Interference effects in resonant magneto-transport

D. Mozyrsky¹, L. Fedichkin², S. A. Gurvitz³, G. P. Berman¹

¹T-13 and CNLS, Los Alamos National Laboratory, Los Alamos, NM 87545, USA
²Physics Department, Clarkson University, NY 13699-5820, USA
³Department of Particle Physics, Weizmann Institute of Science, Rehovot 76100, Israel

We study non-equilibrium magneto-transport through a single electron transistor or an impurity. We find that due to spin-flip transitions, generated by the spin-orbit interaction, the spectral density of the tunneling current fluctuations develops a distinct peak at the frequency of Zeeman splitting. This mechanism explains modulation in the tunneling current at the Larmor frequency observed in scanning tunneling microscope (STM) experiments and can be utilized as a detector for single spin measurement.

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Problems involving transport through low dimensional structures have received significant attention in connection with the rapid development of spintronic ¹ and single electron quantum computing designs ². Apart from being likely candidates for becoming components of future electronic integrated circuits, the use of single electron transistors (SET) as charge detectors have been contemplated in several solid state quantum computing designs ³.

In the present work we demonstrate that the spectral density of current fluctuations of a single electron transistor in the external magnetic field develops a peak at the electron Zeeman frequency generated by spin-orbit interactions. We attribute such effect to the interference between the spin up and spin down components of the transmitted current resulting from the spin flips in the tunneling process.

As a model system we consider a heterostructure (for example Si/Ge) schematically shown in Fig. 1. The two regions, to the right and to the left from the dotted line denoting the interface, have different g-factors, ⁹₁ ≈ 2 for the left region and ⁹₂ ≠ 2 for the right region. There are two contacts/Fermi reservoirs in each of the regions. The left region also contains a quantum dot, so that when a potential difference V is applied between the two reservoirs, electrons can tunnel from left to the right reservoirs via the dot. The energy levels of the dot are spin-split by an external magnetic field. In this case the spin-orbit coupling causes the spin-flip transitions resulting in coherent effects in the tunneling current ⁴.

We describe our system by the Hamiltonian:

\[ H = H_L + H_R + H_S + H_C + H_T \]

where the first two terms represent the unperturbed states of two contacts, \( H_L = \sum_{l,s} \epsilon_l a_{ls}^\dagger a_{ls} \) and \( H_R = \sum_{r,s} \epsilon_r a_{rs}^\dagger a_{rs} \), where \( a_{ls}^\dagger \) creates a fermion/electron at the energy level \( \epsilon_l \) and with spin \( s \) in the left (right) reservoir. We assume that there is a single discrete level in the dot due to spatial quantization. The level is spin-split by the magnetic field \( B \), so that the states in the dot are described by \( H_S = \sum_{s} \epsilon_s n_s \), where \( n_s = a_{ls}^\dagger a_{ls} \) and \( a_{ls}^\dagger \) creates an electron in the dot at the level \( \epsilon_s \) with spin \( s \). We denote \( \epsilon_{-1/2} - \epsilon_{1/2} = gB = E \), Fig. 1, where \( g \) is the electronic g-factor in the dot and \( \beta \) is Bohr’s magneton. The term \( H_C = \sum_{s} \frac{U}{2} n_s n_{-s} \) corresponds to the Coulomb charging energy for the electron in the well. In what follows we will assume the case of complete Coulomb blockade, i.e., \( U \rightarrow \infty \), thus allowing for only one electron to occupy the two spin states in the dot.

The tunneling transitions between the left reservoir, the dot and the right reservoir are represented by the Hamiltonian:

\[ H_T = \sum_{l,s} \Omega_l \left( a_{ls}^\dagger a_s + a_s^\dagger a_{ls} \right) + \sum_{r,s,s'} \Omega_{rss'} \left( a_{rs}^\dagger a_{s'} + a_{s'}^\dagger a_{rs} \right). \quad (1) \]

Fig. 1: Quantum dot coupled to two contacts. The right contact has g-factor different from that of the left contact and the dot. Tunneling with spin flip generates effective coupling between the two Zeeman sublevels in the dot.

