Spin Injection Across a Heterojunction: A Ballistic Picture

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Spin injection across heterojunctions plays a decisive role in the new field of spintronics. Within the ballistic transport regime, we state a general expression for the spin-injection rate in a heterojunction made of two ballistic electrodes. Both the spin-orbit interaction and interface scattering effect are taken into account. Our model is consistent with the well-documented results of ferromagnetic-metal junctions. It explains the recent experimental results of a dilute-magnetic-semiconductor/semiconductor junction and predicts solutions to enhance the spin-injection rate across a ferromagnetic-semiconductor junction.

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Heterojunctions made of spin-polarized electrodes are the building blocks for spintronics [1,2]. Of particular interest is the spin-polarized field-effect transistor (Spin FET) proposed by Datta and Das [3]. It requires spin injection across a ferromagnetic-metal/semiconductor (FM/SC) junction. Results achieved yet are rather controversial [4–16]. Experimentally, the spin-injection rate η measured on a Permalloy/InAs junction is below 10% [4–7], much smaller than the bulk spin-polarization rate $\eta_0 \approx 45\%$ of the Permalloy electrode. In some experiments it is concluded that η is too small to be distinguishable from other spurious effects [8,9]. Theoretically, different approaches are applied to study the influence on η with effects such as the spin polarization of the electrodes [10], spin precession [11], spin-involved scattering [12], electrodes mismatch [13–16], and spin-selective tunneling [14]. Spin-injection rates calculated in different models based on different approximations differ significantly.

The problem of spin injection across a heterojunction is in fact not a new one. Many types of heterojunctions have been investigated, including the ferromagnetic-metal/metal (FM/M) junction [17] with a giant-magnetoresistance (GMR) effect and ferromagnetic-metal/superconductor-metal (FM/SM) junction with spin-dependent Andreev reflections [18]. Recently, spin injection across novel dilute-magnetic-semiconductor/semiconductor (DMS/SC) [19] and ferromagnetic-semiconductor/semiconductor (FS/SC) [20] junctions were demonstrated. Theories for FM/M and FM/SM junctions have been successfully established that show large spin-injection effects [17,18]. The significant different experimental results of spin injection across an all-metal junction [17] and a hybrid junction [4–9] remain to be understood. Effects such as spin polarization, spin-orbit interaction, interface scattering, and band-structure mismatch need to be analyzed on equal footing to find out important physical parameters that determine the spin-injection rate.

In this Letter, based on the quantum mechanical picture, we develop a simple but general model that describes the spin injection across a heterojunction made of two electrodes in the thermodynamic equilibrium. The spin polarization is taken into account by including exchange interaction or large Zeeman splitting in one of the electrodes, and by spin-orbit interaction in the other. Using suitable band-structure parameters, the well-known results for the FM/M (GMR devices) [17] and ideal FM/SC (Spin FET) [3,11] junctions are recovered. Our model qualitatively explains recent experimental data [19] on the DMS/SC junction. The spin-injection rate for a realistic FM/SC junction is analyzed as a function of band structure and junction parameters, which display solutions to enhance η.

We consider a heterojunction with the interface located at $x = 0$. The left electrode contains a three dimensional (3D) spin-polarized electron gas. The right one has a waveguide shape with electrons laterally confined in the x-z plane with a finite width w along the z axis. The left electrode can be made of either a FM, a FS, or a DMS material. For the FM or FS electrode we apply the Stoner model using an effective one-electron Hamiltonian with an exchange interaction h_0. For the DMS electrode, spin polarization is induced by an external magnetic field B that results in a Zeeman shift h_0 due to the large g factor. In both cases the magnetization or the B field is along the x axis. For the right electrode we consider the spin-orbit interaction. For a two dimensional electron gas (2DEG) in a narrow-gap semiconductor that is highly interesting for spintronics, the Rashba effect parametrized by α is the dominant spin-orbit interaction [3,21]. To model the elastic scattering that usually occurs at the interface, we follow the pioneering work of Blonder *et al.* [22] on the metal/superconductor-metal junction to include a δ-function potential $U\delta(x)$. It allows us to describe the crossover from a metallic to a tunnel-junction behavior by changing the parameter U. Assuming a uniform junction at $x = 0$, we have $h(\mathbf{r}) = h_0\Theta(-x)$, $\alpha(\mathbf{r}) = \alpha\Theta(x)$ with $\Theta(x)$ the unit step function. The Schrödinger equation has the form

$$\{H_0\mathbf{I} - h\sigma_x - i[\alpha(\partial/\partial x) + (\partial/\partial x)\alpha]\sigma_z/2 - \alpha(-i\partial/\partial z)\sigma_x + U\delta(x)\}\Psi(\mathbf{r}) = \varepsilon\Psi(\mathbf{r}). \tag{1}$$

