Influence of Spin Relaxation on Trap-assisted Resonant Tunneling in Ferromagnet-Oxide-Semiconductor Structures

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***Abstract*—Spin-dependent resonant tunneling in ferromagnet-oxide-semiconductor structures is currently of great interest due to the promising potential of semiconductors and silicon in particular for spin-driven applications. Trap-assisted tunneling explains the larger than predicted signal in three-terminal spin-injection experiments. However, for realistic comparison to experiments at elevated temperatures the master equation describing the occupation and spin evolution at an electron trap coupled to the contacts must be augmented to include spin relaxation and dephasing. A short spin relaxation time suppresses the "spin blockade", thus reducing the magnetoresistance modulation. However, intensive dephasing does not strongly affect the magnetoresistance. The substantial magnetoresistance modulation is present at an arbitrary trap position relative to the contacts. Finally, an unusual non-monotonic dependence of the magnetoresistance half-width as a function of the perpendicular magnetic field with dephasing increased is observed.**

Keywords*—Spin, trap-assisted tunneling, master equation, spin relaxation, spin dephasing, tunneling magnetoresistance

I. INTRODUCTION

Silicon, the main material of microelectronics, is perfectly suited for spin-driven applications due to its weak spin-orbit interaction and long spin lifetime [1,2]. Spin injection from a ferromagnetic electrode into n-silicon was claimed at room temperature [3] and also at elevated temperatures [4]. However, the amplitude of the signal extracted from a three-terminal injection method [3,4] is orders of magnitude larger than that predicted by a theory [1], provided the signal is caused by spin accumulation in silicon. Possible reasons for this discrepancy are currently heavily debated [1,5-8]. An alternative interpretation of the three-terminal signal magnitude based on spin-dependent magnetoresistance due to trap-assisted resonant tunneling was proposed [5]; however, the effects of spin dynamics and spin relaxation [6], which are important at room temperature, were not taken properly into consideration. Our goal has been to investigate the role of the spin dynamics on a trap including spin relaxation and decoherence in order to determine the trap-assisted tunneling magnetoresistance.

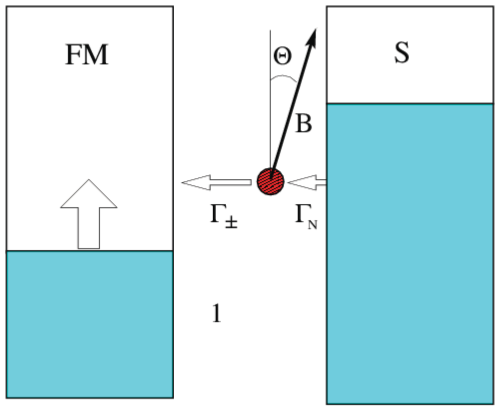

Fig. 1. An electron tunnels with the rate Γ_N on the trap and $\Gamma_\pm$ to the ferromagnet. A magnetic field **B** defines the trap spin quantization axis OZ', which is at an angle Θ to the magnetization orientation OZ in the ferromagnetic contact.

II. METHOD

To highlight the role of spin relaxation and decoherence on the impurity we introduce the corresponding relaxation terms into a Lindblad equation for the density matrix evolution of spin on a trap. Without these relaxation terms included the master equation for the spin density matrix $\rho_{\sigma\sigma'}$, $(\sigma, \sigma' = \pm)$ was recently derived in [5] from the Anderson impurity model in the limit of large on-site interaction. In the basis with the quantization axis chosen along the magnetization direction (Fig.1) in the ferromagnetic contact the corresponding equations are [5]:

$$\frac{d}{dt}\rho_{\sigma\sigma} = \frac{\Gamma_N}{2}(1-\alpha) - \Gamma_\sigma \rho_{\sigma\sigma} + \omega_L \sin(\Theta)\,\mathrm{Im}\,(\rho_{-\sigma\sigma})\,, \qquad \sigma = \pm \quad (1)$$

$$\frac{d}{dt}\rho_{\sigma-\sigma} = i\omega_L(\sin(\Theta)\ (\rho_{-\sigma-\sigma} - \rho_{\sigma\sigma})/2 \pm \cos(\Theta)\rho_{\sigma-\sigma}) - \frac{\Gamma_\sigma + \Gamma_{-\sigma}}{2}\ \rho_{\sigma-\sigma}\ , \qquad -\sigma = \mp \quad (2)$$

