Rashba spin splitting in biased semiconductor quantum wells

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Rashba spin splitting (RSS) in biased semiconductor quantum wells is investigated theoretically based on the eight-band envelope function model. We find that at large wave vectors, RSS is both nonmonotonic and anisotropic as a function of in-plane wave vector, in contrast to the widely used linear and isotropic model. We derive an analytical expression for RSS, which can correctly reproduce such nonmonotonic behavior at large wave vectors. We also investigate numerically the dependence of RSS on the various band parameters and find that RSS increases with decreasing band gap and subband index, increasing valence band offset, external electric field, and well width. Our analytical expression for RSS provides a satisfactory explanation to all these features.

PACS numbers: 71.70.Ej, 73.21.Fg

\[
\begin{align*}
H_k &= \begin{bmatrix}
  k_A \cdot k & 0 & iP_0 k_+ / \sqrt{2} & \sqrt{2/3} P_0 k_z & iP_0 k_- / \sqrt{6} & 0 & iP_0 k_z / \sqrt{3} & P_0 k_- / \sqrt{3} \\
 0 & k_A \cdot k & 0 & -P_0 k_+ / \sqrt{6} & i\sqrt{2/3} P_0 k_z & -P_0 k_- / \sqrt{2} & iP_0 k_+ / \sqrt{3} & -P_0 k_z / \sqrt{3} \\
L - i\sqrt{6} S & P - Q & M & 0 & iL/\sqrt{2} + \sqrt{3} S & -i\sqrt{2} M & i\sqrt{3/2} L - S & i\sqrt{3/2} L^+ + S^+ \\\nL + i\sqrt{6} S & P + Q & -2i\sqrt{3} S & P - Q & M & -i\sqrt{2} Q & i\sqrt{3/2} L^+ + S^+ & -i\sqrt{2} Q \\\nL - i\sqrt{6} S & P - Q & -2i\sqrt{3} S & P + Q & i\sqrt{3/2} L^+ + S^+ & M & -i\sqrt{2} M^+ & 2\sqrt{2} S \\
L + i\sqrt{6} S & P + Q & 0 & -2i\sqrt{3} S & P - Q & i\sqrt{3/2} L^+ + S^+ & M & -i\sqrt{2} M^+ \\
0 & i\sqrt{2} Q & 0 & 2\sqrt{2} S & P & -i\sqrt{2} M^+ & 2\sqrt{2} S & P
\end{bmatrix},
\end{align*}
\]

where \( A_c = \hbar^2/(2m_0) \gamma_c \),

\[ P = -\hbar^2/(2m_0) k \gamma_1 k, \]
\[
Q = -\hbar^2/(2m_0)(\gamma_2 k_y^2 - 2k_z \gamma_3 k_z),
\]
\[
L = i\sqrt{3}\hbar^2/(2m_0)(\gamma_3 k_z + k_z \gamma_3)k_x.
\]
\[
M = -\sqrt{3}\hbar^2/(2m_0)(\gamma_2 k_x^2 - k_y^2) - 2i k_x \gamma_3 k_y,
\]
\[
S = -\hbar^2/(2m_0)(k k_z - k_z k)k_x.
\]
Here \(\gamma_1, \gamma_2, \gamma_3, \kappa\) are modified Luttinger parameters, \((\gamma_1 - 1)\) describes the remote band contribution to the CB effective mass, \(k_z = -i\partial/\partial z\), and \(k_x, k_y\) are c-numbers.

