Spin-orbit interactions in inversion-asymmetric two-dimensional hole systems: A variational analysis

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We present an in-depth study of the spin-orbit (SO) interactions occurring in inversion-asymmetric two-dimensional hole gases at semiconductor heterointerfaces. We focus on common semiconductors such as GaAs, InAs, InSb, Ge, and Si. We develop a semianalytical variational method to quantifiy SO interactions, accounting for both structure inversion asymmetry (SIA) and bulk inversion asymmetry (BIA). Under certain circumstances, using the Schrieffer-Wolff (SW) transformation, the dispersion of the ground state heavy hole subbands can be written as $E(k) = A k^2 - B k^4 + C k^6$ where $A$, $B$, and $C$ are material- and structure-dependent coefficients. We provide a simple method of calculating the parameters $A$, $B$, and $C$, yet demonstrate that the simple SW approximation leading to a SIA (Rashba) spin splitting $\propto k^3$ frequently breaks down. We determine the parameter regimes at which this happens for the materials above and discuss a convenient semianalytical method to obtain the correct spin splitting, effective masses, Fermi level, and subband occupancy, together with their dependence on the charge density, and dopant type, for both inversion and accumulation layers. Our results are in good agreement with fully numerical calculations as well as with experimental findings. They suggest that a naive application of the simple cubic Rashba model is of limited use in either common heterostructures or quantum dots. Finally, we find that for the single heterojunctions studied here the magnitudes of BIA terms are always much smaller than those of SIA terms.

I. INTRODUCTION

The ability to harness the spin degree of freedom is essential for the development of practical semiconductor spintronic devices and quantum information processing. All-electrical spin control may be possible by exploiting the coupling of the spin and orbital degrees of freedom brought about by the strong spin-orbit interactions in certain semiconductor systems. This could lead to faster spin rotations and lower power consumption, as well as the convenience of using solely electric fields, which are easier to apply and localize than magnetic fields. The search for semiconductor systems with strong spin-orbit coupling has led naturally to low-dimensional hole systems. Despite the promising advances of recent years, in particular in the experimental state of the art, functional hole spin-based devices are yet to be realized. In particular, a comprehensive understanding of the interaction between a hole’s spin and its solid-state environment is far from complete.

In group IV and III-V semiconductors, the uppermost valence band is described by wave functions originating from bonding atomic $p$ orbitals with orbital angular momentum $L = 1$. Together with the spin $S = 1/2$ this results in an effective spin $J = 3/2$. The bulk valence band eigenstates are heavy holes (HH) with angular momentum projection $m_J = \pm 3/2$ in the direction of the wave vector and light holes (LH) with $m_J = \pm 1/2$. These are degenerate at the zone center but split by a finite energy at nonzero wave vectors. Confinement to the interface of a heterojunction fixes the hole spin quantization axis in the growth direction $\hat{z}$, which here we take to be parallel to (001), and lifts the degeneracy of the HH and LH states at the subband edge (in-plane wave vector $k = 0$). At this point the eigenstates remain pure HH and LH, while at finite $k$, the $k \cdot p$ interaction causes the HH and LH states to mix. However, for typical Fermi wave vectors $k_F$, the subband states with $k \lesssim k_F$ can still be regarded as approximately HH- or LH-like.

Inversion asymmetry further lifts the spin degeneracies of HH and LH states, resulting in additional $k$-dependent energy level splittings. Inversion asymmetry in semiconductor heterostructures may stem from the asymmetry of the confining potential [structural inversion asymmetry (SIA) or Rashba terms] or from the asymmetry of the underlying crystal structure [bulk inversion asymmetry (BIA) or Dresselhaus terms]. BIA and SIA spin splittings are proportional to odd powers of $k$, with $k$-linear, $k^3$, and $k^5$ terms, frequently representing the dominant contributions. They result in a high degree of nonparabolicity of the hole energy bands. Accounting for the complex couplings between the hole bands is vital if one is to capture all aspects of hole spin dynamics correctly. So far, theoretical studies of two-dimensional hole gases (2DHHs) in group IV and III-V structures have been predominantly numerical and always material-specific. Calculations for single heterojunctions are more complex due to the nature of the confining potential. Unlike quantum wells, where the potential shape is approximately fixed, the shape of the confining potential in single heterojunctions is highly density-dependent, thus requiring...
self-consistent wave functions that produce the potential for a given density.

In this paper, we develop a variational method that enables us to gain a transparent insight into spin-orbit interactions in 2DHGs in III-V and Si-based heterojunctions. We use the Luttinger Hamiltonian\cite{2} and the standard envelope function approximation\cite{2,3,4} combined with a simple self-consistent variational approach\cite{5,6} to calculate the spin splitting and effective masses for semiconductors with zincblende and diamond lattices. The variational approach allows one to easily solve for the confinement potential \( V(z) \). Once the Luttinger Hamiltonian for the 2DHG is constructed, one can use a Schrieffer-Wolff (SW) transformation\cite{7} (in the context of semiconductors also known as L"owdin perturbation theory\cite{8}) to derive analytical expressions for the spin-dependent dispersion of 2D hole systems, which subsequently yields the Fermi level, spin splitting, effective masses and subband occupancy. We apply this method to common semiconductors such as GaAs, InAs, InSb, Ge, and Si, and compare inversion and accumulation layers.

In the axial approximation, i.e., ignoring anisotropic corrections including warping and BIA, the SW transformation enables one to write the dispersion relation in a rather simple form \( E^\pm (k) = A k^2 - B k^4 \pm C k^3 \) where \( A, B, \) and \( C \) are material- and structure-dependent coefficients, and the \( C k^3 \) term represents the Rashba spin splitting\cite{9,10} and the standard spin helix.\cite{10,11,12} It is also highly relevant to the understanding of the spin-Hall conductivity,\cite{13} and the validity of the simple dispersion relation to realistic heterostructures is relevant to the current understanding of the spin-Hall conductivity\cite{13,14,15,16,17,18} and Zitterbewegung\cite{19,20,21} all of which have been derived based on the assumption that the HH spin splitting is proportional to \( k^3 \). Our work can be used to determine spin densities and spin-Hall currents in the same way as for electrons.\cite{22,23} It is also highly relevant to the burgeoning field of hole quantum dots, which are constrained basis set, \cite{24,25,26} existing single-hole quantum dots are contained in the quasitriangular wells. We apply this method to calculate the spin splitting and effective masses for 2DHGs in inversion and accumulation layers in various semiconductors. The effects of the Dresselhaus spin-orbit interaction terms are outlined in Sec. \( V \). We discuss our results in Sec. \( V \) while Sec. \( V I \) contains a summary and conclusions.

Recently the importance of surface termination effects on spin-orbit interactions and the HH spin splitting has been pointed out by Durnev et al\cite{27} who focused on the case of quantum wells. Inclusion of these effects is beyond the scope of our present work. Whereas in heterojunctions, where the wave functions vanish near the interface, surface termination effects are expected to be weaker\cite{28} a complete description will require the systematic inclusion of these contributions.

This paper is structured as follows: In Sec. \( II \) we introduce the variational method employed for 2DHGs in quasitriangular wells. We apply this method in Sec. \( III \) to calculate the spin splitting and effective masses for 2DHGs in inversion and accumulation layers in various semiconductors. The effects of the Dresselhaus spin-orbit interaction terms are outlined in Sec. \( V \). We discuss our results in Sec. \( V \) while Sec. \( V I \) contains a summary and conclusions.

