Spin-orbit interaction in symmetric wells with two subbands

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We investigate the spin-orbit (s-o) interaction in two-dimensional electron gases (2DEGs) in quantum wells with two subbands. From the 8 × 8 Kane model, we derive a new inter-subband-induced s-o term which resembles the functional form of the Rashba s-o – but is non-zero even in symmetric structures. This follows from the distinct parity of the confined states (even/odd) which obliterates the need for asymmetric potentials. We self-consistently calculate the new s-o coupling strength for realistic wells and find it comparable to the usual Rashba constant. Our new s-o term gives rise to a non-zero ballistic spin-Hall conductivity, which changes sign as a function of the Fermi energy (εF), and can induce an unusual zitterbewegung with cycloidal trajectories without magnetic fields.

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The rapidly developing field of spintronics has generated a great deal of interest in s-o coupling in semiconductor nanostructures [1]. For an n-doped zincblende semiconductor quantum well with only the lowest subband occupied, i.e. in a strictly 2D situation, there are two main contributions to the interaction of the spin and orbital degrees of freedom of electrons. One contribution is the Dresselhaus term, which results from the lack of inversion symmetry of the underlying zinc-blende lattice and is of lowest order linear in the crystal momentum [2, 3]. This linearity is shared by the other contribution known as the Rashba term [4], which is due to structural inversion asymmetry and can be tuned by an electric field across the well [3]. These two contributions can lead to an interesting interplay in spintronic systems [8].

In this Letter we consider yet another type of electronic s-o coupling which, as we show, occurs in III-V (or II-VI) zinc-blende semiconductor quantum wells with more than one subband. We derive a new inter-subband-induced s-o interaction which resembles that of the ordinary Rashba model; however, in contrast to the latter, ours is non-zero even in symmetric structures, Fig. 1. We self consistently determine the strength of this new s-o coupling for realistic single and double wells and find it comparable to the Rashba constant, Figs. 2(a)-(b). We have investigated the spin Hall effect and the dynamics of spin-polarized electrons due to this new s-o term. We find (i) a non-zero ballistic spin Hall conductivity which changes sign as a function of εF and (ii) an unusual zitterbewegung [5] with cycloidal trajectories without magnetic fields, Fig. 3. As derived below, for a symmetric well with two subbands our 4 × 4 electron Hamiltonian is

\[ \mathcal{H} = \left( \frac{\mathbf{p}^2}{2m^*} + \epsilon_+ \right) \mathbf{1} - \epsilon_- \mathbf{\tau} \otimes \mathbf{1} + \frac{\eta}{\hbar} \mathbf{\tau} \otimes \left( \mathbf{p}_x \sigma^y - \mathbf{p}_y \sigma^x \right), \]  

where \( m^* \) is the effective mass, \( \epsilon_\pm = (\epsilon_o \pm \epsilon_e) / 2 \), \( \epsilon_e \) and \( \epsilon_o \) are quantized energies of the lowest (even) and first excited (odd) subbands (corresponding to eigenstates |e\rangle and |o\rangle), respectively, measured from the bottom of the quantum well, \( \tau^{x,y,z} \) denote the Pauli matrices describing the subband (or pseudospin) degree of freedom, and \( \sigma^{x,y,z} \) are Pauli matrices referring to the electron spin.

The new inter-subband-induced s-o coupling \( \eta \) is

\[ \eta = - \left( \frac{P^2}{E_g^2} - \frac{1}{(E_g + \Delta)^2} \right) \frac{P^2}{3} \langle e | \partial_z V(z) | o \rangle + \frac{\delta_e}{E_g} - \frac{\delta_\Delta}{(E_g + \Delta)^2} \frac{P^2}{3} \langle e | \partial_z \mathcal{H}(z) | o \rangle, \]  

where \( E_g \) and \( \Delta \) are the fundamental and split-off band gaps in the well region [5]; \( P \) is the Kane matrix element [5]. The parameters \( \delta_e \) and \( \delta_\Delta \) denote valence band off-
sets between the well and the barrier regions: $V(z)$ is the Hartree-type contribution to the electron potential and $h(z)$ is the structural quantum-well profile. Note that $\eta$ can be varied via external gates, Eq. 2. Next we outline the derivation of $\mathcal{H}$ in Eq. (1).