Here, $\mathbf{I}$ is the unit matrix, σ_i are the Pauli matrixes, ε is the energy measured from the Fermi level, and $H_0 = \mathbf{P}^2/2m^* + \mathbf{V} - E_F$ is the single-particle Hamiltonian with $V(\mathbf{r}) = V(z)\Theta(x)$ the confinement potential. We assume $V(z)$ to have a parabolic form. The effective mass m_L as well as the Fermi energy E_F^L for electrons in the left electrode can be different from those of the right electrode with m_R and E_F^R.

In general, spin-orbit interaction couples the motions in all directions. However, as shown in the seminal paper of Datta and Das [3] by restricting to the quasi-1D limit with the condition of $w \ll \hbar^2/\alpha m_R$, the problem is greatly simplified. We will show later that with weak spin-orbit interaction, the result for spin injection into a quasi-1D system with a parabolic confinement potential $V(z)$ is valid likewise to that into a 2D electrode. Using the Datta-Das approximation, the energy states of Eq. (1) are found to be

$$\begin{aligned} E_{\sigma,L} &= E_F^L + \varepsilon_\sigma = \frac{\hbar^2 k^2}{2m_L} + \frac{\hbar^2 k_\parallel^2}{2m_L} - \sigma h_0\,, \\ E_{\sigma,R} &= E_F^R + \varepsilon_\sigma = \frac{\hbar^2 (q + \sigma q_s)^2}{2m_R} + \frac{\hbar^2 q_n^2}{2m_R} - E_s\,, \end{aligned} \tag{2}$$

where $\sigma = \pm 1$ is the spin index, $q_s = m_R\alpha/\hbar^2$ and $E_s = \hbar^2 q_s^2/2m_R$ are the Rashba wave vector and Rashba energies, respectively, $k(k_\parallel)$ and $q(q_n)$ are the spin-dependent wave vectors along (perpendicular to) the x axis in the left (L) and right (R) electrodes, respectively. The quantized value of q_n can be obtained by applying the Bohr-Sommerfeld quantization condition for the confinement potential $V(z)$.

Based on Eq. (2) the contact conductance can be solved as a scattering problem between the incoming and outgoing Bloch waves $(k, k_\parallel)$ and (q, q_n) at the Fermi level with $\varepsilon_\sigma = 0$. Note that in our device configuration, due to the presence of spin-orbit interaction, an incoming wave with spin σ in the left electrode can be transmitted and reflected as waves with both spin indices. The problem described in Eq. (1) is in fact very similar to that of a FM/SM junction, in which Cooper pairing described by Bogoliubov equations couples different spins [18]. For temperatures $k_B T \ll E_F$, the Landauer formula [18]

$$G_\sigma = \frac{e^2}{h} \sum_{n=0}^{N} \sum_{\sigma'=\pm 1} t^*_{\sigma,\sigma'} t_{\sigma,\sigma'} \tag{3}$$

links the conductance G with the transmission amplitude t. Here N is the total number of the transmitted modes. The spin-injection rate across a heterojunction is defined by

$$\eta = \frac{G_+ - G_-}{G_+ + G_-}\,. \tag{4}$$

By using the spin-dependent boundary conditions, the transmission amplitudes can be calculated using the standard quantum mechanic method [23] and we get an analytical result of

$$t_{\sigma,\sigma'} = \frac{\sqrt{2F_\sigma P_0}}{F_\sigma + P_0 + iZ_0} \tag{5}$$

