Current and Noise in a FM/quantum dot/FM System

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(Dated: March 22, 2022)

Using the Keldysh nonequilibrium technique we calculate current, noise and Fano factor in a ferromagnetic(FM)-quantum dot-ferromagnetic(FM) system with Coulomb interaction and spin-flip scattering in the dot. The lead polarizations are considered in both parallel P and antiparallel AP alignments. We show that spin-flip can increase both AP-current and AP-noise, while the P-current and P-noise are almost insensible to it. This fact leads to a suppression of the tunnelling magnetoresistance with increasing spin-flip rate.

I. INTRODUCTION

The emerging field of spintronics [1]-[3], where the electron spin and charge are used to design new devices, has led to fascinating and novel ideas such as spin filters [4]-[6], spin field effect transistors [7], and has offered many proposals for solid state quantum computing [8]. For example, quantum dot systems are useful in the control of the electron spin and are suitable to create quantum bits relevant for quantum gate operations [9].

The study of nonequilibrium transport properties of spintronic devices is of great importance to understand basic physical phenomena and to predict new functionalities. Calculation of the current, for example, can give the conductance/resistance of a state quantum computing [10]. The phenomena and to predict new functionalities. Calculation of the current, for example, can give the conductance/resistance of a quantum bit. This fact leads to a suppression of the tunnelling magnetoresistance with increasing spin-flip rate.

Here we apply the Keldysh nonequilibrium technique [12] to calculate current and its fluctuations (noise) in a quantum dot coupled to two ferromagnetic leads as a function of the applied voltage for parallel and antiparallel lead-polarization alignments. We include Coulomb interaction in the Hartree-Fock approximation as well as spin-flip in the dot. We show that spin-flip makes the alignment of the lead polarizations less important; both P and AP results coincide for large enough spin-flip rates. This fact is due to the granularity of the charge (shot noise [10]), are also relevant because their measurements can provide additional information not contained in the average current [11].

Our paper is organized as follows. In Sec. 2 we describe the system and present its Hamiltonian. In Sec. 3 we apply the Keldysh nonequilibrium technique to determine current and noise in our system. In Sec. 4 we discuss our results for current and noise and Sec. 5 gives our conclusions.

II. SYSTEM

Our system is composed of two ferromagnetic leads coupled to a quantum dot via tunnelling barriers (Fig.1). While the left lead has a fixed polarization (hard lead), the right one can have its polarization switched from parallel P to antiparallel AP.

The Hamiltonian of the dot is

\[ H_D = \sum_\sigma \epsilon_0 d^\dagger_\sigma d_\sigma + U n_\uparrow n_\downarrow + R (d^\dagger_\uparrow d_\uparrow + d^\dagger_\downarrow d_\downarrow), \]

where \( d^\dagger_\sigma \) (\( d_\sigma \)) destroys (creates) an electron in the dot with spin \( \sigma \) and the energy \( \epsilon_0 \) is spin independent [14], [15]. In addition, we assume we have a small enough dot in order to have only one active level \( \epsilon_0 \). In the presence of a voltage the level shifts by \( \epsilon_0 = \epsilon_d - eV \), where \( \epsilon_d \) is the dot level for zero bias (for numerical convenience we use \( \epsilon_d = \frac{eV}{2} \)). This assumption does...
which includes charging effects in a self-consistent way, will be discussed elsewhere [16]. In Eq.(2) the Coulomb interaction is taken into account via the Hubbard term with a correlation parameter. Not taking into account charge accumulation in the dot, which tends to wash out this linear drop. A more sophisticated approach, the system, which is reflected in both current and noise.

FIG. 1: Schematic of the system. It is composed of two ferromagnetic leads and a quantum dot as a spacer. The electrons are allowed to tunnel through the left and right barriers (with tunnelling rate $G_L$ and $G_R$, respectively) in order to generate a tunnelling current when a voltage $V$ is applied. The left lead has a fixed polarization (hard side) while the right lead switches its polarization from parallel (up arrow) to antiparallel (down arrow) alignment. This polarization rotation changes the majority/minority spin population, leading to a variation in the resistance of the system, which is reflected in both current and noise.

not take into account charge accumulation in the dot, which tends to wash out this linear drop. A more sophisticated approach, which includes charging effects in a self-consistent way, will be discussed elsewhere [16]. In Eq.(2) the Coulomb interaction is taken into account via the Hubbard term with a correlation parameter $U > 0$ and spin-flip scattering is described by the last term, where $R$ is the spin-flip scattering amplitude.