**Kane Hamiltonian.** We start from the usual $8 \times 8$ Kane Hamiltonian describing the s-type conduction and the p-type valence bands around the $\Gamma$ point:

$$\mathcal{H}_{8 \times 8} = \begin{pmatrix} H_e & H_{cv} \\ H_{vc} & H_v \end{pmatrix},$$

where $H_e$ is a $2 \times 2$ diagonal matrix with elements $p^2/2m_0 + V_c(r) - E_g$ for the heavy- and light-hole bands and $p^2/2m_0 + V_{\alpha}(r) - E_g - \Delta$ for the split-off band, $V_i(r) [i = c, v, \Delta]$ denote arbitrary potentials (see below), and $H_{cv} = (H_{vc})^\dagger$ is

$$H_{cv} = \begin{pmatrix} \frac{-\tilde{\kappa}}{\sqrt{2}} & \sqrt{\tilde{\kappa}k_z} & \frac{-\tilde{\kappa}}{\sqrt{2}} & 0 \\ \frac{-\kappa}{\sqrt{2}} & \frac{\kappa}{\sqrt{2}} & \frac{-\kappa}{\sqrt{2}} & 0 \\ 0 & \frac{-\kappa}{\sqrt{2}} & \frac{-\kappa}{\sqrt{2}} & \frac{\kappa}{\sqrt{2}} \\ \frac{-\kappa}{\sqrt{2}} & 0 & \frac{-\kappa}{\sqrt{2}} & \frac{-\kappa}{\sqrt{2}} \end{pmatrix},$$

where $\tilde{\kappa} = \tilde{p}k$, $\tilde{p} = p/\hbar$ is the electron wave vector, $k_{\pm} = k_0 \pm ik_y$, and $P = -i[b_i(S)p_xX]/m_0$ parameterizes the conduction-to-valence band coupling; $|S\rangle$ and $|X\rangle$ are the usual periodic Bloch band coupling at the $\Gamma$ point.

**Effective electron Hamiltonian: folding down.** The Kane Hamiltonian acts on an eight-component spinor $\Psi = (\psi_c \psi_v)^\dagger$ in which the last six components $\psi_v$ represent valence-band states. By eliminating the holomorphic components from the Schrödinger equation $\mathcal{H}_{8 \times 8}\Psi = \varepsilon\Psi$, where $\varepsilon$ is the eigenenergy, we can fold down this $8 \times 8$ equation into a $2 \times 2$ effective equation for the conduction-band states only: $\mathcal{H}(\varepsilon)\hat{\psi}_c = [H_e + H_{cv}(\varepsilon - H_e)^{-1} H_{vc}]\hat{\psi}_c$, $\hat{\psi}_c$ is a renormalized conduction-electron spinor.

**s-o in symmetric wells.** Applying the above procedure to a quantum well, defined by the confining potentials $V_i(r) \to V_i(z) = V(z) + \delta_i h(z)$, $i = c, v, \Delta$, we find

$$\mathcal{H}(\varepsilon) = \mathcal{H}_{QW} + \frac{p^2}{3m^*}p - \left[\eta_1^{-1} + \eta_2^{-1}, p_z\right],$$

$$\mathcal{H}_{QW} = p + \frac{1}{2m^*(z, \varepsilon)}p_\perp + \frac{1}{p_\perp} \frac{1}{2m^*(z, \varepsilon)}p_z + V_c(z),$$

where $1/m^*(z, \varepsilon) = 2\pi^2/3(\nu_1 + \nu_2) + 1/m_0$, $\eta_1 = \varepsilon - (p^2/2m_0 + V(z) - \delta_1 h(z) - E_g)$ and $\eta_2 = \varepsilon - (p^2/2m_0 + V(z) - \delta_2 h(z) - E_g - \Delta)$. Equation (5) describes an electron in a quantum well ($\mathcal{H}_{QW}$ term) with spin orbit interaction (last term) (13). The kinetic-energy operators above are complicated due to the position- and energy-dependent effective mass $m^*(z, \varepsilon)$. Since $E_g$ and $E_g + \Delta$ are the largest energy scales in our system, we can simplify (13) and (9) by expanding $1/\eta_1$ and $1/\eta_2$ in the form $1/\eta_1 = E_g\{1 - (\varepsilon - p^2/2m_0 - V(z) + \delta_1 h(z))/E_g + \ldots\}$ and $1/\eta_2 = (E_g + \Delta)^{-1}\{1 - (\varepsilon - p^2/2m_0 - V(z) + \delta_2 h(z))/E_g + \ldots\}$. To zeroth order $\eta_1 = E_g$, $\eta_2 = E_g + \Delta$ and $H_{QW} = p^2/2m^* + p_\perp^2/2m^* + V_c(z)$ with (a constant effective mass)

$$1/m^* = \frac{2\pi^2}{\hbar^2} \left(\frac{2}{\nu_2} + \frac{1}{E_g + \Delta} + \frac{1}{m_0}\right).$$

Since the s-o operators $[\eta_1^{-1} + \eta_2^{-1}, p_z] \to \partial_z(1/\eta_1) + \partial_z(1/\eta_2)$, we need to keep the first-order terms in the expansions of $\eta_1^{-1}$ and $\eta_2^{-1}$, which yield the leading non-zero contribution to the s-o term in (4). We find $[\eta_1^{-1} + \eta_2^{-1}, p_z] = (1/E_g - 1/(E_g + \Delta)^2)\partial_z h(z)$. Finally, we project this s-o operator into the two lowest (spin-degenerate) eigenstates $|i\rangle_{\sigma} = [k_\parallel i\rangle]_{\sigma_z} = (1/E_g - 1/(E_g + \Delta)^2)\partial_z h(z)$.