\section{Theoretical Formalism}

\subsection{Luttinger Hamiltonian for 2DHGs}

Our formulation takes as its starting point the bulk \( 4 \times 4 \) Luttinger Hamiltonian\cite{29} describing holes in the uppermost valence band with an effective spin \( J = 3/2 \)

\begin{equation}
H_L = \begin{pmatrix}
P + Q & 0 & L & M \\
0 & P + Q & M^* & -L^* \\
L^* & M & P - Q & 0 \\
M^* & -L & 0 & P - Q
\end{pmatrix},
\end{equation}

where

\begin{equation}
P = \frac{\mu}{2} \gamma_1 (2k_z^2 - k^2), \quad Q = -\frac{\mu}{2} \gamma_2 \left( 2k_z^2 - k^2 \right),
\end{equation}

\begin{equation}
L = -\sqrt{3} \mu \gamma_3 k_z, \quad M = \frac{\sqrt{3} \mu}{2} \left( \gamma_2 k_x - \zeta k_y \right),
\end{equation}

\begin{equation}
k^2 = k_x^2 + k_y^2, \quad k_\perp = k_x \pm i k_y,
\end{equation}

\begin{equation}
\mu = \hbar^2 / m_0 \text{ with bare electron mass } m_0, \text{ and } \gamma_1, \gamma_2, \text{ and } \gamma_3 \text{ are the Luttinger parameters, see Table I.}
\end{equation}

The wave vector components are defined by the crystallographic orientation. In this work, we consider holes grown on a \((001)\) surface so that \( k_z \parallel (100), \) \( k_y \parallel (010), \) and \( k_z \parallel (001). \) We have expressed \( H_L \) in the basis of \( J_z \) eigenstates \( \{ |\uparrow\rangle, |\downarrow\rangle, |\frac{\uparrow+\downarrow}{2}\rangle, |\frac{\uparrow-\downarrow}{2}\rangle \} \), where \( \hat{z} \) is the unit vector perpendicular to the plane of the interface.

The Luttinger Hamiltonian is further simplified in the axial approximation, where the terms proportional to \( \zeta \) are neglected\cite{30,31}. The axial approximation is appropriate for GaAs, InAs, InSb and Ge, while for Si \( \zeta \) is significant (Table I) and gives rise to a highly anisotropic Fermi contour, as Sec. \( III C \) will show.

The \( 4 \times 4 \) Luttinger Hamiltonian (1) is accurate as long as the spin-orbit split-off band is far away from the
TABLE I. Luttinger parameters and bulk Dresselhaus coefficients used in this work, where $B_{D1}$, $B_{D2}$, $B_{D3}$, and $B_{D4}$ are in eV Å$^3$ and $C_D$ in eV Å.

| Material | $\gamma_1$ | $\gamma_2$ | $\gamma_3$ | $C_D$ | $B_{D1}$ | $B_{D2}$ | $B_{D3}$ | $B_{D4}$ |
|----------|------------|------------|------------|-------|-----------|-----------|-----------|-----------|
| GaAs     | 6.85       | 2.10       | 2.90       | −0.0034| −81.93    | 1.47      | 0.49      | −0.98     |
| InAs     | 20.40      | 8.30       | 9.10       | −0.0112| −50.18    | 1.26      | 0.42      | −0.84     |
| InSb     | 37.10      | 16.50      | 17.70      | −0.0082| −934.8    | 41.73     | 13.91     | −27.82    |
| Si       | 4.28       | 0.34       | 1.45       | 5.69   |           |           |           |           |
| Ge       | 13.38      | 4.24       |           |        |           |           |           |           |

HH and LH bands. The energy gap $\Delta_{SO}$ separating the split-off band from the HH-LH manifold is of the order of 300–800 meV for GaAs, InAs, InSb, and Ge.\(^\text{56}\) For Si, $\Delta_{SO} = 44$ meV, and thus the couplings to the split-off band must be taken into account.

B. Poisson and Schrödinger Equations

We consider a single heterojunction with the interface at $z = 0$. We assume that the wave functions vanish at the interface so that in the following we restrict ourselves to $z \geq 0$ (see end of Sec. V C on why this is a reasonable approximation for the heterojunctions studied here). Our variational calculation is based on two steps, each of which is variational in nature. First we construct the self-consistent potential $\psi_h(z)$ characterizing the heterojunction assuming a parabolic, spin degenerate, 2DHG dispersion. Then we solve $H_L$ for $V(z)$ in a second variational calculation.

The one-dimensional charge distribution giving rise to the confinement potential $V(z)$, consists of two contributions: the hole density is $p|\psi_h(z)|^2$, where $p$ denotes the number density of 2D holes, and $\psi_h(z)$ is the zero-node HH wave function, assuming that only the lowest subband, labeled HH1, is occupied, which is the most common case. The second contribution is the net donor concentration $N_D$ (Ref. 58). The corresponding Poisson equation is thus:

$$\frac{d^2}{dz^2} V(z) = -\frac{e^2}{\epsilon_s \epsilon_0} \left[ p|\psi_h(z)|^2 + N_D \right],$$  (3)

where $\epsilon_s$ is the dielectric constant of the semiconductor and $\epsilon_0$ is the vacuum permittivity.

The Poisson equation (3) is solved with three boundary conditions. Firstly, the zero of energy is chosen to be at $z = 0$:

$$V(z = 0) = 0.$$  (4)

Secondly, the potential $V(z)$ is flat in the bulk, i.e. at $z \geq w$ we have

$$\frac{d}{dz} V(z \geq w) = 0,$$  (5)

where $w$ is the width of the space charge layer.\(^\text{59}\) Thirdly, the Fermi energy $E_F$ is given by the HH1 energy at the Fermi wave vector $k_F$:

$$E_F \equiv E_{H1} + E_{F1},$$  (6a)

where $E_{H1}$ denotes the subband edge $k = 0$ and $E_{F1}$ is the in-plane kinetic energy of the holes in the HH1 subband at $E_F$ \([i.e., \ E_{F1} = h^2 k_F^2/(2m^*)]\) in a system with a simple parabolic dispersion characterized by an effective mass $m^*$. Furthermore, as the system is in equilibrium, $E_F$ is constant throughout the system. Thus we have:

$$V(z \geq w) = E_F + \Phi = E_{H1} + E_{F1} + \Phi$$  (6b)

where the band bending $\Phi$ is the energy difference between the valence band edge and the Fermi energy in the bulk past the space charge layer.

The solution of the Poisson equation (3), in the Hartree approximation,\(^\text{59,60}\) is given by:

$$V(z) = V_{2DHG}(z) + V_D(z)$$  (7)

where $V_{2DHG}(z)$ is the electrostatic potential due to the 2D holes occupying the HH1 subband and $V_D(z)$ is due to the charged donors in the space charge layer.\(^\text{32,39}\) Assuming that the wave functions $\psi_h(z)$ vanish at the interface $z = 0$, the term $V_{2DHG}(z)$ becomes

$$V_{2DHG}(z) = \frac{pe^2}{\epsilon_s \epsilon_0} \left[ z - \int_0^z dz' \int_0^{z'} dz'' |\psi_h(z'')|^2 \right]$$  (8)

whereas the contribution from the space charge layer becomes

$$V_D(z) = \frac{e^2}{\epsilon_s \epsilon_0} N_D \left( wz - z^2/2 \right),$$  (9)

where

$$w = \sqrt{\frac{2\epsilon_s \epsilon_0}{e^2 N_D} \left[ \Phi + E_{H1} + E_{F1} - \frac{e^2}{\epsilon_s \epsilon_0} p(z) \right]},$$  (10)

and the expectation value $\langle z \rangle$ is defined via the wave function $\psi_h(z)$.

The wave function $\psi_h(z)$ entering the Poisson equation (3) is the solution of the Schrödinger equation. Thus one usually solves the Poisson and Schrödinger equations in a self-consistent iterative scheme.\(^\text{36,42–44,46,61}\) Using $V(z)$ from the Poisson equation, the 2D hole density $p|\psi_h(z)|^2$ is obtained from the Hamiltonian, from which one then constructs a new $V(z)$ by solving the Poisson equation. The process is iterated until $V(z)$ converges. In this work, we instead employ a simplified procedure based on the self-consistent variational scheme presented in Ref. 54, which yields good agreement with fully self-consistent numerical calculations. We approximate the wave functions using Fang-Howard variational wave functions, which take the form:

$$\psi_v(z) = 2\lambda_v^{3/2} z \exp(-\lambda_v z)$$  (11)
where $v = h$ represents the zero-node HH1 wave function. For the wave functions entering $V(z)$ we neglect $k$-dependent band mixing, which has only a small effect on $V(z)$. The variational parameter $\lambda_w$ is obtained by minimizing the $k = 0$ ground state HH energy $E_{H1}$, which, neglecting band mixing, is the sum of the diagonal matrix element of the Luttinger Hamiltonian in Eq. (1) for the HH subspace and the expectation value of $V(z)$ in Eq. (7), taking into account that $E_{H1}$ also appears in Eq. (10).

