Magnetic field implementation in multiband $k \cdot p$ Hamiltonians of holes in semiconductor heterostructures

J Planelles and J I Climente

Departament de Quimica Fisica i Analitica, Universitat Jaume I, Box 224, E-12080 Castelló, Spain

E-mail: josep.planelles@uji.es

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Abstract

We propose an implementation of external homogeneous magnetic fields in $k \cdot p$ Hamiltonians for holes in heterostructures, in which we make use of the minimal coupling prior to introducing the envelope function approximation. Illustrative calculations for holes in InGaAs quantum dot molecules show that the proposed Hamiltonian outperforms the standard Luttinger model (Luttinger 1956 Phys. Rev. 102 1030) describing the experimentally observed magnetic response. The present implementation culminates our previous proposal (Planelles et al 2010 Phys. Rev. B 82 155307).

(Some figures may appear in colour only in the online journal)

1. Introduction

The interaction of a magnetic field with a charged particle with spin comes into the Hamiltonian through coupling to the total (orbital plus spin) angular momentum. In crystals, the total angular momentum is the sum of the Bloch angular momentum, which contains atomic orbital and spin contributions, and the envelope orbital angular momentum [1, 2]. Determining the coupling constant ($g$ factor) is an important requirement for the study of the magnetic properties of materials. In bulk systems, the value of the $g$ factor is strongly influenced by band mixing, spin–orbit interaction and crystal anisotropy [3].

In recent years, there has been an increasing interest in controlling and exploiting the $g$ factor of carriers confined in semiconductor quantum dots (QDs) for spin preparation, conservation and manipulation aiming at spintronic and quantum information devices [4–9]. The magnetism of these structures is significantly different from that of bulk crystals because the weak magnetic confinement is supplemented by a strong spatial confinement. The latter has a profound effect on the energy structure, carrier–carrier interactions, band mixing and spin–orbit interactions [10], which, in turn, influence the $g$ factor value. As a matter of fact, it has been shown that quantum confinement in QDs leads to strongly anisotropic $g$ factors for both electrons and holes [11–13], as well as to a quenching of the $g$ factor value [14, 15].

To date, the majority of theoretical studies investigating the magnetic response of QDs rely either on effective mass and $k \cdot p$ models [10] or on effective band orbital models (EBOM) [16]. The standard inclusion of magnetic fields in $k \cdot p$ Hamiltonians consists in replacing the canonical momentum $p$ by the kinetic momentum $p - qA$, supplemented with the spin Zeeman term, in the differential equation fulfilled by the envelope function (here $q$ is the carrier charge and $A$ the potential vector defining the magnetic field) [17–20]. This approximation, hereafter referred to as the Luttinger approximation, has been successful in explaining several experimental observations in heterostructures [10, 21, 22], it is implemented in the widely employed semiconductor software package nextnano [23, 24], and it is currently being used to determine the $g$ factors of confined carriers [14, 24, 25]. However, a number of situations have been identified where it provides qualitatively incorrect predictions. For example, in quantum rings under axial magnetic fields, amongst the methods used to describe the electronic structure of QDs, EBOM is the closest one to $k \cdot p$. However, it incorporates the magnetic field by means of Peierls phase factors in the matrix elements, while the Zeeman effect is included by adding the spin terms to the diagonal matrix elements. In $k \cdot p$ it just comes into the differential equation. Thus, a direct comparison of the $k \cdot p$ implementations we discuss here to EBOM cannot be properly done.
the Luttinger approximation predicts the optical gap to decrease with the field strength [26], contrary to magneto-
photoluminescence observations [27]. Similarly, in vertically coupled QDs, the Luttinger approximation predicts that an axial magnetic field can tune the hole tunneling rate [28], but this effect is not observed in related experiments [29]. The underlying reason is that the Luttinger approximation includes off-diagonal magnetic terms in the Hamiltonian, which artificially enhance the heavy hole–light hole (HH–LH) band mixing [26, 29].

In [30], an alternative formulation of the magnetic interaction was suggested, in which the replacement of the canonical momentum by the kinetic one is carried out prior to the envelope function approximation (EFA). The resulting Hamiltonian has no off-diagonal magnetic terms directly coupling HH and LH, and the results then become consistent with the experimental measurements [26, 29]. The reason for the discrepancy between the Luttinger and this alternative formulation is related with the non-commutativity of the components of the momentum operator $p$ in the presence of magnetic field [31].

