Common trends in the Zeeman splitting of novel wurtzite materials

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The response of semiconductor materials to external magnetic fields is a reliable approach to probe intrinsic electronic and spin-dependent properties. In this study, we investigate the common Zeeman splitting features of novel wurtzite materials, namely InP, InAs, and GaAs. We present values for the effective g-factors of different energy bands and show that spin-orbit coupling effects, responsible for the spin splittings, also have noticeable contributions to the g-factors. Within the Landau level picture, we show that the nonlinear Zeeman splitting recently explained in magneto photoluminescence experiments for InP nanowires are also present in InAs and GaAs. Such nonlinear features stem from the peculiar coupling of the A and B valence bands, as a consequence of the interplay between the wurtzite crystal symmetry and the breaking of time-reversal symmetry by the external magnetic field. Moreover, we develop an analytical model to describe the experimental nonlinear Zeeman splitting and apply it to InP and GaAs data. Extrapolating our fitted results, we found that the Zeeman splitting reaches a maximum value, which is a prediction that could be probed at higher magnetic fields.

I. INTRODUCTION

Novel III-V semiconductor compounds with wurtzite (WZ) crystal structure, such as InP, InAs, and GaAs, can nowadays be synthesized as nanowhiskers or nanowires (NWs) with large diameters. In contrast to the widely studied zinc-blende (ZB) phase— the most stable crystal structure of non-nitride III-V compounds— there are still many unknown, or at least not completely understood, properties of these WZ materials, especially regarding spin-dependent phenomena. For instance, spin-orbit coupling (SOC) parameters and effective g-factors in WZ NWs control the physics behind the exotic Majorana bound states in semiconductor/superconductor setups, spin-laser operation, spin-relaxation mechanisms, and can be drastically modified under lateral quantum confinement.

One of the possibilities to probe the intrinsic spin properties of a semiconductor system is to investigate their response under external magnetic fields, for instance, coupled to optical excitation in magneto photoluminescence (PL) experiments. Recent studies investigated the Zeeman splitting (ZS) from magneto PL and extracted effective g-factors using the conventional linear dispersion of the WZ ZS. This theoretical modeling has two main disadvantages for the magnetic field oriented along the NW axis (with [0001] growth direction): (i) the effective g-factors of electrons and holes cannot be probed separately because of the optical transitions, and (ii) this theory does not account for the unconventional nonlinear ZS observed. Such nonlinear features have recently been observed in quantum dots and quantum wells, i.e., semiconductor systems with strong quantum confinement.

On the other hand, the case of WZ NWs is quite different since the NWs used in these recent experiments have large diameter and effectively behave as a bulk material (with negligible lateral quantum confinement). Particularly for InP WZ, it was unambiguously shown by Tedeschi et al. that these nonlinear features originate from the peculiar coupling of Landau levels (LLs) from different energy states in the valence band, specifically between A and B bands. Although this nonlinear ZS has also been observed in InGaAs and GaAs, it remains to be shown that indeed these nonlinear features have the same origin and could be described in a compact analytical way. Furthermore, InAs WZ NWs have been investigated by recent transport experiments. However, to the best of our knowledge, no theoretical attempt has ever been made to compute the effective g-factors in such material.

In this paper, we analyze the ZS of novel III-V WZ materials, namely InP, InAs and GaAs. We provide the values for effective g-factors of different energy bands and highlight important contributions due to SOC effects originating from the interband SOC interaction. Turning to the LL physics, we apply the theoretical approach presented in Ref. and show that the nonlinear ZS arises solely from the mixing within the valence band and it is indeed a common feature present in the studied materials. Based on this common mechanism responsible for the nonlinear features, we developed an analytical model that reliably fits the available experimental data, especially for InP WZ. We then extrapolate our fitted results and show that the nonlinear feature acts as a limiting effect to the maximum value of ZS. Under higher magnetic fields, such features could be observed experimentally in order to test the limits of our suggested model.

We organize this paper as follows: In Sec. II we discuss...
the effective g-factors calculations and the role of SOC effects. In Sec. III we show the common nonlinear features arising in the valence band from the LL coupling. The effective analytical model for the nonlinear ZS is presented in Sec. IV and, finally, we draw our conclusions in Sec. V.

II. EFFECTIVE G-FACTORS AND SPIN-ORBIT COUPLING EFFECTS

In order to evaluate the effective g-factors within the \( k \cdot p \) framework, we use the standard perturbative approach[23-25] that accounts for the coupling between different energy bands. Here we focus on the energy bands around the band gap at the \( \Gamma \)-point of WZ crystals, namely the conduction band (CB) and the top three valence bands, labeled A, B and C from highest to lowest energy. In Fig. II(a) we depict the bulk WZ band structure and identify the labels for the different energy bands. Within this \( k \cdot p \) perturbative approach, each band (two-fold degenerate) is described by an effective Zeeman term of the form

\[
H_{\text{ZS}}(B_\alpha) = \frac{\mu_B}{2} B_\alpha \tau_\alpha, \quad \alpha = x, y, z, \tag{1}
\]