Here we use gauge in which tunneling amplitudes \( \Omega_l \) and \( \Omega_{rss'} \) are real. As we noted above the key point of our work is that we consider the tunneling transitions accompanied by spin flips. These are generated by the second term in Eq. (1) due to g-factor difference between the dot and the right contact. The mechanism generating such transitions is similar to that of spin scattering by nonmagnetic impurities in semiconductors ⁴. Due to spin-orbit interaction, relatively strong in the right con-
tact in our case, the orbital and spin states of the electron in the right reservoir are mixed, resulting in effective $g$-factors for the electrons there to be different from 2. The eigenstates of $H_R$ are represented by Kramers doublet, \( |\psi_{r,s=1/2}⟩ = u_r \uparrow + v_r \downarrow \) and a Kramers conjugate state \( |\psi_{r,s=-1/2}⟩ \), where $u_r$ and $v_r$ are functions of spatial coordinates only. We have assumed the spin orbit coupling in the left reservoir and the dot is much weaker ($g \approx 2$), so that we can neglect by the spin-orbit mixing effect there.

In order to evaluate the tunneling matrix elements for transitions from the dot to the right reservoir, given by the second term in Eq. (1), one can utilize Bardeen’s formula [3]: \( \Omega_{rss'} = 1/2m \int dS \cdot (\phi^* \nabla \psi_{r,s'} - \psi_{r,s'} \nabla \phi^*) \), where the integral is over any surface lying entirely within the tunneling barrier, separating the dot and the right reservoir, and the wave functions $\phi$, (state with spin $s$ in the dot, \( |\phi⟩ = |s⟩ \)) and $\psi_{r,s'}$ are smoothly continued under the barrier; $m$ is electron’s mass and $h = 1$. It is obvious that the states $\psi_r$ under the barrier are still spin-orbit mixed due to the continuity condition. Therefore the tunneling matrix elements, corresponding to the transitions from the resonant level to the right reservoir without spin flip, are \( \Omega_{rss} = 1/2m \int dS \cdot (\phi^* \nabla u_r - u_r \nabla \phi^*) \), and the matrix elements of transitions accompanied by spin flips are \( \Omega_{rs\bar{s}} = 1/2m \int dS \cdot (\phi^* \nabla v_r - v_r \nabla \phi^*) \); \( \bar{s} \equiv -s \). For relatively small deviations of $g$ factor in the right reservoir from 2, \( |v| \sim O(|\Delta g|) \), \( \Delta g = g - 2 \) [6], and so the two transition amplitudes are related as \( |\Omega_{rss}| \sim O(|\Delta g|) \). For $\Delta g > 1$, the two components $u_r$ and $v_r$ are of the same order of magnitude and so \( \Omega_{rss} \sim \Omega_{rs\bar{s}} \).

In this work we are interested in spectral properties of the tunneling current and calculate its spectral density. Typically calculations of this sort involve evaluation of the two-particle Green’s functions, which is a quite formidable task in non-equilibrium case, beyond the applicability of the linear response theory. Instead, we adopt an alternative approach developed in Refs. [7,8], that allows one to evaluate the transport rate equations from the microscopic Hamiltonian. In this letter we show that one can obtain the spectral density of fluctuations from these equations as well (see below). In the following we outline our calculation of current spectral density and analyze the obtained results.

We construct the time dependent wave function of the system as

\[
|\Psi(t)⟩ = \left\{ b_0(t) + \sum_{l,s} [b_{ls}(t)a_{ls}^†a_{ls} + b_{ls}(t)a_{ls}^†a_{ls}] + \sum_{l,s} [b_{lrs}(t)a_{lrs}^†a_{lrs} + b_{lrs}(t)a_{lrs}^†a_{lrs}] + \ldots \right\} |0⟩ , \tag{2}
\]

where the “ground” state $|0⟩$ corresponds to the situation when all states below Fermi energy in the left contact are filled, while all states above Fermi energy in the right contact are empty. The above wave function is a superposition of all possible particle-hole combinations that can be generated by the Hamiltonian $H$; note that $H$ conserves the total number of particles in the system. Thus the first term in $\Psi$ is the amplitude of the unperturbed state, i.e., when no excitations in the system is present, the second term describes a state in which a hole is created in the left reservoir and a particle with the same spin occupies the resonant level, etc. The above wave function satisfies the Schrodinger equation $i|\dot{\Psi}⟩ = H|\Psi⟩$.