**s-o in symmetric wells.** The above procedure can be repeated for the conduction-band states as well, and the confined wave functions $\varphi_i(z)$, $i = c, v$ of the wells. We then calculate $\langle i \rangle \eta$ via Eq. (2), $\langle ii \rangle$ from equations similar to Eq. (2) for each subband, and $\langle iii \rangle = \gamma_c \langle k_\parallel i\rangle^2 |i\rangle_c$ of the symmetric well ($\mathcal{H}_{QW}$), Fig. 1. This directly leads to the $\mathcal{H}$ in (1) with the s-o coupling $\eta$ (2) (13). Note that this new s-o interaction is non-zero even in symmetric wells as $\eta$ arises from the coupling between the ground state (even) and the first excited state (odd), Eq. (2). We can generalize $\mathcal{H}$ to include the Rashba $\alpha$ and the linearized Dresselhaus $\beta$ s-o couplings. Next we determine the magnitude of $\eta$ (and $\alpha, \beta$) for realistic quantum wells with two subbands.

**Self-consistent calculation of the s-o couplings.** We consider modulation-doped quantum wells similar to those experimentally investigated in Ref. (16). Our wells, however, have two occupied subbands. Similarly to Ref. (12), we study cases with constant chemical potentials (17). By self-consistently solving Poisson and Schrödinger’s equations we determine the energy levels $\varepsilon_c, \varepsilon_v$ and the confined wave functions $\varphi_i(z)$, $i = c, v$ of the wells. We then calculate $\langle i \rangle \eta$ vs. $\varepsilon_c, \varepsilon_v$ and the confined wave functions $\varphi_i(z)$, $i = c, v$ of the wells. We then calculate $\langle i \rangle \eta$ vs. $\varepsilon_c, \varepsilon_v$ and the confined wave functions $\varphi_i(z)$, $i = c, v$ of the wells.
Hamiltonian have eigenvalues \( \eta, \alpha, \beta \). We consider \( \eta \) large such that the Dresselhaus \( \beta \) and the Rashba \( \alpha \) constants are negligible for \( V_b = 0 \). This occurs because the subband splitting \( \epsilon_o - \epsilon_e \) reaches a minimum at \( V_b = 0 \). Upper-right inset of (b): energy dispersions \( \epsilon_{\pm}(k) \) [Eq. (3)] of the symmetric double well.

Having established that the new s-o coupling \( \eta \) is sizable, in what follows we focus on a fully symmetric well to investigate physical effects arising solely from \( \eta \).

**Fully symmetric case: eigensolutions.** Let us consider a two subband well (single or double) described by the Hamiltonian \( \mathcal{H} \) in (1) (we assume a negligible Dresselhaus term [19]). In the basis \( \{|e\uparrow\rangle, |o\downarrow\rangle, |o\uparrow\rangle, |e\downarrow\rangle\} \), \( \mathcal{H} \) becomes

\[
\tilde{\mathcal{H}} = \begin{pmatrix}
\frac{\hbar^2 k^2}{2m_z} + \epsilon_e & -i\eta k_+ & 0 & 0 \\
-i\eta k_+ & \frac{\hbar^2 k^2}{2m_y} + \epsilon_o & 0 & 0 \\
0 & 0 & \frac{\hbar^2 k^2}{2m_z} + \epsilon_e & -i\eta k_+ \\
0 & 0 & i\eta k_+ & \frac{\hbar^2 k^2}{2m_y} + \epsilon_o
\end{pmatrix}.
\]

Both the upper-left (U) and lower-right (L) blocks of \( \tilde{\mathcal{H}} \) have eigenvalues

\[
\epsilon_{\pm}(k) = \epsilon_k \pm \hbar \Omega,
\]

with \( \epsilon_k = \frac{\hbar^2 k^2}{2m} + \epsilon_e + (\hbar \Omega)^2 = \eta^2 k^2 + c^2 \), and eigenvectors

\[
|\psi_1\rangle_L = \sin \left( \frac{\theta_2}{2} \right) |e\uparrow\rangle + \cos \left( \frac{\theta_2}{2} \right) e^{i\phi} |o\downarrow\rangle, \quad (9)
\]

\[
|\psi_2\rangle_L = \cos \left( \frac{\theta_2}{2} \right) |o\downarrow\rangle + \sin \left( \frac{\theta_2}{2} \right) e^{i\phi} |e\uparrow\rangle, \quad (10)
\]

\[
|\psi_3\rangle_L = \cos \left( \frac{\theta_2}{2} \right) |e\uparrow\rangle - \sin \left( \frac{\theta_2}{2} \right) e^{i\phi} |o\downarrow\rangle, \quad (11)
\]

\[
|\psi_4\rangle_L = \sin \left( \frac{\theta_2}{2} \right) |o\downarrow\rangle - \cos \left( \frac{\theta_2}{2} \right) e^{i\phi} |e\uparrow\rangle. \quad (12)
\]