in which the matrices \( \tau_\alpha \) are the Pauli matrices for the two-fold degenerate \( \Gamma \)-point states and the effective g-factor \( g_\alpha \) is obtained after evaluating

\[
g_\alpha \tau_{\alpha m}^{nm} = g_0 \sigma_{\alpha m} - \frac{1}{\hbar^2} \sum_{l \neq n,m} \frac{\Pi_{\alpha}^{l} \Pi_{\alpha m} - \Pi_{\alpha l} \Pi_{\alpha m}}{E_n - E_l}, \tag{2}
\]

with \( g_0 \) \((m_0)\) being the bare electron g-factor (mass), \( n, m \) being the states of a specific energy band at \( \Gamma \)-point, \( E_{n(l)} \) are the energy values at \( \Gamma \)-point and \( \{\alpha, \beta, \gamma\} = \{x, y, z\} \) \((\text{or cyclic permutations})\). The matrix elements of the Pauli matrices acting on the spin 1/2 are given by \( \sigma_{\alpha}^{ab} = \langle a | \sigma \beta | b \rangle \) and the matrix elements for the \( \Pi \) operator are given by \( \Pi_{\alpha}^{ab} = \langle a | \Pi \beta | b \rangle \), with the \( \Pi \) operator written as

\[
\Pi = \frac{\hbar}{m_0} \tilde{p} + \frac{\hbar^2}{4m_0 c^2} \left[ \hat{\sigma} \times \nabla V(\vec{r}) \right], \tag{3}
\]

in which the second term describes the SOC contribution. In Fig. II(b) we show the direction of magnetic fields with respect to the WZ crystal structure.

To compute the g-factors in Eq. (2) we must specify a particular \( k \cdot p \) Hamiltonian that contains the coupling among the different energy bands. For the CB, A, B and C bands including spin, the most general \( 8 \times 8 \) \( k \cdot p \) Hamiltonian that includes both orbital [1st term in Eq. (3)] and SOC [2nd term in Eq. (3)] terms is given in Ref. [32]. It is convenient to notice that the matrix elements \( \Pi_{\alpha}^{ab} \) can be easily obtained by looking at the Hamiltonian terms \( H_{kp}^{(1)} \) and \( H_{kSO}^{(1)} \) (shown in the Appendix B of Ref. [32]). Furthermore, an additional parameter present in the Hamiltonian is the k-independent SOC (\( \sim \left[ \nabla V(\vec{r}) \times \vec{p} \right] \cdot \hat{\sigma} \)) between conduction and valence bands denoted by \( \Delta_4 \) (sometimes also called \( \Delta_{sz} \)). The inclusion of \( \Delta_4 \) prevents the analytical diagonalization of the Hamiltonian at the \( \Gamma \)-point.

![Figure 1](image)

**Figure 1:** (Color online) (a) Schematic band structure for bulk WZ crystals around the \( \Gamma \)-point indicating the different energy bands: CB, A, B and C (from top to bottom). The energies at \( \Gamma \)-point are indicated by the arrows. (b) Scheme of the magnetic field configurations parallel (\( B_z \)) and perpendicular (\( B_x \)) to the NW axis in typical magneto PL experiments. The laser excitation and the collected PL signal are parallel to the NW axis. The inset shows the WZ crystal structure with the orientation of the c-axis in [0001] direction.

The most straightforward way to calculate the g-factors is to evaluate Eq. (2) numerically, especially if the Hamiltonian does not allow analytical solutions. However, to unambiguously identify the contribution of SOC, we present here the analytical expressions for CB and A band g-factors assuming \( \Delta_4 = 0 \), that allows the analytical diagonalization of the WZ Hamiltonian at the \( \Gamma \)-point (see Sec. II.B of Ref. [32] for instance). Rewriting the total g-factor of Eq. (2) as \( g_\alpha = g_0 + \frac{2m_0}{\hbar^2} (L_\alpha + \lambda_\alpha) \) we can identify the orbital contributions in \( L_\alpha \) and the SOC effects in \( \lambda_\alpha \). These terms for CB and A bands read:

\[
L_{xz}^{\text{CB}} = \sqrt{2} P_1 P_{2ab} \left( \frac{1}{\Delta_C} - \frac{1}{\Delta_B} \right), \tag{4}
\]

