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J E. Bunder
judyb@uow.edu.au

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Spin-polarized transport in dilute magnetic semiconductor tunnel junctions

J. E. Bunder^{a)}

Physics Division, National Center for Theoretical Sciences, Hsinchu 300, Taiwan

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The author considers transport properties of a trilayer junction consisting of an insulator sandwiched between two dilute magnetic semiconductors (DMSs). The magnetization directions of the two DMSs are not parallel but at a relative angle of θ . After calculating the transmission probabilities, the author calculates the conductance using the Landauer formula. The author defines a ratio $R(\theta, T)$, related to the tunneling magnetoresistance, which compares the $\theta=0$ to the $\theta \neq 0$ conductance at temperature T . The author also calculates $R(\theta, T)$ semiclassically using the well-known Julliere formula. The author shows that, in general, $R(\theta, T)$ obtained from the Julliere formula poorly approximates $R(\theta, T)$ obtained from the Landauer formula. © 2007 American Institute of Physics. [DOI: 10.1063/1.2775032]

There are a wide variety of devices which consist of a trilayer magnetic junction involving some material sandwiched between two magnetic materials. Many of these magnetic junctions have very promising application potentials because of their magnetic and transport properties. A magnetic tunnel junction¹ (MTJ) usually consists of an insulator (I) between two ferromagnets. The tunneling magnetoresistance (TMR) in a MTJ varies greatly depending on the materials used. For example, a MgO insulator can produce dramatic results, with a TMR close to 500% having been observed in CoFe(B)/MgO/CoFe(B) at room temperature.² Using dilute magnetic semiconductors (DMSs) as the magnetic material can also produce quite large TMR, such as almost 300% for Ga(Mn)As/GaAs/Ga(Mn)As at 0.39 K.^{3–6} The TMR may persist to quite high temperatures, provided the DMS has a high critical temperature.

DMSs exhibit both magnetic and electric properties, making them quite popular in spintronics.^{7,8} They are created by doping group III-V or II-VI semiconductors with a transition metal and these impurity ions couple to the itinerant carriers, giving the DMS some unique magnetic properties. Much theoretical work has been done studying the magnetic properties of these interesting materials, but here we are concerned with transport properties. We are interested in obtaining a more detailed understanding of how the conductance across a DMS-based MTJ varies with relative magnetization orientations. Some experimental work has been done in this area using metal-based MTJ.⁹ We adopt a method originally applied to ferromagnet-based MTJ (Refs. 10–12) but replace both ferromagnets with DMS.^{13,14}

We consider a DMS/I/DMS trilayer structure with layers in the xy plane and the insulator positioned between $z = \pm w/2$. We assume the two DMSs are identical, with the exception of the relative magnetization angle θ . The Hamiltonian of this structure is

$$H = -\frac{\hbar^2}{2m} \partial_r^2 - \frac{\Delta}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \Theta(|z| - w/2) + U \Theta(w/2 - |z|). \quad (1)$$

where U is the insulator potential energy and Δ is the energy gap between the majority (M) spin band and the minority (m) spin band in the two DMSs. The spin matrix is written in

terms of up and down spins, rather than minority and majority bands. The minority and majority bands rotate, while the up and down spins do not so the Hamiltonian contains no explicit rotation. The rotation is explicitly contained in the wave function.

Consider a particle with energy E , measured relative to the chemical potential μ , injected into the left DMS. In either of the DMS, its momentum will be $k_M = \sqrt{(E + \mu + \Delta/2)2m^*/\hbar}$ if it has the same spin as the M band or $k_m = \sqrt{(E + \mu - \Delta/2)2m^*/\hbar}$ if it has the same spin as the m band, where m^* is the reduced mass. In the insulator, this same particle will have momentum $k = \sqrt{(E + \mu - U)2m^*/\hbar}$. A schematic representation of the energy levels is shown in Fig. 1, where we distinguish the majority (minority) bands on the left and right by M and M' (m and m'), respectively.