In the second variational step, we obtain the $k$ and spin dependent eigenfunctions $\Psi_{h,k}(z)$ of the total Hamiltonian $\hat{H} = H_L + V(z)$ for the HH1 sub-band by expanding $\Psi_{h,k}(z)$ in terms of the lowest eigenstates of $\hat{H}$ for $k = 0$, when $\hat{H}$ becomes diagonal. For the $k = 0$ HH1 and LH1 states we use the zero-node wave functions (11) with $v = h, l$. For the one-node HH2, LH2 states we use the form (12).

$$\psi_w(z) = \sqrt{12}\lambda_w^{3/2}z \left[1 - (\lambda_v + \lambda_w) z/3 \right] e^{-\lambda_w z} \sqrt{1 - \lambda_v/\lambda_w + \lambda_v^2/\lambda_w^2}. \quad (12)$$

By construction, these wave functions are orthogonal to the zero-node wave functions (11). The quantities $\lambda_w$ with $w = H, L$ denote additional variational parameters. The introduction of these additional variational parameters improves the accuracy of the method as compared to using a single variational parameter $\lambda_0 = \lambda_w$. The eigenvalues $E(k)$ and the corresponding $k$ dependent expansion coefficients are obtained by diagonalizing the matrix $\hat{H}$, whose elements are given as

$$\hat{H}_{\nu\nu'} = \langle \nu | H_L + V(z) | \nu' \rangle, \quad (13)$$

where $| \nu \rangle$ denotes the wave functions (11) and (12). The two lowest eigenenergies of the $8 \times 8$ matrix (13) correspond to the dispersion of the spin-split HH1 subband. In certain regimes these eigenenergies can also be obtained analytically to a good approximation, as shown in the next section.

C. Schrieffer-Wolff Transformation and Rashba Spin Splitting

It is well established that, under certain circumstances, the HH1 subbands may be described by an effective $2 \times 2$ Hamiltonian formulated as an expansion in powers of the wave vector $k$. The general kinematic structure of such a reduced Hamiltonian can be found from the theory of invariants.\(^{63}\) Retaining terms up to fourth order in $k$ and postponing the discussion of Dresselhaus terms until Sec. [XI] the effective $2 \times 2$ Hamiltonian for the subspace spanned by the spin-split HH1 subbands takes the form

$$H_{2\times2} = [Ak^2 - Bk^4 - d(k_+^2 - k_-^2)^2] \mathbb{I}_{2\times2} + i\alpha_R1(k_+\sigma_+ - k_-\sigma_-) + i\alpha_R2(k_+^3\sigma_+ - k_-^3\sigma_-) + i\alpha_R3(k_+\sigma_+ - k_-\sigma_-)k^2 \quad (14)$$

Up to fourth order in $k$, the Hamiltonian $H_{2\times2}$ includes all possible terms. The terms weighted by $A, B,$ and $d$ describe the orbital motion, whereas the terms weighted by $\alpha_R1$ represent the Rashba spin-orbit coupling. More specifically, the term $Ak^2$ describes the usual parabolic component of the dispersion, while the term $Bk^4$ represents the lowest-order nonparabolic correction, which remains isotropic and often has a sizable effect on the dispersion of hole systems, as discussed below. The term $d(k_+^2 - k_-^2)/2$ characterizes the warping of the energy contours. As can be seen from Eq. (14), the most general form of the Rashba SO coupling includes a term linear in $k$ proportional to $\alpha_R1$ and two terms cubic in $k$ weighted by $\alpha_R2$ and $\alpha_R3$. The terms weighted by $d, \alpha_R1,$ and $\alpha_R3$ break axial symmetry, which implies that these prefactors are zero when the axial approximation $\zeta = 0$ is employed in Eq. (1). Moreover, to lowest order the prefactor $\alpha_R1$ stems from the $k \cdot p$ coupling between the bonding and antibonding atomic $p$ orbitals (the latter give rise to the first excited conduction band).\(^6\) For the systems discussed here, the $k$-linear Rashba term thus contributes not more than $\sim 1\%$ of the total spin splitting, consequently this term is not considered further.

To obtain analytical expressions for the prefactors appearing in Eq. (14), one can apply a Schrieffer-Wolff transformation\(^{60}\) (Löwdin perturbation theory\(^{62}\)) to Eq. (14). The coefficients $A, B, d, \alpha_R1, \alpha_R2,$ and $\alpha_R3$ are evaluated to lowest order in the perturbation expansion: Explicit expressions are given in the Appendix. In the axial approximation, with $d = \alpha_R1 = \alpha_R3 = 0$, the dispersion for the HH1 subband takes the simple form

$$E_{\pm}(k) = Ak^2 - Bk^4 \pm Ck^3, \quad (15)$$

where $C \equiv |\alpha_R2|$. Numerical values for $A, B$, and $C \equiv |\alpha_R2|$ for typical experimental densities are given in Table [II]. The resulting subbands, denoted as HH1+ and HH1−, have unequal subband populations $p_\pm$ and density of states (DOS) effective masses $m_\pm$.

To characterize the strength of the Rashba spin-orbit interaction, we use the dimensionless quantity

$$\Delta p \equiv \frac{|p_+ - p_-|}{p} \quad (16)$$

where $p_\pm$ denotes the spin subband densities with $p = p_+ + p_-$. Experimentally, the quantity $\Delta p$ is usually inferred by analyzing the beating pattern of Shubnikov-de Haas (SdH) oscillations.\(^{61,64-66}\) For the single heterojunctions studied here, it can be manipulated by tuning the density $p$. At low temperature, $p_\pm$ is given by

$$p_\pm = \int \frac{d^2k}{(2\pi)^2} \theta[E_F - E_{\pm}(k)]. \quad (17)$$

where $\theta$ is the Heaviside step function. For hole systems with isotropic Fermi contours, Eq. (17) becomes

$$p_\pm = \frac{k_F^2}{4\pi}. \quad (18)$$
where \( k_{F\pm} \) denotes the Fermi wave vectors for the spin-split bands. Using the coefficients in Eq. (15), this translates to

\[
p_{\pm} = \frac{p}{2} \pm \frac{pc}{\sqrt{2X}} \sqrt{p\pi \left( 6 - \frac{4}{X} (1 - 4p\pi b) \right)}
\]

(19)

where \( X \equiv 1 - 4p\pi b + \sqrt{1 - 4p\pi(2b + c^2 - 4b^2p\pi)} \) \( (20a) \)

\[ b \equiv B/A \quad c \equiv C/A \]

(20b)

so that the Rashba spin splitting \( \Delta p \) is given by

\[
\Delta p = \frac{\sqrt{2c}}{X} \sqrt{p\pi \left( 6 - \frac{4}{X} (1 - 4p\pi b) \right)}.
\]

(21)

The DOS effective masses \( m_{\pm} \) of the spin-split subbands at the Fermi energy \( E_F \) takes the form

\[
m_{\pm} = \frac{\mu}{2\pi} \int d^2k \delta[E_F - E_{\pm}(k)],
\]

(22)

where \( \delta \) is the Dirac \( \delta \) function. For isotropic bands, this becomes

\[
m_{\pm} = \frac{\mu}{2\pi} \left( \frac{1}{k} \frac{dE_{\pm}(k)}{dk} \right)^{-1} \bigg|_{k=k_{F\pm}},
\]

(23a)

which can be further evaluated for the dispersion \( (15) \)

\[
m_{\pm} = \frac{\mu}{2A - 4Bk_{F\pm}^2 \pm 3Ck_{F\pm}},
\]

(23b)

where the Fermi wave vectors \( k_{F\pm} \) for a given total density \( p \) are evaluated using Eqs. \( (18) \) and \( (19) \).

D. Comparison with Numerical Results

To illustrate our approach, Fig. 1 shows a comparison between the results obtained using our variational calculation and those obtained in Ref. \( [42] \) using an iterative Fang-Howard and Luttinger Hamiltonian scheme. The 2DHG considered in Ref. \( [42] \) is a hole GaAs single heterojunction with a density of \( 5 \times 10^{15} \) m\(^{-2} \) and a net dopant concentration of \( N_D - N_A = 1 \times 10^{21} \) m\(^{-3} \). The confinement potential \( V(z) \) obtained from solving Eq. \( (3) \) is shown in the inset of Fig. 1. Our variational approach slightly overestimates the ground state heavy hole energy \( E_{H1} \) compared to the numerical results, as expected for a variational calculation. The corresponding DOS effective masses, obtained from Eqs. \( (13) \) and \( (22) \), are \( m_+ = 0.52 \) \( m_0 \) and \( m_- = 0.12 \) \( m_0 \). These numbers are in close agreement with the full-numerical calculations in Ref. \( [42] \) where \( m_+ = 0.46 \) \( m_0 \) and \( m_- = 0.12 \) \( m_0 \). We also find good agreement between our variational results for the Rashba spin splitting \( \Delta p \) and those obtained using the numerical method described in Refs. \( [49] \) and \( [57] \) (see Table 1).

