Spin Density Matrix of Spin-3/2 Hole Systems

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For hole systems with an effective spin \( j = 3/2 \), we present an invariant decomposition of the spin density matrix that can be interpreted as a multipole expansion. The charge density corresponds to the monopole moment and the spin polarization due to a magnetic field corresponds to a dipole moment while heavy hole–light hole splitting can be interpreted as a quadrupole moment. For quasi two-dimensional hole systems in the presence of an in-plane magnetic field \( B_\parallel \) the spin polarization is a higher-order effect that is typically much smaller than one even if the minority spin subband is completely depopulated. On the other hand, the field \( B_\parallel \) can induce a substantial octupole moment which is a unique feature of \( j = 3/2 \) hole systems.

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I. INTRODUCTION

A powerful approach to the quantum many-body problem is density functional theory. Hohenberg and Kohn showed that the (nondegenerate) ground state of a system of interacting particles is a unique function of the corresponding ground state density \( \rho \). The ground state of the system is thus fully characterized by its density \( \rho \) (Ref. 2). For electrons with spin \( j = 1/2 \) the density \( \rho \) must be replaced by a \( 2 \times 2 \) spin density matrix \( \rho \). It is well-known that \( \rho \) can be parameterized by the density \( \rho = \text{tr} \rho \) and (the magnitude of) the spin polarization. The spin polarization at a magnetic field \( B > 0 \) is thus an important quantity for our understanding of many-particle phenomena. Recently, the interest in this subject has been renewed because experiments have indicated that the spin polarization of quasi two-dimensional (2D) systems due to a magnetic field \( B_\parallel \) parallel to the 2D plane affects the apparent metallic behavior of these systems. Furthermore, the spin polarization is an important parameter for possible applications in the field of spintronics. In quasi two-dimensional (2D) systems the spin polarization has been studied by applying a magnetic field \( B_\parallel \) parallel to the 2D plane.\(^5_6,7,8,9,10,11,12,13,14\)

If the Zeeman splitting due to \( B_\parallel \) becomes sufficiently large, the minority spin subband is completely depopulated. In such a situation, electron systems are fully spin-polarized. This approach has been used by several groups to study the spin polarization in low-density 2D electron systems.\(^7,8,9,10\)

Recently, there has been considerable interest in the spin polarization of quasi 2D hole systems.\(^11,12,13,14\) Hole systems in the uppermost valence band of many common semiconductors such as Ge and GaAs are different from electron systems due to the fact that the hole states have an effective spin \( j = 3/2 \) (Ref. 12). Usually, hole states in quasi 2D systems are discussed using a basis of angular momentum \( j = 3/2 \) eigenfunctions with quantization axis perpendicular to the 2D plane. Subband quantization yields so-called heavy hole (HH) states with \( z \) component of angular momentum \( m = \pm 3/2 \) and light hole (LH) states with \( m = \pm 1/2 \). Often it is assumed that the spin degree of freedom of these HH and LH states behaves similar to the spin of \( j = 1/2 \) electron states. However, recently it has been shown that the spin polarization of quasi 2D HH systems in the presence of an in-plane magnetic field behaves rather different from the more familiar case of \( j = 1/2 \) electron systems.\(^3\) For example, the spin polarization of quasi 2D HH systems can change its sign at a finite value of \( B_\parallel \).

Similar to the case of \( j = 1/2 \) electron systems, the fundamental object for the characterization of \( j = 3/2 \) hole systems is the spin density matrix \( \rho \) from which we can derive, e.g., the spin polarization. The dominant character of the occupied eigenstates of hole systems depends on the quantization axis of the underlying \( j = 3/2 \) basis functions. Obviously, all observable quantities such as the spin polarization may not depend on this choice. Therefore, it is necessary to formulate the spin density matrix in a way such that observable quantities can be calculated independent of the particular choice for the basis functions that are used. It is the goal of this paper to present such a theory. Using the theory of invariants\(^17,18\) we will derive an invariant decomposition of the spin density matrix of \( j = 3/2 \) hole systems that can be interpreted as a multipole expansion.

II. INVARIANT DECOMPOSITION OF THE SPIN DENSITY MATRIX

A. General theory

In general, the single-particle states in quasi 2D systems with effective spin \( j \) (the Kohn-Sham states) can be characterized by multicomponent envelope functions:

\[
\Psi_{\alpha\sigma k_l}(r) = \frac{e^{i{\mathbf{k}_l \cdot \mathbf{r}}}}{2\pi} \sum_m \xi_{\alpha\sigma k_l}^m(z) \ u_m(r) .
\]

Here \( \xi_{\alpha\sigma k_l}^m(z) \) denotes the \( m \)th component of the envelope function that modulates the band-edge Bloch function \( u_m(r) \), \( m \) labels the \( z \) components of \( j \), \( \alpha \) is the subband index, \( \sigma \) is the spin index, and \( \mathbf{k}_l = (k_z, k_y, 0) \).
is the in-plane wave vector. The \((2j + 1)\)-dimensional Hermitian, positive definite spin density matrix \(\rho\) has then the matrix elements (temperature \(T = 0\))

\[
\langle m|m'\rangle = \sum_{\alpha,\sigma} \int \frac{dk}{2\pi} \theta[\pm(E_F - E_{\alpha\sigma}(k))] \\
\times \int dz \xi_{\alpha \alpha k||}(z) \xi_{\sigma' \sigma k||}(z).
\]

(2)

Here \(E_{\alpha\sigma}(k)\) is the spin-split subband dispersion and \(E_F\) is the Fermi energy. The upper (lower) sign in Eq. (2) applies to electron (hole) systems. We integrate over all orbital degrees of freedom that are irrelevant in the present discussion. The density is given by the trace of \(\rho\). Obviously, the trace is independent of the particular choice for the set of basis function \(u_m(r)\).