In the present work, we extend the theory of [30] in order to account for the spin Zeeman term, and identify the coefficients that should accompany the magnetic terms in this approximation, which are pending clarification [29]. The remote band influence is considered through the zero-field approximation, which are pending clarification [29]. The underlying reason is that the Luttinger approximation predicts the optical gap to decrease with the field strength [26], contrary to magneto-
photoluminescence observations [27]. Similarly, in vertically coupled QDs, the Luttinger approximation predicts that an axial magnetic field can tune the hole tunneling rate [28], but this effect is not observed in related experiments [29]. The underlying reason is that the Luttinger approximation includes off-diagonal magnetic terms in the Hamiltonian, which artificially enhance the heavy hole–light hole (HH–LH) band mixing [26, 29].

2. Theory

2.1. The Hamiltonian

The classical Hamiltonian of a charged particle subject to the action of a magnetic field defined by a potential vector $A$ is

$$\mathcal{H} = \frac{\pi^2}{2m} = \frac{(p - q A)^2}{2m},$$

where $p$ is the canonical momentum, $q$ the charge and $m$ the mass.

If the charged particle has anisotropic mass response to external forces, by employing the notation $\bar{\pi}_i = \frac{\pi_i}{\sqrt{m_i}}$, the Hamiltonian reads as

$$\mathcal{H} = \frac{\bar{\pi}^2}{2} = \sum_i \frac{\pi_i^2}{2m_i} = \sum_i \frac{(p_i - q A_i)^2}{2m_i},$$

where $m_i, i = x, y, z$ is the anisotropic mass.

Elemental particles, in addition to charge, have spin. In the presence of magnetic field, spin introduces an extra Zeeman term, so that the kinetic energy (1) turns into

$$\mathcal{H}_D = \frac{(p - q A)^2}{2m} - \frac{qh}{2m} \sigma \cdot B,$$

where $\sigma$ is a vector which components are the Pauli matrices and $B = \nabla \times A$ is the magnetic field.

Starting from equation (1) we can introduce heuristically spin by making the formal replacement $\pi \to \sigma \cdot \pi$ (i.e., replacing $\pi^2$ by $(\sigma \cdot \pi)^2$ in equation (1)) and taking into account the next identity involving vectorial operators and Pauli matrices:

$$(\sigma \cdot a)(\sigma \cdot b) = a \cdot b + i\sigma \cdot (a \times b),$$

which, in the case $a = b = \pi = (p - q A)$, turns into

$$(\sigma \cdot \pi)/(\sigma \cdot \pi) = \pi^2 + i\sigma \cdot (\pi \times \pi) = (p - q A)^2 - qh\sigma \cdot B,$$

the last equality coming from

$$\pi \times \pi = (p - q A) \times (p - q A) = -q(p \times A + A \times p) = iqh\nabla \times A = iqhB.$$ 

We see then that (3) may come from (1) by means of the formal replacement $\pi \to \sigma \cdot \pi$.

If the mass is anisotropic, we should start from (2) and carry out the formal replacement $\bar{\pi} \to \sigma \cdot \bar{\pi}$. The analogue of the mixed product in (5) now reads as

$$\sigma \cdot (\bar{\pi} \times \bar{\pi}) = \sigma_x \frac{1}{\sqrt{m_x m_z}} [\pi_y, \pi_z] + \sigma_y \frac{1}{\sqrt{m_y m_z}} [\pi_x, \pi_z] + \sigma_z \frac{1}{\sqrt{m_y m_x}} [\pi_x, \pi_y],$$

where $[\pi_x, \pi_y] = \pi_x \pi_y - \pi_y \pi_x$.

We may define $\bar{\sigma}$ with components $\tau_{ij} = \sigma_i \tau_j$, where $i, j$ represent a cyclic permutation of $x, y, z$. Then, using (7) we may write that $\sigma \cdot (\bar{\pi} \times \bar{\pi}) = \bar{\sigma} \cdot (\pi \times \pi)$. Now, by employing (6) we have

$$i\sigma \cdot (\bar{\pi} \times \bar{\pi}) = i\bar{\sigma} \cdot (\pi \times \pi) = -qh\bar{\sigma} \cdot B,$$

and then

$$(\sigma \cdot \bar{\pi})(\sigma \cdot \pi) = \pi^2 - qh\sigma \cdot B,$$

showing that by means the formal replacement $\bar{\pi} \to \sigma \cdot \bar{\pi}$ Hamiltonian (2) turns into

$$\mathcal{H}_D = \sum_i \frac{(p_i - q A_i)^2}{2m_i} - \frac{qh}{2} \sigma \cdot B.$$
operator acting on the envelope vector function can be written as:

\[ \mathcal{H} = \sum_{\alpha = \pm, \zeta} (p_{\alpha} - q A_{\alpha}) \frac{1}{2m_{\alpha}} (p_{\alpha} - q A_{\alpha}) - \frac{q h}{2m_{\parallel}} \sigma_{z} B_{0}, \]

