Negative tunneling magneto-resistance in quantum wires with strong spin–orbit coupling

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Abstract
We consider a two-dimensional magnetic tunnel junction of the FM/I/QW(FM+SO)/I/N structure, where FM, I and QW(FM+SO) stand for a ferromagnet, an insulator and a quantum wire with both magnetic ordering and Rashba spin–orbit coupling (SOC), respectively. The tunneling magneto-resistance (TMR) exhibits strong anisotropy and switches sign as the polarization direction varies relative to the quantum-wire axis, due to interplay among the one-dimensionality, the magnetic ordering, and the strong SOC of the quantum wire.

Keywords: tunneling magneto-resistance, quantum wire, LAO/STO

1. Introduction
The magnetic tunneling junction (MTJ) consisting of two ferromagnetic electrodes (FM) separated by a thin insulating barrier (I) is a prototype structure in the rapidly developing field of spintronics [1]. The tunneling magneto-resistance (TMR), depending on the relative magnetic polarization of the two ferromagnets, is a key issue not only for the spintronic applications but also for the study of fundamental magnetic properties [2, 3]. Due to the spin selection rule the TMR, if any, is typically positive. Two exceptional cases have been known. One involves magnetic impurities in the tunnel barriers and is not surprising. The other (more important) case is associated with the resonant tunneling and spin-dependent interfacial phase shift in double-barrier FM/I/N/I/FM structures, where N represents a non-magnetic normal metal [4–8].

In this work we explore another non-trivial example of negative TMR in a two-dimensional (2D) double-barrier MTJ of the FM/I/QW(FM+SO)/I/N structure (see figure 1(a)), where QW(FM+SO) stands for a quantum wire (QW) with both magnetic ordering and Rashba spin–orbit coupling (SOC). Our MTJ structure should be distinguished from more common 1D MTJs of the FM/I/QW/I/FM structure such as in [5], where the QW is non-magnetic and the junction interface is perpendicular to the quantum-wire axis. In our case, the QW itself has a magnetic ordering and the junction interface is parallel to its axis. Thus, transport occurs across, not along the quantum wire. We find that the TMR exhibits strong anisotropy and even changes sign as the polarization direction of the ferromagnets varies relative to the quantum-wire axis. This sign-switching anisotropic TMR is attributed to the interplay among the one-dimensionality, the magnetic ordering, and the strong SOC of the QW. It is interesting to recall that anisotropic TMR was previously studied in the FM/I/FM structure where the insulating barrier (not the ferromagnets) had SOC (see [9] and references therein), but the TMR remained positive without switching its sign.

Our MTJ structure is peculiar in that the nanoscale quantum wire has both strong SOC and magnetic ordering. One important motivation for our MTJ structure is (but is not limited to) the recent experiment [10] on the transition metal oxide interface between LaAlO₃ (LAO) and SrTiO₃ (STO) (see figure 1(b)), where the measured TMR is strongly anisotropic and switches sign as the magnetization direction varies in the interface plane. Since the LAO/STO interface...
was demonstrated a decade ago [11] to be metallic even though both LAO and STO are typical band insulators, it has attracted ever-growing interest by exhibiting superconductivity [12], ferromagnetism [13] and even coexistence of both effects [14, 15]. Despite a number of experimental studies of the system, the origins of magnetic ordering and superconductivity remain controversial [16, 17] and further studies are imperative. The sign-switching anisotropic TMR [10] adds a fresh intriguing question concerning the magnetic properties of the LAO/STO interface. Our results below discuss the characteristics of the single interface between the ferromagnetic top electrode and the quantum wire. Then, the behavior of the TMR ratio found in section 3. First, section 4 analytically and qualitatively the sign-switching anisotropic TMR effects. (Figure 1). The direction of the effective field (‘Rashba field’) due to the Rashba SOC is along the y-axis, as it arises from the structural inversion symmetry breaking and should be perpendicular to both x- and z-axis. The Rashba SOC is present only on the QW (0 < z < d): 

\[
\sigma(z) = \begin{cases} 
\sigma_0 & (0 < z < d) \\
0 & \text{(otherwise)}
\end{cases}
\]

where \(d \sim 1 \text{ nm}\) represents the diameter of the QW or the thickness of the LAO/STO interface. The Zeeman field \(\Delta(z)\) is due to the ferromagnetism on the top electrode and the QW and is modeled as a vector in the xy plane