For 3D \textit{inhomogeneous} hole gases \((B = 0)\) the matrix \(\rho\) is proportional to the unit matrix, i.e., we have no preferential direction for the quantization axis of angular momentum \(\mathbf{\ell}\). (This was overlooked in Ref. 20.) For \textit{inhomogeneous} systems such as quasi-2D systems, the matrix \(\rho\) has a more complicated structure, even at \(B = 0\). In principle \(\rho\) contains all information about the ground state of the system. However, as the Hermitian \(4 \times 4\) matrix, \(\rho\) is characterized by 16 independent parameters, it appears impractical to characterize a \(j = 3/2\) system by its density matrix. Thus, Bobbert et al.\textsuperscript{21} suggested to parameterize the mixed HH-LH character of inhomogeneous hole gases by the ratio between the LH and HH Fermi wave vectors. Enderlein et al.\textsuperscript{22} proposed to use partial densities for \(\text{HH}\) and \(\text{LH}\) states. The latter approach was criticized by Bobbert et al.\textsuperscript{19} because the partial hole densities depend on the set of basis function \(u_m(r)\). Recently, Kärrkäinen et al.\textsuperscript{23} suggested to treat mixed HH-LH systems as two-component systems where the HH and LH components are essentially independent of each other. Until today, the interpretation of the \(4 \times 4\) spin density matrix \(\rho\) of particles with \(j = 3/2\) has remained an open problem.

We show here that the theory of invariants\textsuperscript{17,18} allows to decompose \(\rho\) for systems with arbitrary point group \(G\) into symmetry-adapted irreducible tensors which provide a rigorous yet physically transparent classification of the different terms in \(\rho\) — independent of the particular choice for the set of basis functions. We assume that the system is characterized by an \(N \times N\) multiband Hamiltonian \(H\). The basis functions of \(H\) transform according to an \(N\)-dimensional representation \(\Gamma_\alpha\) of \(G\). For simplicity, we assume that the representation \(\Gamma_\alpha\) is irreducible. The density matrix \(\rho\) of this system can be written in the form

\[
\rho = \sum_{\mu,\nu} M_{\mu\nu} \rho_{\mu\nu}.
\]

(3)

Here \(M_{\mu\nu}\) are \(N \times N\) matrices with all elements equal to zero, except for the element \((\mu,\nu)\) that equals one. The components \(\{\rho_{\mu\nu}\}\) and the matrices \(\{M_{\mu\nu}\}\) transform according to the product representation \(\Gamma_\alpha \times \Gamma_\alpha\).

In general, this representation is reducible, i.e., we have

\[
\Gamma_\alpha \times \Gamma_\beta^* = \sum_\beta \Gamma_\beta.
\]

(4)

Equation (4) implies that we can decompose the set of matrices \(\{M_{\mu\nu}\}\) (the components \(\{\rho_{\mu\nu}\}\)) into irreducible tensors \(\{M_\beta\}\) (\(\{\rho_\beta\}\)) that transform according to the representations \(\Gamma_\beta\) of \(G\). The symmetry-adapted expansion of the density matrix \(\rho\) is then given by\textsuperscript{17}

\[
\rho = \sum_\beta M_\beta \cdot \rho_\beta \equiv \sum_{\beta,\lambda} M_{\beta\lambda} \rho_{\beta\lambda}^\prime,
\]

(5)

where \(\lambda\) labels the elements of the irreducible representation \(\Gamma_\beta\). The terms \(\rho_{\beta\lambda}\) can be interpreted as the projection of \(\rho\) on the basis matrices \(M_{\beta\lambda}\). If the matrices \(\{M_{\beta\lambda}\}\) are orthonormalized we thus have

\[
\rho_{\beta\lambda} = \text{tr}(M_{\beta\lambda} \rho).
\]

(6)

According to Eq. (4), we get a decomposition of the density matrix \(\rho\) in terms of invariants \(M_\beta \cdot \rho_\beta\). Often, these invariants provide already a clear interpretation of the different terms in \(\rho\). A second advantage of the invariant expansion (5) is the following. Using the Clebsch-Gordan coefficients for the irreducible representations \(\{\Gamma_\beta\}\) of \(G\) we can construct \textit{scalar} quantities \(\{\rho_s\}\) from the irreducible tensors \(\{\rho_\beta\}\) which transform according to the unit representation \(\Gamma_1\) (Ref. 17). These scalars are sums of products of the elements \(\{\rho_{\beta\lambda}\}\). By definition, they are independent of the particular choice for the set of basis functions that was used to evaluate the spin density matrix. Therefore, the scalars \(\{\rho_s\}\) represent a convenient set of independent variables for a parameterization and characterization of the spin density matrix of a system with point group \(G\).