By employing the symmetric gauge \( A = \frac{B_{0}}{z} [-y, x, 0] \), we see that \( A_{\perp} = 0 \). Then, the \( z \) component of the kinetic energy is not affected by the field, \( T_{z} = p_{\perp} \frac{1}{2m_{\perp}} p_{\perp} \), while the in-plane component is

\[ T_{\perp} = p_{\perp} \frac{1}{2m_{\perp}} p_{\perp} + \frac{q^{2}A_{\perp}^{2}}{2m_{\perp}} - \frac{q A_{\perp}}{2m_{\perp}} \cdot p_{\perp} = -\hbar^{2} \nabla_{\perp} \cdot 1 \frac{q^{2}B_{0}^{2}\rho^{2}}{8m_{\perp}} \]

Since \( m_{\perp}(\rho, z) \), then \( p_{\perp} \frac{1}{m_{\perp}} = -\hbar^{2} \rho \left( \frac{\partial}{\partial \rho} \right) \frac{1}{m_{\perp}} \) and \( p_{\perp} \cdot A_{\perp} = \frac{A_{\perp}}{m_{\perp}} \cdot \rho \psi, \) so that the in-plane component of the kinetic energy is

\[ T_{\perp} = p_{\perp} \frac{1}{2m_{\perp}} p_{\perp} + \frac{q^{2}A_{\perp}^{2}}{2m_{\perp}} - \frac{q m_{\perp}}{2m_{\perp}} A_{\perp} \cdot p_{\perp} = -\hbar^{2} \nabla_{\perp} \cdot \frac{q B_{0}}{2m_{\perp}} (\hat{\rho}_{y} - \rho_{y}) \]

and the complete Hamiltonian is in turn

\[ \mathcal{H} = -\sum_{\alpha = \pm, \zeta} \nabla_{\alpha} \cdot \frac{1}{2m_{\alpha}} \nabla_{\alpha} + \frac{q^{2}B_{0}^{2}\rho^{2}}{8m_{\perp}} - \frac{q B_{0}}{2m_{\perp}} \hat{L}_{z} - \frac{B_{0}}{2m_{\perp}} (\hat{L}_{z} + \sigma_{z}). \]

This equation particularized to effective electrons \( m > 0, q = -1 \) is

\[ \mathcal{H}_{e} = -\sum_{\alpha = \pm, \zeta} \nabla_{\alpha} \cdot \frac{1}{2m_{\alpha}} \nabla_{\alpha} + \frac{B_{0}^{2}\rho^{2}}{8m_{\perp}} + \frac{B_{0}}{2m_{\perp}} (\hat{L}_{z} + \sigma_{z}). \]

What about holes \( m = -|m| < 0, q = 1 \)? Holes are tricky particles that require care to tackle. We know that in the case of a one-band model, electron and hole energy dispersions are mirror images of each other. Thus, assume that

\[ \mathcal{H}_{h} = \sum_{\alpha = \pm, \zeta} \nabla_{\alpha} \cdot \frac{1}{2m_{\alpha}} \nabla_{\alpha} - \frac{B_{0}^{2}\rho^{2}}{8m_{\perp}} - \frac{B_{0}}{2m_{\perp}} (\hat{L}_{z} + \sigma_{z}). \]

2.2. Envelope and Bloch functions

In solid state physics the wavefunction \( |\Psi(\tau)\rangle \) is expressed as a sum of products \( |\Psi(\tau)\rangle = \sum_{i} |\Psi_{i}(\tau)\rangle|f_{i}\rangle \), where \( |\Psi_{i}(\tau)\rangle \) are the Bloch band-edge and \( |f_{i}\rangle \) are the envelope functions [2, 18]. Let us denote \( \mathcal{H}^{0} \) the Hamiltonian, equation (16), in the absence of magnetic field and \( \mathcal{H}_{e}^{0} \) the second and third terms of this equation describing the action of the external magnetic field. The Luttinger–Kohn \( \mathcal{H}_{H}^{0} \) matrix Hamiltonian operator [17] acting on the envelope vector function can be obtained by applying \( \mathcal{H}_{H}^{0} \) onto \( |\Psi(\tau)\rangle \), then left-multiplying by the different Bloch functions \( |\Psi_{i}(\tau)\rangle \) and integrating over the unit cell. Afterwards, the effect of remote bands is incorporated by replacing the actual mass by effective masses in the matrix elements of \( \mathcal{H}_{H}^{0} \).