The tunnelling Hamiltonian is

$$H_T = \sum_{k\nu\sigma} (t_{k\nu\sigma} c_{k\nu\sigma}^\dagger d_{\nu\sigma} + t_{k\nu\sigma} c_{k\nu\sigma} d_{\nu\sigma}),$$

where $t_{k\nu\sigma}$ couples an electronic state in lead $\eta$ to one in the dot. We consider a spin conserving tunnelling; the spin-flip process is assumed to be confined in the dot. In the nonequilibrium Green function technique $H_T$ is the nonequilibrium part of the Hamiltonian because it couples contacts with different chemical potential (if $eV \neq 0$), thus allowing for charge flow. Next we apply the Keldysh technique [17] to determine the average current and the noise.

III. CURRENT AND NOISE

Current. The average current from the left contact into the dot is defined as $I_L = -e \langle \dot{N}_L \rangle$, where $N_L = \sum_{k\sigma} c_{kL\sigma}^\dagger c_{kL\sigma}$ is the number operator for lead $L$. To find the time evolution of the occupation-number operator, we use the Heisenberg equation $\dot{N}_L = i[H, N_L]$. The only term of the Hamiltonian which does not commute with $N_L$ is $H_T$. Using Eq.(3) we obtain

$$I_L = \frac{2e}{\hbar} \text{Re} \sum_{k\sigma} t_{kL\sigma} i\langle c_{kL\sigma}^\dagger(t)d_{\sigma}(t) \rangle. \quad (4)$$

To avoid further complications in the analysis due to the spin-flip term, we perform a canonical transformation [15],

$$\left(\begin{array}{c} d_1^\dagger \\ d_2^\dagger \end{array}\right) = \frac{1}{\sqrt{2}} \left(\begin{array}{cc} 1 & 1 \\ -1 & 1 \end{array}\right) \left(\begin{array}{c} d_\uparrow \\ d_\downarrow \end{array}\right), \quad (5)$$

in terms of which Eq.(4) becomes

$$I_L = \frac{2e}{\hbar} \frac{1}{\sqrt{2}} \text{Re} \sum_k \text{Tr}\{c^\dagger_{kL\uparrow} c_{kL\downarrow} \left(\begin{array}{cc} t_{kL\uparrow} & t_{kL\downarrow} \\ -t_{kL\downarrow} & t_{kL\uparrow} \end{array}\right) \left(\begin{array}{cc} G_{1,kL\uparrow}^c & G_{1,kL\downarrow}^c \\ G_{2,kL\downarrow}^c & G_{2,kL\uparrow}^c \end{array}\right)\}, \quad (6)$$

where $G^c_{i,k\nu\sigma}(t,t) = i\langle c_{i,k\nu\sigma}(t)d_{i}(t) \rangle$. Applying the Keldysh technique as described in [17] we find

$$I_\eta = \frac{2e}{\hbar} \text{Re} \int dt_2 \text{Tr}\{G^r(t,t_2)\Sigma^{\eta<}(t_2,t) + G^<(t,t_2)\Sigma^{\eta>}(t_2,t)\}, \quad (7)$$

where $G^r$ and $G^<$ are the nonequilibrium dot Green functions, with elements $G^c_{ij}(t,t_2) = i\langle d_i(t_2)d_j(t) \rangle$ and $G^r_{ij}(t,t_2) = -i\theta(t-t_2)\langle d_i(t_2)d_j(t_2) \rangle$. Here the averages are taken over the initial ($t = -\infty$) equilibrium density matrix [18]. The lesser
(retarded, advanced) self-energy is given by

$$\Sigma^{L<} (t_2, t) = \frac{1}{2} \sum_k |t_{kL}^2| \left( \begin{array}{cc}
g^{<}(c\sigma)(t_2, t) + g^{<}(c\sigma)(t_2, t) & g^{<}(c\sigma)(t_2, t) - g^{<}(c\sigma)(t_2, t) \\
g^{<}(kL\sigma)(t_2, t) - g^{<}(kL\sigma)(t_2, t) & g^{<}(kL\sigma)(t_2, t) + g^{<}(kL\sigma)(t_2, t) \end{array} \right), \tag{8}$$