\[
\lambda_{xz}^{\text{CB}} = \frac{1}{\Delta_B} \left[ 2b \beta_1 \left( a \beta_1 - \sqrt{2} b \beta_2 \right) + b P_1 \left( 2b \beta_2 - \sqrt{2} a \beta_1 \right) + 2a^2 \beta_1 P_2 \right] + \frac{1}{\Delta_C} \left[ 2b \beta_1 \left( b \beta_1 + \sqrt{2} a \beta_2 \right) + a P_1 \left( 2a \beta_2 + \sqrt{2} b \beta_1 \right) + 2b^2 \beta_1 P_2 \right],
\]
\[ L_z^{\text{CB}} = P_2 \left( \frac{b^2}{\Delta_C} + \frac{a^2}{\Delta_B} - \frac{1}{\Delta_A} \right), \]  
\[ \lambda_z^{\text{CB}} = \frac{1}{\Delta_A} \beta_1 (2P_2 - \beta_1) + \frac{1}{\Delta_B} \left[ (a \beta_1 - \sqrt{2} b \beta_2)^2 + 2a P_2 (a \beta_1 - \sqrt{2} b \beta_2) \right] + \frac{1}{\Delta_C} \left[ (b \beta_1 + \sqrt{2} a \beta_2)^2 + 2b P_2 (b \beta_1 + \sqrt{2} a \beta_2) \right], \]  
\[ L_z^A = \frac{P_2}{\Delta_A} + 2A_7^2 \left( \frac{b^2}{\Delta_{AB}} + \frac{a^2}{\Delta_{AC}} \right), \]  
\[ \lambda_z^A = -\frac{1}{\Delta_A} (\beta_1^2 - 2\beta_1 P_2) + \frac{1}{\Delta_{AB}} \left[ (ba_1 + \sqrt{2} a \alpha_2)^2 - 2a A_7 (2a \alpha_2 + \sqrt{2} b a_1) \right] + \frac{1}{\Delta_{AC}} \left[ (a a_1 - \sqrt{2} b a_2)^2 + 2a A_7 (2b a_2 - \sqrt{2} a a_1) \right], \]

with the energy differences given by \( \Delta_A = E_{\text{CB}} - E_A, \) \( \Delta_B = E_{\text{CB}} - E_B, \) \( \Delta_C = E_{\text{CB}} - E_C, \) \( \Delta_{AB} = E_A - E_B \) and \( \Delta_{AC} = E_A - E_C. \) The values \( E_{\text{CB}}, E_A, E_B \) and \( E_C \) are the energies at \( \Gamma \)-point for the bands considered, as indicated in Fig. (1a). The \( a \) and \( b \) coefficients read \( a = \delta^2 / [\delta^2 + 2(\Delta_1)^2] \) and \( b = 2(\Delta_2)^2 / [\delta^2 + 2(\Delta_1)^2] \) with \( \delta = (\Delta_1 - \Delta_2) / 2 + \sqrt{(\Delta_1 - \Delta_2)^2 + 4(\Delta_3)^2}. \) The energy parameters \( \Delta_1, \Delta_2, \Delta_3 \) represent the crystal field splitting energy and the valence band SOC energies in WZ, respectively. The parameters \( P_1 \) and \( P_2 \) couple conduction and valence bands via the linear momentum operator, \( A_7 \) is the intra valence band coupling also mediated by \( \vec{p}, \beta_1 \) and \( \beta_2 \) are SOC terms between conduction and valence bands while \( \alpha_1 \) and \( \alpha_2 \) are SOC terms within the valence band only. For the precise definition of these couplings, please refer to the Appendix B of Ref. [36].

The SOC corrections to the g-factors, shown in Eqs. (1)-(5), take into account the same parameters that control the spin splitting of the energy bands (see for instance Eq. (10) in Ref.[34] for the CB spin splitting parameters). Therefore, since the spin splittings of the energy bands are different (either in magnitude or \( k \)-dependence), so are the SOC corrections to the g-factors. We point out that \( g_{x}^* \) is not shown simply because it is zero due to the symmetry of the A bands (they do not couple via the \( \Pi_x \) operator to any other band and their different spin projections also do not couple by \( \sigma_x \)). Furthermore, we emphasize that by removing the SOC contribution (setting \( \lambda_0 = 0 \)) we recover the known result for the conduction band presented by Hermann and Weissbuch.

Now we turn to the calculated values of the effective g-factors for InP, InAs, and GaAs WZ. For InP and InAs we used the parameters (which contain SOC effects) available in Ref. [36] and for GaAs we used the parameters (without any SOC effects) from Ref. [39]. We emphasize here that the SOC effects we refer to in the \( k \cdot p \) Hamiltonians are related to the terms that contribute to the g-factor as shown in Eqs. (11) and (12) and the additional interband k-independent SOC term \( \Delta_1 \). Furthermore, in both \( k \cdot p \) models\[26,28,32\] the usual SOC in the valence band is included via the parameters \( \Delta_2 \) and \( \Delta_3 \). In Table I we show the calculated g-factors in the absence of SOC and with SOC (if the \( k \cdot p \) model allows). As a general trend, \( g_x = g_y \neq g_z \) (highlighting the anisotropy of the WZ structure), and the valence bands have larger g-factors (in absolute value) than the CB. Taking into account the SOC effects, only available for InP and InAs, we notice that their correction to the g-factor values are, in general, not negligible and with values within the typical experimental precision. For instance, the influence of SOC can reach contributions of \( \sim 20\% \) in CB g-factors. It is also worth mentioning the g-factors for ZB phase. Restricting ourselves to the CB, the most commonly investigated case, the ZB g-factor is \( g^x = 1.26 \) for InP, \( g^y = -14.9 \) for InAs and \( g^z = -0.44 \) for GaAs (with values taken from Ref. [40]). We notice that indeed the effective g-factor values are quite different for ZB and WZ crystal phases.