In the presence of magnetic field \( \mathcal{H}_{H} \) must be supplemented by \( \mathcal{H}_{B} \) coming from \( \mathcal{H}_{e}^{0} \) and \( |\Psi(\tau)\rangle \), through a similar procedure. Since all terms in \( \mathcal{H}_{e}^{0} \) act as pure multiplicative operators on the envelope function components except for \( \hat{L}_{z} \), we have that [30]

\[ \mathcal{H}_{e}^{0}(|\Psi_{i}(\tau)\rangle) = \langle j | \mathcal{H}_{e}^{0} | j \rangle = \langle j | \mathcal{H}_{e}^{0} | j \rangle - \frac{B_{0}}{2|m_{\perp}|} \hat{L}_{z} |j\rangle. \]

Axially symmetric systems have well defined \( z \)-component \( F_{z} \) of the total angular momentum and, additionally, the components of the envelope function associated with the Bloch function \( |\Psi_{i}(\tau)\rangle \) also have a well defined \( M = (F_{z} - J_{z}) \) orbital angular momentum [36, 37], so that \( \hat{L}_{z} |j\rangle = (F_{z} - J_{z}) |j\rangle \). Then, we calculate the \( (J'J_{z}) \) matrix element of \( \mathcal{H}_{B}^{0} \) as follows:

\[ (J'J_{z}) | \mathcal{H}_{B}^{0} (|JM\rangle) \rangle = (J'J_{z}) \left( \mathcal{H}_{e}^{0} - \frac{F_{z} - J_{z}}{2|m_{\perp}|} B_{0} \right) \times |J_{z}\rangle \cdot |\rangle \]

i.e.,

\[ \mathcal{H}_{B}^{0} = -\frac{B_{0}^{2}\rho^{2}}{8|m_{\perp}|} \frac{F_{z} - J_{z}}{2|m_{\perp}|} - \frac{B_{0}}{2|m_{\perp}|} (\hat{L}_{z} + \sigma_{z}). \]

Next, we incorporate the effect of the remote bands as for electrons: the mass \( m_{j} \), arising in the two first terms of \( \mathcal{H}_{B}^{0} \) is replaced by the effective mass parameter appearing in the corresponding matrix elements of \( \mathcal{H}_{H}^{0} \), while the third term in \( \mathcal{H}_{B}^{0} \) becomes \( -2\kappa \mu_{B} B_{0} \frac{F_{z} - J_{z}}{2|m_{\perp}|} \). The procedure yields the following non-zero matrix elements for the \( 6 \times 6 \) valence Hamiltonian for zinc-blende crystals, which includes heavy hole \((1/2, \pm 1/2)\), light hole \((1/2, \pm 1/2)\) and split-off \((1/2, \pm 1/2)\) bands:

\[ (11) = -\gamma_{1} + \gamma_{2} \left[ \frac{B_{0}^{2}\rho^{2}}{8} + \frac{B_{0}}{2(F_{z} - 3/2)} \right] - \frac{3}{2}\kappa \mu_{B} B_{0} \]

\[ (22) = -\gamma_{1} - \gamma_{2} \left[ \frac{B_{0}^{2}\rho^{2}}{8} + \frac{B_{0}}{2(F_{z} - 1/2)} \right] + \frac{1}{2}\kappa \mu_{B} B_{0} \]

\[ (33) = -\gamma_{1} - \gamma_{2} \left[ \frac{B_{0}^{2}\rho^{2}}{8} + \frac{B_{0}}{2(F_{z} + 1/2)} \right] + \frac{1}{2}\kappa \mu_{B} B_{0} \]

\[ (44) = -\gamma_{1} + \gamma_{2} \left[ \frac{B_{0}^{2}\rho^{2}}{8} + \frac{B_{0}}{2(F_{z} + 3/2)} \right] + \frac{3}{2}\kappa \mu_{B} B_{0} \]

\[ (55) = -\gamma_{1} \left[ \frac{B_{0}^{2}\rho^{2}}{8} + \frac{B_{0}}{2(F_{z} - 1/2)} \right] - \frac{1}{2}\kappa \mu_{B} B_{0} \]