Neglecting the off-diagonal elements in the valence bands (VB’s) and eliminating the VB components of the envelope function, the effective CB Hamiltonian is obtained as
\[
H_{\text{eff}}(k) = E_{\text{e}}(z) + V(z) + \frac{\hbar^2}{2m^*(z)}k^2 + \alpha_0(z)(k_x e_z)\cdot\sigma,
\]
where \(E_p = 2m_0P^2/\hbar^2\) and \(m^*(z)\) is the effective mass given by
\[
\frac{m_0}{m^*(z)} = \gamma_c + \frac{2E_p}{3m_0} + \frac{E_p}{3U_0},
\]
with \(U_{\text{ih}}(z) = E - H_{\text{ih}}, U_{\text{so}}(z) = E - H_{\text{so}}, H_{\text{ih}} = E_{\text{e}} + V + P - Q\), and \(H_{\text{so}} = E_{\text{e}} - \Delta + V + P\). Here \(E\) is the eigenenergy, and the operators \(k^2\) in \(P\) and \(Q\) have been replaced by \(\pi/W\) (\(W\) is the well width). The Rashba spin-orbit interaction strength \(\alpha_0(z) = \hbar^2/(6m_0)\partial \gamma(z)/\partial z\), where \(\gamma(z) = E_p[1/U_{\text{ih}}(z) - 1/U_{\text{so}}(z)]\). It is interesting to notice that RSS at small wave vectors comes from the coupling to the light hole and spin-orbit split-off VB’s, while the heavy hole bands do not contribute. This is because the basis functions for the electron \(S\) \(\uparrow\), \(S\downarrow\) and those for the heavy hole \(3/2, \pm 3/2\) are spin eigenstates, while the \(\mathbf{k} \cdot \mathbf{p}\) interaction between the CB and VB’s is independent of spin. The last term of Eq. (2) leads to spin-dependent boundary conditions. To obtain an analytical expression for RSS, we neglect its influence on the envelope function but keep it in the effective Hamiltonian (we have checked numerically that this approximation would not change the qualitative behavior of the resulting analytical expression at large wave vectors), then the RSS of the n-th subband is given by
\[
\Delta E_n(k) = \Delta E_n^{(1)}(k) + \Delta E_n^{(2)}(k),
\]
where
\[
\Delta E_n^{(1)}(k) = \frac{\hbar^2}{3m_0}k_x \sum_j |F_n(z_j)|^2 [\gamma(z_j^+) - \gamma(z_j^-)],
\]
\[
\Delta E_n^{(2)}(k) = \frac{\hbar^2}{3m_0}E_{pF} F_{k_x} \int dz |F_n(z)|^2 (U_{\text{ih}}^2 - U_{\text{so}}^2).
\]
Here \(F_n(z)\) is the envelope function of the n-th subband along the \(z\) axis, \(z_j^\pm = z_j \pm 0^+\), and \(\{z_j\}\) denote the \(z\) coordinates of the interfaces. \(\Delta E_n^{(1)}(k)\) can be viewed as the \(\Gamma_8\) and \(\Gamma_7\) VBO’s-induced interface electric field contribution, while \(\Delta E_n^{(2)}(k)\) is roughly proportional to the external electric field. For small \(V(z)\) compared with the band gap, we obtain \(\Delta E_n^{(2)}(k)\) analytically as
\[
\Delta E_n^{(2)}(k) = \frac{\hbar^2}{3m_0}E_p e F_k \sum_j P_n^j \left((U_{\text{ih}}^j)^2 - (U_{\text{so}}^j)^2\right).
\]
Here \(P_j^\delta = \int_{\text{layer}} d\zeta |F_n(z)|^2\) is the probability of the electron in the \(j\)-th layer, \(U_{\text{ih}}^j, U_{\text{so}}^j\) [in which \(V(z)\) has been dropped] are for the \(j\)-th layer. Further, if \(\gamma_c\) and the wave function penetration into the barriers are neglected, and \(U_{\text{ih}}, U_{\text{so}}\) are replaced by \(1/E_g\) and \((1/E_g + \Delta)\) \(E_g\) and \(\Delta\) refer to the well material), respectively, then we recover the result of Ref. 12,
\[
\Delta E_n^{(2)}(k) = \frac{\hbar^2}{m^*} \frac{\Delta}{E_g + \Delta} \frac{2E_g + \Delta}{3E_g + 2\Delta} e F_k,
\]
where \(m^*\) is the CB effective mass of the well. We notice, however, that a factor of 3/2 is missing in the definition of \(m^*\) in Ref. 12. Further, Eq. (6) is invalid for narrow-gap semiconductors or narrow quantum wells, where the subband energy is comparable to the band gap.

From the above discussions, we see that RSS comes from (i) spin-dependent kinetic and potential energy; (ii) expectation value of the total electric field (including the external and interface electric fields) in the \(\Gamma_8\) and \(\Gamma_7\) VB’s; (iii) variation of band parameters across the interfaces. The above analytical expressions show that RSS is determined by the total electric field in the \(\Gamma_8\) and \(\Gamma_7\) VB’s, in agreement with Ref. 11. As a result, we see that the Ando argument\textsuperscript{6} fails due to an incorrect assumption that RSS is proportional to the total electric field in the CB. This deepens the previous argument\textsuperscript{12} that the failure of the Ando argument is caused by the spin-dependent boundary conditions or the vanishing barrier penetration.

To estimate the validity of our analytical expressions, we solve the 8×8 Hamiltonian numerically for a biased CdTe/HgCd\textsubscript{1-x}Cd\textsubscript{x}Te/CdTe quantum well and compare the full numerical solutions with the analytical results in Fig. 1. The band parameters can be found in Refs. 14 and 20. First, we see that our analytical expressions [Eqs. (3) and (5)] agree better with the numerical results than the previous analytical expression\textsuperscript{12} [Eq. (6)] does at small \(k\). Second, RSS begins to decrease for \(k\) larger than a critical value \(k_0\). This nonmonotonic behavior is correctly reproduced by our analytical expression, while the previous analytical expression only gives a linear behavior. The decrease of RSS at large \(k\) arises as follows. With increasing \(k\), the subband energy \(E_n(k)\) \(\approx E_{n0} + \hbar^2 k^2/2m^*\) in \(U_{\text{ih}}\) and \(U_{\text{so}}\) increases and becomes comparable to \(E_g(HgCdTe)\) when \(k_0 \approx k_0\).
The further increase of \( k_\parallel \) leads to the decrease of \( k_\parallel \gamma(z) \) and \( k_\parallel (U_m^2 - U_\infty^2) \) in Eqs. 4 and 5. Consequently, RSS begins to decrease when \( k_\parallel > k_0 \). Further, when \( E_g(\text{HgCdTe}) \) decreases from 0.8 to 0.2 eV, the critical wave vector \( k_0 \) decreases, since a smaller \( k_0 \) is required for \( E_g(k_0) \) to become comparable to \( E_g(\text{HgCdTe}) \). Here we see that the nonmonotonic behavior of RSS at large \( k_\parallel \) comes from the energy dispersion of the subband. Physically, the coupling to the VB’s and, consequently, RSS are reduced by the increasing energy difference between the CB and VB’s.