with $F_\sigma = \sqrt{1 + \sigma\eta_0 - m\mu(1 + r_0)(n/N)}$ and $P_0 = \sqrt{\mu/m}\sqrt{(1 - n/N)(1 + r_0)}$ being restricted to positive values. Here $\sigma = \pm 1$ and $\sigma' = \pm 1$ are spin indices. Spin injection across arbitrary heterojunctions is hence determined by five dimensionless parameters defined as $m = m_R/m_L$, $\mu = E_F^R/E_F^L$, $\eta_0 = h_0/E_F^L$, $r_0 = E_s/E_F^R$, and $Z_0 = (U/\hbar)\sqrt{2m_L/E_F^L}$ in our model. Note that m and μ describe the mismatch of the effective mass and Fermi energy, respectively, η_0 and r_0 describe the spin polarization in the left and right electrodes, respectively, and Z_0 describes the strength of the elastic scattering at the interface. It is interesting to find that in the quantum mechanical picture, the effect of electrode mismatch [13–16], spin polarization in the electrodes [10], and interface scattering [14], that have previously been separately studied under various approximations, are now unified in a simple picture expressed by the analytical Eqs. (3)–(5). We are now going to study the spin injection in various types of heterojunctions based on this unified picture.

Let us first test the reliability of our result using the well-documented FM/M junction [17] by assuming $m = 1$, $\mu = 1$, $r_0 = 0$, and $Z_0 = 0$. Figure 1(a) shows the result of G_σ and η calculated as a function of η_0 using

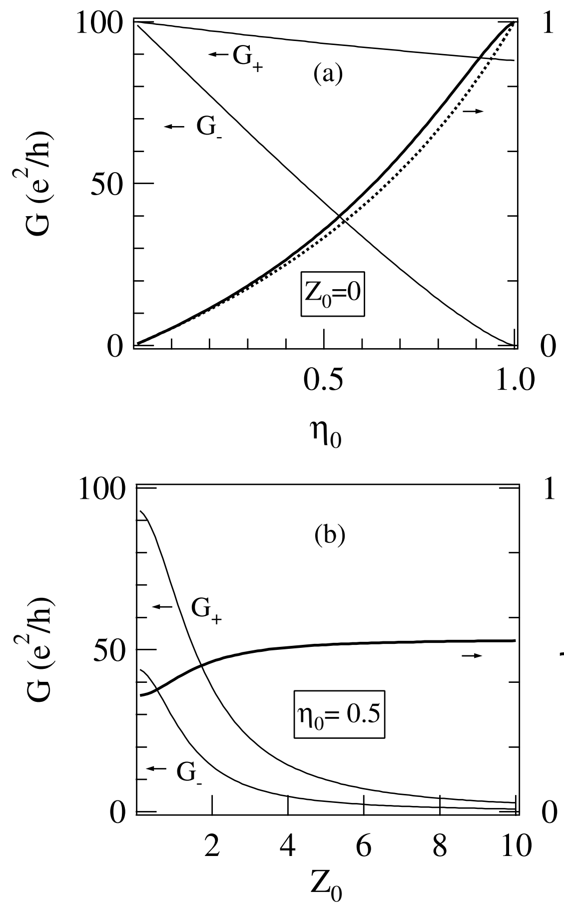

FIG. 1. Dependence of G_σ and η on (a) η_0 and (b) Z_0 for matched electrodes ($m = 1$ and $\mu = 1$) in either a FM/M or a DMS/SC junction with $r_0 = 0$. The dotted line is the semiclassical result.

Eqs. (3)–(5). As has been confirmed by many experiments, η increases with increasing η_0. The result can be illustrated in an instructive semiclassical picture proposed by Bauer for a junction with 2D interface [17]: based on the Stoner model for FM, the exchange interaction changes the potential energy of the two spin states at the Fermi level, so that at the interface, the available number of modes ($k_{\|}$ states) in the FM electrode is $N_\sigma \propto (E_F \pm h_0)$ for up (+) and down (−) spins. In the metal electrode however, the maximum number of modes that can be accepted is $N \propto E_F$. Therefore the number of transmitted modes is $N_+ \propto E_F$ and $N_- \propto (E_F - h_0)$. It follows that $\eta = \eta_0/(2 - \eta_0)$. We plot this semiclassical result in Fig. 1(a) as a dotted line. It seems surprising that our result of a quasi-1D junction agrees so well with that of a 2D junction. The reason lies in the parabolic confinement $V(z)$ we choose, with which we have $N \propto E_F$. Indeed, if we choose a square potential, η scales slightly differently with η_0, however it keeps the same behavior. We find that for weak spin-orbit interaction our results apply for both a quasi-1D junction with parabolic potential and a 2D junction [24].