\[ (66) = -\gamma_{1} \left[ \frac{B_{0}^{2}\rho^{2}}{8} + \frac{B_{0}}{2(F_{z} + 1/2)} \right] + \frac{1}{2}\kappa \mu_{B} B_{0} \]

where labels 1, 2, ..., 6 refer to the basis elements \([3/2, 3/2], [3/2, 1/2], [3/2, -1/2], [3/2, -3/2], [1/2, 1/2], [1/2, -1/2] \).
and \( |1/2, -1/2\), respectively, \( \mu_B = |q|/2m \) is the Bohr magneton, while \( \kappa \) and \( \kappa' \) are effective \( g \) factors for holes which become \( 4/3 \) and \( 2/3 \) respectively if we remove the contribution of the remote bands.

Note that the magnetic terms in equation (20) differ from those of the Luttinger approximation (see table 3 in [30]). In particular, as shown in equation (20), no off-diagonal magnetic terms mixing HH and LH subbands result. We may ascribe this difference to the fact that, contrary to the Luttinger procedure, the magnetic field has been implemented incorporating the minimal coupling \( p \rightarrow p - qA \) prior to the EFA, rather than after it. The magnetic terms in equation (20) also differ from our previous proposal [30] in two aspects: (i) the spin degree of freedom is now included, and (ii) the remote bands’ contribution to the linear-in-\( B \) term coming from the Bloch function (third term in equation (19)) is now included through hole \( g \) factors \( (\kappa, \kappa') \).

### 3. Illustrative calculations

In this section we implement the magnetic terms described above in a 4-band \( k \cdot p \) Hamiltonian coupling HH and LH states. Hereafter we refer to this as \( \mathcal{H}_x \). For comparison, we also implement the magnetic terms following the Luttinger approximation, \( \mathcal{H}_\text{lutt} \) (table 3 of [30] but adding diagonal spin terms, \( -\kappa \mu_B B_0 |j_3\rangle \langle j_3| \), and our previous proposal \( \mathcal{H}_\text{mass} \) (four-band Hamiltonian taken from [38]).

As stated and justified in [30], \( \mathcal{H}_\text{lutt} \) gives similar results to those of \( \mathcal{H}_\text{mass} \). Likewise, it gives similar results to those of the present implementation, \( \mathcal{H}_x \), which is a refinement of \( \mathcal{H}_\text{mass} \). However, in some situations, the off-diagonal magnetic field terms arising in \( \mathcal{H}_\text{lutt} \), which overestimate the subband mixing, may even lead to qualitatively incorrect predictions. These terms do not appear in our Hamiltonian. In this section we study one such case and will show that while \( \mathcal{H}_\text{lutt} \) fails, our Hamiltonian yields a correct physical description. We compare the performance of the different Hamiltonians with available experimental data for an InGaAs/GaAs QD molecule subject to a longitudinal magnetic field [29]. The Hamiltonian is solved numerically for a structure formed by two vertically stacked cylindrical QDs. The QDs have radius \( R = 15 \) nm and height \( H = 2 \) nm, with an interdot barrier of thickness \( S = 2.8 \) nm. InGaAs Luttinger parameters are used for the masses \( (\gamma_1 = 11.01, \gamma_2 = 4.18, \text{and } \gamma_3 = 4.84) \) [39], and a valence band offset of 0.2 eV is taken at the interfaces.

In bulk, the \( \kappa \) constant takes a value of 7.68 (for pure InAs) [40]. However, as noted in [25], quantum confinement severely quenches this value. In QDs, one should disregard the contribution from remote bands, and simply consider that coming from the HH–LH subband coupling. Therefore, following [25], we take \( \kappa = 4/3 \).

Figure 1 shows the energy of the highest valence band states. These are the \( |F_e| = 3/2 \) hole states with bonding (solid lines) and antibonding (dashed lines) molecular character [41]. Panels (a), (b) and (c) correspond to estimates obtained with \( \mathcal{H}_\text{lutt} \), \( \mathcal{H}_\text{mass} \), and \( \mathcal{H}_x \), respectively. One can see there are conspicuous differences in the energy spectra. For example, both \( \mathcal{H}_\text{lutt} \) and \( \mathcal{H}_\text{mass} \) predict that for the ground state, the \( B \)-linear term dominates over the \( B \)-quadratic (diamagnetic) one, so that its energy increases with the field. This would imply a decrease of the excitonic gap, in sharp contrast with photoluminescence experiments of InGaAs QDs, where the gap increases quadratically, indicating that the diamagnetic term is dominant. This is precisely the situation predicted by \( \mathcal{H}_x \), figure 1(c).