While the simple dispersion in Eq. \( (15) \) affords a convenient way to calculate DOS properties such as effective masses and spin splittings, the validity of the Schrieffer-Wolff transformation is limited to certain sets of densities and dopant concentrations. When the separation between subband energies is small, the coefficients \( A, B \) and \( C \) are overestimated (refer to the Appendix for the dependence of \( A, B \) and \( C \) on the energy separations) and one can no longer describe the HH1+ and HH1− bands by Eq. \( (15) \). For example, using the values in Table 1 for a GaAs inversion layer with \( p = 2.5 \times 10^{15} \) m\(^{-2} \) and \( N_D - N_A = 3 \times 10^{20} \) m\(^{-3} \), the Rashba term \( Ck^3 \) be-
comes larger than $Ak^2 - Bk^4$ so that the heavier HH1+ band bends down for $k > k_{\text{bend}} = 1.7 \times 10^8 \text{ m}^{-1}$. As $k_{F+} = 1.5 \times 10^8 \text{ m}^{-1}$ is very close to HH1+ turning point $k_{\text{bend}}$, the HH1+ dispersion is almost flat at $k_{F+}$, which means that the HH1+ effective mass is overestimated. The Schrieffer-Wolff results for GaAs inversion layers with $N_D - N_A = 3 \times 10^{20} \text{ m}^{-3}$ and $p \gtrsim 2.5 \times 10^{15} \text{ m}^{-2}$ are invalid and we resort to a numerical diagonalization of Eq. (13) to obtain the energy dispersion. Note that unlike Eq. (13), dispersion curves obtained from a numerical diagonalization of Eq. (13) include spin splitting to all orders in $k$. Therefore, the dispersions from Eq. (13) are a reasonable approximation for any wave number $k$ (and hence for any density $p$), so long as only the zero-node heavy hole subbands HH1± are occupied. Indeed, in all the structures discussed in this paper, at the densities we consider, only the HH1+ and HH1− bands are occupied (Tables I, III, and V).

### III. Full Rashba Spin-Splittings and Effective Masses

Generally, spin splittings for holes are much larger than for electrons: For electron inversion layers with the same doping concentration, the spin splittings are about two orders of magnitude smaller. Below we focus first on GaAs inversion and accumulation layers, which are distinguished by the position of the Fermi level $E_F$ towards the substrate: in an inversion (accumulation) layer, $E_F$ is pinned near the conduction (valence) band. Finally, we discuss the spin splitting and effective masses in InAs, InSb, Ge, and Si hole inversion layers.

#### A. GaAs Inversion and Accumulation Layers

The type of background dopant determines the location of the Fermi level $E_F$ in the substrate and hence the amount of valence band bending $\Phi$ at the heterojunction interface [Fig. 2(a)]. For an accumulation layer, the band bending is less pronounced than for an inversion layer. Consequently, in accordance with Gauss’ law, for the same density, the confinement potential for an accumulation layer is less steep than in an inversion layer [Fig. 2(b)]. This means that the spacing between subbands is smaller (Fig. 3 and Table II), hence, according to the expressions in the Appendix, the Rashba SO interaction is stronger in an accumulation layer.

The variational approach followed in this work is designed to yield the energies of the HH1± subbands. Although it is not intended to give reliable values for the higher subbands, some qualitative observations can be made concerning the HH1-LH1 spacing in inversion and accumulation layers. In Table II and Fig. 3, the HH1-LH1 separation $\Delta_{11} E \equiv |E_{H1} - E_{L1}|$ at $k = 0$ is smaller in an
accumulation layer than in an inversion layer at the same density (Table II). Since the Rashba coefficient increases as the subbands get closer together, it is larger in an accumulation than an inversion layer at a given density (see Appendix for the dependence of the Rashba coefficient on the subband energy separations). The Rashba coefficient increases with density, which is consistent with the experimental results reported in Ref. 65 (Fig. 1).

We compare the different trends in the Rashba spin splitting $\Delta p$ as a function of density in inversion and accumulation layers in Fig. 5a) and (b). As expected, $\Delta p$ increases with density in both inversion and accumulation layers. For inversion layers with $N_D - N_A = 3 \times 10^{20} \text{ m}^{-3}$ and $p$ ranging from $5 \times 10^{14} \text{ m}^{-2}$ to $3 \times 10^{15} \text{ m}^{-2}$, the Rashba spin splitting increases with density in an almost linear fashion. In the accumulation layer counterparts, however, the spin splitting increases in an almost linear fashion at lower densities but saturates at higher densities. This feature can be attributed to the fact that, in an accumulation layer, the HH1-LH1 separation is smaller than in an inversion layer (see Appendix) such that the HH1− band anticrosses with the next highest energy subband (LH1) at a lower $k$ than in an inversion layer at the same density (Fig. 3). Consequently, for an accumulation layer with a higher density, $k_{F-}$ can be near the HH1-LH1 anticrossing. In the anticrossing region the HH1− band is pushed down in energy, hence the separation between the HH1− and HH1+ bands is reduced.

The strength of the Rashba SOI is also evident in the difference between the HH1+ and HH1− effective masses. Figures 5c) and 5d) show the variation of the effective HH1+ and HH− masses with density. As the figures show, there is a remarkable distinction in the dependence of the $m_+$ and $m_-$ on density for the inversion and accumulation layers we consider. For the inversion layers studied here, the HH1+ effective mass also increases in an almost linear fashion with density, whereas $m_-$ is essentially constant. The increase in the difference between the effective masses $m_+$ and $m_-$ with density again implies that the strength of the Rashba SO interactions increase with density. Comparison between numerical and SW results for inversion layers with densities up to $p = 2 \times 10^{15} \text{ m}^{-2}$ shows the SW approach works well. However, at a density $p = 2.5 \times 10^{15} \text{ m}^{-2}$, the HH1+ effective mass, calculated using the values in Table II is overestimated [Fig. 5(c)], which signifies that SW breaks down. For the accumulation layers considered here, however, with densities ranging from $5 \times 10^{14} \text{ m}^{-2}$ to $3 \times 10^{15} \text{ m}^{-2}$, the HH1+ effective mass increases, then saturates, and becomes increasingly lighter as the density increases. The SW approach is only valid for densities up to $\sim 5 \times 10^{14} \text{ m}^{-2}$ for the accumulation layers. That SW fails at lower densities in accumulation layers is expected as the separation between subband energies in an accumulation layer is smaller than in an inversion layer at

![FIG. 3.](image)

![FIG. 4.](image)
that the HH1+ band curvature becomes slightly steeper as the density increases, the Fermi energy increases, and the fact that the HH1+ band structure (Fig. 3). As the den-
m

\[ \text{Fig. 5(d).} \]
The dependence of the HH1+ effective mass \( m^+ \) on density is due to the HH1-LH1 anticrossing. In (c) we show the effective masses \( m^\pm \) for GaAs inversion layers and in (d) for accumulation layers. The heavier mass \( m^+ \) increases with density whereas \( m^- \) is nearly density-independent. In accumulation layers \( m^+ \) saturates with density due to the proximity of \( k_{F^-} \) to the HH1-LH1 anticrossing. The doping concentration is \( N_D - N_A = 3 \times 10^{20} \text{ m}^{-3} \) for the inversion layers and \( N_D = 3 \times 10^{20} \text{ m}^{-3} \) for the accumulation layers.

\[ \text{Fig. 6.} \]
(Color online) (a) Rashba spin splitting \( \Delta p \) and (b) effective masses \( m^\pm \) for various inversion layers. The results are obtained from a numerical diagonalization of Eq. (13), with \( N_D - N_A = 3 \times 10^{20} \text{ m}^{-3} \).

\[ \text{at} k > 1 \times 10^8 \text{ m}^{-1} \text{ means that the HH1+ effective mass at the Fermi energy decreases slightly with increasing density. The behavior of HH1−, on the other hand, reflects the anticrossing between the HH1-LH1 bands. As explained above, at a sufficiently high density, } k_{F-} \text{ can be very close to the HH1-LH1 anticrossing. In this region, the HH1− band becomes flatter, hence the corresponding effective mass } m^- \text{ increases slightly.} \]