Here, \( e^{i\phi} = (-k_y + ik_x)/k \), \( \cos(\theta) = 1/\sqrt{1 + (\eta k/\epsilon_e)^2} \), and \( \tilde{k} = k(\sin \phi, -\cos \phi) \). For \( \eta k << 2\epsilon_e \) we can expand \( \epsilon_{\pm}(\tilde{k}) \) in (3) and define effective masses \( m^*_e = m^*/[1 \pm 2\epsilon_{so}/\epsilon_e] \), where \( \epsilon_{so} = \eta^2 m^*/2\hbar^2 \) is the energy scale of the new s-o coupling. For the double well of Fig. 2(b), \( m^* \) is reduced by \( \sim 5\% \) compared to the bulk value \( m_e^* \). This could be measured via, e.g., cyclotron-resonance experiments [23].

**Novel Zitterbewegung.** The dynamics of electron wave packets in wells with s-o interaction exhibit an oscillatory motion [2] – the zitterbewegung. For our new s-o interaction, a wave packet \( |\psi\rangle \) moves according to \( \langle \chi | \hat{r}_H(t) | \chi \rangle \) where \( \hat{r}_H(t) = U^\dagger \hat{U} \) is the position operator in the Heisenberg picture \([U = \exp(-i\hat{H}t/\hbar)] \) with components

\[
x_{H}(t) = 1 \otimes 1 x(0) + 1 \otimes \frac{p_x}{m_x} t + \frac{\eta}{\hbar} \tau_t \otimes \sigma_y - \frac{\eta}{2(\hbar \Omega)^2} \left[ \epsilon_y \tau_y \otimes \sigma_y + \frac{\eta p_y}{\hbar} 1 \otimes \sigma_z \right] (\cos(2\Omega t) - 1)
\]

\[
+ \frac{\eta}{2(\hbar \Omega)^3} \left[ \epsilon_y \tau_y \otimes \sigma_y + \frac{\eta}{\hbar} \tau_t \otimes 1 p_x \right] + \left( \frac{\hbar}{\eta} \right)^2 p_y \tau_y \otimes (p_x \sigma_y + p_y \sigma_x)
\]

and \( y_{H}(t) \), obtained from Eq. (13) via the replacements \((p_x, \sigma_z) \rightarrow (p_y, \sigma_y), (p_y, \sigma_y) \rightarrow (-p_x, -\sigma_z) \) [i.e., a \( \pi/2 \) rotation about the z-axis]. Similar expressions can be derived for the spin components \( \sigma_i |\psi(t)\rangle \), \( i = x, y, z \).

For simplicity, we evaluate the expectation value of \( \hat{r}_H(t) \) for planes waves (“wide wave packets”). For a spin-up electron injected into the lowest subband along the \( y \)-axis with (group) velocity \( V_y = (h k_{0y}/m^*) \dot{y} \) we find

\[
x_{H}(t) = \frac{\eta^2 k_{0y}}{2(\hbar \Omega)^2} \left[ 1 - \cos(2\Omega t) \right], \quad (14)
\]

\[
y_{H}(t) = \frac{h k_{0y}}{m^*} t + \frac{\eta^2 k_{0y} \epsilon_e}{2(\hbar \Omega)^2} \left( \sin(2\Omega t) - 2\Omega t \right), \quad (15)
\]

assuming \( x(0) = y(0) = 0 \). Equations (14) and (15) show that cycloidal motion is possible in our system. This differs qualitatively from the Rashba s-o zitterbewegung which is always perpendicular to the initial \( V_y \).

Figure 3 shows trajectories for three distinct \( V_y = (h k_{0y}/m^*) \dot{y} \) – all with \( k_{0y} > 0 \). We find motion opposite to and along the \( y \)-axis (orbits I and III, resp.) and even a closed path (II). To understand this behavior we note that for \( \eta k_{0y} << \epsilon_e - \epsilon_o \) the linear-in-\( t \) terms in \( \langle y_{H}(t) \rangle \) can be recast into \( h k_{0y} t/m^* \Rightarrow \) the injected wave moves...
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