B. \textbf{Multipole expansion of the density matrix for systems with point group SU(2)}

For a system with spherical symmetry we have \(G = SU(2)\). We denote the irreducible representations of \(SU(2)\) by \(D_j\) where \(j\) is the angular momentum. Here the invariant expansion (5) is equivalent to a multipole expansion of the density matrix. It follows from the well-known relation for the addition of angular momenta\textsuperscript{24}

\[
D_j \times D_{j'} = \sum_{j'' = |j - j'|}^{j + j'} D_{j''},
\]

(7)

that for a system with angular momentum \(j\) the invariant expansion (5) contains multipole moments \(\rho_j\) up to the order \(2j\). The squared magnitude of the \(j\)th multipole moment is given by\textsuperscript{24}

\[
\rho_j^2 = \sum_{m=-j}^{j} (-1)^m \rho_{jm} \rho_{-m}.
\]

(8)
TABLE I: Invariant decomposition of the spin density matrix of a system with spin \( j = 1/2 \).

| \( D_l \) | \( m \) | \( M_{lm} \) | \( \rho_{lm} \) |
|------|------|------|------|
| \( D_0 \) | 0 | \( \frac{1}{\sqrt{2}} \mathbb{I}_{2 \times 2} \) | \( \frac{1}{\sqrt{2}} \left( \left\langle \frac{1}{2} \mid \frac{1}{2} \right\rangle + \left\langle -\frac{1}{2} \mid -\frac{1}{2} \right\rangle \right) \) |
| \( D_1 \) | 1 | \( -\frac{1}{\sqrt{2}} \sigma_x + \frac{i}{\sqrt{2}} \sigma_y \) | \( -\frac{1}{\sqrt{2}} \left( \left\langle \frac{1}{2} \mid \frac{1}{2} \right\rangle - \left\langle -\frac{1}{2} \mid -\frac{1}{2} \right\rangle \right) \) |
| \( D_2 \) | \( \sigma_z \) | \( \frac{1}{\sqrt{2}} \left( \left\langle \frac{1}{2} \mid \frac{1}{2} \right\rangle - \left\langle -\frac{1}{2} \mid -\frac{1}{2} \right\rangle \right) \) |

TABLE II: Tensor operators \( K_{lm} \) for the point group \( SU(2) \).

| \( D_l \) | \( m \) | \( K_{lm} \) |
|------|------|------|
| \( D_0 \) | 0 | \( k^2 = \{k_+, k_-\} + k_z^2 \) |
| \( D_1 \) | 1 | \( -\frac{1}{\sqrt{2}} B_z \) |
| \( D_2 \) | 2 | \( -\frac{1}{2} k_z^2 + \{k_+, k_-\} \) |
| \( D_3 \) | \( \sigma_z \) | \( \frac{1}{\sqrt{2}} \left( 2k_z^2 - \{k_+, k_-\} \right) \) |

By definition, these scalars are independent of the quantization axis of angular momentum that is used for the basis functions \( u_m(r) \) in Eq. (1).

1. \( j = 1/2 \) Electron systems

First we apply the above formalism to the well-known case of a density matrix for systems with angular momentum \( j = 1/2 \). Using standard angular momentum algebra, we obtain the invariant decomposition listed in Table I, where \( \sigma_x \), \( \sigma_y \), and \( \sigma_z \) are the Pauli spin matrices. We have omitted the terms with \( m < 0 \) which can be obtained using \( M_{i,-m} = (-1)^{i+m} M_{i,m}^* \) and \( \rho_{i,-m} = (-1)^{i+m} \rho_{i,m}^* \) (Ref. 24). We note that the terms \( \rho_{lm} \) can be obtained either from Eq. (3) or by using the Clebsch-Gordan coefficients of \( SU(2) \) (Ref. 24). By summing over the invariants \( M_j \cdot \rho_i \) it is easy to check that these invariants provide a decomposition of the spin density matrix \( \rho \).

Using Eq. (5) we obtain the scalars

\[
\rho_0 = \frac{1}{\sqrt{2}} \left( \left\langle \frac{1}{2} \mid \frac{1}{2} \right\rangle + \left\langle -\frac{1}{2} \mid -\frac{1}{2} \right\rangle \right) \tag{9a}
\]

\[
\rho_1^2 = \frac{1}{2} \left( \left\langle \frac{1}{2} \mid \frac{1}{2} \right\rangle - \left\langle -\frac{1}{2} \mid -\frac{1}{2} \right\rangle \right)^2 + 2 \left\langle \frac{1}{2} \mid \frac{1}{2} \right\rangle \tag{9b}
\]

Apart from a prefactor \( 1/\sqrt{2} \), the magnitude of the monopole moment, \( \rho_0 \), is equal to the density. (We remark that by definition \( \rho_0 \) is already a positive scalar that transforms according to \( D_0 \) so that we always have \( \rho_0 = \sqrt{\rho_0^0} \equiv \rho_0 \).) Apart from a prefactor \( 1/2 \), the (squared) magnitude of the dipole moment, \( \rho_1^2 \), is equal to the (squared) magnitude of the polarization. Due to the rotational invariance implied by \( G = SU(2) \), the density matrix is completely characterized by \( \rho_0 \) and \( \rho_1^2 \).