In Fig. 1(b) we fix $\eta_0 = 50\%$ and study the effect of interface scattering. The effect is twofold: scattering reduces the total conductance but increases η. This is again known for GMR devices [17]. Although here scattering effect improves only modestly η that is mainly restricted by η_0, we will see in the following that it has a dominant influence on spin injection across a FM/SC junction.

Coming to the FM/SC junction, let us first consider the ideal device proposed by Datta and Das [3] followed by a comprehensive study by Tang *et al.* [11]. In both cases, the problem is treated in two steps: spin injection across an ideal FM/SC junction followed by spin precession within SC. The ideal junction can be defined as $m = 1$, $\eta_0 = 1$, $\mu = 2$ [25], $r_0 = 0$, and $Z_0 = 0$. Equation (5) yields $t_{+,+} = t_{+,-} = \sqrt{2}/2$ and $t_{-,+} = t_{-,-} = 0$, which means a spin-up wave from the ferromagnetic electrode splits equally into the two spin states of the 2DEG, while there is no spin-down wave transmitted across the interface. This is exactly what has been suggested [3,11]. Consequently the spin-injection rate $\eta = 100\%$.

The realistic FM/SC junction is not so nice. In Fig. 2 we show the results calculated for a typical device [5] with a FM electrode of $m_L = m_e$, $E_F^L = 3.5$ eV and a 2DEG electrode with $m_R = 0.05\ m_e$, $E_F^R = 100$ meV, and $N = 100$. Figure 2(a) shows the dependence of η on η_0. Unlike in a FM/M junction, increasing η_0 now helps little to increase η unless η_0 approaches 100%. This is because the number of modes N that a 2DEG can accept is much less than the number of modes N_σ coming from the FM electrode. Therefore the information of the spin-dependent number of states in the FM is lost. This effect, first pointed out by Grundler [15], is implicated in Eq. (5). Note the dependence of η on η_0 in Fig. 2(a) is qualitatively similar to that found by Schmidt *et al.* [13] in a diffusive approach. It is not surprising since the conductivity mismatch [13] originates from the effective mass and Fermi energy mismatch.

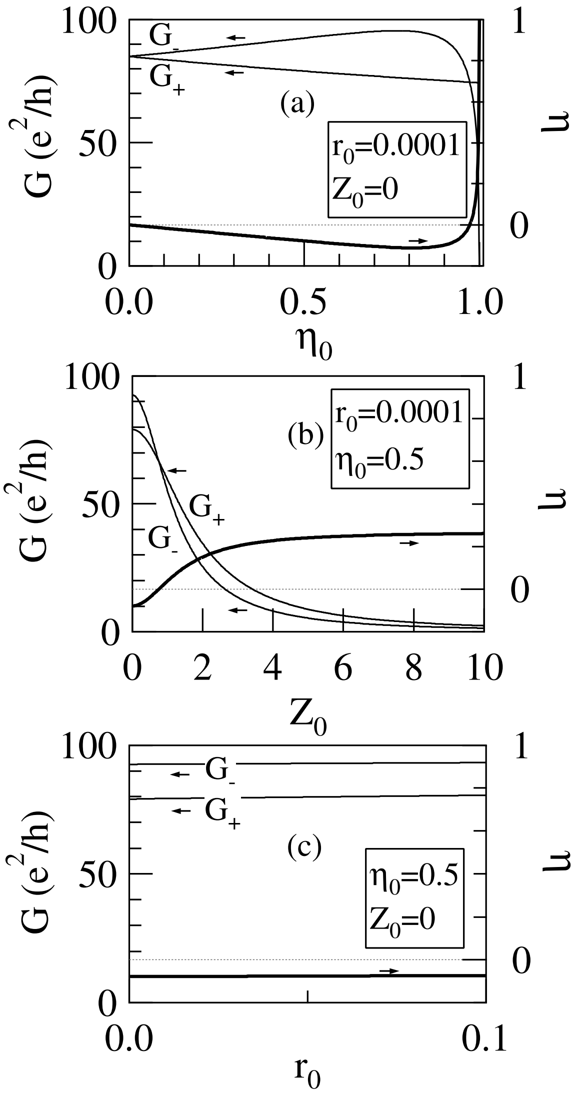

FIG. 2. Dependence of G_σ and η on (a) η_0, (b) Z_0, and (c) r_0 for mismatched electrodes with $m = 0.05$ and $\mu = 0.029$ that is typical for a FM/SC junction.