Here the tunneling rate Γ_N from silicon to a trap does not depend on spin, while the tunneling rate from the trap to a ferromagnet depends on the spin projection σ = ± on the magnetization direction:

$$\Gamma_{\pm} = \Gamma_F(1 \pm p) \tag{3}$$

The current polarization at the interface of the ferromagnet $p \leq 1$ is defined as

$$p = \frac{\Gamma_+ - \Gamma_-}{2\Gamma_F}. \tag{4}$$

The external magnetic field **B** at the impurity position applied in the XZ plane is assumed to form an angle Θ with the magnetization direction in the ferromagnetic lead. The magnetic field **B** enters into the equations (1,2) via the spin Larmor precession frequency

$$\omega_L = |\boldsymbol{\omega}_L| = \left|\frac{e\mathbf{B}}{mc}\right|, \tag{5}$$

where e and m are the electron charge and the mass, c is the velocity of light. In (1) Im denotes the imaginary part and in (2) i is the imaginary unit.

Let us briefly discuss the terms appearing on the right-hand side of the equations (1,2). The time dependence of the diagonal elements of the density matrix (1) is governed by the balance of the first influx term from the normal electrode on the trap and the second outflux term to the ferromagnet The influx term is proportional to the tunneling rate Γ_N multiplied by the probability

$$P_0 = 1 - \alpha \tag{6}$$

that the site is empty, where $0 \leq \alpha \leq 1$ is the probability of the trap to be occupied. The one-half coefficient in the first term is due to the fact that the electron tunneling from the normal electrode can occupy the site with equal probabilities for the spin projection σ to be up or down.

The second outflux term is proportional to the probability that the state with a certain spin projection is occupied multiplied by the corresponding tunneling rate. It is also assumed for simplicity that a relatively high voltage U is applied between the electrodes, so the trap is located at such an energy E that the corresponding state in the normal electrode is always occupied, while the state in the ferromagnet is empty. A generalization to lower voltages and finite temperatures is straightforwardly accomplished by weighting the tunneling rates Γ_N and Γ_σ with the Fermi distribution $f(E)$ and $(1 - f(E+U))$, respectively.

In order to interpret the third term in the right-hand side of (1) let us express the density matrix ρ in terms of the spin projections s_x, s_y, and s_z, on the coordinate axis X, Y, and Z, correspondingly, in the form

$$\rho = \frac{1}{2}\left(\alpha I + s_x\sigma_x + s_y\sigma_y + s_z\sigma_z\right), \tag{7}$$

where I is the unity matrix and $\sigma_i,\ i = x, y, z$ are the Pauli matrices. The difference of the equations (1) for σ = ± can be written as:

$$\frac{d}{dt}s_z = -\Gamma_F s_z - p\Gamma_F\alpha - \omega_L\sin(\Theta)s_y \tag{8}$$

For completeness we also provide the equation for the site occupation probability α following from summing up the equations (1):

$$\frac{d}{dt}\alpha = \Gamma_N(1-\alpha) - \Gamma_F\alpha - p\Gamma_F s_z \tag{9}$$

In case $p = 0$ one obtains the standard balance equation for the occupation decoupled from the spin. The non-zero spin polarization of the drain electrode involves the spin degree of freedom into the equation for the site occupation, thus affecting the current which results in the resistance dependence on the magnetic field.

Similarly, the sum and difference of equations (2) produce the following equations:

$$\frac{d}{dt}s_x = \omega_L\cos(\Theta)s_y - \Gamma_F s_x \tag{10}$$

$$\frac{d}{dt}s_y = -\,\omega_L\cos(\Theta)s_x + \omega_L\sin(\Theta)s_z - \Gamma_F s_y \tag{11}$$

