A Monte Carlo Evaluation of the Current and Low Frequency Current Noise at Spin-Dependent Hopping

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Abstract. Monte Carlo methods are convenient to model the electron transport due to single electron hopping. The algorithm allows to incorporate a restriction that due to the Coulomb repulsion each trap can only be occupied by a single electron. With electron spin gaining increasing attention, the trap-assisted electron transport has to be generalized to include the electron spin, especially in the presence of an external magnetic field and with transport between ferromagnetic contacts. An innovative Monte Carlo method to deal with the spin-dependent hopping is presented. When the electron spin is taken into account, the escape transition rates are described by transition matrices which describe the coupled spin and occupation relaxation from the trap. The transport process is represented by a cyclic repetition of consecutive electron hops from the source to a trap and from the trap to the drain. The rates do not depend on the previous hops nor on time. The method allows to evaluate the electron current as well as the low frequency current noise at spin-dependent hopping. Our Monte Carlo approach resolves a controversy between theoretical results found in literature.

1 Introduction

An elementary particle, the electron, plays the most important role in improving the human life. The property of the electron charge to interact with the electric field is exploited in every electric device from energy generation to microelectronics. As the transistor is currently approaching its smallest ultimate limits, another electron intrinsic characteristic, the electron spin, attracts increasing attention as a supplementary degree of freedom to be used in upcoming nanoelectronic devices. Spin-dependent transport properties play increasingly important role in applications. Recently, an extremely large magnetic response on light emission caused by spin-charge correlated transport was observed at room temperature [1]. Resonant spin-dependent tunneling plays an important role in

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defining the large resistance modulation with magnetic fields observed in three-terminal spin accumulation experiments [2]. However, the expressions for the magnetoresistance dependencies obtained in [2] were challenged [3]. To resolve the controversy, we developed a numerical Monte Carlo approach for the trap -assisted spin tunneling in tunnel junctions.

2 Method

To develop the Monte Carlo approach for spin-dependent trap-assisted transport, we at first briefly outline the algorithm for spin-independent hopping. Single electron hopping between the trap levels is the main transport mechanism in non-degenerate semiconductors. In the case of spin-independent hopping the master equation for the trap occupations is conveniently solved by a Monte Carlo method. The transition rate of hopping between two given sites defines the frequency of an electron to travel between the two sites. Importantly, before the transition the initial site must be occupied by an electron while the final site is empty. The fact that the final site must be empty for a successful transition is the manifestation that each site can only be occupied by a single electron. The single occupation is a consequence of the Coulomb blockade, when the strong on-site Coulomb repulsion prevents two charged electrons to occupy the same site. Knowing the transition rate Γ between the two sites, the *random* time t distribution of an electron hop is determined by the exponential probability $P(t) = \exp(-\Gamma t)$. Using a random number r uniformly distributed between zero and one, the random time t is conveniently found [4] as

$$t = \frac{-\ln(r)}{\Gamma}. \tag{1}$$

Given the transition rates between the traps, the rate of an electron to escape from a certain trap i is the sum $\sum_j \Gamma_{ij}$ of the rates Γ_{ij} to all the traps j which are empty [5]. The transport process is then conveniently modeled as follows. For given sites' occupations the sum of all possible transition rates $\Gamma = \sum_{ij} \Gamma_{ij}$ is computed. The sum of all rates Γ is substituted into (1) to determine the transition time for an electron to perform a hop. Which particular transition ij happens is determined by the probability

$$P_{ij} = \frac{\Gamma_{ij}}{\Gamma}. \tag{2}$$

The approach described above also can treat contacts. The source contact is modeled as a site which always supplies an electron for hopping, while the drain contact is modeled as a site where an electron can always escape. In order to do so it is sufficient to lift the restriction of single occupancy of the drain site.

In the case of single electron hopping through a trap between the metal source and ferromagnetic drain, the escape rates from the trap depend on the spin orientation of the electron on the trap relative to the drain magnetization direction. When a voltage between the electrodes is applied, current flows, and an average spin at the trap appears. This spin influences the trap occupation $n(t)$ and the current. The average spin $\mathbf{s}(t)$ at the trap is determined by the drain magnetization orientation. It is built up slowly as a result of many electron hops from the trap to the drain. It then appears that both probabilities of an electron, to hop from the source to the trap and to escape from the trap to the drain, depend on the history of the previous hops. This violates the picture of the spin-independent charge transfer as a series of consecutive *independent* hops from the source to the trap and further to the drain each described by a time-independent transition rate and inhibits using traditional Monte Carlo techniques to evaluate the current.

