Enhanced Shot Noise as a Signature of Trap-Assisted Tunneling in Magnetic Tunnel Junctions: a Monte Carlo Approach

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Abstract. A numerical Monte Carlo approach to evaluate transport due to spin-dependent trap-assisted tunneling in magnetic tunnel junctions has been developed. The current and the low frequency current noise is calculated. It is shown that the shot noise at spin-dependent hopping is significantly enhanced due to the Pauli spin blockade. This provides an additional characteristic for identifying spin-dependent trap-assisted tunneling as a cause of large magnetoresistance observed in three-terminal spin accumulation experiments.

Introduction

With magnetic tunnel junctions scaling down, many interesting phenomena due to the correlated charge transport are anticipated. The Coulomb interaction leads to a strong repulsion on a trap - a Coulomb blockade - and results in pronounced charge transport correlations, when electrons are transferred through the trap \cite{1}. Indeed, an electron from a contact cannot jump on the trap before the electron from the trap escapes to a lead.

The Pauli exclusion principle - forbidding two electrons with the same spins to occupy the same quantum state on the trap - results in yet another correlation effect during the transport through quantum dots and traps \cite{2}. Spin correlations are responsible for large magnetoresistance and magnetoluminescence effects observed at room temperature in organic semiconductors and in organic light-emitting diodes \cite{3}.

Spin-dependent resonant tunneling is also believed to be responsible for the large resistance modulation with the magnetic field \cite{4} observed in three-terminal spin accumulation experiments \cite{5}. However, the phenomenon remains puzzling \cite{6}, and even the expression for the magnetoresistance dependence obtained in \cite{4} was recently challenged \cite{7}.

To resolve the controversy, we present a numerical Monte Carlo approach capable of evaluating the current due to trap-assisted tunneling. We also calculate the shot noise at spin-dependent hopping and demonstrate that, due to the Pauli spin blockade in a magnetic field parallel to the magnetization of the ferromagnetic contacts, the Fano factor is significantly enhanced relative to the direct tunneling case. This provides an additional characteristic for distinguishing spin-dependent trap-assisted tunneling as a possible cause of the large magnetoresistance \cite{5} in spin accumulation experiments.

1. Method and Results

To describe the spin-independent hopping it is sufficient to provide the transition rates to/from a trap, and the stationary current and its low-frequency fluctuations can then be evaluated by a Monte Carlo algorithm \cite{8, 9}. In contrast to spin-independent tunneling, the transition rates with spin depend on the magnetic field and the magnetization direction of the electrodes. In the case when an electron tunnels from a normal electrode to the trap with the rate $\Gamma_N$ and from a trap to the ferromagnetic electrode characterized by the polarization vector $\mathbf{p} = (\Gamma_+ + \Gamma_-)/(2\Gamma_F)\mathbf{M}/M$ with the rates $\Gamma_\pm$ for the spin parallel (anti-parallel) to the magnetization $\mathbf{M}$ (Fig.1), the trap occupation $0 \leq n \leq 1$ dynamics depends on the electron spin $s$ \cite{10}:

\[
\frac{dn}{dt} = \Gamma_N(1-n) - \Gamma_F n - \Gamma_F ps
\]  
\[
\frac{ds}{dt} = -\Gamma_F s - p\Gamma_F n + [s \times \omega].
\]

Here $\omega = \frac{\hbar \omega}{mc}$ is the Larmor frequency vector pointing in the direction of the external field $\mathbf{B}$. The escape probability $P(t) = 1 - n(t)$ from the trap is determined by the matrix differential equation resolved for $n(t)$:

\[
\frac{d}{dt} \begin{pmatrix} n \\ s_x \\ s_y \\ s_z \end{pmatrix} = A \begin{pmatrix} n \\ s_x \\ s_y \\ s_z \end{pmatrix}
\]

with $A$ defined as:

\[
A = \begin{pmatrix} -\Gamma_F & -p\Gamma_F \sin \Theta & 0 & -p\Gamma_F \cos \Theta \\ -p\Gamma_F \sin \Theta & -\Gamma_F & -\omega & 0 \\ 0 & \omega & -\Gamma_F & 0 \\ -p\Gamma_F \cos \Theta & 0 & 0 & -\Gamma_F \end{pmatrix}
\]