Let us now compare our theoretical g-factor values to experiments. In Table II we compare our calculated WZ g-factors with the available magneto PL experimental data for InP and GaAs NWs (with diameters large
enough to be considered a bulk system). Let us first discuss the InP case. For both $g^{CB}_{z}$ and $g^{CR}_{z} - g^{A}_{z}$, our calculated values including the SOC contributions provide an excellent agreement to the reported experimental values. We also point out the apparent inconsistency between the two experimental $g$-factors by showing the range of magnetic field used in the fitting. Since for magnetic fields along the z direction the ZS is nonlinear, the larger the range used in the fitting the smaller the $g$-factors will be in order to account for the sublinear features. Therefore, we emphasize that $g$-factors should be fitted only at the limit of small magnetic fields where the linear regime holds. For GaAs, although the comparison for $g^{CB}_{z}$ looks reasonable, the theoretical value obtained for $g^{CR}_{z} - g^{A}_{z}$ is nearly twice as large as the experimental value. This clearly indicates that the $k \cdot p$ parameters for GaAs are not completely consistent and further theoretical efforts are required to build a more realistic model.

### Table II: Comparison between calculated and experimental values of the effective $g$-factors.

| Material | Experimental Ref. | $g^{CB}_{z}$ | $g^{CR}_{z} - g^{A}_{z}$ |
|----------|--------------------|--------------|--------------------------|
| InP      | Ref. [22]          | 1.3          | 4.4$^a$                  |
|          | Ref. [1]           | 1.4          | 3.4$^b$                  |
|          | Ref. [36] (with SOC) | 1.29        | 4.66                     |
|          | Ref. [36] (no SOC) | 1.72         | 5.26                     |
| GaAs     | Ref. [39] (no SOC) | 0.28$^c$     | 5.4$^d$                  |

$^a$fitting up to 5 T  
$^b$fitting up to 15 T  
$^c$Ref. [5], fitting up to 0.4 T  
$^d$Ref. [6], fitting up to 15 T (still linear regime)

Although there is, to the best of our knowledge, no magneto PL reported in pure InAs WZ NWs, it is important to mention that this material has recently been investigated in several transport experiments\textsuperscript{13,14,32,41}. Specifically, the conductance experiments by Vaitiekėnas et al.\textsuperscript{32} using 100 nm InAs WZ NWs showed that for negative gate voltages the effective $g$-factor of CB electrons saturates to $|g^*| \sim 5$. This is significantly different from the bulk InAs ZB value of $g^* = -14.9$ but much closer to our calculated value for InAs WZ of $g^{CB}_{z} = -6.23(-5.33)$ with (without) SOC effects. Furthermore, the recent theoretical analysis of ZB NWs by Winkler et al.\textsuperscript{13} showed that orbital effects play a large role in the effective $g$-factors of different subbands. However, the lowest subband still retains much of the bulk information, especially at 100 nm (see for instance Figs.(b),(d) in Ref. \textsuperscript{19}). Although our theoretical value for the InAs WZ $g$-factor seems consistent with recent experiments and, more importantly, it is substantially different than the ZB value, further investigations that account for the electrostatic environment and quantum confinement in WZ NWs are still required, as pointed out in the conclusions of Ref. \textsuperscript{32}.

### III. NONLINEAR FEATURES IN LANDAU LEVELS

Following the theoretical approach discussed in Ref. \textsuperscript{22} to model the nonlinear ZS of InP WZ, we show in this section that indeed such nonlinear features are a common trend and also appear in the LLs of InAs and GaAs WZ. To calculate the LLs, we use the general description of an external magnetic field within the $k \cdot p$ framework which considers the envelope function approximation (EFA), combined with the minimal coupling and the Zeeman term\textsuperscript{35,42,43}. The mathematical procedure of the EFA leads to the general Hamiltonian

\begin{equation}
H = H_{\text{bulk}} \left\{ \vec{k} \rightarrow -i \vec{\nabla} + \frac{e}{\hbar} \vec{A}(\vec{r}) \right\} + g_0 \frac{\mu_B}{2} \vec{\Sigma} \cdot \vec{B},
\end{equation}

in which $H_{\text{bulk}}(\vec{k})$ is the $k \cdot p$ bulk Hamiltonian, the replacement $\vec{k} \rightarrow -i \vec{\nabla} + \frac{e}{\hbar} \vec{A}(\vec{r})$ takes into account the EFA procedure, $g_0$ is the bare electron $g$-factor and $\vec{\Sigma}$ is a vector of the Pauli matrices describing the Zeeman term for the spins of the bulk Bloch functions\textsuperscript{35,42,43}. By choosing the vector potential with a single spatial dependence, we can solve the Hamiltonian \textsuperscript{(7)} numerically by introducing the finite differences approach\textsuperscript{44}, similar to a quantum well treatment. The solution provides the LL spectra of the system, with energies denoted by $E_\lambda(k_B, k_A)$ and wave functions

\begin{equation}
\psi_{\lambda,k_B,k_A}(\vec{r}) = \frac{e^{i(k_B \vec{r} + k_A \vec{r}_A)}}{\sqrt{\Omega}} \sum_l f_{\lambda,k_B,k_A,l}(\rho) u_l(\vec{r}),
\end{equation}