B. Zinblende Materials and Ge Inversion Layers

Figure 6 shows the spin splitting \( \Delta p \) and effective masses \( m^\pm \) as functions of density for inversion layers in GaAs, Ge, InSb, and InAs. The strength of the SO interaction is reflected in the difference between the subband populations and effective masses of the HH1+ and HH1− subbands. In Ge, InAs, and InSb, the Rashba spin splitting and HH1+ effective mass \( m^+ \) saturate at a lower density compared to GaAs. The saturation of the spin splitting and \( m^+ \) indicates that HH1 and LH1 are close enough such that the HH1-LH1 anticrossing occurs near \( E_F \). This indicates that Ge, InSb, and InAs exhibit a stronger SO interaction than GaAs, which is consistent with the known fact that SO coupling is stronger in compounds containing elements with larger atomic numbers \( Z \). The corollary of this is that SW breaks down at different densities for various materials, which implies that Eq. (15) is valid only for low densities for heavy materials. For example, using the values for \( A \), \( B \), and \( C \) listed in Table II, one can get a reasonable estimate for the HH1+ and HH1− effective masses of InAs and Ge at a density of \( 5 \times 10^{14} \text{ m}^{-2} \). The SW effective masses of InAs are obtained as \( m^+ = 0.094 \text{ m}_0 \) and \( m^- = 0.036 \text{ m}_0 \), which are close to \( m^+ = 0.113 \text{ m}_0 \) and \( m^- = 0.036 \text{ m}_0 \) obtained by numerically diagonalizing Eq. (13). For Ge, the SW effective masses are \( m^+ = 0.108 \text{ m}_0 \) and \( m^- = 0.059 \text{ m}_0 \), which are in excellent agreement with the numerical diagonalization results \( m^+ = 0.118 \text{ m}_0 \) and \( m^- = 0.059 \text{ m}_0 \). For InSb, the SW results are valid at densities \( \lesssim 4 \times 10^{14} \text{ m}^{-2} \). Using the values in Table VII for \( 3.3 \times 10^{14} \text{ m}^{-2} \), the SW effective masses are \( m^+ = 0.087 \text{ m}_0 \) and \( m^- = 0.019 \text{ m}_0 \), which also compare well with the numerical diagonalization results of \( m^+ = 0.095 \text{ m}_0 \) and \( m^- = 0.020 \text{ m}_0 \).

C. Silicon Inversion Layers

In Si, the hole density is usually of the order of \( 10^{16} \text{ m}^{-2} \), so that \( k_F \sim 5 \times 10^{-8} \text{ m}^{-1} \). In this regime, the term \( CK^3 \) in Eq. (13) becomes dominant, SW breaks down, and only numerical diagonalization gives reliable results. As pointed out above, due to the large cubic terms, it is necessary to include the spin-orbit split-off band, hence the Luttinger Hamiltonian is now projected onto a 12 x 12 subspace. In this work, we consider densities up to \( 2 \times 10^{16} \text{ m}^{-2} \) (Table VII), since for larger den-

\[ \text{dinisa} \]
TABLE III. Values for material-dependent constants $A$ (in $10^{-16}$ meV m$^2$), $B$ (in $10^{-32}$ meV m$^4$), and $C$ (in $10^{-24}$ meV m$^3$) in the dispersion relation $E(k) = Ak^2 - Bk^4 + Ck^6$ for GaAs, InAs, and Ge inversion layers with $N_D - N_A = 3 \times 10^{20}$ m$^{-3}$. All densities below are in $10^{15}$ m$^{-2}$. The Schrieffer-Wolff approach breaks down for densities exceeding $0.5 \times 10^{15}$ m$^{-2}$ for InAs as well as for Ge.

| Density | GaAs | InAs | Ge |
|---------|------|------|----|
|         | $A$  | $B$  | $C$ | $A$  | $B$  | $C$ | $A$  | $B$  | $C$ |
| 0.5     | 2.99 | 0.27 | 0.33 | 9.02 | 1.94 | 3.60 | 5.84 | 1.13 | 1.60 |
| 1.0     | 2.92 | 0.25 | 0.58 |       |      |      |      |      |      |
| 1.5     | 2.86 | 0.23 | 0.61 |       |      |      |      |      |      |
| 2.0     | 2.80 | 0.22 | 0.64 |       |      |      |      |      |      |
| 2.5     | 2.74 | 0.20 | 0.67 |       |      |      |      |      |      |
| 3.0     |      |      |      |       |      |      |      |      |      |

TABLE IV. The energy spacing (in meV) between the HH1 and LH1 levels, as well as the Fermi energy for GaAs, InAs, and Ge hole inversion layers at various densities (in $10^{15}$ m$^{-2}$) and $N_D - N_A = 3 \times 10^{20}$ m$^{-3}$. In all cases considered below LH1 is far above the Fermi energy, thus validating the assumption that only the HH1 band is occupied.

| Density | GaAs | InAs | Ge |
|---------|------|------|----|
|         | $E_{H1}$ | $\Delta_{HH}^{H1}$ | $E_{F1}$ | $E_{H1}$ | $\Delta_{HH}^{H1}$ | $E_{F1}$ | $E_{H1}$ | $\Delta_{HH}^{H1}$ | $E_{F1}$ |
| 0.5     | 16.12 | 8.32 | 0.91 | 12.87 | 10.87 | 2.27 | 14.72 | 7.74 | 1.63 |
| 1.0     | 19.24 | 8.73 | 1.67 | 16.38 | 11.42 | 3.47 | 18.04 | 8.16 | 2.72 |
| 1.5     | 22.12 | 9.04 | 2.30 | 19.54 | 11.79 | 4.33 | 21.08 | 8.46 | 3.50 |
| 2.0     | 24.83 | 9.27 | 2.83 | 22.47 | 12.06 | 5.12 | 23.91 | 8.69 | 4.18 |
| 2.5     | 27.40 | 9.46 | 3.26 | 25.21 | 12.28 | 5.88 | 26.58 | 8.87 | 4.80 |
| 3.0     | 29.85 | 9.62 | 3.64 | 27.82 | 12.45 | 6.61 | 29.13 | 9.02 | 5.43 |

Due to the significant size of the prefactor $\zeta$ in Eq. 1, the SO interaction and hence spin splitting (17) is anisotropic: It has a minimum along the (100) direction and a maximum along (110). The anisotropy of the SO strength is shown in Fig. 7(a): The difference in the Fermi wave vectors $k_{F+}$ and $k_{F-}$ is $6 \times 10^6$ m$^{-1}$ along (100) and $1 \times 10^6$ m$^{-1}$ along (110). The equienergy lines for Si ground state HHs [Figs. 7(b) and 7(c)] show that Si valence bands are in general warped, and the warping becomes more pronounced as the density increases.

The spin splitting in Si [Fig. 7(d)] also increases with density, which again reflects the fact that the strength of spin-orbit interaction increases with density. However, spin splittings in Si holes are smaller than in both zincblende materials and Ge, discussed in the previous section. This is expected since amongst all the materials considered in this paper, Si is the lightest element with atomic number $Z = 14$. Nevertheless, the spin splitting in Si hole systems is considerably larger than in Si electron systems.

IV. DRESELHAUS SPIN-ORBIT INTERACTION

In semiconductor crystals which lack a center of inversion, such as GaAs, InAs, and InSb, Dresselhaus spin-orbit interaction terms are present.22 In this section, we discuss the spin splitting as a function of density and material parameters in GaAs, InAs, and InSb accounting for both the Rashba and the Dresselhaus interactions. The Dresselhaus spin-orbit coupling in bulk semiconductor hole systems is characterized by a variety of terms, whose relative importance depends on the parameter regime under study. In what follows we establish a hierarchy among these terms in heterojunctions at realistic experimental densities.