Consistent with the invariant expansion of the density matrix one can perform an invariant expansion of the Hamiltonian \( H_{2 \times 2} \) of \( j = 1/2 \) electron systems. In lowest order of \( k \) and \( B = (i\hbar/e)k \times r \) we obtain the tensor operators listed in Table II. Here \( k_\pm \equiv k_x \pm ik_y \), and \( \{\ldots\} \) denotes the symmetrized product of its arguments, e.g., \( \{A, B\} = \frac{1}{2}(AB + BA) \). We then obtain

\[
H_{2 \times 2} = \frac{k^2}{\sqrt{2}m^*} M_0 + \frac{g^*\mu_B}{\sqrt{2}} M_1 \cdot \mathcal{K}_1 + V(r) \mathbb{I}_{2 \times 2} \tag{10}
\]

Here \( V(r) \) is the external potential. The kinetic energy operator with effective mass \( m^* \) transforms like a monopole and the Zeeman term with effective \( g \) factor \( g^* \) transforms like a dipole. The symbol \( \mu_B \) denotes the Bohr magneton. We see here that for \( j = 1/2 \) systems the \( j \)th invariant in \( H_{2 \times 2} \) characterizes the dynamics of the \( j \)th invariant of the spin density matrix. However, we want to emphasize that this simple correspondence between the different terms in the Hamiltonian (10) and the multipole moments (9) is valid only because we can factorize the eigenfunctions of \( H_{2 \times 2} \) into an orbital part and a spin part. In general, no such factorization can be performed for \( j = 3/2 \) hole states. This is the reason why we will find below that hole systems can have an octupole moment even though the corresponding Hamiltonian does not contain any octupole term.

2. \( j = 3/2 \) Hole systems

We now perform the invariant decomposition of the density matrix for a system with \( j = 3/2 \). According to Eq. (5) it contains multipole terms up to \( j = 3 \). Using standard angular momentum algebra, we obtain the invariant decomposition listed in Table III. Here \( J_x, J_y \), and \( J_z \) are the angular momentum matrices for \( j = 3/2 \) and \( J_x \equiv J_x \pm iJ_y \). Once again, the (squared) magnitudes of the multipole moments can readily be calculated by means of Eq. (5). We obtain
\[ \rho_0 = \frac{1}{3} \left( \langle \frac{1}{2}, \frac{1}{2} \rangle + \langle -\frac{1}{2}, -\frac{1}{2} \rangle + \langle -\frac{1}{2}, \frac{1}{2} \rangle \right) \]

\[ \rho_1^2 = \frac{1}{3!} \left( 3 \langle \frac{1}{2}, \frac{1}{2} \rangle + \langle -\frac{1}{2}, -\frac{1}{2} \rangle - 3 \langle -\frac{1}{2}, \frac{1}{2} \rangle \right)^2 + \frac{1}{4} \left( \sqrt{3} \langle \frac{1}{2}, \frac{1}{2} \rangle + 2 \langle -\frac{1}{2}, \frac{1}{2} \rangle + \sqrt{3} \langle -\frac{1}{2}, \frac{1}{2} \rangle \right)^2 \]

\[ \rho_2^2 = \frac{1}{4} \left( \langle \frac{1}{2}, \frac{1}{2} \rangle - \langle -\frac{1}{2}, -\frac{1}{2} \rangle - \langle -\frac{1}{2}, \frac{1}{2} \rangle \right)^2 + \left( \langle \frac{1}{2}, -\frac{1}{2} \rangle - \langle -\frac{1}{2}, \frac{1}{2} \rangle \right)^2 \]

\[ \rho_3^2 = \frac{1}{30} \left( \langle \frac{1}{2}, \frac{1}{2} \rangle - 3 \langle \frac{1}{2}, \frac{1}{2} \rangle + 3 \langle -\frac{1}{2}, -\frac{1}{2} \rangle - \langle -\frac{1}{2}, -\frac{1}{2} \rangle \right)^2 + \frac{2}{5} \left( \langle \frac{1}{2}, \frac{1}{2} \rangle - \sqrt{3} \langle \frac{1}{2}, -\frac{1}{2} \rangle + \langle -\frac{1}{2}, -\frac{1}{2} \rangle \right)^2 \]

Apart from a prefactor 1/2, the monopole moment \( \rho_0 \) is equal to the density, and apart from a prefactor 9/20, the squared dipole moment \( \rho_1^2 \) is equal to the squared magnitude of the polarization. The quadrupole moment \( \rho_2 \) and the octupole moment \( \rho_3 \) have no equivalent in \( j = 1/2 \) systems. The magnitude \( \rho_2 \) of the quadrupole moment quantifies the effect of HH-LH splitting. If only the diagonal elements \( \langle m|m \rangle \) of \( \rho \) are nonzero, \( \rho_2 \) is equal to the difference between the partial HH and LH densities used by Enderlein et al. (Ref. 26) (apart from a prefactor 1/2).