in which $\lambda$ is the LL label, $f_{\lambda,k_B,k_A,l}(\rho)$ is the envelope function, the summation in $l$ runs over the bulk basis states denoted by $u_l(\vec{r})$, $\Omega$ is the area of the system perpendicular to the confinement direction, $k_B$ is the wave vector parallel to the magnetic field, $k_A$ is parallel to the vector potential and the spatial dependence of the vector potential is denoted by the coordinate $\rho$. For the two directions of magnetic field investigated here [indicated in Fig. \textsuperscript{11}b)], we have $\vec{B} = B_\perp \vec{z} \Rightarrow \vec{A} = B y \hat{z}, k_B = k_z, k_A = k_z, \rho = y$ and $\vec{B} = B_\parallel \vec{z} \Rightarrow \vec{A} = B x \hat{y}, k_B = k_x, k_A = k_y, \rho = x$. To simplify the notation we use $\vec{B} = B \hat{z}$ as $B_x$ and $\vec{B} = B \hat{z}$ as $B_z$ in the remainder of the paper. We note that in experimental papers\textsuperscript{16,21,22}, $B_x$ and $B_z$ are typically called Voigt and Faraday configurations, respectively. For the numerical implementation of the Hamiltonian \textsuperscript{41} we considered the system to have a size of $L = 200$ nm with 401 discretization points (with approximately 1 point every 0.5 nm). For InP and InAs we used the bulk $8 \times 8$ $k \cdot p$ model from Ref. \textsuperscript{39} and for GaAs we used the $6 \times 6$ $k \cdot p$ model from Ref. \textsuperscript{39}.

Due to the coupling of the A and B bulk energy bands
induced by the external magnetic field, the valence band LLs show a markedly nonlinear behavior\textsuperscript{22}. This common feature can be seen in Figs. 2(a)-(c) for InP, InAs and GaAs, respectively. We notice the clear nonlinear features in the different LLs whenever the B band mixing is present (indicated by the color code). Although for the B\textsubscript{x} configuration this mixing is drastically reduced, partially because of the zero g-factor of the A band, the A-B mixing is indeed responsible for the slight nonzero ZS observed. As revealed in Ref. \textsuperscript{22}, the topmost LL (with branches indicated by 1+ and 1- in Fig. 2) provides the main contribution to the excitonic effects and therefore the nonlinear features in the magneto PL for the B\textsubscript{x} configuration originate from the mixing of A and B valence bands. We point out here that although the 6\times6 Hamiltonian for GaAs WZ\textsuperscript{39} is not sufficient to describe the linear Zeeman splitting correctly, since the P\textsubscript{1} and P\textsubscript{2} parameters are not included, the nonlinear features in the LLs are clearly visible. In fact, this is an additional support to the fact that these nonlinear features are beyond the linear g-factor approach, which is mainly ruled by the P\textsubscript{1} and P\textsubscript{2} parameters as shown in Eqs. \textsuperscript{4}–\textsuperscript{6}.

Figure 2: (Color online) (a) Calculated Landau level spectra for the A band at k\textsubscript{F} = k\textsubscript{F} = 0 as function of the magnetic field for (a) InP, (b) InAs and (c) GaAs. The color code indicates the contribution of the B valence band to the total state. The upper (lower) branch of the topmost LL is indicated by the 1+ (1-). We denote with positive (negative) values in the x-axis the magnetic field configuration B\textsubscript{x} along z (B\textsubscript{x} along x) direction.

In order to complete our analysis of the common nonlinear features of the valence band, we now discuss how the LL coupling manifests in the envelope functions. We show in Fig. 3 the probability density of the envelope functions for the topmost LL (the 1+ and 1- branches shown in Fig. 2) in both magnetic field configurations at 30 T. Due to the interplay of the WZ symmetry and the external magnetic field, the mixing of A and B bands has a peculiar form that couples envelope functions with different numbers of nodes, i.e., 0 node for A bands and 2 nodes for B bands (further details on this coupling can be found in Ref. \textsuperscript{22} and its Supplemental Material). In fact, due to strong SOC in InAs we also notice the contribution of B states with 1 node, see Figs. 3(f) and 3(h). Moreover, for the B\textsubscript{y} configuration the coupling between envelope functions is spin dependent, which means that the nonlinear feature is associated to one specific type of circular polarization (due to the conservation of angular momentum, spins in conduction and valence band define the allowed transitions of circularly polarized light\textsuperscript{16,46}). Indeed, this is exactly the case observed in recent magneto PL experiments in InP WZ\textsuperscript{22} that identified a strong nonlinear feature arising for a specific circular polarization of the PL spectra. On the other hand for the B\textsubscript{x} configuration, both spin components contribute equally.