\[
\Delta(z) = \begin{cases} 
\Delta_1(-\sin \phi, \cos \phi, 0) & (z > d) \\
\Delta_2(-\sin \phi, \cos \phi, 0) & (0 < z < d) \\
0 & (z < 0)
\end{cases}
\]

where the angle \(\phi (0 < \phi < \pi)\) is measured from the y-axis (Rashba field direction). We assume that \(\Delta_1 > 0\) and that \(\Delta_2 > 0\) and \(\Delta_2 < 0\) for the parallel (P) and anti-parallel (AP) configuration of the magnetic polarization directions, respectively. The chemical potentials (carrier densities) in different regions are described by potential steps and the thin insulating barriers by \(\delta\)-potentials, giving the potential profile \(U(z)\) of the form

\[
U(z) = U_1 \theta(z-d) + U_2 [\Theta(z-d) - \Theta(z)]
\]

\[
+ a_b U_0 \delta(z-d) + a_b' U_0' \delta(z).
\]

\(U_b\) is responsible for the insulating layer of LAO, \(a_b\) is the effective width of the barrier (\(a_b \sim 1-5 \text{ nm}\)), \(U_0'\) is responsible for the junction between the QW and the normal electrode and \(a_b'\) is its effective length scale. Experimentally, \(U_1\) and \(U_2\) correspond to chemical potentials in the corresponding regions. For a typical LAO/STO interface [16, 20–22], the Fermi energy \(E_F \sim 40 \text{ meV}, a_0 \sim \hbar v_F^0/8\) with \(v_F^0 = \sqrt{2E_F/m}, \Delta_2 \sim E_F/16, \text{ and } d \sim 1 \text{ nm}\).

The model in section 1 has been constructed mainly focusing on the device of the form in figure 1(a) and hence ignoring the motion in the y-direction. However, it is still relevant for more realistic devices like figure 1(c). In such a case, one has only to integrate over the transverse momentum \(k_y\) in the regions \(z > d\) and \(z < 0\), without affecting the qualitative features of our findings to be discussed below. The results are also insensitive to the width of the QW in the y-direction as long as it is small compared with the thickness in the z-direction and the Fermi wavelength.

The momentum in the x-direction is preserved over a tunneling process; here the junction (QW) is assumed to be infinitely wide (long). We thus seek a wave function of the form
$\Psi(x, z) = e^{i\phi z} \psi(z)$, where $\psi(z)$ satisfies the 1D Schrödinger equation $H_z \psi(z) = (E - \hbar^2 q^2/2m) \psi(z)$. The 1D effective Hamiltonian $H_z$ is given by

$$H_z = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \left( \frac{\hbar^2}{2m} \frac{d^2}{dz^2} + U_1 \right) - \Delta_1 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

in the region $z > d$, by

$$H_z = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \left( \frac{\hbar^2}{2m} \frac{d^2}{dz^2} + U_2 \right) - \frac{i}{\alpha_0 q} \sin \phi + \Delta_2 \begin{pmatrix} \alpha_0 q \cos \phi + \Delta_2 & -i \alpha_0 q \sin \phi \\ i \alpha_0 q \sin \phi & -(\alpha_0 q \cos \phi + \Delta_2) \end{pmatrix}$$

in the region $0 < z < d$, and by

$$H_z = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \left( -\frac{\hbar^2}{2m} \frac{d^2}{dz^2} \right)$$

in the region $z < 0$. Here the spin part of $H_z$ has been represented in the eigenbasis $|\chi_{\uparrow} \rangle, |\chi_{\downarrow} \rangle$ of $\sigma_z \cos \phi - \sigma_x \sin \phi$ corresponding to the Zeeman field of the ferromagnetic top electrode (region $z > d$). In the region $z > d$, the plane waves of the form

$$|\chi_{\uparrow/(\downarrow)} \rangle = e^{ik_{\uparrow/(\downarrow)} z}$$

with $k_{\uparrow/\downarrow} = \sqrt{2m(E - U_1 \pm \Delta_1)/\hbar^2 - q^2}$ compose the wave function $\psi(z)$. In the region $0 < z < d$, $\psi(z)$ is a linear combination of the plane waves of the form

$$|\chi_{\pm} \rangle = e^{ik_{\pm} z}, \quad |\chi_{\pm} \rangle = e^{-ik_{\pm} z}$$

where $k_{\pm} = \sqrt{2m(E - U_2 \pm \Delta_2)/\hbar^2 - q^2}$ and

$$|\chi_{+} \rangle = \cos(\theta/2) |\chi_{\uparrow} \rangle + i \sin(\theta/2) |\chi_{\downarrow} \rangle$$

$$|\chi_{-} \rangle = i \sin(\theta/2) |\chi_{\uparrow} \rangle + \cos(\theta/2) |\chi_{\downarrow} \rangle.$$  