The master equation for the spin density matrix at the trap can be derived from the stochastic Liouville equation [6]. In the basis with the quantization axis chosen along the magnetization direction (Fig. 1) in the ferromagnetic contact the corresponding equations for the trap occupation $n(t)$ and the spin $\mathbf{s}(t)$ are [7]:

$$\frac{dn(t)}{dt} = \Gamma_N(1 - n(t)) - \Gamma_F n(t) - \Gamma_F \mathbf{p}\mathbf{s}(t) \tag{3}$$

$$\frac{d\mathbf{s}(t)}{dt} = -\Gamma_F \mathbf{s}(t) - \Gamma_F \mathbf{p} n(t) + [\mathbf{s}(t) \times \omega_{\mathbf{L}}] \tag{4}$$

Here Γ_N is the tunneling rate from the metal source to the trap and $\Gamma_F = (\Gamma_+ + \Gamma_-)/2$ is the average tunneling rate from the trap to the ferromagnetic drain with a polarization $p \leq 1$. Electrons with spins parallel/antiparallel to the drain polarization vector $\mathbf{p}$ tunnel with the rates $\Gamma_\pm = \Gamma_F(1 \pm |\mathbf{p}|)$, correspondingly. Although the particular expressions for the transition rates depend on the microscopic transport mechanism, the use of the transition rates as parameters of the problem allows to describe both the resonant tunneling [2] and the single-electron hopping [8] on equal footing. The Larmor frequency vector $\omega_{\mathbf{L}} = e\mathbf{B}/(mc)$ direction is defined by the magnetic field $\mathbf{B}$ which forms an angle

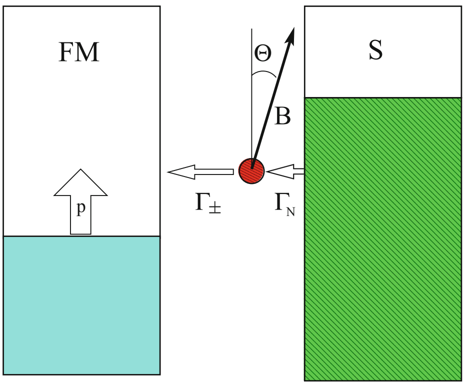

Fig. 1. An electron tunnels with the rate Γ_N on the trap and $\Gamma_\pm$ to the ferromagnet. A magnetic field $\mathbf{B}$ forms the angle Θ with the ferromagnetic drain polarization $\mathbf{p}$.

Θ with $\mathbf{p}$ (Fig. 1). Equation (3) determining $n(t)$ contains the influx contribution and the escape term. The influx term from the normal source does not depend on the spin and can be treated in a way similar to the spin-independent hopping. Namely, the random time distribution to jump from the normal source on the empty trap is determined by the exponential distribution (1) with the transition rate Γ_N.

The escape rate depends also on the spin $\mathbf{s}(t)$. In order to find the escape rate we assume that the probability $P_{out}(t)$ to escape from the occupied trap is equal to

$$P_{out}(t) = 1 - n(t), \tag{5}$$

where the probability $n(t)$ of the trap to be occupied at the time t is determined by

$$\begin{pmatrix} \frac{dn(t)}{dt} \\ \frac{ds_x(t)}{dt} \\ \frac{ds_y(t)}{dt} \\ \frac{ds_z(t)}{dt} \end{pmatrix} = - \begin{pmatrix} \Gamma_F & p\Gamma_F \sin(\Theta) & 0 & p\Gamma_F \cos(\Theta) \\ p\Gamma_F \sin(\Theta) & \Gamma_F & \omega_L & 0 \\ 0 & -\omega_L & \Gamma_F & 0 \\ p\Gamma_F \cos(\Theta) & 0 & 0 & \Gamma_F \end{pmatrix} \cdot \begin{pmatrix} n(t) \\ s_x(t) \\ s_y(t) \\ s_z(t) \end{pmatrix}. \tag{6}$$

This is the first important assumption.

Equation (6) must be complemented with an initial condition. Since electrons are tunneling on the trap from a non-magnetic source, they have an equal probability to have their spin projection up or down on any axis, so their initial spin before tunneling to the drain is zero. This is the second non-trivial assumption which contradicts the intuition that an average spin at the trap depends on the drain magnetization polarization and thus must be finite. We now demonstrate that the results obtained with this assumption are correct.