Figure 3: (Color online) Probability density of the envelope functions at 30 T for the first LL (indicated by the labels 1+ and 1- in Fig. 2) along B\textsubscript{x} and B\textsubscript{y} for (a-d) InP, (e-h) InAs and (i-l) GaAs. The B band envelope functions are multiplied by a factor of 8, as indicated in the legend. The spin notation for the energy bands is identified with respect to the leading contribution of the bulk basis states\textsuperscript{15}.
and, as a consequence, the output light cannot be resolved in different circular polarizations.

IV. EFFECTIVE MODEL FOR THE NONLINEAR ZEEMAN SPLITTING

Based on the LL calculations, we showed that the physical mechanism behind the nonlinear ZS in the valence band is a common feature in WZ materials due to the mixing of A and B bands induced by magnetic field. It would be valuable to incorporate these features in an analytical expression that could be used to fit the experimental data beyond the linear ZS regime. In order to capture the nonlinear effects present in the LL branch with spin up, we can restrict ourselves to the important contributions of the A-B mixing by using the basis set \{f_{0,\uparrow} A\}, \{f_{2,\downarrow} \}, \{B\}, in which the subindices 0 and 2 refer to the number of nodes in the envelope functions.

\[
E_{A\uparrow}(B) = \frac{1}{2} \left[ E_B + \frac{\mu_B}{2} B g + d_B + \sqrt{\left( E_B - \frac{\mu_B}{2} B g - d_B \right)^2 + 4d_{AB}^2 B^2} \right],
\]

with \(g = g_A \pm g_B\) and \(d_B = d_A \pm d_B\). For the A\downarrow branch that does not couple to any other states, unlike A\uparrow, we have simply the linear dependence in B, i.e.,

\[
E_{A\downarrow}(B) = -\frac{\mu_B}{2} B g_A + B d_A,
\]

in which the first term is related to the ZS, with opposite sign in the g-factor as compared to the A\uparrow branch and the second term is spin-independent with the same form as the A\uparrow branch.

In order to model the ZS obtained from the experimental PL peaks, we must take into account not only the ZS of valence but also of the conduction band, since they are coupled via the optical transition. The total ZS can be written as the difference of the ZS of the conduction and valence bands, i.e., \(Z_{\text{CB}} = Z_{\text{A}} + Z_{\text{B}}\). For the conduction band we can use the linear g-factor ZS, \(Z_{\text{CB}} = \mu_B B g_{\text{CB}}\), and for the A band we use \(Z_{\text{A}} = E_{A\uparrow}(B) - E_{A\downarrow}(B)\) [shown in Eqs. (10) and (11)]. Finally, the total ZS is given by

\[
ZS(B) = \mu_B B \left( g_{\text{CB}}^2 - g_A^2 \right) - \frac{1}{2} \left[ E_B - \frac{\mu_B}{2} B g - d_B + \sqrt{\left( E_B - \frac{\mu_B}{2} B g - d_B \right)^2 + 4d_{AB}^2 B^2} \right],
\]

in which the unknown parameters are only \(d_B\) and \(|d_{AB}|\) if we assume the values for the effective g-factors and the energy separation of A and B bands given by theory or found experimentally by other means. We emphasize that if we set the coupling parameter \(d_{AB}\) to zero in Eq. (12), we recover the linear ZS already established in the literature by Refs. [23,24]. Furthermore, if we set the energy separation of A and B bands to zero (\(E_B \rightarrow 0\), then all the terms in Eq. (12) become linear in the magnetic field and the nonlinearities vanish. This condition would be equivalent to the case of ZB crystals that have degenerate heavy and light hole bands at the \(\Gamma\)-point and therefore would present a linear ZS (see for instance the experimental ZS of InP ZB in the Supplemental Material of Ref. [22]).

Applying the effective analytical ZS of Eq. (12) to the magneto PL data of InP [23,24] and GaAs [25], we show in Fig. 4 that this model successfully captures the experimental trends, particularly for InP WZ. In the fitting, we assumed the g-factors and energy separations to be known from theory and obtained the values for \(d_B\) and \(|d_{AB}|\) (given in the caption of Fig. 4). For GaAs we notice that the fitted parameters \(d_B\) and \(|d_{AB}|\) are nearly one order of magnitude larger than the values obtained for InP. We assign this feature to the overestimation of the GaAs g-factors in comparison with the experimental data in the
Figure 4: (Color online) Comparison between the fitting of Eq. (12) to the experimental Zeeman splitting for (a) InP and (b) GaAs. We use the calculated g-factors of Table I and the theoretical values of $E_0 = -35.4$ meV for InP and $E_0 = -99.4$ meV for GaAs. The fitting procedure provides $d_\perp = 0.16$ meV/T, $|d_{AB}| = 0.43$ meV/T for InP and $d_\perp = 17.63$ meV/T, $|d_{AB}| = 2.82$ meV/T for GaAs. The experimental data for InP is taken from Ref. [22] and for GaAs from Ref. [23].

linear regime, shown in Table II. We emphasize that it is beyond the scope of this study to provide reliable interband couplings of GaAs WZ since additional theoretical efforts are required, such as ab initio calculations with the correct conduction band ordering and a proper fitting of the $k \cdot p$ parameters, possibly including the SOC effects. Finally, we show that extrapolating our fitted curve up to 40 T, we observe that the ZS of InP reaches a maximum value and then starts to decrease. This indicates that the nonlinear features act as a limiting factor to the maximum ZS that can be observed. For GaAs, this feature is not visible due to the overestimated g-factors. Therefore, additional experimental data at magnetic fields higher than 30 T could provide useful insight and also test the limits of the effective model presented in this study.