In order to describe transport in our model we introduce probabilities for the dot to be empty or occupied, provided that a certain number of electrons have passed through the junction. The level can be either empty, with probability $\sigma_{aa}^0$, where the subscript $aa$ indicates that there is no electrons in the dot and the superscript $n$ describes that $n$ electrons have arrived in the right reservoir/collector, or the level can be filled with probabilities $\sigma_{bb}^n$ and $\sigma_{cc}^n$, where $bb$ indicates that the lower Zeeman sublevel $s = 1/2$ is filled, while $cc$ stands for the upper Zeeman sublevel $s = -1/2$ being filled. Occupation of both Zeeman levels in the dot by two electrons is prohibited in our model by the infinite charging energy $U$; see Refs. [7,8] for detailed discussion. We also introduce the off-diagonal elements $\sigma_{bc}^n$, describing coherent superpositions of states on the upper and lower Zeeman levels of the electron in the dot. $\sigma_{ij}^n$’s are related to the wave function $|\Psi⟩$ as $\sigma_{aa}^0 = |b_0|^2$, $\sigma_{bb}^0 = \sum_{l,s=1/2} |b_{ls}|^2 + \sum_{l,s=−1/2} |b_{ls}|^2$, $\sigma_{aa}^1 = \sum_{l,s} |b_{ls}|^2 + |b_{lrs}|^2$, etc.

Following steps of Refs. [7,8] one derives the rate equations for the density matrix $\sigma$ from the Schrodinger equation for the wave function $|\Psi⟩$. These rate equations for a general case are presented in [8]. One finds for our case:

\[
\dot{\sigma}_{aa}^n = -2\Gamma_L \sigma_{aa}^n + \Gamma_R (\sigma_{aa}^{n-1} + \sigma_{aa}^{n+1}) + \Delta \Gamma_R (\sigma_{bc}^{n−1} + \sigma_{cb}^{n−1}) , \tag{3a}
\]

\[
\dot{\sigma}_{bb}^n = -\Gamma_R \sigma_{bb}^n + \Gamma_L \sigma_{aa}^n - \frac{\Delta \Gamma_R}{2} (\sigma_{bc}^n + \sigma_{cb}^n) , \tag{3b}
\]

\[
\dot{\sigma}_{cc}^n = -\Gamma_R \sigma_{cc}^n + \Gamma_L \sigma_{aa}^n - \frac{\Delta \Gamma_R}{2} (\sigma_{bc}^n + \sigma_{cb}^n) , \tag{3c}
\]

\[
\dot{\sigma}_{bc}^n = iE\sigma_{bc}^n - \Gamma_R \sigma_{bc}^n - \frac{\Delta \Gamma_R}{2} (\sigma_{bb}^n + \sigma_{cc}^n) . \tag{3d}
\]

Here $\Gamma_{L,R}, \Delta \Gamma_R = 2\pi\Omega_{L,R}^2 (\epsilon) \rho_{L,R}(\epsilon)$ and $\Delta \Gamma_R = 2\pi\Omega_{L,R}^2 (\epsilon) \rho_{L,R}(\epsilon)$, where we denote $\sigma_{rss} \equiv \sigma_{rr}, \Omega_{rss} \equiv \Omega$. In derivation of Eqs. (3) we assumed that the coupling constants $\Omega$’s and the densities of states $\rho$’s are weakly dependent on energy, and so $\rho_{L,R}(\epsilon) = \rho_{L,R}(\epsilon)\rho_{L,R}(\epsilon)$, $\Omega_{L,R}(\epsilon) = \Omega_{L,R}(\epsilon)$ and thus rates $\Gamma_{L,R}$ for the electrons tunneling into and out of the dot are independent of energy. We also assumed that $\Gamma_L, \Gamma_R \geq \Delta \Gamma_R$ and the bias voltage condition, $V \gg \Gamma_{L,R}$, which is essential for derivation of Eqs. (3). We point out that Eqs. (3) are derived in the limit of small $\delta \Omega_R$, therefore terms of order $\delta \Omega_R^2$ and higher are neglected in (3). One sees from
Eqs. (3) that similar to Bloch equations the two Zeeman levels in the dot are coupled with each other by the off-diagonal terms (“coherences”) due to spin-flip transitions through continuum with the rate $\Delta \Gamma_R$.