where $g^{<}(c\sigma)$ is the lesser (retarded, advanced) uncoupled Green function for lead $L$. These are defined as $g^{<}_{kL\sigma}(t_2, t) = i(\bar{c}_{kL\sigma}(t)\bar{c}_{kL\sigma}(t_2))$, $g^{<}_{kL\sigma}(t_2, t) = -i\theta(t_2 - t)\{\bar{c}_{kL\sigma}(t_2), \bar{c}_{kL\sigma}(t)\}$ and $g^{<}_{kL\sigma}(t_2, t) = i\theta(t - t_2)\{\bar{c}_{kL\sigma}(t_2), \bar{c}_{kL\sigma}(t)\}$, where the tilde denotes that the operator is in the interaction picture; its time evolution is governed entirely by Eq. (1). In Eq. (8) we assume a spin-independent amplitude $t_{kL}$ for simplicity.

For a time-independent Hamiltonian the Fourier transform of Eq. (7) yields

$$I_L = \frac{e}{\hbar} \int \frac{d\omega}{2\pi} \text{Tr}\{\Sigma^{L<}(\omega)[G^\sigma(\omega) - G^\alpha(\omega)] - G^<(\omega)[\Sigma^{L<}(\omega) - \Sigma^{La}(\omega)]\}, \tag{9}$$

where $\Sigma^{\gamma<}(\omega)$ and the difference $\Sigma^{\gamma<}(\omega) - \Sigma^{\gamma<}(\omega)$ are calculated using the expressions $g^{<}_{k\gamma\sigma}(\omega) = \frac{1}{\omega - \epsilon_{k\gamma\sigma} + i\eta}$ and $g^{<}_{k\gamma\sigma}(\omega) = 2\pi i n_\eta(\omega)\delta(\omega - \epsilon_{k\gamma\sigma})$, $n_\eta(\omega)$ is the Fermi distribution function of the lead $\eta$. We find $\Sigma^{\gamma<} = i\eta \Gamma^\gamma$ and $\Sigma^{\gamma<} - \Sigma^{\gamma<} = -i\Gamma^\gamma$, with

$$\Gamma^\gamma = \frac{1}{2} \left( \Gamma^\gamma + \Gamma^\gamma - \Gamma^\gamma + \Gamma^\gamma \right). \tag{10}$$

where $\Gamma^{\gamma'} = 2\pi \sum_k \{t_{kL}\}^2 \delta(\omega - \epsilon_{k\gamma\sigma})$.

Accounting for Coulomb interaction in the Hartree-Fock approximation, we can write down a matrix Dyson equation for the retarded Green function, $G^r = G^{0r} + G^{0r}\Sigma^r G^r$, and a Keldysh equation for the lesser Green function $G^< = G^r\Sigma^< G^r$, where $G^{0r}$ is the uncoupled dot Green function. In these equations the self energies are the sum of the left and right self energies, i.e., $\Sigma^{(r,<)} = \Sigma^{L(r,<)} + \Sigma^{R(r,<)}$. A self consistent calculation is required to calculate $\langle n_\eta \rangle$ and $\langle \delta n_\eta \rangle$, which are given by the lesser Green function, $\langle d_i^\dagger d_i \rangle = \int \frac{d\omega}{2\pi} \text{Im} G_{ij}^<(\omega)$.

Noise. The current operator can be written as its average value plus some fluctuation, i.e., $\bar{I}_\eta = I_\eta + \delta \bar{I}_\eta$. In our system there are two sources of noise, namely, thermal noise and shot noise. The first one is due to thermal fluctuations in the occupations of the leads. It vanishes for zero temperature and $eV \neq 0$, but can be finite for $T \neq 0$ and $eV = 0$. On the other hand, shot noise is due to the granularity of the electron charge and is a nonequilibrium property of the system in the sense that it is nonzero only when there is a finite current ($eV \neq 0$). To calculate the noise (thermal+shot noise) we use the standard definition $S_{\eta\eta'}(t - t') = \langle \delta \bar{I}_\eta(t), \delta \bar{I}_{\eta'}(t') \rangle$, which can also be written as $S_{\eta\eta'}(t - t') = \langle \bar{I}_\eta(t), \bar{I}_{\eta'}(t') \rangle - 2T \delta(t - t')$. After a straightforward calculation, which will be presented elsewhere [13], we find for the noise power spectrum (dc limit) [12],