V. CONCLUSIONS

In summary, we theoretically investigated the common features of the Zeeman splitting in novel III-V wurtzite materials, namely InP, InAs and GaAs, using the $k \cdot p$ method. Specifically, we calculated the effective g-factors for the important energy bands around the band gap at the Γ-point (CB, A, B and C) and showed that spin-orbit coupling effects have appreciable contribution to the total g-factor values (contributing up to $\sim 20\%$ of CB, for instance). Our calculated values for InP and InAs g-factors are in very good agreement with the available experimental values. Within the Landau level picture, following the prescription of Ref. [22], we showed that the nonlinear Zeeman splitting for the $B_\parallel$ direction is a common feature of wurtzite materials due to the mixing of A and B valence bands induced by the external magnetic field. Relying on the main mechanism behind the origin of this nonlinear feature allowed us to develop an effective analytical description of the Zeeman splitting that describes the experimental data with very good agreement, particularly for InP WZ. By extrapolating our fitted model, we found that the nonlinear Zeeman splitting reaches a maximum value that could be investigated experimentally under magnetic fields higher than 30 T.

Furthermore, our study shows that the $k \cdot p$ approach is very versatile but it requires reliable parameter sets for quantitative comparison with the experimental data. For instance, the calculated g-factors we presented for GaAs do not provide a good description of the experimental data, indicating that further theoretical efforts in extracting reliable $k \cdot p$ parameters are needed. With the ongoing interest in these novel III-V WZ materials, with recent reports on high-quality samples of GaP and GaSb, we believe our findings could guide future experiments and motivate further theoretical efforts to characterize these materials.

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1. M. De Luca, A. Polimeni, H. A. Fonseka, A. J. Meaney, P. C. M. Christianen, J. C. Maan, S. Paiman, H. H. Tan, F. Mura, C. Jagadish, and M. Capizzi, Nano Lett. 14, 4250 (2014).

2. D. Tedeschi, M. De Luca, A. Granados del Águila, Q. Gao, G. Ambrosio, M. Capizzi, H. H. Tan, P. C. M. Christianen, C. Jagadish, and A. Polimeni, Nano Lett. 16, 6213 (2016).

3. M. Möller, M. M. de Lima Jr., A. Cantarero, T. Chiaramonte, M. A. Cotta, and F. Ikawa, Nanotechnology 23, 375704 (2012).

4. M. B. Rota, A. S. Ameruddin, H. A. Fonseka, Q. Gao, F. Mura, A. Polimeni, A. Miriametro, H. H. Tan, C. Jagadish and M. Capizzi, Nano Lett. 16, 5197 (2016).

