+ recombination, respectively, of the heavy-hole exciton, and $m_s^{lh}=+1/2$, $m_s^e=+1/2$, and $m_s^{lh}=-1/2$, $m_s^e=-1/2$ for σ^- and σ^+ recombination, respectively, of the light-hole exciton, with the proviso that the extra hole remains unaffected by the recombination process. The consequence is eight optically allowed transitions, two with σ^- recombination involving the heavy hole and leaving the light hole and two with σ^- recombination involving the light hole and leaving the heavy hole, and similarly for σ^+. However, since the light-heavy hole X^+ is really a heavy or a light-hole exciton plus a second hole, it means that the spin state of the excess hole does not affect the PL energy. Thus, the σ^- transitions 1 and 4 involving recombination of a heavy-hole exciton (plus a light hole with $m_s^{lh}=\pm 1/2$) are indistinguishable in PL, as are 1 and 3, and similarly for the light-hole exciton (plus heavy hole). There are therefore four optically distinguishable transitions, with experimental Zeeman splittings of $\Delta E_Z=(-g_e+g_h)\mu_B B$ and $\Delta E_Z=(g_e$

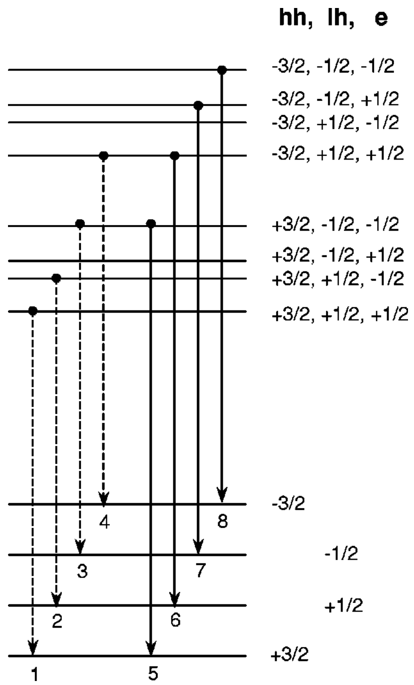

FIG. 3. Zeeman-level diagram of the heavy-light hole X^+. Note that there are no coupled hole states, just a ladder of spin states which can be determined by summing the spins of the individual particles. Transitions 1, 4, 5, and 8 correspond to recombination of a light-hole exciton (plus a heavy hole), and transitions 2, 3, 6, and 7 correspond to a heavy-hole exciton (plus a light hole). The heavy light X^+ has only four optically distinguishable PL transitions, corresponding to σ^+ and σ^- heavy- and light-hole excitons recombination.

$+3g_h)\mu_B B$, which are naturally defined depending on whether the recombination is from a light-hole exciton (plus a heavy hole) or from a heavy-hole exciton (plus a light hole).

V. DISCUSSION AND COMPARISON WITH EXPERIMENT

Having derived the four possible Zeeman-level diagrams, it is interesting to speculate as to which of these would be the most likely to be observed experimentally, and furthermore, try to use the Zeeman-level diagrams to interpret experimental data, as has been achieved for X^-.[9] In order to do so we have to make some judgement as to whether heavy or light holes, or both, are likely to be involved in the formation of X^+. In most theoretical and experimental studies of low-dimensional III–V semiconductors in which holes are involved, it is either implicitly or explicitly assumed that the holes are heavy and not light. There are two justifications for this. The first is that the heavy holes have a greater density of states due to their larger effective mass than light holes. The second is that as a result of symmetry breaking, due to confinement effects, strain etc., the degeneracy between heavy and light holes is lifted such that the heavy-hole band is above the light-hole band. This gives us good grounds for the exclusion of the light hole X^+ as a realistic option; even if the hole bands are degenerate, an exclusively light hole X^+ is very unlikely. If we assume that the heavy- and light-hole bands are degenerate, we are left with the remaining three possibilities. The density of states argument would lead us to suppose that the heavy-light hole X^+ is not likely, but it should be noted that the density of states argument cannot be used to exclude the band degenerate X^+ for the reason that in this case nearly all X^+ spin states are a mixture of both heavy and light holes; they only take on heavy- or light-hole (spin) character after recombination. If the hole bands are not degenerate, then the heavy hole X^+ is the only realistic candidate.