We assume that the component of the momentum which is parallel to the barrier, i.e., in the xy plane, is constant throughout the structure and so need only consider the z dependent part of the wave functions. Firstly, we consider a particle injected into the M band so that the wave functions in the left and right DMSs are

$$\Psi_L(z) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{ik_M z} + C_{MM} \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-ik_M z} + C_{Mm} \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{-ik_m z},$$

$$\Psi_R(z) = \hat{R} \left[C_{MM'} \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{ik_{M'} z} + C_{Mm'} \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{ik_{m'} z} \right], \quad (2)$$

respectively. The matrix

$$\hat{R} = \begin{pmatrix} \cos(\theta/2) & \sin(\theta/2) \\ -\sin(\theta/2) & \cos(\theta/2) \end{pmatrix} \quad (3)$$

rotates the spin bands in the right DMS by θ . The wave function in the insulator will be

FIG. 1. Schematic diagram of the two spin band models for a DMS/I/DMS tunnel junction with a particle of energy $E + \mu$ in the insulator. The M' and m' bands are rotated by an angle θ relative to the M and m bands.

^{a)}Electronic mail: bunder@phys.cts.nthu.edu.tw

$$\Psi_I(z) = \begin{pmatrix} A_1^+ \\ A_2^+ \end{pmatrix} e^{ik^z z} + \begin{pmatrix} A_1^- \\ A_2^- \end{pmatrix} e^{-ik^z z}. \quad (4)$$

The coefficients C_{ab} describe transmission of an a -band particle into the b band. The M -band incident particle's ability to generate a m' -band particle is due to the θ rotation.

By matching the wave functions and derivatives at the boundaries $z = \pm w/2$, we can solve for $C_{MM'}$ and $C_{Mm'}$,

$$C_{MM'} = 4Dk_M^z k^z e^{iw(k^z - k_M^z)} S_{mm} \cos(\theta/2),$$

$$C_{Mm'} = 4Dk_M^z k^z e^{iw(2k^z - k_M^z - k_m^z)/2} S_{Mm} \sin(\theta/2), \quad (5)$$

where

$$D^{-1} = S_{MM} S_{mm} \cos^2(\theta/2) + S_{Mm}^2 \sin^2(\theta/2)$$

$$= S_{MM} S_{mm} + 4(k^z)^2 (k_M^z - k_m^z)^2 e^{2ik^z w} \sin^2(\theta/2)$$

$$S_{MM} = (k_M^z + k^z)^2 - (k_M^z - k^z)^2 e^{2ik^z w},$$

$$S_{mm} = (k_m^z + k^z)^2 - (k_m^z - k^z)^2 e^{2ik^z w},$$

$$S_{Mm} = (k_M^z + k^z)(k_m^z + k^z) - (k_M^z - k^z)(k_m^z - k^z) e^{2ik^z w}. \quad (6)$$

When a m -band particle is injected into the left DMS, one can simply invert the spins of the above results to find the coefficients for transmission into the m' band or the M' band,

$$C_{mm'} = 4Dk_{zm}^z k^z e^{iw(k^z - k_m^z)} S_{MM} \cos(\theta/2),$$

$$C_{mM'} = 4Dk_m^z k^z e^{iw(2k^z - k_M^z - k_m^z)/2} S_{Mm} \sin(\theta/2), \quad (7)$$

respectively.

If a voltage drop of V is maintained across the insulator, the total current density through the insulator is $J = J_{MM'} + J_{Mm'} + J_{mm'} + J_{mM'}$, where $J_{ab'}$ can be found from the Landauer formula¹¹

$$J_{ab'} = e \int \frac{d^3 k_a}{(2\pi)^3} [f(E_a) - f(E_a + eV)] T_{ab'} v_{za}, \quad (8)$$