Up to third order in $k$, the Dresselhaus SO interaction in bulk systems is described by the following invariants.

\[ H_D = -\frac{2}{3} C_D \left[ x \{ J_x, J_y^2 - J_z^2 \} + \text{cp} \right] + B_{D1} \left[ x \{ k_y^2 - k_z^2 \} J_x + \text{cp} \right] + B_{D2} \left[ k_x \{ k_y^2 - k_z^2 \} J_y^2 + \text{cp} \right] + B_{D3} \left[ k_x \{ k_y^2 + k_z^2 \} \{ J_x, J_y^2 - J_z^2 \} + \text{cp} \right] + B_{D4} \left[ k_x^2 \{ J_x, J_y^2 - J_z^2 \} + \text{cp} \right], \]

(24)
TABLE V. The energy spacing (in meV) between the HH1 and LH1 levels, as well as the Fermi energy $E_{F1}$ for an InSb hole inversion layer with $N_D - N_A = 3 \times 10^{20} \text{ m}^{-3}$. At the densities below (in $10^{15} \text{ m}^{-2}$), only the HH1+ and HH1− subbands are occupied. Here the material- and structure-dependent coefficients $A$, $B$, and $C$ are listed for $p = 0.33 \times 10^{15} \text{ m}^{-2}$. $A$ is given in multiples of $10^{-16} \text{ meV m}^2$, $B$ in multiples of $10^{-32} \text{ meV m}^4$, and $C$ in multiples of $10^{-24} \text{ meV m}^3$.

| Density | $E_{H1}$ | $\Delta_{H1}^{LL}$ | $E_{F1}$ | $A$ | $B$ | $C$ |
|---------|----------|---------------------|----------|-----|-----|-----|
| 0.33    | 9.69     | 11.72               | 2.26     | 15.76 | 5.84 | 10.06 |
| 0.50    | 10.87    | 12.00               | 2.87     |       |     |     |
| 0.67    | 12.02    | 12.23               | 3.33     |       |     |     |
| 0.83    | 13.05    | 12.42               | 3.74     |       |     |     |
| 1.00    | 14.11    | 12.59               | 4.15     |       |     |     |

FIG. 7. Panel (a) shows the dispersion for Si holes along (100) and (110), indicating that the strength of the spin-orbit interaction is a maximum along (110) and minimal along (100). The inset shows that the spin splitting is only $6 \times 10^6 \text{ m}^{-2}$ along (100), compared to $1 \times 10^{16} \text{ m}^{-2}$ along (110). Here, the density is $2 \times 10^{16} \text{ m}^{-2}$ and the doping concentration is $N_D - N_A = 3 \times 10^{23} \text{ m}^{-3}$. The equienergy contours (separated by 5 meV) for the (b) HH1+ and (c) HH1− subbands in the inversion layer discussed in panel (a) show a strong valence band warping. Panel (d) shows the spin splitting for Si hole inversion layers at various densities with $N_D - N_A = 3 \times 10^{23} \text{ m}^{-3}$. Here, the dispersion is obtained by numerically diagonalizing Eq. (13).

TABLE VI. Si hole inversion layer energy level spacings (in meV) for various densities (in $10^{16} \text{ m}^{-2}$), showing that only the HH1+ and HH1− bands are occupied. The dopant concentration $N_D - N_A$ for the inversion layer is $3 \times 10^{23} \text{ m}^{-3}$.

| Density | $E_{H1}$ | $\Delta_{H1}^{LL}$ | $E_{F1}$ |
|---------|----------|---------------------|----------|
| 0.83    | 152.81   | 15.36               | 6.62     |
| 1.00    | 157.13   | 15.51               | 7.64     |
| 1.33    | 165.36   | 15.73               | 9.36     |
| 1.67    | 173.63   | 15.96               | 10.87    |
| 2.00    | 181.48   | 16.12               | 12.17    |

To evaluate the prefactors in Eq. (25), we first project Eq.
onto the subspace spanned by the zero- and one-node hole states. Then, by means of the SW transformation, we obtain an effective $2 \times 2$ Hamiltonian describing the Dresselhaus interactions in the HH1± subspace, so that the prefactors can be obtained by comparison with Eq. 25. Analytical expressions for the prefactors $\gamma_D, \beta_{D1}$, and $\beta_{D2}$ are listed and discussed in the Appendix, complemented by typical numerical values.

Strictly speaking, our treatment of Dresselhaus SO coupling relies implicitly on a hierarchy of steps. The first step, carried out in detail in Ref. 6, is the projection of the bulk $14 \times 14$ Hamiltonian yielding the bulk $4 \times 4$ Luttinger Hamiltonian, which includes all the possible bulk Dresselhaus terms with the prefactors listed in Table II. In the second step the bulk Luttinger Hamiltonian is projected onto the subspace spanned by the (spin-split) ground state HH1 sub-band. In this sense our approach is comparable to that of Ref. 34 which directly projects from the bulk $14 \times 14$ Hamiltonian to the HH1 subspace.

When only the dominant Rashba and Dresselhaus terms are retained the energy dispersion relation becomes

$$E(k) = Ak^2 - Bk^4 + 2dk^4(1 - \cos 4\phi) \pm \sqrt{(\alpha_{R2}^2 + \beta_{D1}^2)k^6 + 2\beta_{D1}\gamma_D k^4 + \gamma_D^2k^2 - 2|\alpha_R^2|(k^2\beta_{D1} + \gamma_D)k^4 \sin 2\phi}$$

for

$$\alpha_{R2}^2 = 1/\kappa^4, \beta_{D1}^2 = \frac{1}{(2\kappa^2)^4}$$

$$\beta_{D2}^2 = \frac{1}{(2\kappa^2)^4}, \gamma_D = \frac{1}{2}(\kappa^2\beta_{D1} + \gamma_D)k^4 \sin 2\phi$$

where $\phi = \arctan(k_y/k_z)$. We find that, for the single heterojunctions studied here, the Dresselhaus terms contribute at most one order of magnitude less than the Rashba term to the total spin splitting at the Fermi energy. Nevertheless, the contribution due to the Dresselhaus coupling is visible in the term proportional to $\sin 2\phi$, which causes the difference $\Delta k_F \equiv |k_{F+} - k_{F-}|$ to be anisotropic in $\kappa$. The anisotropic terms in Eq. (14) are likewise sizable. In accordance to Eq. (25), the extrema of $\Delta k_F$ occur when $\phi = \pi/4$ or $\phi = 3\pi/4$. The anisotropy of the spin splitting, which we define here as the ratio $\kappa \equiv \Delta k_F(\phi = 3\pi/4)/\Delta k_F(\phi = \pi/4)$, depends on the density as well as on material-specific parameters, as Fig. 8 shows. For example, one can infer from Fig. 8a) that $\kappa = 2.24$ for a GaAs inversion layer with $p = 5 \times 10^{14}$ m$^{-2}$ and $\kappa = 1.77$ with $p = 3 \times 10^{15}$ m$^{-2}$. The fact that the anisotropy $\kappa$ decreases with density implies that the Rashba coefficient increases faster with density than the cubic and linear Dresselhaus coefficients combined (see Appendix). Comparing different materials [Fig. 8b)], one can deduce that $\kappa = 1.89, \kappa = 1.42, \kappa = 1.48$ for GaAs, InAs, and InSb inversion layers with $p = 1 \times 10^{15}$ m$^{-2}$, respectively. This implies that, amongst the materials considered here, the effect of Dresselhaus SOI is weakest in InAs but strongest in GaAs, an observation that is rather counterintuitive considering the relative values of the bulk Dresselhaus prefactors in these materials. Indeed, this reflects the fact that the relative importance of specific spin-orbit interaction terms is determined by their ratio to the spin-independent terms in the dispersion relation, rather than the absolute magnitude of their corresponding numerical prefactors.

V. DISCUSSION

A. Breakdown of the SW method

The analysis presented in this work is consistent with the known general trend that SO coupling in 2DHGs increases with the carrier number density. We have characterized the strength of the Rasha SO interaction using both the relative spin-split population difference $\Delta p$ and the effective masses $m_\pm$. We have found that $\Delta p$ and $m_\pm$ are expected to increase almost linearly with density whereas $m_-$ is approximately constant. While the simple dispersion found using the SW transformation provides a good approximation for certain systems, e.g. GaAs inversion layers with $N_D - N_A = 3 \times 10^{20}$ m$^{-3}$ and densities $p < 2.5 \times 10^{15}$ m$^{-2}$, there are many parameter regimes in which SW breaks down. The fact that the simple dispersion can fail for realistic parameters challenges the current theories on electric dipole spin resonance (EDSR), effective spin conductivity, hole spin helix, and Zitterbewegung, which assume that hole spin-orbit coupling is simply cubic in wave vector.