$$S_{\eta\eta'}(0) = \frac{e^2}{\hbar} \int \frac{d\omega}{2\pi} \text{Tr}\{\delta n_\eta \Gamma^\eta G^r - \delta n'_\eta i(1 - n_\eta)\Gamma^\eta G^< + G^< \Gamma^\eta G^r \Gamma^\eta' - n_\eta(1 - n_\eta)G^< \Gamma^\eta G^r \Gamma^\eta' \}
- n_\eta(1 - n_\eta)G^< \Gamma^\eta G^r \Gamma^\eta' - n_\eta(1 - n_\eta)G^< \Gamma^\eta G^r \Gamma^\eta' \}
- n_\eta(1 - n_\eta)G^< \Gamma^\eta G^r \Gamma^\eta' - (1 - n_\eta)G^< \Gamma^\eta G^r \Gamma^\eta' + (1 - n_\eta)G^< \Gamma^\eta G^r \Gamma^\eta' \}. \tag{11}$$

The dc noise (zero frequency) is position independent, and it is possible to show that $S_{LL}(0) = S_{RR}(0) = -S_{LR}(0) = -S_{RL}(0)$ [14]. In the next section we use the component $S_{LL}$.

IV. RESULTS.

Using Eqs. (3) and (11) we calculate current and noise for the system in Fig.1. We assume $\Gamma^\eta$ to be independent of energy, but polarization dependent with values $\Gamma^\uparrow_\downarrow = \Gamma^\uparrow_0[1 + (-1)^{\sigma}p]$, $\Gamma^\uparrow_\uparrow = \Gamma^\downarrow_\downarrow$ and $\Gamma^\uparrow_\downarrow = \Gamma^\downarrow_\uparrow$ if the leads have parallel alignment or $\Gamma^\uparrow_\uparrow = \Gamma^\uparrow_\uparrow$ and $\Gamma^\downarrow_\downarrow = \Gamma^\downarrow_\downarrow$ if they are antiparallel aligned. The parameter $p$ gives the spin-splitting of the ferromagnetic band. For example, for $p = 0$ the system is unpolarized while for $p = 1$ the system is fully polarized. The parameter $\Gamma_0$ fixes the coupling strength between leads and dot. The sign +/- in $\Gamma^\uparrow_\uparrow$ corresponds to majority/minority spins, respectively. Here we take $\sigma = \uparrow$ ($\sigma = \downarrow$) as majority (minority) spins in the lead $L$ and assume $\Gamma_0 = 0.01U$ and $p = 0.5$ as in Ref. [14]. The majority/minority spin population in the right lead switches from one to the other according to the lead polarization, which can be controlled via an external magnetic field. This simple form for $\Gamma^\eta_\uparrow$ is reasonable when the band is wide compared to others energies of the system.

The temperature is assumed to be $k_B T = \Gamma_0(1 + p)$. Our approximation (Hartree-Fock) does not include correlations of the Kondo type, however we do not expect these to change our results in the present range of parameters.

A relevant quantity in transport is the spectral function, for the present spin-dependent case defined as $A(\omega) = i\text{Tr}[G^r(\omega) - G^<(\omega)]$, whose poles give the resonant levels which work as conduction channels. Figure 2 shows $A(\omega)$ for different applied voltages and for $R = 0$ (upper panel) or $R = 0.1$ (lower panel). For $R = 0$ we have only one peak when $eV = 0$ (labelled 1).
and two peaks when $eV = 1.5U$ or $eV = 3U$ (labelled 2,2' or 3,3', respectively). When $eV = 0$ the dot is empty because the level $\epsilon_0 = \epsilon_d = 0.5U$ is above the Fermi energies $\mu_L$ and $\mu_R$ (set equal to zero), so Coulomb interaction plays no role. When $eV = 1.5U$ or $3U$, $\epsilon_0$ is below the Fermi energy of the left lead (peaks 2 or 3), consequently the electrons could go inside the dot, creating the high energy peak at $\epsilon_0 + U$ (peaks 2' or 3'), due to Coulomb interaction. The levels in the dot shift linearly with the bias, following the assumption $\epsilon_0 = \epsilon_d - eV/2$. As mentioned above, this linear drop does not account for charging effects. However, it gives reasonable qualitative results here. For $R = 0.1U$ we have similar behaviors but each peak in the $R = 0$ case is now split due to spin-flip. The peaks are located at $\epsilon_1$, $\epsilon_2$, $\epsilon_1 + U$ and $\epsilon_2 + U$ [Fig.2(b)].