where $v_{za} = \hbar k_a^z / m^*$ and Fermi distribution function $f(E_a) = [\exp \beta(E_a - a\Delta/2 - \mu) + 1]^{-1}$, with $\beta = 1/k_B T$, $E_a = \hbar^2 k_a^2 / 2m^*$, and $a\Delta = \pm\Delta$ for $a=M$ and m , respectively. The transmission probability is defined by $T_{ab'} = |C_{ab'}|^2 k_b^z / k_a^z$, provided both k_b^z and k_a^z are real and positive. If not, $T_{ab'} = 0$. After converting into polar coordinates, integrating over the azimuthal angle, and defining $u = k_a^z / k_a = \cos \phi$, where ϕ is the polar angle, we write the conductance as

$$G(\theta) = \frac{c}{eV} \sum_{ab} \int_0^\infty dk_a k_a^3 [f(E_a) - f(E_a + eV)] \int_0^1 du T_{ab'} u, \quad (9)$$

where $c = e^2 \hbar / (2\pi)^2 m^*$. We define a relative conductance ratio by

$$R(\theta, T) = \frac{G(\theta) - G(0)}{G(0)}. \quad (10)$$

Although this ratio is sometimes referred to as the TMR, the TMR is more commonly defined by $\text{TMR} = R(\pi, T)G(0)/G(\pi)$.

FIG. 2. $R(\theta, T)$ ratio for $n_h = 0.3 \text{ nm}^{-3}$.

We obtain Δ and μ from a self-consistent Green's function approach¹⁵⁻¹⁸ for parameters suitable for GaAs doped with Mn. The carrier magnetization $\langle \sigma^z \rangle$ and impurity magnetization $\langle S^z \rangle$ obtained from this method are shown in Figs. 2 and 3 of Ref. 18 and Fig. 2 of Ref. 19 for various carrier concentrations n_h . In our calculations, we set the impurity concentration at $n_I = 1 \text{ nm}^{-3}$ and the exchange coupling between impurities and carriers is $J = 0.15 \text{ eV nm}^3$. The energy gap is defined by $\Delta = J \langle S^z \rangle$. We substitute these results into Eqs. (9) and (10) to find the conductance and $R(\theta, T)$. We use $U = 0.55 \text{ eV}$, which is suitable for AlAs, $V = 1 \text{ meV}$, and $w = 1.5 \text{ nm}$, which are both typical experimental values.³

In Ga(Mn)As a six-band model is generally much more accurate than a two-band model as spin-orbit effects can be significant.²⁰⁻²² However, the two-band model can sometimes give a qualitative description, especially when the carrier concentration is small. The TMR, in particular, is not significantly affected by the spin-orbit coupling, provided the carrier concentration remains small, and even when the carrier concentration is not small, the qualitative behavior is still captured.²³ Therefore, as we are mostly interested in the general shape of $R(\theta, T)$ the two-band model is an acceptable approximation.

Figure 2 shows $R(\theta, T)$ when the hole concentration in the two DMS is $n_h = 0.3 \text{ nm}^{-3}$. The Green's function technique requires that $n_h \ll n_I$ as this allows us to assume translational invariance, and so $n_h = 0.3 \text{ nm}^{-3}$ is approximately the upper limit of n_h for this method. This case describes a DMS with typical mean-field properties, i.e., the magnetization declines gradually as the temperature increases, both for the impurities and carriers. This pattern is reflected in the shape of the $R(\theta, T)$ curve, with a maximum $R(\theta, T)$ of 50% when $\theta = \pi$ and the temperature approaches zero.

If the hole concentration is decreased to $n_h = 0.1 \text{ nm}^{-3}$, a far more interesting situation occurs. The magnetization no longer has the classic mean-field shape, instead declining slowly as the temperature increases and diving suddenly near the critical temperature. Figure 3 shows that the maximum possible $R(\theta, T)$ is 100%, attained when $\theta = \pi$ over a large range of temperatures. The shape of the $R(\theta, T)$ curve for a given θ is very close to the shape of the $\langle \sigma^z \rangle$ curve. Decreasing the hole concentration further leaves the $R(\theta, T)$ ratio much the same as for $n_h = 0.1 \text{ nm}^{-3}$.

