Spin-dependent trap-assisted tunneling in magnetic tunnel junctions: A Monte Carlo study

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Spin-dependent resonant tunneling is responsible for the large resistance modulation with magnetic fields observed in three-terminal spin accumulation experiments [1]; however, the expression for the magnetoresistance dependence was questioned [2]. To resolve the controversy, we developed a numerical Monte Carlo approach for the trap-assisted spin tunneling in tunnel junctions. In contrast to spin-independent tunneling [3,4], the transition rates depend on the magnetic field **B** and the magnetization **M** direction of the electrodes. In the case, when an electron can jump from a normal electrode to the trap with the rate Γ_N and from the trap to the ferromagnetic electrode (characterized by the polarization vector $\mathbf{p} = \frac{\Gamma_+ - \Gamma_-}{2\Gamma_F}\frac{\mathbf{M}}{|\mathbf{M}|}$) with the rates $\Gamma_\pm = \Gamma_F(1 \pm |\mathbf{p}|)$ for the spin parallel (anti-parallel) to **M** (Fig.1), the trap occupation n depends on the electron spin **s** [5]:

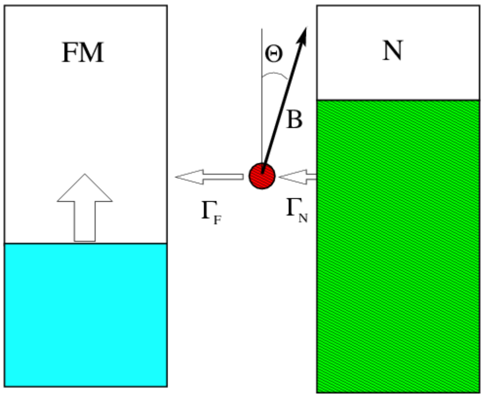
$$\frac{d}{dt}n = \Gamma_\mathrm{N}(1-\mathrm{n}) - \Gamma_F\mathrm{n} - \Gamma_F\mathbf{ps}, \quad \frac{d}{dt}\mathbf{s} = -\Gamma_\mathrm{F}\mathbf{s} - \mathbf{p}\Gamma_\mathrm{F}\mathrm{n} + [\mathbf{s}\times\boldsymbol{\omega}_L].$$

Here $\boldsymbol{\omega}_\mathrm{L} = \frac{\mathbf{eB}}{\mathrm{mc}}$ is the Larmor frequency vector pointing along the magnetic field **B**. The escape probability P(t)= 1-n(t) from the trap is determined by the matrix differential equation (1) (Fig.2). Since the electrons tunnel to the trap from the normal spin-unpolarized electrode, the initial conditions for Eq.1 are n(t=0)=1 and **s**(t=0)=0.

Fig.3 shows the typical probability distributions for escape times from the trap. In contrast to spin-independent tunneling, the probability is not determined by a single exponential and has a more complex behavior. For further calculations the probabilities are stored to evaluate the escape times later.

The charge transport consists of a series of repeated cycles: An electron jumps from the normal electrode to the trap with the rate Γ_N, followed by the electron hop from the trap to the ferromagnetic electrode with the probability P(t). Double occupancy of the trap is prohibited by the Coulomb repulsion. One electron charge is transferred at each cycle during the time $T=T_1+T_2$. The fluctuating time T_1 is evaluated by a direct Monte Carlo technique according to the distribution probability $P_1(t)= \exp(-t/\Gamma_\mathrm{N})$. The time T_2 is distributed according to $P_2(t) = n(t)$ and is evaluated with the rejection technique. The total current I is computed as $\mathrm{I} = \mathrm{eN}/\sum_{\mathrm{i}=1}^{\mathrm{N}}(\mathrm{T}_1 + \mathrm{T}_2)_\mathrm{i}$, where N is a large number of cycles i.

Current simulation results are shown in Fig.4. They are in good agreement with the results from [1]. The current values from [2] are too large for all the directions of the magnetic field except the one, when **B** is parallel to **p**. This implies that escape times used in [2] are shorter. The escape time distribution probability in [2] is determined by the two tunneling rates from each of the Zeeman levels renormalized by coupling to the ferromagnetic contact (Fig.5, dashed lines). This approximation [2] is appropriate only in the case, when the magnetic field is aligned with the magnetization. Fig.6 shows the error reduction for a shorter time while solving the matrix equation (Fig.2) for this case. The consideration based on the matrix equation (Fig.2) is necessary to reproduce the correct transition probabilities and currents.



$$\frac{d}{dt}\begin{pmatrix} n \\ s_x \\ s_y \\ s_z \end{pmatrix} = A\begin{pmatrix} n \\ s_x \\ s_y \\ s_z \end{pmatrix}, \ (1)$$

$$A = \begin{pmatrix} -\Gamma_F & -|\mathbf{p}|\Gamma_F\sin(\Theta) & 0 & -|\mathbf{p}|\Gamma_F\cos(\Theta) \\ -|\mathbf{p}|\Gamma_F\sin(\Theta) & -\Gamma_F & -\omega_L & 0 \\ 0 & \omega_L & -\Gamma_F & 0 \\ -|\mathbf{p}|\Gamma_F\cos(\Theta) & 0 & 0 & -\Gamma_F \end{pmatrix}$$

Fig.1 Electrons tunnel from the normal electrode to the trap with the rate Γ_N and from the trap to the ferromagnetic electrode with the rates $\Gamma_+(\Gamma_-)$ for the spin parallel (anti-parallel) to **M.**

Fig.2 Matrix equation which describes the trap occupation and the spin. To find the escape rates the equation is solved numerically with the initial conditions n(t=0)=1 and **s**(t=0)=0.