Third, RSS is dominated by the mean external electric field contribution \( \Delta E^{(2)} \). This trend becomes more pronounced when \( E_g(\text{HgCdTe}) \) is decreased from 0.8 to 0.2 eV. It can be understood since the interface contribution \( \Delta E^{(1)} \) is roughly proportional to \( 1/E_g \) through \( \gamma(z^2_j) \) in Eq. 4, while the mean external electric field contribution \( \Delta E^{(2)} \) is roughly proportional to \( 1/E_g^2 \) through \( U_m^2 \) and \( U_\infty^2 \) in Eq. 5. Fourth, both \( \Delta E^{(1)} \) and \( \Delta E^{(2)} \) increase significantly when \( E_g(\text{HgCdTe}) \) is decreased from 0.8 to 0.2 eV, in agreement with Eq. 6. Physically, the increasing RSS is caused by the increasing coupling between the CB and VB’s with decreasing band gap.

In the above, we see that our analytical expression gives a better description for RSS than the previous analytical expression. Next, by numerically solving the 8×8 Hamiltonian, we investigate the dependence of RSS on the band gap \( E_g(\text{HgCdTe}) \), VBO, subband index, external electric field, and well width. The previous analytical expressions \( 12,13 \) can only explain the dependence of RSS on the band gap and external electric field, while our analytical expression can explain all the dependences, as we shall show below.

In Fig. 2, we plot the RSS of the lowest three sub-bands for different band gaps and VBO’s. First, in addition to the increase of RSS with decreasing band gap, it also increases with increasing VBO. This can be understood from Eqs. 8 and 9, because the subband energy \( E_n(k_\parallel) \) decreases with increasing VBO. As a result, \( \gamma(z^2_j) \), \( U_m^2 \), and \( U_\infty^2 \) in Eqs. 8 and 9 increases. Second, RSS decreases with increasing subband index, due to the increase of the subband energy \( E_n(k_\parallel) \) and the decrease of the asymmetry of the envelope function at the two interfaces, because the orthogonality requirement between different eigenstates serves as an effective repulsive force, which reduces the potential asymmetry produced by the external electric field.
Finally, RSS is isotropic at small $k_{\parallel}$ but anisotropic at large $k_{\parallel}$. This interesting behavior is in contrast to the current understanding that RSS is always isotropic. From Fig. 3, it can be seen that RSS has a four-fold anisotropy in the $k_{\parallel}$ space. This anisotropy comes not from the macroscopic potential, but from the $C_{4v}$ symmetry group of the quantum well structure (neglecting the bulk inversion asymmetry).

The dependence of the RSS at $k_{\parallel}=0.1$ nm$^{-1}$ on the electric field and well width is shown in Fig. 4. The RSS increases almost linearly with increasing electric field, in agreement with Eq. 3, while it increases with increasing well width and saturates at large well width. The latter can be explained through the dependence of $\gamma(z)$, $U_{lh}^{-2}$, and $U_{so}^{-2}$ on the subband energy $E_{n}(k_{\parallel})$. With increasing well width, $E_{n}(k_{\parallel})$ decreases due to the decrease of the confining energy $E_{n0}$, such that $\gamma(z)$, $U_{lh}^{-2}$, $U_{so}^{-2}$ and, therefore, RSS increase until $E_{n0}$ vanishes and $E_{n}(k_{\parallel})$ approaches a constant value $\hbar^2k_{\parallel}^2/(2m^*)$. Afterwards, $\gamma(z)$, $U_{lh}^{-2}$, and $U_{so}^{-2}$ do not vary appreciably and RSS saturates. This behavior is quite different from that of asymmetric AlAs/GaAs/Al$_{0.15}$Ga$_{0.85}$As quantum wells, where RSS shows a peak and then decreases with increasing well width. It was argued that such behavior comes from the competition between confinement and barrier penetration. Using our analytical expression, however, the origin of such behavior is transparent. That is, increasing the well width leads to two competing effects: the decrease of the subband energy (which increases RSS) and the asymmetry of the envelope function at the two interfaces (which decreases RSS).

In summary, based on the full numerical solutions to the eight-band envelope function model, we have found that at large wave vectors, RSS is both nonmonotonic and anisotropic, in contrast to the widely used linear and isotropic model. We have derived an analytical expression, which can correctly reproduce such nonmonotonic behavior at large wave vectors. It shows that the nonmonotonic behavior comes from the energy dispersion of the subband. We have also investigated numerically the dependence of RSS on the various band parameters and found that RSS increases with decreasing band gap and subband index, increasing VBO, external electric field, and well width. Our analytical expression gives better descriptions to all these dependences than the previous analytical expressions.
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