For \( j = 3/2 \) systems, a complete characterization of the density matrix by means of scalar quantities requires to take into account additional terms beyond those obtained from Eq. (3). They characterize, e.g., the interaction between different multipole moments. It follows from Eq. (7) that these scalars are of higher order in \( \langle m|m \rangle \).

The dynamics of \( j = 3/2 \) hole systems is characterized by the \( 4 \times 4 \) Luttinger Hamiltonian \( \mathcal{H}_{4 \times 4} \) (Ref. 15). Using Tables II and III we express \( \mathcal{H}_{4 \times 4} \) in terms of spherical tensor operators.26,27

\[ \mathcal{H}_{4 \times 4} = -\frac{\hbar^2}{m_0} \gamma_1 M_0 \cdot \mathcal{K}_0 - 2\sqrt{5} \kappa g_B M_1 \cdot \mathcal{K}_1 \]

\[ + \sqrt{6} \frac{\hbar^2}{m_0} 2\gamma_2 + 3\gamma_3 M_2 \cdot \mathcal{K}_2 + \zeta M_3 \cdot \mathcal{K}_3 \]

\[ + V(r) \mathbb{I}_{4 \times 4}, \]

where \( \gamma_1, \gamma_2, \) and \( \gamma_3 \) are the Luttinger parameters and \( \kappa \) is the isotropic effective \( g \) factor. We neglect here the small terms with cubic symmetry. They are considered in the numerical calculations discussed below. Once again, the magnetic field is acting in spin space as a dipole field (the operator \( \mathcal{K}_1 \)). Obviously, the quadrupole and the octupole term in \( \mathcal{H}_{4 \times 4} \) have no equivalent in \( j = 1/2 \) systems. The quadrupole operator \( \mathcal{K}_2 \) is responsible for the HH-LH splitting.26 We note that in bulk material, uniaxial or biaxial strain also gives rise to a splitting of HH and LH states because analogous to \( \mathcal{K}_2 \) the strain tensor contains a term \( \mathcal{K}'_2 \) that transforms according to \( D_2 \) so that we get another invariant \( \propto M_2 \cdot \mathcal{K}'_2 \) (Ref. 27).

In Eq. (12), the symbol \( \zeta \) denotes the prefactor of the octupole term. Starting from the 8 \( \times \) 8 Kane model we obtain in fourth order perturbation theory28

\[ \zeta = \frac{\sqrt{2}}{3} \frac{e}{\hbar} \frac{P^4}{E_0^2} \left( \frac{1}{E_0} - \frac{1}{\Delta_0} \right), \]

where \( P \) is Kane’s momentum matrix element, \( E_0 \) is the fundamental gap, and \( \Delta_0 \) is the spin-orbit split-off gap. If we insert typical values for \( P, E_0, \) and \( \Delta_0 \) it can be seen that \( \zeta \) is rather small so that the octupole term in \( \mathcal{H}_{4 \times 4} \) can safely be neglected. However, we show below that, nonetheless, the spin density matrix of hole systems can have a large octupole moment.

III. SPIN DENSITY MATRIX OF QUASI 2D SYSTEMS

A. \( j = 1/2 \) Electron systems

As an example we consider next the spin density matrix of quasi 2D electron and HH systems in the presence of an in-plane magnetic field \( B \). For \( j = 1/2 \) electron systems at \( B \geq 0 \) we can choose the eigenstates independent of \( B \)

\[ |\Psi_{\alpha \pm}(z)\rangle = \frac{e^{ik_1 r_1}}{2\pi} \zeta^\alpha (z) \left( \begin{array}{c} 1 \\ \pm 1 \end{array} \right) , \]

Using Eq. (10) we then obtain for the dipole moment normalized with respect to the total 2D density

\[ \rho_1^2 = \begin{cases} \frac{1}{2} \left( \frac{m^* g^* g_B}{2\pi N} \right)^2 & B \perp B_p \\ \frac{1}{2} & B \parallel B_p \end{cases} \]

where we have assumed that only the lowest orbital subband \( \alpha = 1 \) is occupied, \( N \) denotes the total density in the 2D system, and \( B_p = 2\pi h^2 N/(m^* g^* g_B) \) is the magnetic field at which the system becomes fully spin-polarized.29 In Eq. (14) the index \( z \) at the spinor indicates that we have chosen the spin quantization axis in \( z \) direction perpendicular to \( B \). Of course, the dipole moment \( \rho_1^2 \) may not depend on this seemingly inconvenient choice. It is easy to check that we get the same result if the spin quantization axis is chosen parallel to \( B \).
TABLE III: Invariant decomposition of the spin density matrix of a system with \( j = 3/2 \).