The last terms in equations (10), (11) describe the escape probabilities of the spin being in the XY plane into the ferromagnet. Because the XY plane is perpendicular to the magnetization orientation in the ferromagnet along the OZ axis, the escape probability is the sum of the two probabilities $\frac{\Gamma_+}{2}$ and $\frac{\Gamma_-}{2}$ to tunnel into the states with the spin up and spin down in the ferromagnet, respectively. Their sum $\frac{\Gamma_+ + \Gamma_-}{2}$ results, according to (3) in the total rate Γ_F. The equations (9-11) are conveniently written in the vector form

$$\frac{d}{dt}\mathbf{s} = -\Gamma_F\mathbf{s} - \mathbf{p}\Gamma_F\alpha + [\mathbf{s}\times\boldsymbol{\omega}_L], \tag{13}$$

where $\mathbf{s} = (s_x,\ s_y,\ s_z)$ and $\mathbf{p} = (0,\ 0\ ,\ p)$. Equation (13) describes the dynamics of the spin in the presence of a magnetic field on the impurity coupled to the leads, one of which is ferromagnetic. Without the terms proportional to Γ_F the equation resembles the Bloch equation for spin dynamics, however, without relaxation and dephasing included. Spin relaxation and dephasing can become quite important, especially at elevated temperatures, where experiments on spin injection in semiconductor by pushing the electrical current through a ferromagnet-oxide-semiconductor structure are performed. Similar to the Bloch equation, one can generalize (13) to include the spin lifetime T_1 and the dephasing time T_2.

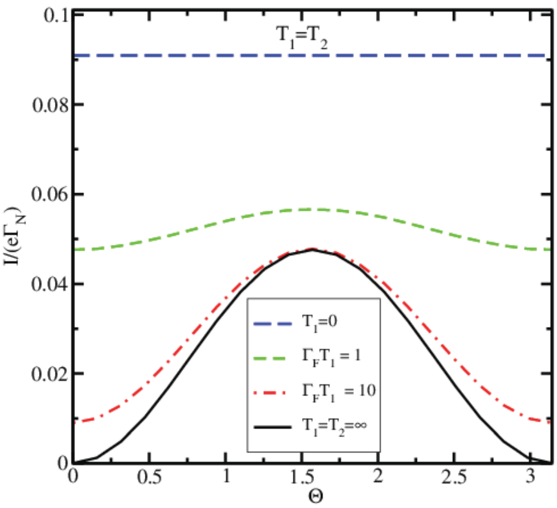

Fig. 2. Current in units of $e\Gamma_N$ as a function of Θ for p=1 Γ_N/Γ_F = 10, ω_L/Γ_F = 1, and several values of T_2=T_1

The spin dynamics is then described by

$$\frac{d}{dt}\mathbf{s} = -\Gamma_F\mathbf{s} - \mathbf{p}\Gamma_F\alpha + [\mathbf{s}\times\boldsymbol{\omega}_L] - \left(\frac{1}{T_1}-\frac{1}{T_2}\right)\frac{(\mathbf{s}\cdot\boldsymbol{\omega}_L)}{\omega_L}\frac{\boldsymbol{\omega}_L}{\omega_L} + \frac{1}{T_1}s_0\frac{\boldsymbol{\omega}_L}{\omega_L} - \frac{1}{T_2}\mathbf{s} \quad (14)$$

Thereby it is guaranteed that the spin component along the magnetic field **B** relaxes with the time T_1 to an equilibrium value s_0, while the perpendicular component dephases with the time T_2. The master equation (14) includes the spin lifetime T_1 and coherence time T_2. Typically $T_2 \leq T_1$, however, at elevated room temperature $T_2 \cong T_1$.

In order to analyze (14), we assume that the temperature is high compared to the Zeeman energy $kT \gg \hbar\omega_L$ so that one can neglect s_0. It is also more convenient to change the basis to x',y',z' axes so that the z' axis is along the direction of the magnetic field on the trap. The density matrix in this basis is written as

$$\rho = \alpha I + a\sigma'_x + b\sigma'_y + c\sigma'_z \quad (15)$$

with a, b, c being the spin expectation value projections on the axes x',y',z'. To find a stationary solution of (14) we set $\frac{d}{dt}\mathbf{s} = 0$. Then (14) results in the following equations

$$b\omega_L + c\left(\frac{1}{T_2}+\Gamma_F\right) = 0\,, \quad (16a)$$

$$c\,\omega_L\cos(\Theta) - a\sin(\Theta)\left(\frac{1}{T_1}+\Gamma_F\right) - b\cos(\Theta)\left(\frac{1}{T_2}+\Gamma_F\right) = 0\,, \quad (16b)$$

$$b\sin(\Theta)\left(\frac{1}{T_2}+\Gamma_F\right) - a\cos(\Theta)\left(\frac{1}{T_1}+\Gamma_F\right) - c\,\omega_L\sin(\Theta) = p\Gamma_F\alpha\,, \quad (16c)$$