By summing Eqs. (3) over the number of electrons in the right reservoir one obtains the “standard” Bloch-type equations for the reduced density matrix $\sigma_{ij} = \sum_n \sigma_{ij}^n$ with $i,j = a,b,c$. These equations, which look essentially identical to Eqs. (3), describe the state of the resonant level independently of the states of the reservoirs.

From Eqs. (3) one can derive the dynamics for the expectation value of the tunneling current in the right (left) reservoir, $\langle I_{R,L}(t) \rangle = i\epsilon(\Psi(t)|[H, \hat{N}_{R,L}]|\Psi(t))$, where $H$ is the total Hamiltonian and $\hat{N}_{R,L}$ are the operator of the electron (hole) numbers is the right (left) reservoirs. For instance, by using $\hat{N}_R = \sum_{n,r} a^\dagger_r a_r$ and one easily finds from Eq. (3) that the average current in the right reservoir can be written as $\langle I_R(t) \rangle = \epsilon(\langle \hat{N}_R(t) \rangle)$, where $\langle \hat{N}_{R} \rangle = \sum_n n(\sigma_{aa}^n + \sigma_{bb}^n + \sigma_{cc}^n)$. Using Eqs. (3) for $\sigma^n$, one can sum over $n$ thus obtaining

$$\langle I_R(t) \rangle = \epsilon \Gamma_R [\sigma_{bb}(t) + \sigma_{cc}(t)] + \epsilon \Delta \Gamma_R [\sigma_{bc}(t) + \sigma_{cb}(t)].$$

It is easy to check that the transient behavior of the average current is an oscillatory one (due to coherence terms $\sim \sigma_{bc}$) with frequency equal to $E$ and approaching stationary value

$$\langle I(\infty) \rangle = \frac{2\epsilon \Gamma_L \Gamma_R \left( E^2 + \Gamma^2_R - \Delta \Gamma^2_R \right)}{(2\Gamma_L + \Gamma_R)(2E^2 + \Gamma_R^2) - 2\Gamma_R \Delta \Gamma^2_R}. \quad (4)$$

Actually one measures a circuit current, given by $\langle I(t) \rangle = \alpha \langle I_R(t) \rangle + \beta \langle I_L(t) \rangle$ where the coefficients $0 \leq \alpha, \beta \leq 1$ and $\alpha + \beta = 1$ are depending on a circuit geometry (3). Obviously, the stationary current, $\langle I(\infty) \rangle$ is independent of $\alpha$ and $\beta$, Eq. (4). Yet, the transient current, $\langle I(t) \rangle$ and so the current spectral density are depending on a circuit geometry. For simplicity we consider such a case where only the collector current is measured ($\alpha = 1, \beta = 0$).

In order to evaluate current spectral density, $S_I(\omega) = \int_0^\infty d\tau \cos(\omega \tau) \langle I(t) I(t + \tau) \rangle$, from rate equations (3), we utilize MacDonald’s formula, that relates $S_I$ to the dispersion of charge accumulated on the collector (right reservoir) (4):

$$S_I(\omega) = \frac{\epsilon^2 \omega / \pi}{\int_0^\infty dt \sin(\omega t) \langle \dot{\hat{N}}^2_R(t) \rangle}. \quad (5)$$