We can use a semiclassical analysis to approximate $R(\theta, T)$. Adjusting the Julliere model^{1,11,23} to take the rotation into account gives

FIG. 3. $R(\theta, T)$ ratio for $n_h = 0.1 \text{ nm}^{-3}$.

$$R(\theta, T) = \frac{2P^2}{1 + P^2} \sin^2(\theta/2), \quad (11)$$

where P is the polarization of the carriers in either DMS. The angular dependence of Eq. (11) can be shown to be approximately true for $R(\theta, T)$ obtained from the Landauer equation. Generally, $k_z^2(k_{zm} - k_{zm'})^2 e^{2ik_z w} \ll S_{MM} S_{mm}$ so that from Eq. (6), $D^{-1} \sim S_{MM} S_{mm}$. After some straightforward algebra, it can be shown that $R(\theta, T) \sim \sin^2(\theta/2)$. This is comparable to $\delta G \sim \sin \theta \delta \theta$, which was derived from experimental data in Ref. 9. When the DMSs are fully polarized so that the minority bands are empty $T_{mm'} = T_{mM'} = T_{mM} = 0$ and we only need to consider the conductance between the two majority bands which leads directly to $R(\theta, T) = \sin^2(\theta/2)$, as seen in Fig. 3 when T is not close to T_c .

We compare the semiclassical Julliere formula with the results obtained from the Landauer formula in Fig. 4, where $R(T) = R(\theta, T) / \sin^2(\theta/2)$. To calculate the polarization, we use two different methods.²³ We firstly define P in terms of the total number of carriers n_M and n_m in the two bands, $P = (n_M - n_m) / (n_M + n_m) = 2\langle \sigma^z \rangle$. Then, we define P in terms of the density of states in both bands, or equivalently, the Fermi momenta $k_{FM} = k_M(E=0)$ and $k_{Fm} = k_m(E=0)$, so the polarization is $P = (k_{FM} - k_{Fm}) / (k_{FM} + k_{Fm})$. The semiclassical approximation is good when the DMS is fully polarized, as can be seen for $n_h/n_l = 0.1$ when T is not close to T_c . However, for unpolarized DMS, the semiclassical approximation for $R(T)$, particularly for larger carrier concentrations, is not good. Calculating the polarization from the total number of carriers generally gives a better result than when the density of states at the Fermi energy is used. This is not surprising as

FIG. 4. (Color online) $R(T)$ ratio from both the Landauer formula (solid line) and the Julliere formula with polarization calculated using the total number of states (dashed line) and the density of states at the Fermi energy (dash-dotted line) for two different carrier concentrations.

the Landauer formula is dependent on all particles and not just those at the Fermi energy. The discrepancy between results obtained from the Landauer and Julliere formulas was noted in Ref. 23 in a similar system but with a quantum well approximation for the DMS. The quantization of the quantum well makes the Fermi energy approximation for the polarization more accurate and so the Julliere formula is a better approximation in this case.

In conclusion, we have used the transmission probability through a DMS/I/DMS trilayer structure to determine the conductance and a TMR-like ratio $R(\theta, T)$. We assume the two DMSs are identical, except for their magnetization orientation, defined by the angle θ . The $R(\theta, T)$ dependence on θ is very simple, being proportional to $\sin^2(\theta/2)$. Consequently, tuning to a specific $R(\theta, T)$ and hence TMR is theoretically at least very simple. For low carrier concentrations, tuning is particularly simple as the full polarization of the carrier spin sets $R(\theta, T) = \sin^2(\theta/2)$ for a large range of temperatures. This has quite interesting consequences for the realization of the Datta-Das spin field effect transistor^{24–26} Experimentally, obtaining an extremely high $R(\theta, T)$ would be unlikely due to temperature induced fluctuations and disorder. We also show that the Julliere formula is generally not a good approximation for this system.

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