| \( D_j \) | \( m \) | \( M_{im} \) | \( \rho_{im} \) |
|---|---|---|---|
| \( D_0 \) | 0 | \( \frac{1}{2} \) | 4, \( 4 \times 4 \) |
| \( D_1 \) | 1 | -\( \frac{1}{\sqrt{6}} \) | \( J_3 \) |
| 0 | \( \frac{1}{\sqrt{3}} \) | \( J_2 \) |
| \( D_2 \) | 2 | \( \frac{1}{\sqrt{6}} \) | \( J_1 \) |
| 1 | \( \frac{1}{\sqrt{3}} \) | \( J_0 \) |
| 0 | \( \frac{1}{2} (J_2^2 - J_0^2) \) |
| \( D_3 \) | 3 | \( \frac{1}{\sqrt{6}} \) | \( J_3 \) |
| 2 | \( \frac{1}{\sqrt{3}} \) | \( J_2 \) |
| 1 | \( \frac{1}{\sqrt{2}} \) | \( J_1 \) |
| 0 | \( \frac{1}{2} (2J_2^2 - 3J_0^2) \) |

\[ \rho_{im} = \frac{1}{2} \left( \begin{array}{c} 1 \\ 0 \\ 0 \end{array} \right) \left( \begin{array}{c} 1 \\ \sqrt{2} \\ \pm 1 \end{array} \right) \] \( (16) \)

Here we have assumed that the Luttinger Hamiltonian \( H \) is expressed in a basis of \( j = 3/2 \) angular momentum eigenfunctions in the order \( m = 3/2, 1/2, -1/2, \) and \(-3/2\); and the index \( z \) at the spinor indicates that the quantization axis of these basis functions is perpendicular to the 2D plane. For simplicity we have neglected HH-LH mixing due to a nonzero in-plane wave vector \( k_\parallel \) and we also neglected the \( k_\parallel \) dependence of the envelope functions \( e^{\text{HH}}_\alpha (z) \). These aspects are fully taken into account in the numerical calculations discussed below. A finite in-plane magnetic field \( B_\parallel \) gives rise to a mixing of HH and LH states. In first order degenerate perturbation theory we obtain the following expressions \( \Phi \) for the quasi 2D HH states in an in-plane field \( B_\parallel \)

\[ \rho_{im} = \frac{1}{2} \left( \begin{array}{c} 1 \\ 0 \\ 0 \end{array} \right) \left( \begin{array}{c} 1 \\ \sqrt{2} \\ \pm 1 \end{array} \right) \] \( (17) \)

Here \( E_{\alpha}^0 \) is the energy of the \( \alpha \)th HH (LH) subband at \( B_\parallel = 0 \), and we have used the gauge \( A = 0, -zB_\parallel, 0 \).

The expression for \( G \) in Ref. 14 differs slightly from our Eq. (13) because we have used here the spherical approximation \( H^{4\times 4} \) of \( H_\parallel \). As discussed in Ref. 14 we can often treat the HH-LH mixing characterized by \( K \) and \( G \) as a small parameter even if \( B_\parallel \) is so large that only the majority spin subband is occupied. This is a consequence of the frozen angular momentum of HH states in quasi 2D systems.

Using Eq. (14) we then obtain for the multipole moments normalized with respect to the total 2D density

\[ \rho_1^2 = \frac{9}{5} (K + G \delta N)^2 \] \( (19a) \)
\[ \rho_2^2 = \frac{1}{4} + 3K^2 \left[ \delta N)^2 - 1 \right] \] \( (19b) \)
\[ \rho_3^2 = \frac{(\delta N)^2}{2} - K^2 \left[ 3(\delta N)^2 - \frac{6}{5} \right] - \frac{18}{5} G K \delta N \] \( (19c) \)

where \( \delta N = (N_+ - N_-)/(N_+ + N_-) \) denotes the normalized difference between the 2D densities \( N_\pm \) in the majority and the minority spin subband (with \( N = N_+ + N_- \)), and we have assumed that only the lowest HH subband \( \alpha = 1 \) is occupied (which is usually the case for 2D hole systems). We note that prior to deriving the multipole moments \( \rho_1, \rho_2, \rho_3 \) one must normalize the perturbed wave functions \( \Phi \).

HH-LH mixing gives rise to a dipole moment \( \rho_1^2 \) proportional to the small parameters \( K \) and \( G \) (Ref. 14). In lowest (i.e., zeroth) order of the HH-LH mixing, the quadrupole moment \( \rho_2^2 \) is equal to \( 1/4 \), i.e., \( \rho_2^2 \) is essentially independent of \( B_\parallel \), which is a consequence of HH-LH splitting. Finally, we also get a substantial octupole moment even though we assumed \( \zeta = 0 \) in the
Luttinger Hamiltonian \[\text{(12)}\]. If the minority spin subband is completely depopulated the normalized octupole moment equals 1/2 in lowest (i.e., zeroth) order of the HH-LH mixing. We note that the Zeeman energy splitting of the HH states in the presence of an in-plane magnetic field \(B_\parallel\) is proportional to \(B_\parallel^3\) (Ref. \[15\]). Neglecting the nonparabolicity of the HH energy dispersion we thus have \(\delta N \propto B_\parallel^3\).