Here the angle $\theta$ $(0 < \theta < \pi)$ switches between $\theta_P$ and $\theta_{AP}$ upon the P $(\theta = \theta_P)$ and AP $(\theta = \theta_{AP})$ configuration, which are defined by

$$\tan \theta_{P/AP} = \frac{\alpha_0 q \sin \phi}{\alpha_0 q \cos \phi \pm \Delta_2}.$$ 

Imposing proper matching conditions over $\delta$-potentials at $z = 0$ and $d$, we determine (both with numerically exact method and with analytically approximate method) the scattering wave function $\psi(z)$ and calculate the TMR ratio, $TMR = 1 - R_P/R_{AP}$, where $R_{P/AP}$ is the resistance for the P/AP polarization.

The analytical solution of the full double-barrier problem with proper matching conditions should be straightforward in principle. However, in practice it leads to a lengthy expression of the transmission even for a given direction of the incidence momentum, and it should additionally be integrated over the incidence angle. As it does not provide a clear physical insight, below we discuss qualitative features of the analytical approach, as well as the numerical exact results.

3. Exact results

Figure 2 shows the numerically exact results of the TMR as a function of $U_2$ and $\phi$ for $d = 4.5/k_0$ $(k_0^2 \equiv \sqrt{2mE_F/\hbar^4})$, $\alpha_0 = \hbar v_F/8 \sqrt{\gamma}$, $\Delta_1 = E_F/8$, $\Delta_2 = E_F/16$ and $U_1 = E_F/4$. (b) Cuts along $\phi = 0$ (black dots, $y$ polarization) and $\phi = \pi/2$ (red-gray dots, $x$-$z$ polarization). (c) Cuts along $\phi$ for the indicated fixed values of $U_2 = -0.17E_F$ and $U_2 = -0.40E_F$. 

Figure 2. (a) Numerical results of the TMR as a function of $U_2$ and $\phi$ for $d = 4.5/k_0$ $(k_0^2 \equiv \sqrt{2mE_F/\hbar^4})$, $\alpha_0 = \hbar v_F/8 \sqrt{\gamma}$, $\Delta_1 = E_F/8$, $\Delta_2 = E_F/16$ and $U_1 = E_F/4$. (b) Cuts along $\phi = 0$ (black dots, $y$ polarization) and $\phi = \pi/2$ (red-gray dots, $x$-$z$ polarization). (c) Cuts along $\phi$ for the indicated fixed values of $U_2 = -0.17E_F$ and $U_2 = -0.40E_F$. 

3. Exact results

Figure 2 shows the numerically exact results of the TMR as a function of $U_2$ and $\phi$ for a typical set of parameters consistent with the LAO/STO interface [16, 20–22]. The numerical method involves the integration of the transmission probabilities over the angle of the incident wave. The algorithm has been devised in such a way as to ensure a sufficient precision for the angular integrals. The details of the numerical method are described in a previous work by one of the authors [23].

It is shown in figure 2 that the TMR can be negative, as much as $-10\%$. Further, it reveals two additional interesting features: first, the TMR depends rather strongly on $U_2$ (figure 2(b)). Experimentally, $U_2$ corresponds to the backgate voltage and controls the carrier density on the QW (or the LAO/STO interface). In the recent experiment [10], on the
other hand, the TMR did not depend much on the gate voltage. However, the actual gate capacitance was not known and it is not clear how large is the actual energy range covered by the gate voltage variation. The gate voltage dependence needs to be tested further. Moreover, in real samples (even if there are twin boundaries) the electric conduction is not completely confined to the narrow paths.