Since the electrons tunnel to the trap from the spin-unpolarized electrode, the initial conditions are taken as

\[
n(t = 0) = 1 \quad s(t = 0) = 0
\]

The charge transport consists of a series of repeated cycles of electron hops from the non-magnetic electrode onto the trap with the rate $\Gamma_N$ followed by a hope from the trap to the ferromagnetic electrode with the time-dependent probability $P(t)$. Double occupancy of the trap is prohibited by the Coulomb repulsion. The next electron can only tunnel onto the trap if it is empty. A single electron charge is transferred during each cycle.

The time of each cycle $T = T_1 + T_2$ fluctuates. The random time $T_1$ is evaluated by a direct Monte Carlo technique according to the distribution $P_1(t) = \exp(-t\Gamma_N)$. The time $T_2$ is distributed according to $P_2(t) = 1 - n(t)$. The probability $P_2(t)$ is determined by solving (3-5) numerically for fixed $B$ and $p$.

The stored $P_2(t)$ is used to evaluate the escape time $T_2$ from the trap with the rejection technique. The total current

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I and the Fano factor $F$ (characterizing the strength of the shot noise spectral density $S = 2eIF$) are computed as

$$ I = \frac{eN}{\sum_i N_i (T_1 + T_2)_i}, \quad F = \frac{N \sum_i (T_1 + T_2)_i^2}{\left(\sum_i (T_1 + T_2)_i\right)^2} - 1, $$

where $N$ is a large number of the cycles numbered by $i$. In the case of spin-independent transport ($p=0$), $F$ is given by $F = \frac{(\Gamma_F - \Gamma_o)/\Gamma_F}{(\Gamma_F + \Gamma_o)/\Gamma_F}$. The Fano factor characterizes the regularity of the current flow. Importantly, in the most irregular case, when one of the rates is much smaller than the other, it reaches the maximum value of one for spin-independent tunneling.

Fig.1 shows the typical dependences of the probability of the escape times from the trap determined by solving (3-5) numerically, for several values of the angle $\Theta$ between $\mathbf{B}$ and $\mathbf{p}$, for $\omega = 2\Gamma_F$ and $p=0.9$. In contrast to spin-independent tunneling, the probability is not determined by a single exponential. It is also different from the rates determined by the two tunneling rates from each of the Zeeman levels renormalized by their coupling to the ferromagnetic contact (dashed lines) in [7] and displays a more complex behavior. This approximation [7] is appropriate only for the case, when the magnetic field is aligned with the magnetization of the ferromagnetic contact.

Current simulation results are shown in Fig.2. They reproduce the results from [4]. At the same time, the current values from [7] are too large for all the directions of the magnetic field except the one when $\mathbf{B}$ is parallel to $\mathbf{p}$. This is due to the fact that the escape time used in [7] is too short as is shown in Fig.1. The approximation with tunneling from the two Zeeman levels [7] is incomplete in the case, when the magnetic field is not aligned with the magnetization and the consideration based on the matrix equation (3) is necessary to reproduce the correct transition probabilities and currents.

Fig.3 shows the Fano factor for the same parameters as in Fig.2. It can be seen that the value of $F$ is larger than one for magnetic fields and angles $\Theta$, where the current is suppressed due to the Pauli blockade (see Fig.2). This demonstrates that, due to the Pauli spin blockade in the magnetic field parallel to the magnetization of the ferromagnetic contact, the Fano factor is significantly enhanced relative to the direct tunneling case. This provides an additional characteristic, capable of recognizing whether spin-dependent trap-assisted tunneling is the reason for a large magnetoresistance signal in magnetic tunnel structures.

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References