It is interesting to trace back the physical origin of the multipole moments \(\rho_2\) and \(\rho_3\). In spite of the fact that we do not have a simple correspondence between the multipoles in the Luttinger Hamiltonian [Eq. \[12\]] and the multipole moments \(\rho_i\) of the spin density matrix [Eq. \[19\]], we get nonzero multipole moments \(\rho_2\) and \(\rho_3\) only if the Hamiltonian \[12\] contains a quadrupole term \(\propto M_2 \cdot K_2\). If the quadrupole term in Eq. \[12\] were zero the HH eigenstates \[16\] at \(B = 0\) were degenerate with the corresponding LH states. Similar to the electron states \[14\] these four degenerate states could be factorized into a scalar orbital part times a spinor that depends only on \(B\), and we would have \(\rho_2 = \rho_3 = 0\). To the best of our knowledge, the quadrupole term \(\propto M_2 \cdot K_2\) is a unique feature of the Hamiltonian for the extended valence band states in semiconductors.\[15,26,27\]

It is instructive to check that the scalars \(\tilde{\rho}_i^2\) in Eq. \[18\] are indeed independent of the quantization axis \(\hat{e}\) of angular momentum used in Eqs. \[16a\] and \[14\]. If \(\hat{e}\) is chosen parallel to \(B_\parallel\) Eq. \[14\] must be replaced by\[28\]

\[
|\Psi_{\alpha+}^{\text{HH}}\rangle = \frac{e^{ik_|| \tau_||}}{2\pi} s_\alpha^{\text{HH}}(z) \left( \frac{-1 + 3K + 3G}{\sqrt{3}(1 + K + G)} \right)_x \quad (20a)
\]

\[
|\Psi_{\alpha-}^{\text{HH}}\rangle = \frac{e^{ik_|| \tau_||}}{2\pi} s_\alpha^{\text{HH}}(z) \left( \frac{0}{\sqrt{3}(-1 + K - G)} \right)_x \quad (20b)
\]

In this basis the dominant spinor components of the HH states have \(|n| = 1/2\). Nonetheless, we obtain the multipole moments \[19\].

C. Numerical results

To confirm the qualitative results in Eq. \[19\], we show in Fig. 1 the self-consistently calculated multipole moments \(\rho_i^2\) as a function of the in-plane magnetic field \(B_\parallel\) for a symmetric (100) GaAs-Al\(_{0.3}\)Ga\(_{0.7}\)As quantum well with hole density \(N = 5 \times 10^{10}\) cm\(^{-2}\) and well width \(w = 150\) Å. The numerical calculations follow Ref. \[18\]. We evaluate Eq. \[2\] by means of analytic quadratic Brillouin zone integration.\[30\] The solid lines in Fig. 1 have been obtained using the spherical approximation \[12\] of the Luttinger Hamiltonian \(H_{4\times 4}\). However, we have neglected the small octupole term in Eq. \[12\]. For comparison we also show the results based on the 8 \(\times\) 8 Kane Hamiltonian \(H_{8\times 8}\) which includes implicitly the octupole term. The dashed lines in Fig. 1 are based on the spherical approximation of \(H_{8\times 8}\) while the dotted lines also take into account the cubic terms \[28\].

We can see in Fig. 1 that the complete depopulation of the HH minority spin subband due to \(B_\parallel\) does not imply full spin polarization of the system.\[16\] In Fig. 1 (solid lines), the minority spin subband is completely depopulated at \(B_D \approx 23.9\) T while \(\rho_i^2(B_D) \approx 0.0093\). The latter value is much smaller than \(9/20 = 0.45\), the value of \(\rho_2^2\) in
a consequence of the
The derivative of \( \rho \) in a pure HH system. This is a consequence of the \( k_\parallel \)-induced HH-LH mixing which was fully taken into account in Fig. 1. For \( B_\parallel > 0 \) we observe only a small decrease of \( \rho_2 \). This is due to the fact that the HH-LH splitting \( E_4^h - E_i \approx 6.7 \text{ meV} \) [i.e., the denominators in Eq. (18)] is the largest energy scale in the system so that the HH states have a frozen angular momentum perpendicular to the 2D plane. For comparison, we note that the Zeeman energy splitting of the HH subband at \( B_D \) is \( \sim 0.4 \text{ meV} \). The spin polarization due to \( B_\parallel \) is thus a higher-order effect in 2D HH systems.

It is remarkable that the octupole moment \( \rho_3 \) at \( B_\parallel = B_D \) is close to 1/2, the largest possible value of \( \rho_3 \) in a 2D HH system. This value is essentially independent of whether we use \( H_{4\times 4} \) without an octupole term or whether we use \( H_{8\times 8} \) which includes implicitly the octupole term \( \propto M_3 \cdot K_3 \). For \( B_\parallel \geq B_D \), the octupole moment \( \rho_3^2 \) remains essentially constant, consistent with Eq. (19c). These findings suggest that an in-plane magnetic field \( B_\parallel \) provides an efficient tool to study 2D HH systems with a large octupole moment but with a small dipole moment (i.e., with a small spin polarization). We can obtain a 2D HH system with a large spin polarization but with a small octupole moment if the magnetic field is applied perpendicular to the 2D plane.