Further insight is obtained by comparing energy differences within each spectrum. We first compare the energy splitting between the bonding and antibonding states, \( \Delta_{\text{bab}} \), as a function of the magnetic field. Figure 2 shows \( \Delta_{\text{bab}} \) calculated with the three Hamiltonians. \( \mathcal{H}_\text{lutt} \) (dashed line) predicts that the energy splitting decreases with \( B_0 \), becomes zero at \( B_0 = 5.3 \) T and negative afterwards, which means that the ground state has changed from bonding to antibonding character. This ground state crossing is indicated by a green arrow in figure 1(a). The modulation of \( \Delta_{\text{bab}} \) with longitudinal magnetic fields is a consequence of the off-diagonal magnetic terms in \( \mathcal{H}_\text{lutt} \) [28]. However, no such behavior is found in experiments, where \( \Delta_{\text{bab}} \) remains roughly constant with the field. This is shown by the symbols in figure 2, which represent experimental data taken from [29]. Clearly, both
\[ H_{t} \text{ (dashed–dotted line) and } H_{\kappa} \text{ (solid line) succeed in reproducing the approximately constant value of } \Delta_{\text{hab}}. \]

In order to discriminate between \( H_{\text{mass}} \) and \( H_{\kappa} \), in figure 3 we compare the Zeeman splitting of the ground state, \( \Delta_{z} \), calculated with all three Hamiltonians and the experimental values, represented by symbols. It can be seen that \( H_{\text{mass}} \) (dashed–dotted line) vastly overestimates the Zeeman splitting, while \( H_{\kappa} \) (solid line) offers the closest description. It is worth noting that the experimental values of \( \Delta_{z} \) are even smaller than those predicted by \( H_{\kappa} \). The inclusion of strain and piezoelectric effects may be relevant for a quantitatively improved description [25, 42].

Finally, we compare the envelope angular momentum admixture obtained with the different Hamiltonians. In a four-band model, the hole states of cylindrical QDs are four-component spinors of the form

\[ |F_{z}, n\rangle = \sum_{J_{z}=-3/2,3/2} |\hbar t\rangle \left| \frac{3}{2} J_{z} \right\rangle, \]

(21)

where \( n \) is the main quantum number and \( M = F_{z} - J_{z} \) is the envelope azimuthal angular momentum of a given component. We calculate the expectation value of the ground state envelope angular momentum at different fields and plot the results in figure 4. At zero field \( \langle M \rangle = 0.02 \), indicating that the ground state largest component is by far the HH \((|J_{z}| = 3/2)\) with \( M = 0 \), with a small admixture with finite \( M \) components. When the magnetic field is switched on, \( H_{t} \) predicts a faster increase of \( \langle M \rangle \) than \( H_{\text{mass}} \) or \( H_{\kappa} \) (the bump at \( B_{0} = 5.4 \) T is due to the bonding–antibonding reversal). Since the degree of envelope angular momentum admixture is critical in determining the effective \( g \) factor of holes [25], and we have shown that only \( H_{\kappa} \) provides a consistent description of the magnetic response, figure 4 implies that the widely used Luttinger approximation is likely to overestimate the \( g \) factor values in confined systems.

4. Summary

We have derived a multiband \( k \cdot p \) Hamiltonian for valence holes confined in heterostructures subject to an external magnetic field. The magnetic field has been implemented incorporating the minimal coupling \( p \rightarrow p - qA \) prior to introducing the EFA. The inclusion of the remote bands has been considered through effective masses for the envelope function terms and effective \( g \) factors for the magnetic terms originating in the (unit cell) Bloch functions. For QDs, owing to the strong confinement, the latter have been replaced by the bare hole values, disregarding the influence of remote bands.

The resulting Hamiltonian has been compared with the widely employed Luttinger approximation and our previous proposal. When tested against experimental data for coupled InGaAs QDs under axial magnetic fields, the Hamiltonian presented in this work clearly outperforms the others. In particular, it succeeds in simultaneously describing the increase of the constant splitting between bonding and antibonding states and the reduced Zeeman splitting observed in photoluminescence experiments, with no fitting parameters.

The Hamiltonian we have formulated is expected to improve current attempts to estimate the \( g \) factors of holes confined in QDs for spintronic, quantum information and optical applications.
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