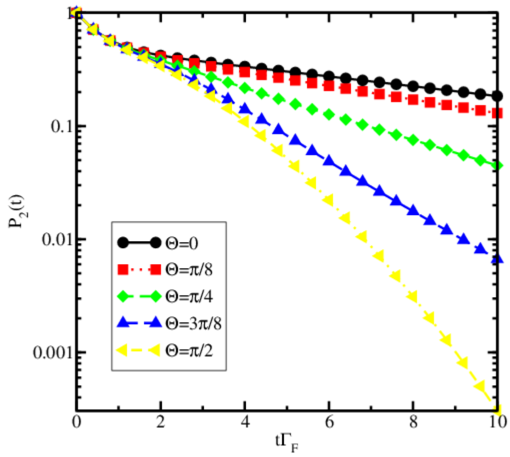


Fig.3 Probability distribution of escape times for $\Gamma_F = \omega_L$ and |**p**|=0.9 .

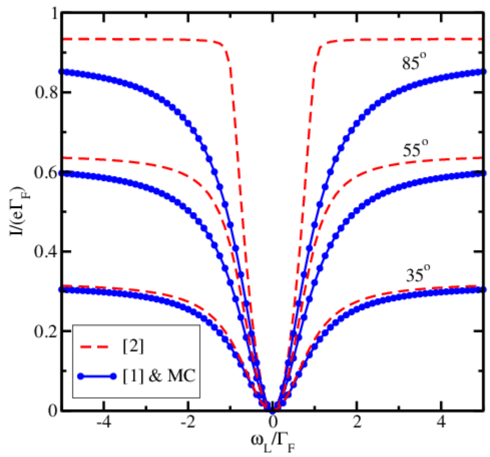


Fig.4 Comparison of Monte Carlo results (symbols) with the results from [1] and [2].

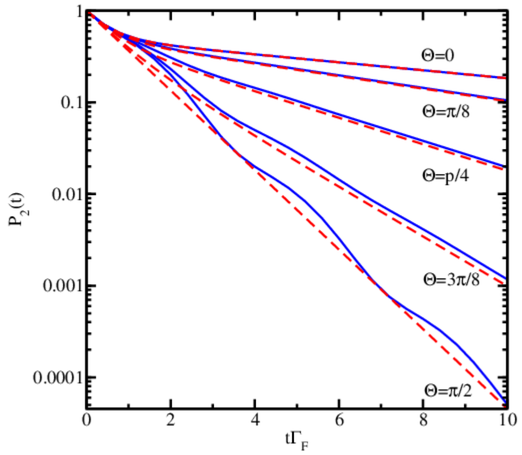


Fig.5 Probability distribution of escape times for ω_L=2Γ_F, |**p**|=0.9 compared to those computed with the method from [2].

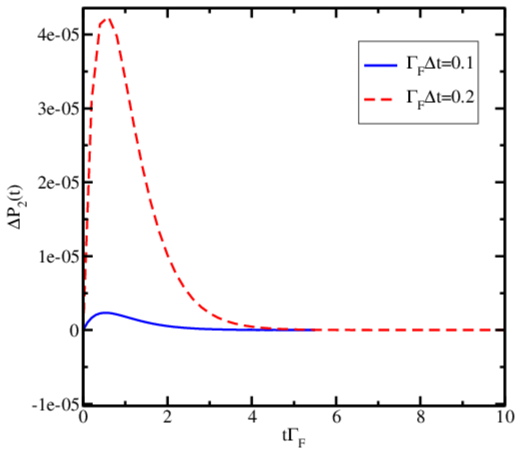


Fig.6 Validation of the numerical rates for two different time steps by comparing with the analytical results from [2] for $\Theta = 0$.

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Full band Monte Carlo simulation of high-field transport in si nanowires

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The effect of collision broadening on the number of impact events has previously been studied in bulk materials. It was shown that incorporating collision broadening increases the number of impact events in the bulk [1]. In this paper, we study the effect of collision broadening in nanowires, where it is expected to have more significance due to the 1D nature of the density of states. In this initial study, a simple Lorentzian broadening is employed and its effects on the velocity field and impact ionization events are studied. A full band impact ionization rate for nanowires is also presented for the first time within the tight binding scheme.

The band structure of the Si nanowires along the [100] direction is calculated according to the empirical tight binding method (TB) [2]. The deformation potential scattering rates are calculated using Fermi's golden rule from the TB coefficients using the method outlined in [3]. At high electric fields multiband tunneling during the free-flight process becomes important [4]. This is taken into account by solving the Krieger and Iafrate equations using the Magnus expansion method [5]. The impact ionization rate is derived for nanowires within the TB scheme and is given by eqn. (1) $k_{1,n}$ represents the high energy electron/hole impacting with a valence band electron/conduction band hole, $k_{4,m}$ creating two new electrons/holes, $k_{2,n'}$ and $k_{3,m'}$.