Figure 1 shows that the cubic terms are only small corrections in \( H_{8\times 8} \). They can safely be neglected in a discussion of the main features in Fig. 1. This is consistent with the fact that the cubic terms in \( H_{4\times 4} \) (and \( H_{4\times 4} \)) are proportional to \( \gamma_3 - \gamma_2 \) which is typically a small parameter.\(^{72} \) On the other hand, it was important for the results shown in Fig. 1 that the numerical calculations took into account HH-LH mixing due to a nonzero in-plane wave vector \( k_\parallel \). As the analytical expressions in Eq. (19) neglect this effect, we do not present a direct comparison between Eq. (19) and the numerical results in Fig. 1. We remark that it is straightforward to include the \( k_\parallel \)-induced HH-LH mixing in Eq. (19). However, we do not reproduce here the lengthy formulas.

IV. OTHER SYSTEMS AND OUTLOOK

The numerical calculations shown in Fig. 1 have neglected many-particle effects beyond the Hartree approximation. These effects will be important for a quantitative analysis of the spin multipole moments in the density regime discussed here. However, to the best of our knowledge an appropriate theory for particles with \( j = 3/2 \) is currently not available. It represents a formidable task to develop such a theory. We note that the symmetry arguments developed here are not affected by many-particle effects. The multipole expansion of the spin density matrix can thus provide a useful starting point for a more quantitative theory. We expect that the essential features in Fig. 1 will be confirmed by such an investigation.

Our results can readily be generalized to spherically symmetric systems with arbitrary \( j \), both half integer and integer\(^{24} \) as well as to systems characterized by the crystallographic point groups\(^{21} \). As an example, we consider a \( j = 1/2 \) electron system in a spatial environment with point group \( G \). Here the \( 2 \times 2 \) spin density matrix is completely characterized by five independent scalars

\[
\rho_0 = \langle \frac{1}{2} | \frac{1}{2} \rangle + \langle -\frac{1}{2} | -\frac{1}{2} \rangle \quad (21a)
\]
\[
\rho_1 = |\langle \frac{1}{2} | -\frac{1}{2} \rangle + \langle -\frac{1}{2} | \frac{1}{2} \rangle|^2 \quad (21b)
\]
\[
\rho_2 = |\langle \frac{1}{2} | -\frac{1}{2} \rangle - \langle -\frac{1}{2} | \frac{1}{2} \rangle|^2 \quad (21c)
\]
\[
\rho_3 = |\langle \frac{1}{2} | \frac{1}{2} \rangle - \langle -\frac{1}{2} | -\frac{1}{2} \rangle|^2 \quad (21d)
\]
\[
\rho_4 = |\langle \frac{1}{2} | -\frac{1}{2} \rangle - \langle -\frac{1}{2} | \frac{1}{2} \rangle|^2 \quad (21e)
\]

Each term in Eq. (21) has a clear physical interpretation. Once again, the scalar \( \rho_0 \) is the charge density. The scalars \( \rho_1, \rho_2, \) and \( \rho_3 \) describe the magnitude of the spin polarization in \( x, y, \) and \( z \) direction, respectively. These quantities must be distinguished from each other in a system with point group \( G \). Finally, \( \rho_4 \) describes the relative sign of the spin polarization in \( x, y, \) and \( z \) direction. The five scalars \( \rho_4 \) thus form a decomposition of the four independent parameters of a Hermitian \( 2 \times 2 \) matrix into their magnitudes and their relative signs. For the explicit formulas in Eq. (21) we have assumed that the angular momentum quantization axis of the basis functions is parallel to the symmetry axis of the point group \( G \). We emphasize that the magnitude of the scalars \( \rho_4 \) in Eq. (21) does not depend on this choice.

Finally, we want to briefly address the question of how one can measure the multipole moments of the spin density matrix of hole systems. The polarization of \( j = 1/2 \) electron systems can be probed by measuring the hyperfine interaction between the electrons and the atomic nuclei. Electrons in the conduction band of common semiconductors like GaAs originate in \( s \)-like atomic orbitals. Therefore, the electrons have a large probability density at the atomic nuclei so that the hyperfine interaction is large. The \( j = 3/2 \) hole states in the valence band, on the other hand, originate in \( p \)-like atomic orbitals which have a vanishing probability density at the atomic nuclei. The hyperfine interaction is therefore much weaker\(^{25} \) so that it will be difficult to use this technique to measure the polarization of \( j = 3/2 \) hole states.

Indirect evidence for the unusual features of the spin density matrix of hole systems can be obtained by varying the confinement of quasi 2D HH systems perpendicular to the 2D plane. This will change the HH-LH splitting \( E_\alpha^h - E_\alpha^l \) in the denominators of Eq. (18). Here our results are in good qualitative agreement with the trends
observed in recent experiments. A detailed comparison with experimental results will be the subject of a future publication.

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\[ V_{\pm 1} = \mp \frac{1}{\sqrt{2}} (V_x \pm iV_y) \]  

\[ V_0 = V_z. \] (22a)

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