The transport process is represented as a cyclic repetition of the two tunneling processes from the source to the trap and from the trap to the drain. The first process is described by a random time defined with the help of Eq. (1) with the replacement of Γ by Γ_N. The second tunneling process from the trap to the drain is described by the tunneling time found with the help of Eqs. (5) and (6). Therefore, Eq. (6) is applicable, if the trap is occupied by an electron. Equation (6) is then solved with the initial conditions

$$n(t=0) = 1; \mathbf{s}(t=0) = 0. \tag{7}$$

3 Results

The numerical solution for $n(t)$ is shown in Fig. 2. In contrast to tunneling to a normal electrode, the dependence is more complex as it is not determined by an exponential dependence with a single rate. By generating a random number r uniformly distributed between zero and one, the random tunneling time t_F is found by solving $n(t_F) = r$. The current I is evaluated with respect to N transport cycles as

$$I = e\frac{N}{\sum_{i=1}^{N}(t_N + t_F)}. \tag{8}$$

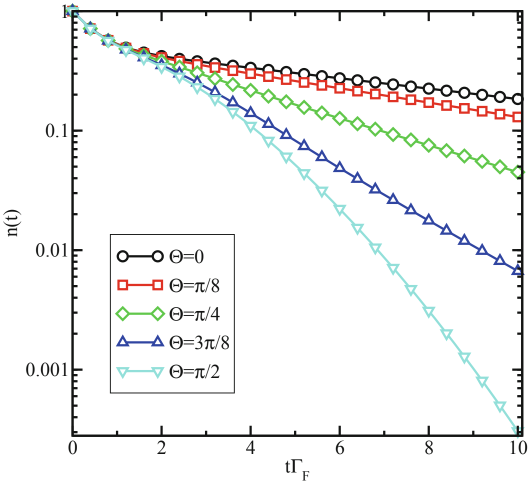

Fig. 2. Probability of trap occupancy. $p = 0.9$, $\omega_L = \Gamma_F$.

The results of the current I are compared with the current computed as a stationary solution of (3, 4) [2] (solid lines) in Fig. 3. The perfect agreement between the results proves that the Monte Carlo algorithm suggested to treat the spin-dependent tunneling is correct. Figure 4 demonstrates the comparison of the current Eq. (8) with the results obtained in [3]. The reason for the discrepancy is clarified in Fig. 5 where the dependence of the occupation $n(t)$ defining the

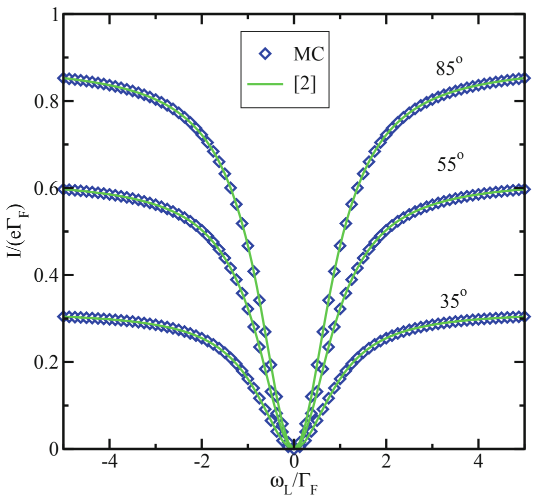

Fig. 3. Comparison of the current I computed as the stationary solution [2] (solid lines) and by the suggested Monte Carlo method using Eq. (8) (symbols). $p = 1$, $\Gamma_N = 8\Gamma_F$.

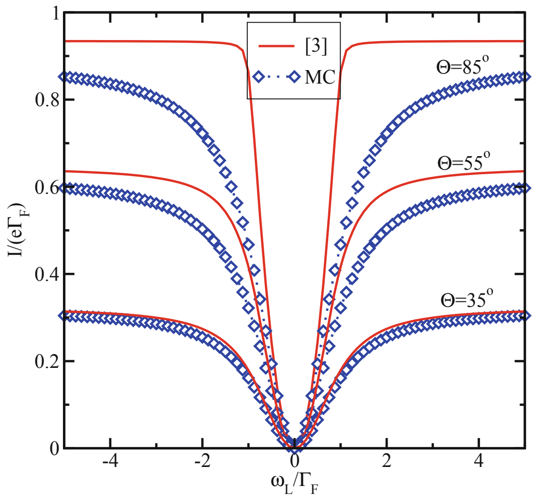

Fig. 4. The current I computed with Eq. (8) is compared with the results from [3], for several angles Θ. A large discrepancy is observed if the magnetic field $\mathbf{B}$ is not parallel to $\mathbf{p}$. $p = 1$, $\Gamma_N = 8\Gamma_F$.

escape probability and the escape tunneling time computed with the method from [3] (solid lines) are compared with $n(t)$ evaluated from Eq. (6). Therefore, the assumption that the tunneling rates from the trap are determined by the two Zeeman spin levels adopted in [3] is valid only, if the magnetic field $\mathbf{B}$ is parallel to the ferromagnetic drain polarization $\mathbf{p}$. In a general case of an arbitrary orientation between $\mathbf{B}$ and $\mathbf{p}$ the tunneling rates must be evaluated from the more general expression Eq. (6) which contains a 4×4 relaxation matrix. Shorter tunneling times obtained by considering only two Zeeman levels result in the larger current observed in Fig. 4.