![Figure 2: Spectral function $A(\omega)$ against energy $\omega$ for $R = 0$ and $R = 0.1U$. The peaks correspond to the dot levels. For $R = 0$ there is one peak for $eV = 0$ (peak 1) and two peaks for $eV = 1.5U$ and $eV = 3U$ (peaks 2,2' and 3,3'). The extra peak (2' or 3') is due to Coulomb interaction, since the lowest level (2 or 3) is already below the Fermi energy (here at zero), thus allowing electrons to go into the dot. For $R = 0.1U$ the peaks are split and given by $\epsilon_0 \pm R$ and $\epsilon_0 \pm R + U$. The insets show the integral $I(\omega)$ of the spectral function. Each step gives the area under a peak. Since the total area is normalized the last step is at one.]

The inset in Fig.2(a) shows the integrals of the spectral function, namely $I(\omega) = \frac{1}{4\pi} \int_{-\infty}^{\infty} A(\omega')d\omega'$ for the three voltages used. Observe that $I(\omega) \rightarrow 1$ as $\omega$ increases. This is due to the normalization of the spectral function. For $eV = 0$ the whole area is essentially under the peak at 0.5U (peak 1), which explains the single step in $I(\omega)$. For $eV = 1.5U$ and $eV = 3U$ the total normalized area should be distributed under the two peaks (2 and 2' or 3 and 3'), in order to keep the normalization of $A(\omega)$. It leads to a reduction of the area of the lowest peak (2 or 3) in comparison to its $eV = 0$ value. This area is given by the first step in $I(\omega)$.

Figure 3 shows current (a) and noise (b) as a function of the bias with $R = 0$ (solid line) and $R = 0.1U$ (dotted line) for both P and AP configurations. Because P and AP curves for $R = 0.1U$ coincide, we plotted only the AP case. The first enhancement of the current and noise at $eV = U$ happens when $\epsilon_0$ crosses the left chemical potential, allowing electrons to tunnel from the emitter (left lead) to the dot and then to the collector (right lead). The current and noise remain constant until the second level $\epsilon_0 + U$ reaches $\mu_L$ at $eV = 3U$, when another enhancement is observed. In terms of differential conductance ($\sigma_{\text{diff}}$) each enhancement corresponds to a peak in $\sigma_{\text{diff}}$. These peaks reflect the spectral function plotted in Fig.2.
When the system changes from parallel (P) to antiparallel (AP) configurations the current is reduced. This is a typical behavior of tunnelling magnetoresistance (TMR): the resistance increases when the system switches from P to AP configuration. The noise is also affected by this resistance variation, showing a similar reduction. Contrasting behaviors between current and noise will be explored elsewhere [16] for another set of parameters.

Looking at the effects of spin-flip on current and noise we see that the AP curves with $R = 0.1U$ (dotted lines) tend to be on the P curves with $R = 0$, thus showing that lead alignments are less important when spin-flip plays a part. This AP current enhancement due to spin-flip gives rise to a reduction of the TMR: since $TMR = (I_P - I_{AP})/I_{AP}$, when $I_{AP} \to I_P$ we have $TMR \to 0$. W. Rudziński et al. [14] found a similar behavior for TMR.