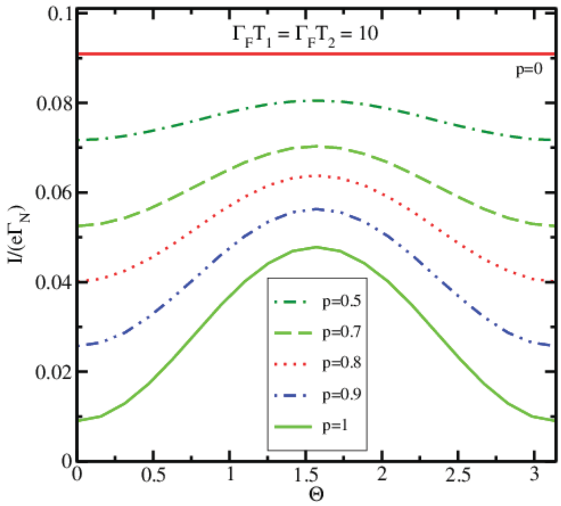

Fig. 3. Current as a function of Θ, for Γ_N/Γ_F = 10, ω_L/Γ_F = 1, $\Gamma_F\, T_1 = \Gamma_F\, T_1$ = 10, and several values of p.

while (9) after setting $\frac{d}{dt}\alpha = 0$ results in

$$(\Gamma_F + \Gamma_N)\alpha + p\Gamma_F(a\cos(\Theta) - b\sin(\Theta)) = \Gamma_N. \quad (16d)$$

The current I due to tunneling via a trap is computed as

$$I = e\,\Gamma_F(1-\alpha). \quad (17)$$

III. RESULTS

Solving equations (16,17) results in the following expression for the current:

$$I = e\frac{\Gamma_F(\Theta)\,\Gamma_N}{\Gamma_F(\Theta)+\Gamma_N} \quad (18a)$$

$$\Gamma_F(\Theta) = \Gamma_F\left(1 - p^2\,\Gamma_F T_1\left\{\frac{\cos^2\Theta}{\Gamma_F T_1 + 1} + \frac{T_2}{T_1}\frac{\sin^2\Theta(\,\Gamma_F T_2 + 1)}{\omega_L^2 T_2^2 + (\,\Gamma_F T_2 + 1)^2}\right\}\right) \quad (18b)$$

The current I differs from $I_0 = \Gamma_F\,\Gamma_N / (\Gamma_F + \Gamma_N)$, the current value when both electrodes are nonmagnetic metals. It depends on the angle Θ between the spin quantization axis and the magnetization orientation.

In the case T_1=T_2→∞, when relaxation and dephasing are ignored, one obtains

$$\Gamma_F(\Theta) = \Gamma_F\left(1 - p^2\left\{\cos^2\Theta + \frac{\sin^2\Theta}{\omega_L^2/\Gamma_F^2 + 1}\right\}\right). \quad (19)$$

With this result the corresponding expression for the current obtained in [5] is reproduced.

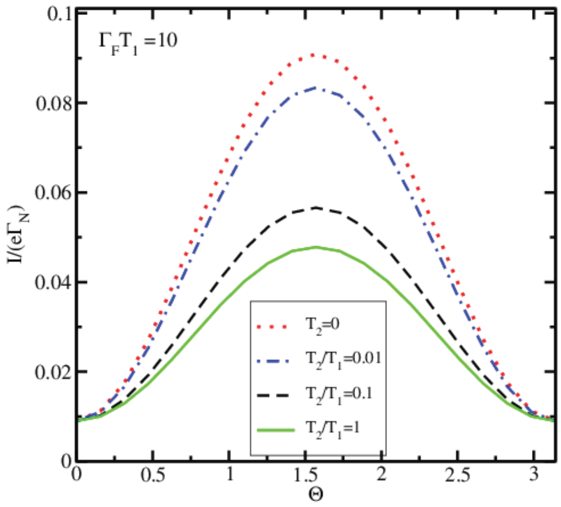

Fig. 4. Current as a function of Θ, for p=1, Γ_N/Γ_F = 10, ω_L/Γ_F = 1, $\Gamma_F T_1$ = 10, and several values of T_2/T_1.