A second remarkable thing about figure 2 is the change of the $\phi$ dependence from a $\cos(\phi/2)$ to a $-\cos(\phi/2)$ behavior by tuning the value of $U_2$ (figure 2(c)). This is seen as a reversed change of sign of the TMR when going from $\phi = 0$ to $\phi = \pi/2$; from positive to negative for $U_2 = -0.4E_F$, and reversed for $U_2 = -0.17E_F$.

As we discuss below, both features of the exact results can be understood qualitatively by means of an analytical (but approximate) method.

### 4. Qualitative features of single-barrier tunneling

We first examine the transmission over the first barrier at $z = d$. Before going further, recall the transmission problem of a spinless particle with energy $E$ over a potential barrier $U_b$, $U(z) = U_1\Theta(-z) + U_2\Theta(z) + a_0U_0\delta(z)$. The transmission amplitude $t$ is given by

$$t(q_b; k_1, k_2) = \frac{\sqrt{k_1k_2}}{(k_1 + k_2)/2 + iq_b}, \quad (12)$$

where $k_j = \sqrt{2m(E - U_j)/\hbar^2}$ and $q_b = ma_0U_b/\hbar^2$. When the barrier is sufficiently high ($U_b \gg E$), it can be approximated as

$$t(q_b; k_1, k_2) \approx \frac{\sqrt{k_1k_2}}{iq_b}. \quad (13)$$

Consider now a scattering state $\psi_s(z)$ of the form

$$\psi_s(z) = \begin{cases} \sum_{s=\uparrow, \downarrow} (A_s|\chi_s\rangle e^{-iksz} + B_s|\chi_s\rangle e^{iksz}) & (z > d) \\ C_s|\chi_s\rangle e^{-iksz} & (z < d) \end{cases} \quad (14)$$

Here we have imposed a boundary condition such that in the region $z < d$ there is only one propagating spin channel $|\chi_s\rangle$ of fixed $\mu = \pm$. On the one hand, the coefficients $A_s$ and $C_s$ are related through the transmission coefficients $t_{\mu}$ by $C_s = \sum_{\pm} t_{\mu}|\chi_s\rangle$.

The transmission probability is given by $T = \sum_{\mu=\pm} |t_{\mu}|^2$. We discuss below, both features of the exact results can be understood qualitatively by means of an analytical (but approximate) method.

### 5. Qualitative features of the double-barrier structure

Now we investigate the full double-barrier structure for all possible values of $q_b$. For high tunnel barriers, the wave number $k_\pm$ in the central region ($0 < z < d$) is quantized to $k_\pm = \pi n/d (n = 1, 2, \cdots)$ and the wave function takes the form $\Psi(x, z) = \chi_{\pm}(q_\pm^{\prime\prime}) \sin(k_\pm z)e^{i\phi_\pm\pi/2}$. For each $k_\pm$ and a given energy $E$, the allowed values $q_\pm^{\prime\prime}$ ($v = \pi/2$) is determined by the dispersion relation

$$E = \frac{\hbar^2}{2m} \left[ k_\pm^2 + (q_\pm^{\prime\prime})^2 \right] + U_2$$

Due to narrow confinement ($d \sim 1$ nm) and strong SOC ($aq_b \sim E/8$), typically only one $k_\pm$ is allowed for each $\pm$. Hereafter we thus drop the subscript $n$: $k = k_\pm$, $q_\pm^{\prime\prime}$, and $|\chi_{\pm}\rangle = \chi_{\pm}(q_\pm^{\prime\prime})$. The total transmission probability is given by $T = \sum_{\mu=\pm} |t_{\mu}(q_\pm^{\prime\prime})|^2$.

For $\phi = \pi/2$, the Zeeman field is perpendicular to the Rashba field and the dispersion relation is particularly simple. Especially, one has $q_\pm^{\prime\prime} = -q_\pm^{\prime\prime}$, $q_\pm^{\prime\prime} > 0$, $\cos \theta_{\pm\mp}(q_\pm^{\prime\prime}) < 0$, and $T = \frac{1}{2} \left[ T_\uparrow(q_\pm^{\prime\prime}) + T_\downarrow(q_\pm^{\prime\prime}) \right]$.