The dispersion for the number of electrons in the right reservoir can be found from Eqs. (3) as $\langle \hat{N}^2_R \rangle = \sum_n n^2(\sigma_{aa}^n + \sigma_{bb}^n + \sigma_{cc}^n)$. The latter must be averaged with respect to the stationary state distribution in the dot. Evaluation of the above sum is tedious but can be performed exactly from Eqs. (3). Here we quote the final expression for spectral density $S_I(\omega)$. The general result is rather cumbersome. In the region of interest, $E \geq \Gamma_L, \Gamma_R \geq \Delta \Gamma_R$, expanding $S_I$ in powers of $\Delta \Gamma_R$ up to $O(\Delta \Gamma^2_R)$, we obtain:

$$S_I(\omega) = \frac{\epsilon^2}{\pi} \frac{2\Gamma_L \Gamma_R}{2\Gamma_L + \Gamma_R} \frac{4\Gamma^2_R + \omega^2}{(2\Gamma_L + \Gamma_R)^2 + \omega^2} + \frac{8e^2 \Gamma^3 R \Delta \Gamma_R}{\pi E^2 (2\Gamma_L + \Gamma_R)^2 \Gamma_R^2 + (\omega - E)^2}. \quad (6)$$

The spectrum (6) is shown in Fig. 2. The first term in (6) is the shot noise approaching the “Schottky” limit $S_I = \epsilon \langle I \rangle / \pi \omega$ for $\omega \gg \Gamma_L, \Gamma_R$. For frequencies $\omega \leq \Gamma_L, \Gamma_R$ there is a dip in the spectrum - the result merely consistent with Refs. (10). The second term, representing a distinct peak, arises due to spin-flip transitions between the Zeeman-split sublevels in the dot. It is roughly of Lorentzian shape centered approximately at $\omega = \Gamma_R$ and having width $\Gamma_R$. Importantly, the width of the peak is governed by $\Gamma_R$, while the width of the dip is controlled by $\Gamma_L$ for $\Gamma_L \gg \Gamma_R$. Such condition guarantees that the peak is sufficiently distinct and thus can be resolved. A similar situation takes place in case of a current tunneling through a double well structure (12), where a peak in the fluctuation spectrum appears to be located at the tunneling frequency for the double well structure.

The ratio of the peak’s height to the noise pedestal (the signal to noise ratio) given by Eq. (6) is $S/N = 4\Gamma^2_R \Delta \Gamma^2_R / E^2 \Gamma_R (2\Gamma_L + \Gamma_R)$. The $S$ to $N$ ratio can be significantly increased in heterostructures with greater $g_1 - g_2$ difference, and thus greater spin transition rate $\Delta \Gamma_R$, or in asymmetric SETs with $\Gamma_L \gg \Gamma_R$.

The above described spin-coherence mechanism can be used for single spin detection. Suppose that nuclear spins in the dot are polarized. From Eqs. (3), (6) one can evaluate the orders of magnitude for parameters needed for observation of the distinct peak in the fluctuations spectrum in magnetic field generated by a few nuclear spins. The width of the peak in (6) is defined by the value of current through the structure, $\Gamma_R \simeq \langle I \rangle / \epsilon$ for $\Gamma_L > \Gamma_R$.  

**Fig. 2:** Power spectrum of tunneling current fluctuations; Eq. (6). Here $E = 50\Gamma_R$, $\Delta \Gamma_R = 0.4 \Gamma_R$, $\Gamma_L = 20 \Gamma_R$. 

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Therefore in order to resolve a peak due to spin flip transitions one needs to satisfy condition $E > \Gamma_R$, though $E$ should not be too great as signal to noise ratio decreases with growth of $E$. Assuming that the Zeeman splitting $E$ is solely due to hyperfine coupling, which is typically of order $10^2$ MHz per single nuclear spin, the measurable tunneling current through the structure would be of order $10^3$ pA. This number is well within the capabilities of today’s single-electronics. We thus conclude that the interference effect in resonant magneto-transport can naturally be explained by the tunneling current, which have been observed in a set of scanning tunneling microscope (STM) experiments [15]. Impurities at semiconductor surfaces are known to form resonant levels that can influence the STM tunnel current [16]. In contrast to previous attempts to explain experiments [15], the tunnel current flows through a cluster of impurities having a number of resonant levels.

As a result the current through a single resonant level rather than by the principal conclusions of this work.

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