Complementary to [5], (18) includes the effects of spin relaxation. When $\Gamma_F T_1 = \Gamma_F T_2 \ll 1$, the resistance dependence on the magnetic field is a Lorentzian function with the half-width determined by the inverse spin lifetime. A short spin relaxation time suppresses the "spin blockade" [5], which appears at small Θ (Fig.2), in a similar fashion as the reduction of spin current polarization p (Fig.3). Due to the suppression of the last term in (19) at short T_2 with T_1 fixed, the amplitude of the current I(Θ) modulation with Θ becomes more pronounced (Fig.4), in contrast to the intuitive expectation that strong decoherence should reduce the effect. At finite T_1 the modulation of I(Θ) is present at an arbitrary trap position relative to the contacts (Fig.5), complementary to [5]. Finally, with T_2 decreasing an unusual non-monotonic dependence of the magnetoresistance as a function of the perpendicular magnetic field **B**, with the linewidth decreasing, at shorter T_2 is shown in Fig.6.

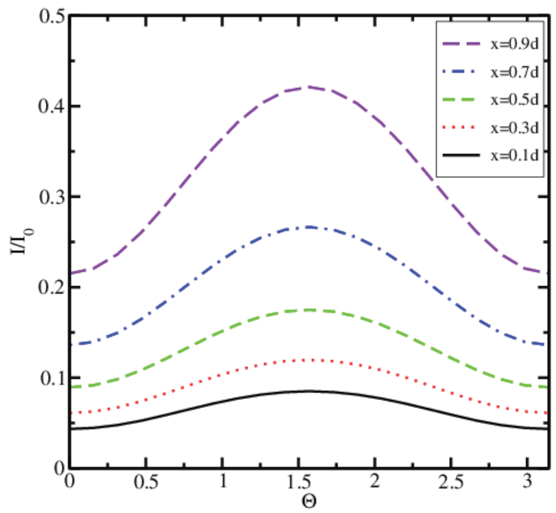

Fig. 5. *Normalized current as a function of the position x*, for p=1, $\Gamma_N=\Gamma_0 \exp(-x/d)$, $\Gamma_F=\Gamma_0 \exp(-(d-x)/d)$, $T_2=T_1$, $\omega_L T_2 = \Gamma_0 T_2 = 10$,

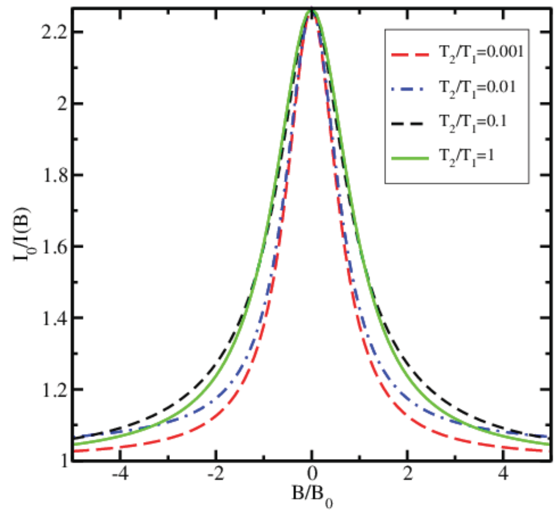

Fig. 6. Magnetoresistance signal as a function of the perpendicular magnetic field **B** for several T_2/T_1, for p=0.8 and $\Gamma_F T_1$=10. The field $\mathbf{B}_0$ is parallel to the magnetization in the ferromagnet.

IV. Summary

The master equation describing the dynamics of the electron spin on a trap in oxide sandwiched between a ferromagnetic and a normal metal contact is augmented to include the spin relaxation and dephasing. Strong spin relaxation reduces the magnetoresistance modulation, however, strong dephasing has a lower effect on the magnetoresistance. At finite spin relaxation the substantial magnetoresistance modulation is present at an arbitrary trap position relative to the contacts. An unusual non-monotonic dependence of the magnetoresistance as a function of dephasing is observed.

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