The $q_\pm^{\prime\prime}$ channel contributes a positive (negative) TMR. As $q_\pm > q_\mp$, $k_\uparrow(q_\pm^{\prime\prime}) < k_\uparrow(q_\mp^{\prime\prime})$ and $k_\downarrow(q_\pm^{\prime\prime}) + k_\downarrow(q_\mp^{\prime\prime})$ and the positive contribution from $q_\pm^{\prime\prime}$-channel dominates. When $q_\pm^{\prime\prime}$-channel is not allowed (figure 3(b)), $T_\downarrow(q_\pm^{\prime\prime})$ is the sole contribution and the TMR becomes negative.

For $\phi = 0$ ($\pi$), $\theta_{\pm\mp}(q_\pm^{\prime\prime}) = \theta_{\mp\pm}(q_\pm^{\prime\prime}) = 0$ and the total transmission reads as (equation 18) with $k_\pm = k$

$$T = \frac{k}{q_\mp^{\prime\prime}} \left[ k_\uparrow(q_\mp^{\prime\prime}) + k_\downarrow(q_\mp^{\prime\prime}) + k_\uparrow(q_\pm^{\prime\prime}) + k_\downarrow(q_\mp^{\prime\prime}) \right]. \quad (21)$$
Note that $q_+^\pi > -q_-^\pi > -q_-^\sigma > q_+^\sigma > 0$ in the P polarization configuration (figures 3(c) and (d)). The TMR is then given by

$$\text{TMR} \propto [k_+(q_+^\pi) - k_-(q_-^\pi)] - [k_-(q_-^\pi) - k_+(q_-^\sigma)]$$

$$+ [k_+(q_-^\pi) - k_+(q_-^\sigma)] - [k_+(q_-^\pi) - k_-(q_-^\sigma)] \quad (22)$$

where the terms have been arranged in decreasing order (all values within square brackets are positive) and all $q_{\pm}^\pi$ have been defined for the P polarization configuration. As $U_2$ (the chemical potential in the central region) varies, the $q_+^\pi$ channel may become disallowed (figure 3(d)). In such a case, there are more negative contributions to the TMR. As $U_2$ varies further, the $q_-^\pi$ channel is also disallowed, and the TMR becomes positive again. As $U_2$ varies even further, the $q_-^\pi$ channel stops contributing to the transport and the TMR becomes negative once more.

Putting all together, with $U_2 \to -\infty$, TMR is positive both at $\phi = 0$ and $\phi = \pi/2$. As $U_2$ moves up, the $q_-^\pi$-mode at $\phi = \pi/2$ gets disallowed first at $U_2 \approx -0.6E_F$; the TMR($\phi = \pi/2$) becomes negative but TMR(0) remains positive. At $U_2 \approx -0.5E_F$, the $q_+^\pi$ mode at $\phi = 0, \pi$ gets disallowed and both TMR($\pi/2$) and TMR(0) become negative. But quite soon at $U_2 \approx -0.45E_F$, the $q_-^\pi$ mode gets disallowed and TMR(0) quickly becomes positive again. Therefore, until $U_2 \approx -0.2E_F$, where both spin channels get disallowed, TMR($\pi/2$) and TMR(0) remain negative and positive, respectively. As a function of $\phi$, the TMR is expected to behave like $\cos(\phi/2)$. This is consistent with figures 2(b) and (c) for $U_2 \lesssim -0.2E_F$.

We stress that in these qualitative arguments, evanescent waves have been ignored completely. In particular, for $U_2 \gtrsim -0.2E_F$ (with other parameters fixed as given), both spin channels are evanescent in the central region ($0 < z < d$) and cannot be addressed within the approximate analytical method. (Even if the energy is positive, evanescent waves appear already for negative $U_2$ because of the strong Rashba SOC in the central region.) Quite interestingly, as we have seen above, the contributions of the evanescent waves are highly nontrivial in this parameter range and give rise to $-\cos(\phi/2)$ behavior.

6. Conclusion

We have considered a double-barrier MTJ consisting of a ferromagnetic electrode, a QW with magnetic ordering and strong Rashba spin-orbit coupling, and a normal metal electrode where the junction is formed on the cylindrical shell of the QW. The structure may have a relevance as a simplified model for the magnetic tunnel junction with a LAO/STO transition metal oxide interface including twin boundaries. The latter has been reported to exhibit sign-switching anisotropic TMR. By means of both qualitative analysis and numerically exact calculations, we have shown that our model exhibits a sign-switching anisotropic TMR. The negative TMR occurs as a combined effect of one-dimensionality, magnetic order, and strong SOC in the QW.

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