In the inset of Fig.3 we plot the Fano factor $S_{LL}/2eI_L$. For the parallel case the Fano factor remains around 0.5 for voltages between $U$ and $5U$, except at $eV = 3U$ where it has a small peak. This average value around 0.5 is a consequence of the symmetry of the double-barrier structure in the P case. A similar behavior is observed for the AP case with its average value above the P case. When spin-flip is included ($R = 0.1U$) the AP Fano factor is shifted down, becoming close to the P result for $R = 0$, with the addition of a peak close to $eV = U$ and a double peak around $eV = 3U$. This peculiar double structure is a consequence of the splitting of the dot levels when $R \neq 0$ as observed in the spectral function.
FIG. 3: Current and noise as a function of the bias for parallel (P) and antiparallel (AP) alignments and with $R = 0$ and $0.1U$. The curves for $R = 0.1U$ are only for the AP alignment; observe that these are almost on top of the P curves, except within the sloping region around $U$ and $3U$. Both current and noise are reduced when the right lead changes its polarization from P to AP, following the typical behavior of TMR. The inset shows a suppression of the AP-Fano factor due to spin-flip.

V. CONCLUSION

Using the Keldysh nonequilibrium technique we calculated current and noise in a ferromagnetic-quantum dot-ferromagnetic system with Coulomb interaction and spin-flip relaxation. We have shown that the lead alignments affect both current and noise. These are reduced when the leads rotate from the P to the AP configuration, following the typical magnetoresistance behavior. The spin-flip relaxation is crucial to drive the current and noise in the AP case close to their values in the P case. In a way, we can say that spin-flip makes the P and the AP configurations “degenerate” thus reducing the effect of the lead-polarization alignment on transport. We also showed that TMR is reduced due to spin-flip, corroborating previous results in the literature.

FMS acknowledges support from the funding agencies CAPES and FAPESP (Brazil). JCE acknowledges financial support from the Swiss NSF, DARPA and ARO.
References

[1] D. D. Awschalon, M. E. Flatté and N. Samarth, Sci. Am. 286(6), 66 (2002).
[2] S. A. Wolf, D. D. Awschalom, R. A. Buhrman, J. M. Daughton, S. von Molnár, M. L. Roukes, A. Y. Chchelkanova and D. M. Treger, Science 294, 1488 (2001).
[3] G. A. Prinz, Science 282, 1660 (1998).
[4] R. Fiederling, M. Keim, G. Reuscher, W. Ossau, G. Schmidt, A. Waag and L. W. Molenkamp, Nature 402, 787 (1999).
[5] J. C. Egues, Phys. Rev. Lett. 80, 4578 (1998).
[6] T. Koga, J. Nitta, H. Takayanagi and S. Datta, Phys. Rev. Lett. 88, 126601 (2002).
[7] S. Datta and B. Das, Appl. Phys. Lett. 56, 665 (1990).
[8] D. P. DiVincenzo, Science 270, 255 (1995).
[9] H. A. Engel, P. Recher and D. Loss, Solid State Commun. 119, 229 (2001).
[10] For a review on shot noise see Ya. M. Blanter and M. Büttiker, Phys. Rep. 336, 2 (2000).
[11] For an example in the context of fractional charge, see C. L. Kane and M. P. A. Fisher, Nature 389, 119 (1997).
[12] L. V. Keldysh, Soviet. Physics JETP 20, 1018 (1965).
[13] For an illustrated explanation of this kind of effect and many potential applications see [3].
[14] W. Rudziński and J. Barnaś, Phys. Rev. B 64, 085318 (2001).
[15] F. Zhang, Q. K. Xue and X. C. Xie, cond-mat/0201465 (2002).
[16] F. M. Souza, J. C. Egues and A. P. Jauho, in preparation.
[17] For a text-book treatment, see, e.g., H. Haug and A. P. Jauho, Quantum Kinetics in Transport and Optics of Semiconductors, Springer Solid-State Sciences 123 (1996).
[18] The density matrix is defined as \( \rho = \frac{e^{-\beta h}}{Tr(e^{-\beta h})} \), where \( h = H_L + H_R + H_D \). The coupling Hamiltonian is not included in this definition because it is considered the nonequilibrium part of the Hamiltonian which is turned on at \( t = -\infty \). For further discussion about this definition and its implications we refer the reader to [17] and references therein.
[19] A scalar version of Eq.[14] was obtained by B. Dong and X. L. Lei, J. Phys.: Condens. Matter 14, 4963 (2002).
[20] R. Świrkowicz, J. Barnaś and M. Wilczyński, J. Phys. Condens. Mat. 14, 2011 (2002).