Further clues can perhaps be found by a comparison with the experimental data. After all, the band degenerate X^+ has a very large number of states and possible optical transitions, whereas the heavy-hole X^+ Zeeman-level diagram has features which are essentially indistinguishable from that of X^-. Magneto-PL experiments on three *p*-type GaAs single quantum wells were recently reported in which the neutral and positively charged exciton were observed from 0 to 50 T.[12] In each case, just two lines from X^+, one for each polarization, arising from a single spin-split state were observed. In Ref. 12, this transition was associated with the singlet state of X^+. Such an assignment would be correct irrespective of whether the X^+ consisted entirely heavy holes or whether it was a band degenerate X^+. In the latter case one would, according to Fig. 1, expect to see four lines from the singlet rather than two that are observed, although it is quite possible that transitions 1 and 4, which leave behind a light hole, are strongly suppressed due to the reduced number of available final states that results from the small density of states for the light hole. Moving onto the higher-energy states, both the heavy hole and the band degenerate X^+ have triplet states. There are two optically distinguishable transitions from the triplet state of the heavy hole X^+ and four from the band degenerate X^+, regardless of whether we exclude light holes in the final state or not. Examining the triplet PL might therefore distinguish between heavy hole and band degenerate X^+. However, as mentioned above, no triplet-state PL was observed in these experiments. We do not consider angular momentum here, but it is well known that the lowest-energy triplet spin state for X^- is ''dark'' (z component of angular momentum is -1),[2,4] and not generally observable in experiments.[10] If the same were true for the X^+ triplet spin state,[15] this would explain the data. An alternative explanation is that heavy- (or light-) hole exciton recombination in a heavy-light hole X^+ was measured, leaving a light (heavy) hole in the valence band. One might imagine that in such a system, the heavy hole is more closely bound to the electron than the light hole. In this case the PL would be dominated by heavy-hole ($-$ electron) recombination, and there would be one σ^- and one σ^+ peak, as was found. We also note that when the heavy- and light-hole bands are degenerate, but heavy and light holes are distinguishable (e.g. via their effective mass), the formation of the heavy-light hole X^+ is favored over the band degenerate X^+.

On the other hand, other groups have reported the observation of both polarization components of the X^+ triplet spin state in a magnetic field,[7,13] which would exclude the heavy-light hole X^+. The band degenerate X^+ also has quintuplet and septet states, which have certainly not been observed in any experiment. However, since these states have high total spin, and are therefore assumed to be higher-energy states than the triplet, it is quite possible that they are not bound, and so not observed in PL experiments. Some type of absorption experiment may be a more discerning way to experimentally determine which type of X^+ is present, and such experiments were reported by Shields *et al.*[13] They observed features due to the singlet and triplet states of X^+ and due to heavy- and light-hole excitons in their spectra, the latter two being split by some 2.5 meV. Thus, in that particular experiment, the heavy hole X^+ is the only viable candidate. Similarly, in any other experiment, the valence-band degeneracy would be a crucial factor in determining the type of X^+ observed. Indeed, given the fact that the Zeeman-level diagrams of the various types of X^+ differ substantially with respect to Zeeman levels with high total spin, absorption would seem to be a good method to determine which X^+ is present in any particular sample.

VI. CONCLUSIONS

We have studied the spin states of X^+ considering the four different possibilities for combinations of heavy- and light- holes. When the heavy and light hole bands are degenerate, the X^+ Zeeman-level diagram has a rich hierarchy of states with quintuplet and septet spin states in addition to the singlet and triplet states observed for X^-, and a very large number of possible PL transitions. These properties are a direct result of the higher total spin of the hole. When the problem is restricted to entirely heavy holes, the Zeeman-level diagram reduces to one that is completely analogous to X^-, with two PL transitions from the singlet state and four from the triplet, two of which are optically distinguishable. For the light hole X^+, we expect two singlet transitions and six triplet transitions, though only four of these are distinguishable in PL. X^+ which consists of a heavy and a light hole that are quantum-mechanically distinguishable has no coupled spin states, but only a ladder of energy levels that arise by summing the spins of the individual particles. This situation can truly be considered as a heavy- (or light-) hole exciton plus a light (heavy) hole. We consider that the heavy-hole X^+ is the most likely to be observed in experiment, although the band-degenerate and heavy-light hole X^+ cannot be excluded in most experiments.

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