5. S. Furthmeier, F. Dirnberger, M. Gmitra, A. Bayer, M. Forsch, J. Hubmann, C. Schüller, E. Reiger, J. Fabian, T.
Korn, and D. Bougeard, Nature Commun. 7, 12413 (2016).
6 M. De Luca, S. Rubini, M. Felici, A. Meaney, P. C. M. Christianen, F. Martelli, and A. Polimeni, Nano Lett. 17, 6540 (2017).
7 V. Dubrovskii, G. Cirlin, and V. Ustinov, Semiconductors 43, 1539 (2009).
8 P. Caroff, K. A. Dick, J. Johansson, M. E. Messing, K. Depertt, and L. Samuelson, Nat. Nanotechnol. 4, 50 (2009).
9 I. Vurgaftman, J. R. Meyer and L. R. Ram-Mohan, J. Appl. Phys. 89, 5815 (2001).
10 I. Zutić, J. Fabian, and S. Das Sarma, Rev. Mod. Phys. 76, 23 (2004).
11 R. M. Lutchyn, J. D. Sau, and S. Das Sarma, Phys. Rev. Lett. 105, 077001 (2010).
12 Y. Oreg, G. Refael, and F. von Oppen, Phys. Rev. Lett. 105, 177002 (2010).
13 A. Das, Y. Ronen, Y. Most, Y. Oreg, M. Heiblum and H. Shtrikman, Nat. Phys. 8, 887 (2012).
14 S. Albrecht, A. Higginbotham, M. Madsen, F. Kuemmeth, Y. Oreg, G. Refael, and F. von Oppen, Phys. Rev. Lett. 121, 037703 (2018).
15 J.-Y. Chen, T.-M. Wong, C.-W. Chang, C.-Y. Dong, and Y.-F. Chen, Nat. Nanotechnol. 9, 845 (2014).
16 P. E. Faria Junior, G. Xu, Y.-F. Chen, G. M. Sipahi, and I. Zutić, Phys. Rev. B 95, 115301 (2017).
17 M. Kammermeier, P. Wenk, F. Dirnberger, D. Bougeard and J. Schliemann, Phys. Rev. B 98, 035407 (2018).
18 F. Dirnberger, M. Kammermeier, J. König, M. Forsch, P. E. Faria Junior, T. Campos, J. Fabian, J. Schliemann, C. Schüller, T. Korn, P. Wenk, and D. Bougeard. arXiv:1809.08009 (2018).
19 G. W. Winkler, D. Varjas, R. Skolasinski, A. A. Soluyanov, M. Troyer, and M. Wimmer, Phys. Rev. Lett. 119, 037701 (2017).
20 T. Campos, P. E. Faria Junior, M. Gmitra, G. M. Sipahi and J. Fabian, Phys. Rev. B 97, 245402 (2018).
21 M. De Luca, A. Polimeni, M. Capizzi, A. J. Meaney, P. C. M. Christianen, J. K. Maan, F. Murra, S. Rubini, and F. Martelli, ACS Nano 7, 10717 (2013).
22 D. Teodesi, M. De Luca, P. E. Faria Junior, A. Granados del Águila, Q. Gao, H. H. Tan, B. Scharf, P. C. M. Christianen, C. Jagadish, J. Fabian and A. Polimeni, arXiv:1811.04922 (2018).
23 K. Cho, Phys. Rev. B 14, 4463 (1976).
24 H. Venghaus, S. Suga and K. Cho, Phys. Rev. B 16, 4419 (1977).
25 V. Jovanov, T. Eisfeller, S. Kapfinger, E. C. Clark, F. Klotz, M. Bichler, J. G. Keizer, P. M. Koenraad, M. S. Brandt, G. Abstreiter, and J. J. Finley, Phys. Rev. B 85, 165433 (2012).
26 D. Y. Oberli, Phys. Rev. B 85, 155305 (2012).
27 R. Kotlyar, T. L. Reinecke, M. Bayer, and A. Forchel, Phys. Rev. B 63, 085310 (2001).
28 M. V. Durnev, M. M. Glazov, and E.L. Ivchenko, Physica E 44, 797 (2012).
29 A. Mishra, L. V. Titova, T. B. Hoang, H. E. Jackson, L. M. Smith, J. M. Yarrison-Rice, Y. Kim, H. J. Joyce, Q. Gao, H. H. Tan, and C. Jagadish, Appl. Phys. Lett. 91, 263104 (2007).
30 P. E. Faria Junior and G. M. Sipahi, J. Appl. Phys. 112, 103716 (2012).
31 L. C. O. Dalac and A. Cantarero, Sci. Rep. 6, 33914 (2016).
32 S. Vaitiekūnas, M. T. Deng, J. Nygård, P. Krogstrup, and C. M. Marcus, Phys. Rev. Lett. 121, 037703 (2018).
33 L. M. Roth, B. Lax, and S. Zwerdling, Phys. Rev. Lett. 114, 90 (1959).
34 C. Herrmann and C. Weisbuch. Phys. Rev. B 15, 823 (1977).
35 L. C. Lew Yan Voon, M. Willatzen, The k · p method: electronic properties of semiconductors (Springer, Berlin, 2009).
36 P. E. Faria Junior, T. Campos, C. M. O. Bastos, M. Gmitra, J. Fabian and G. M. Sipahi, Phys. Rev. B 93, 235204 (2016).
37 J. Y. Fu and M. W. Wu, J. Appl. Phys. 104, 093712 (2008).
38 S. L. Chuang and C. S. Chang, Phys. Rev. B 54, 2491 (1996).
39 T. Cheiwchanchamnanji and W. R. Lambrecht, Phys. Rev. B 84, 035203 (2011).
40 R. Winkler, Spin-orbit Coupling Effects in Two-Dimensional Electron and Hole Systems, (Springer, New York, 2003).
41 A. Iorio, M. Rocci, L. Bours, M. Carrega, V. Zannier, L. Sorba, S. Roddaro, F. Giazotto and E. Strambini, arXiv:1807.03341 (2018).
42 C. E. Pryor and M. E. Flätté, Phys. Rev. Lett. 96, 026804 (2006).
43 J. van Bree, A. Yu, Silov, P. M. Koenraad, M. E. Flatté, and C. E. Pryor, Phys. Rev. B 85, 165233 (2012).
44 S. L. Chuang and C. S. Chang, Semicond. Sci. Technol. 12, 252 (1997).
45 Here we denote the bulk basis states as \{|c_1\rangle, \ldots, |c_8\rangle\}, representing the Bloch functions at Γ-point without SOC interaction. From these 8 states, 1-6 represent the valence band and 7-8 the conduction band. Regarding spin 1/2 projections, the states 1,2,3 and 7 have spin up, while 4,5,6 and 8 have spin down. The bulk energy bands with SOC (the so-called CB, A, B and C) are now described as a mixing of the 8 basis states. Here, we use the following convention: CB ⇒ (c_8), A ⇒ (c_7), B ⇒ (c_6) refers to the contribution of c_7 (c_8), A ⇒ (c_4), B ⇒ (c_3) refers to the contribution of c_3 (c_4). For the details of the basis states, please refer to Refs. 26,38.