B. Inversion vs. accumulation layers

Comparing GaAs inversion and accumulation layers, the strength of the Rasha SO interaction is very sensitive to the type of background dopant. Owing to the fact that the confinement potential for inversion layers is steeper than that for accumulation layers, the HH1-LH1 splitting for inversion layers is larger than that for accumulation layers. Consequently, the strength of SO interaction is stronger in an accumulation layer than in an inversion layer (see Appendix for the relation between Rashba or Dresselhaus coefficients and the HH1-LH1 splitting).

In both inversion and accumulation layers, the spin splitting $\Delta p$ increases with density, yet the dependence of the spin splitting and effective mass on density is quite
different. In an accumulation layer, both $\Delta p$ and $m_+$ increase almost linearly with $p$ at low densities, and both saturate at higher densities. These trends can be attributed to the fact that in an accumulation layer, the HH1-LH1 anticrossing occurs at a lower $k$, so that the spin splitting near the anticrossing is reduced. Correspondingly, in accumulation layers SW breaks down at much lower densities than in inversion layers.

We compare our results for GaAs, InAs, InSb, Ge and Si inversion layers. The spin splitting and effective mass profiles show that the Rashba SO interaction is stronger in Ge, InAs, and InSb than in GaAs, though the Fermi contour remains isotropic in the absence of Dresselhaus terms. The Si dispersion, on the other hand, is very anisotropic owing to the large cubic contribution stemming from the bulk Luttinger Hamiltonian. The term $\propto \zeta$ in the Luttinger Hamiltonian Eq. 1 is sizable and is responsible for the highly anisotropic Fermi contour. The spin splitting is a maximum along the (110) and (110) directions but a minimum along (100) and (010).

We have considered the Dresselhaus spin-orbit interaction in zincblende semiconductors GaAs, InAs, and InSb. While the magnitude of BIA is always much smaller than SIA, it causes the spin splitting to be anisotropic in $k$. Figure 8 shows that the spin splitting is a maximum along (110) but a minimum along (110), in accordance with Eq. 26.

C. Relative importance of the $k$-linear and $k$-cubic spin-orbit interaction terms

In general, spin-orbit interaction terms in the system Hamiltonian are characterized by invariants, with each invariant associated with a specific power of $k$ and having a particular functional form. The fact that spin-orbit interactions preserve time reversal symmetry suggests that only odd powers of the wave vector are admissible. To date spin-orbit interaction terms of orders linear and cubic in $k$ have received the most attention. The identification of the relevant powers of the wave vector characterizing a specific form of the spin-orbit interaction depends on the underlying mechanism (BIA, SIA, and interface asymmetry), on the dimensionality of the system, and on whether the carriers are electrons or holes. For example, in bulk electron systems the leading-order Dresselhaus term is $\propto k^3$, while in bulk hole systems as well as in 2D electron and hole systems Dresselhaus terms linear in $k$ are present. Broadly speaking, one expects terms involving smaller powers of $k$ to dominate at low densities, while terms involving higher powers of $k$ are expected to dominate at higher densities.

In the structures we have studied, although $k$-linear Rashba terms of the form $i\alpha R(k_+\sigma_+ - k_-\sigma_-) \equiv -2\alpha R (k_y\sigma_x + k_x\sigma_y)$ are allowed by symmetry, we find the $k$-linear Rashba coefficient to be zero since our model does not include excited bulk conduction bands, as discussed in Sec. II C. Correspondingly, $k$-linear Rashba terms have not been included in our analytical (SW) results. Thus, when the SW transformation is applicable, the Rashba spin splitting is described by Eq. 13, which is consistent with Ref. 6. In contrast, the Dresselhaus spin-orbit interaction is characterized by terms proportional to both $k$ and $k^3$ which are comparable in mag-
We would like to comment on the relative importance of the linear-$k$ and cubic-$k$ Dresselhaus terms for the systems studied in this work. For GaAs inversion layers with the 2DHG densities considered here, the linear-$k$ and cubic-$k$ Dresselhaus terms are of the same order of magnitude (see Appendix). For example, for a GaAs inversion layer with $p = 5 \times 10^{14}$ $m^{-2}$ and $k_F = 5.6 \times 10^7$ $m^{-1}$, we find $\beta_{D1} = 0.08 \times 10^{-24}$ $meV m^3$, and $\gamma_D = 0.03 \times 10^{-8}$ $meV m$, so that the ratio $\xi_D \equiv \frac{\beta_{D1} k_F^3}{\gamma_D} \cdot$ of the $k$-linear and $k$-cubic Dresselhaus terms is $\xi_D = 1.19$. As the density increases, the relative importance of the linear-$k$ term decreases. For example, for $p = 2 \times 10^{15}$ $m^{-2}$ corresponding to $k_F \approx 1.12 \times 10^8$ $m^{-1}$, we find $\beta_{D1} = 0.084 \times 10^{-24}$ $meV m^3$, and $\gamma_D = 0.029 \times 10^{-8}$ $meV m$, yielding $\xi_D = 0.32$, which is four times less than when $p = 5 \times 10^{14}$ $m^{-2}$. Since $\beta_{D1}$ and $\gamma_D$ are almost constant at the densities considered in this work, we can easily estimate the density $p_D$ above which the cubic-$k$ Dresselhaus term dominates. Taking $\beta_{D1} = 0.08 \times 10^{-24}$ $meV m^3$ and $\gamma_D = 0.03 \times 10^{-8}$ $meV m$, we find that $\xi_D \ll 1$ when $k_F \gg 6.1 \times 10^7$ $m^{-1}$, which corresponds to $p_D \gg 6 \times 10^{14}$ $m^{-2}$.

We have performed a similar analysis of the $k$-linear and $k$-cubic Dresselhaus terms for InAs and InSb inversion layers. For an InAs inversion layer with $p = 5 \times 10^{14}$ $m^{-2}$ we obtain $\xi_D = 5.2$, which implies that the linear-$k$ term is much more important than the cubic-$k$ Dresselhaus term for the densities considered here. For InAs we find $p_D = 2.6 \times 10^{15}$ $m^{-2}$. On the other hand, for an InSb inversion layer with $p = 3.3 \times 10^{14}$ $m^{-2}$, $\xi_D = 0.16$. We obtain $p_D = 5.4 \times 10^{13}$ $m^{-2}$, so that the linear-$k$ contribution is essentially negligible for our range of densities.

The Dresselhaus interaction is absent in semiconductors with a diamond structure such as Si and Ge. At the same time terms of the same symmetry may appear depending on the termination at the interface. The interface-induced spin splitting depends on the coupling to the conduction and split-off bands. The dominant contribution from this mechanism is linear in $k$ and has the same symmetry as the $k$-linear Dresselhaus term, i.e. $H_{int} \propto k_n \sigma_+ + k_\sigma + k_\sigma_+ \sigma_+$. A quantitative description of interface asymmetry terms is beyond the scope of the present work. We may expect that for the heterojunctions studied here the effect of interface asymmetry is weaker than in quantum wells, since the wave functions experience a strong confinement at the heterointerface, but only a weak confinement towards the substrate. Thus even in a refined model permitting the wave functions to tunnel into the barrier, the wave functions are less pushed into the barrier than in a quantum well. The smaller probability of finding the carriers at the interface then implies a smaller effect of interface asymmetry on spin splitting. Consistent with this qualitative reasoning, initial studies reveal that in heterojunctions the terms due to interface asymmetry are considerably smaller than the Rashba spin-orbit interaction.

VI. SUMMARY AND OUTLOOK

We have performed a variational analysis of spin-orbit interactions in 2D hole gases in inversion-asymmetric heterojunctions in a number of cubic semiconductors. We have quantified our findings in terms of experimentally accessible quantities: carrier number density, effective masses, and spin splitting. We find that for a broad range of experimentally relevant parameters the frequently used lowest-order expansion of the dispersion breaks down. To address this shortcoming we have provided a simple quasianalytical scheme for calculating spin-orbit related quantities that is in good agreement with numerical studies and experimental data. We recover the known general trend that the spin splitting and $HH1+$ effective mass $m_1$ increase as functions of density. We have found that in heterojunctions the Rashba SO coupling is in general much stronger than the Dresselhaus SO coupling. More specifically, Rashba SO coupling is much stronger in accumulation layers than in inversion layers, and it is very sensitive to the density of background dopants. Finally, in Si, due to the strong cubic terms already present in the bulk, the Fermi contour is strongly anisotropic.