At spin-independent single-electron tunneling the charge is transferred by instantaneous electron hops between the electrodes and the traps separated by long waiting times. The discreteness of the charge transfer is conveniently described by current fluctuations. The low frequency current noise is called the shot noise. To quantitatively characterize the charge transfer discreteness, the ratio of the spectral density of the current fluctuations to the current, or the Fano factor F [5] is introduced. If the transport is due to consecutive single electron hops between the two contacts, the charge transfer resembles shots of single electrons. The charge transfer is due to discrete electrons, and the Fano factor equals to one. If the charge transfer between the electrodes is due to trap-assisted hopping via a single trap, the charge transfer is performed in two steps, the transport is less discrete, and the Fano factor is less than one [5].

The Fano factor for the case of spin-dependent trap-assisted hopping between the normal metal source and the ferromagnetic drain is shown in Fig. 6. The results indicate that, in contrast to the spin-independent hopping, the shot noise

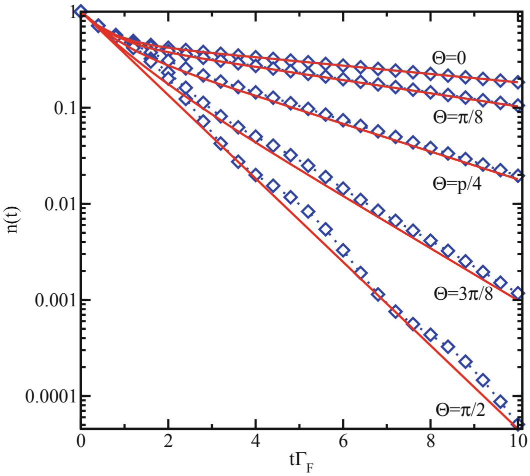

Fig. 5. Time dependence of $n(t)$ evaluated by using the two escape rates from the Zeeman levels to the drain [3] (solid lines) and as a result of numerical solution of Eq. (6) (symbols). $p = 0.9$, $\omega_L = 2\Gamma_F$.

is enhanced above one at small magnetic fields. The maximal value of the Fano factor equals three. It implies that the electrons are transferred in bunches of three electrons in average separated by longer waiting times. A Fano factor larger than one is characteristic for spin-dependent trap-assisted hopping.

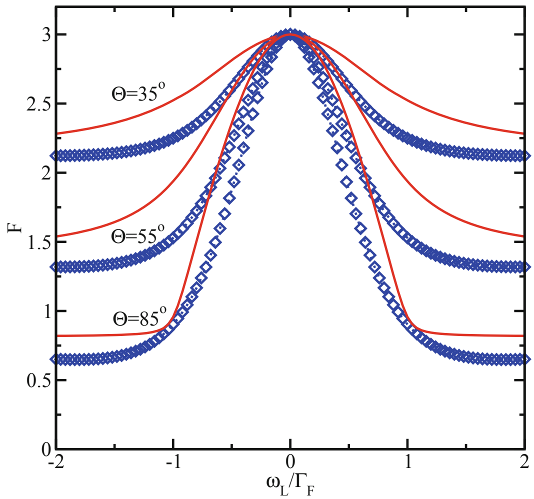

Fig. 6. Fano factor F at spin-dependent trap-assisted tunneling evaluated by using the escape rates from the two Zeeman levels [3] (solid lines) and by the suggested Monte-Carlo method (symbols). $p = 1$, $\Gamma_N = 8\Gamma_F$.

4 Summary and Conclusion

A Monte Carlo method describing spin-dependent trap-assisted hopping is developed. Peculiarities of the current and the shot noise at spin-dependent trap-assisted hopping are investigated. It is shown that the escape probability from a trap to a ferromagnetic electrode is determined by a 4×4 matrix. In contrast to spin-independent hopping, the Fano factor characterizing the charge transfer discreteness can be larger than one. This implies that due to the spin correlations the electrons are transferred in bunches separated by longer waiting times. The results are important for evaluating the role of oxide defects in magnetic tunnel junctions used in modern nonvolatile magnetoresistive random access memory.

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