What is unseen in a diffusive approach is the fact that η is negative over a large range of η_0, which reflects the characteristic difference between the spin injection across an all-metal and a hybrid junction. In the all-metal junction, η is determined by the spin-polarization rate η_0, while in the hybrid junction η is determined by the spin-dependent scattering of Bloch waves across a heterojunction. We note that based on our model, for an inject-detect experiment on the hybrid junction [5,6] the spin-dependent conductance that is proportional to η^2 is small but indeed measurable.

In order to find out solutions to improve η, we show in Figs. 2(b) and 2(c) the dependence of η on the scattering strength and on the Rashba effect. In both cases we fix η_0 with 50%. Again the main effect of scattering is to reduce the total conductance. However we find it can either decrease or increase $|\eta|$ depending on its strength. This is probably the main reason that causes controversy in experimental results on FM/SC junctions [4–9]. In the strong scattering limit η is enhanced by a factor of about 3, which increases the normalized spin-dependent conductance of about 1 order of magnitude in an inject-detect experiment. Intuitively, when Z_0 is large, the FM/SC junction can be viewed as a FM/I/SC tunneling structure with a thin insulating barrier I. Tunneling conductance is well known to be proportional to the product of the states available on both sides of the barrier. Therefore information on spin-dependent numbers of states in the FM that was smeared by the mismatch effect is reinstalled and η is enhanced. The Rashba effect, as shown in Fig. 2(c), does not strongly influence η.

Another way to remove the mismatch obstacle is to replace FM with DMS [19] or FS [20] to get $m \approx 1$ and $\mu \approx 1$. Very recently, a drastic increase of resistance upon increasing an external B field was observed in a diffusive DMS/SC/DMS device [19] that can be regarded as two DMS/SC junctions connected in a series. We plot in Fig. 3 the normalized resistance R together with η for a DMS/SC junction calculated as a function of η_0 that is proportional to B. Our model describes qualitatively both the electrical and optical spin-injection experiments [19] on a DMS/SC junction that measured R and η, respectively.

One of the advantages of SC over M or FM is that the electron mean free path and the Fermi wavelength of electrons in SC is much larger. Microdevices made of a DMS/SC junction can show interesting ballistic spin-polarized transport phenomena. For example, we show in the insertion of Fig. 3 the zoomed-up plot of the η_0 dependence of G_σ and η. Steplike increasing of η is found upon changing the B field. It is because the number of transmitted spin-down modes decreases discretely with increasing B field, while the number of spin-up modes is less affected.

In summary, we study spin injection across a heterojunction by analyzing effects of spin polarization, spin-orbit interaction, interface scattering, and band-structure mismatch on the quantum mechanic footing. An explicit analytical formula is obtained that enables an easy estimation of the spin-injection rate. We find that the spin-injection rate of hybrid FM/SC junctions is determined by the spin-dependent scattering of Bloch waves. It can be either reduced or enhanced if additional interface scattering potential is introduced.

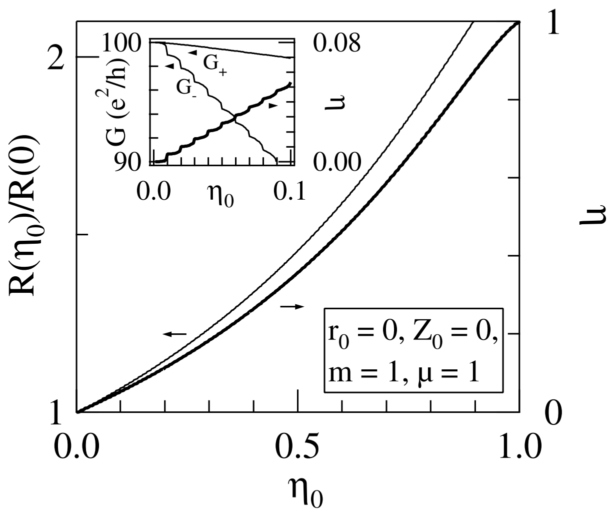

FIG. 3. Dependence of the nomalized resistance R and the spin-injection rate η on η_0 calculated for clean matched electrodes. The inset shows the dependencies of G_σ and η on η_0.

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