The approach presented in this work can be extended to study spin-orbit interactions on surfaces other than (001), while the choice of basis functions can be tailored to the system under consideration. For example, the bulk $k^3$-Dresselhaus interaction applied to a low-symmetry surface includes terms $\propto k_n^3$, which can be problematic depending on one’s choice of basis functions. Reference thus avoids dealing directly with the Dresselhaus terms in determining the spin splitting for 2D hole systems. Instead, this work resorts to the bulk $14 \times 14$ extended Kane Hamiltonian, which avoids powers of $k_z$ higher than second, offering considerable computational flexibility. Nevertheless, although higher powers of $k_z$ require some care, they can easily be treated if the basis functions are sufficiently smooth (e.g., plane waves or Fock-Darwin states). This consideration can become important if in certain systems terms $\propto k_z^3$ turn out to be significant, which is not the case in the present work.

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Appendix: The material- and structure-dependent parameters

In the following we evaluate the prefactors up to second-order perturbation theory. The first-order terms are given by the expectation values of the diagonal elements in the $2 \times 2$ submatrix spanned by the states $\{ | \pm 3/2 \}$ in the Luttinger Hamiltonian (13). The second-order terms are mediated by couplings to intermediate states in the usual way. In all formulas in this section, the index $i$ implies a summation over $i = 1, 2$.

The prefactors for the orbital terms take the form

$$A = \frac{\mu}{2} (\gamma_1 + \gamma_2) + 3\mu^2 \gamma_3^2 \frac{|\langle H_1 | k_2 | L_4 \rangle|^2}{\Delta_{HL}^i},$$

(A.1)

$$B = -\frac{3}{4} \mu^2 (\gamma - \zeta) \frac{|\langle H_1 | L_4 \rangle|^2}{\Delta_{HL}^i},$$

(A.2)

d$ = \frac{3}{4} \gamma \zeta \frac{|\langle H_1 | L_4 \rangle|^2}{\Delta_{HL}^i},$

(A.3)

where $\Delta_{\rho q}^i \equiv E_{\rho}^i - E_{\rho}^q$. Typical values for $A$, $B$ and $d$ for GaAs inversion layers are given in Table VII.

The Rashba coefficient $\alpha_{R2}$ reads

$$\alpha_{R2} = -\frac{3}{2} \mu^2 \gamma_3 \frac{\langle H_1 | L_4 \rangle \langle L_4 | k_2 | H_1 \rangle - \langle H_1 | k_2 | L_4 \rangle \langle L_4 | H_1 \rangle}{\Delta_{HL}^i},$$

(A.4)

while the Rashba coefficient $\alpha_{R3}$ is given by

$$\alpha_{R3} = \frac{3}{2} \mu^2 \gamma_3 \frac{\zeta \langle H_1 | L_4 \rangle \langle L_4 | k_2 | H_1 \rangle - \langle H_1 | k_2 | L_4 \rangle \langle L_4 | H_1 \rangle}{\Delta_{HL}^i},$$

(A.5)

implying $\alpha_{R2}/\alpha_{R3} = -\tilde{\gamma}/\zeta$. Note that these expressions emerge in second order in the SW transformation. This is in contrast to Ref. [6], where these prefactors arose only in third order. This difference is due to the fact that in Ref. [6], the prefactors were expressed in terms of basis functions for inversion symmetric systems such as the infinite square well and the simple harmonic oscillator, treating the asymmetric component of the confining potential $V(z)$ explicitly as a perturbation. In this work, the asymmetry of $V(z)$ is encoded in the asymmetric Fang-Howard functions (11) and (12), so that the expressions (A.4) and (A.5) for Rashba prefactors depend implicitly on the asymmetry of $V(z)$.

The $k$-linear Dresselhaus coefficient has the form:

$$\gamma_D = \frac{\sqrt{3}}{2} C_D + 2\sqrt{3} \mu_0 \gamma_3 C_D \frac{|\langle H_1 | k_2 | L_4 \rangle|^2}{\Delta_{HL}^i},$$

(A.6)

$$-\frac{3}{4} \left( B_{D2} + B_{D3} \right) \langle H_1 | k_2 | H_1 \rangle.$$}

The prefactors of the cubic Dresselhaus terms become

$$\beta_{D1} = \frac{\sqrt{3}}{2} \mu_0 \gamma C_D \frac{|\langle H_1 | L_4 \rangle|^2}{\Delta_{HL}^i} - \frac{3}{16} \left( B_{D2} - B_{D3} + 3B_{D4} \right)$$

$$+ \frac{3}{4} \mu_0 \gamma \beta_{D1} \left( \langle H_1 | L_4 \rangle \langle L_4 | k_2^2 | H_1 \rangle + \langle H_1 | k_2^2 | L_4 \rangle \langle L_4 | H_1 \rangle \right) \frac{\Delta_{HL}^i}{\Delta_{HL}^i},$$

(A.7)

and

$$\beta_{D2} = -\frac{\sqrt{3}}{2} \mu_0 \gamma C_D \frac{|\langle H_1 | L_4 \rangle|^2}{\Delta_{HL}^i} + \frac{3}{16} \left( B_{D2} - B_{D3} + 3B_{D4} \right)$$

$$- \frac{3}{4} \mu_0 \gamma \beta_{D1} \left( \langle H_1 | L_4 \rangle \langle L_4 | k_2^2 | H_1 \rangle + \langle H_1 | k_2^2 | L_4 \rangle \langle L_4 | H_1 \rangle \right) \frac{\Delta_{HL}^i}{\Delta_{HL}^i},$$

(A.8)

For the $k$-linear coefficient $\gamma_D$, the bulk prefactors $B_{D2}$ and $B_{D3}$ give rise to sizable first-order contributions at low densities. On the other hand, interestingly, there are no contributions proportional to the bulk prefactors $B_{D2}$, $B_{D3}$, and $B_{D4}$ from second order in SW perturbation theory. The smallness of $B_{D2}$, $B_{D3}$, and $B_{D4}$ implies approximately $\beta_{D1}/\beta_{D2} \approx -\tilde{\gamma}/\zeta$. Nonetheless, for the prefactors $\beta_{D1}$ and $\beta_{D2}$, we retained the contributions up to second order in SW perturbation theory. Here we note that within the extended Kane model we have the relation $B_{D4} = B_{D3} - B_{D2}$ (see Table IV and Ref. [6]), so that the first-order contributions from the coefficients $B_{D2}$, $B_{D3}$, and $B_{D4}$ to the coefficient $\beta_{D2}$ cancel. While the contributions from the bulk Dresselhaus terms proportional to $B_{D2}$, $B_{D3}$, and $B_{D4}$ are generally small, the terms obtained in first and second-order SW perturbation theory are similar in magnitude. This reflects the fact that the second order yields mixed terms still linear in $B_{D2}$ and $B_{D3}$, but also proportional to the large Luttinger coefficients.

Typical values for the Rashba and Dresselhaus coefficients obtained from the above equations are given in Table VII.
TABLE VII. Typical values for $A$ (in $10^{-16}$ meVm$^2$), $B$, $d$ (both in $10^{-32}$ meVm$^3$), $\alpha_{R2}$, $\alpha_{R3}$ (both in $10^{-24}$ meVm$^3$), $\gamma_D$ (in $10^{-8}$ meVm), $\beta_{D1}$ and $\beta_{D2}$ (both in $10^{-24}$ meVm$^3$), for 2DHG GaAs hole inversion layers with $N_D - N_A = 3 \times 10^{12} \text{ m}^{-2}$.

Superscripts (1) and (2) distinguish contributions from first- and second-order perturbation theory to the respective coefficients. The density is given in multiples of $10^{12} \text{ m}^{-2}$.

| density | $A^{(1)}$ | $A^{(2)}$ | $B$ | $d$ | $\alpha_{R2}$ | $\alpha_{R3}$ | $\gamma_D^{(1)}$ | $\gamma_D^{(2)}$ | $\beta_{D1}$ | $\beta_{D2}$ |
|---------|---------|---------|-----|----|-----------|-----------|------------|------------|--------|--------|
| 0.5     | 3.41   | -0.42  | 0.27 | 0.70 | -0.53     | 0.084     | 0.022      | 0.008      | 0.083  | -0.013 |
| 2.0     | 3.41   | -0.61  | 0.22 | 0.56 | -0.64     | 0.103     | 0.017      | 0.010      | 0.086  | -0.014 |

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