Spin-current rectification through a quantum dot using temperature bias

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Abstract
We analyze spin-dependent transport through a spin-diode in the presence of spin-flip and under influence of temperature bias. The current polarization and the spin accumulation are investigated in detail by means of reduced density matrix. Results show that the spin accumulation is linearly increased when the metallic electrode is warmer whereas, its behavior is more complicated when the ferromagnetic lead is warmer. Furthermore, spin-flip causes that the current polarization becomes not only a function of spin-flip rate but also a function of temperature. The current polarization is reduced up to 90% if the time of spin-flip is equal to the tunneling time. The behavior of spin-dependent current is also studied as a function of temperature, spin-flip rate, and polarization.

1 Introduction
Study of electron transport through devices fabricated from quantum dots (QDs) has attracted a lot of attention during two recent decades. Transport through QDs exhibits novel and interesting phenomena such as Coulomb and spin blockade effects, Kondo effect, negative differential conductance, and so on. Coupling of QD to different leads such as, normal metal, ferromagnet, or superconductor, is now feasible due to recent progress in nanotechnology. One of the most interesting configurations is a quantum dot coupled to a normal metal(NM) and a ferromagnetic (FM) lead. In recent years the configuration has been extensively studied experimentally and theoretically. With regard to spin-current rectification effect observed in the device, it can work as a spin-diode.

the most studies done about the spin-diode have been focused on the behavior of the system in the presence of electric bias. Due to recent advance in the field of thermoelectricity, it is now possible to produce the spin current by applying temperature bias across a ferromagnetic semiconductor or a magnetic insulator. Very recently, F. Qi and co-workers have studied the transport through a QD coupled to a normal metal and a ferromagnetic
electrode under influence of the temperature bias. They have reported that the temperature gradient results in a rectification effect in the current polarization. In this article, we analyze the behavior of the system in the presence of spin-flip. Transverse magnetic field [28], spin-orbit interaction [29] and etc can cause the spin-flip. With regard to the structure of the device, it is completely possible that the electron of the QD interacts with the polarized nucleus of the sublayer. Current polarization, spin accumulation, and spin current are analyzed in detail by means of reduced density matrix approach [30, 31]. It is found that spin-flip affects current polarization significantly.

In the next section, model Hamiltonian and equations used for calculations are presented. Using density matrix approach and wide band limit, formal expressions of electron density and current are given. Numerical results and analytical expressions for the spin accumulation and the current polarization are presented in section 3. In the end, some sentences are given as conclusion.

Figure 1: Schematic diagram of a spin diode. $\Delta T$ denotes the temperature difference between leads. The left lead is warmer if $\Delta T > 0$ and $\Delta T < 0$ means the right lead is warmer. The increase of temperature causes that the electrons of the lead occupy the states above the chemical potential shown as gray space.

2 Model

We consider a single level quantum dot coupled to a normal metal (NM) and a ferromagnetic (FM) lead as fig. 1. The Hamiltonian describing the system is
given as follows

\[ H = \sum_{\alpha k} \varepsilon_{\alpha k} c_{\alpha k}^\dagger c_{\alpha k} + \sum_{\sigma} \varepsilon_{\sigma} n_{\sigma} + U n_{\uparrow} n_{\downarrow} \]  

where non-interacting quasi-particle approximation is used to describe the 

electrodes, \( c_{\alpha k} (c_{\alpha k}^\dagger) \) destroys (creates) an electron with 

wave vector \( k \), spin \( \sigma \), and energy \( \varepsilon_{\alpha k} \) in the lead \( \alpha \) (\( \alpha = L, R \)). \( d_{\sigma} (d_{\sigma}^\dagger) \) is 

annihilation (creation) operator in the QD which destroys (creates) an electron with 

spin \( \sigma \) in the QD. \( U \) denotes on-site Coulomb repulsion and \( n_{\sigma} = d_{\sigma}^\dagger d_{\sigma} \) is occupation operator. The fourth 
term describes spin-flip process and \( R \) is spin-flip rate which is spin-independent.

The last term describes tunneling between the QD and the electrodes and \( V_{\alpha k} \) 

stands for the coupling strength.

It is clear that the QD can be in : empty state \(| 0 \rangle \), singly occupied state \(| \sigma \rangle \) \((\varepsilon_{\sigma})\), or doubly occupied state \(| 2 \rangle \) \((\varepsilon_{2} = \varepsilon_{\uparrow} + \varepsilon_{\downarrow} + U)\). States \(| \uparrow \rangle \) and \(| \downarrow \rangle \) are not the eigenstates of the isolated QD Hamiltonian because of spin-flip. 

Using Markov approximation the time evolution of the density matrix elements 

are given as [30, 31]

\[ \frac{dP_{ss'}}{dt} = -i <s| [H_{s.f}, P]|s' > + \delta_{ss'} \sum_{k \neq s} [W_{ks} P_{kk} - W_{sk} P_{ss}] \]  

where \( H_{s.f} \) denotes the fourth term in Eq.(1). \( P_{ss} \) is probability of being in 

the state \( s \) \((s = 0, \sigma, 2)\) whereas, \( P_{ss'} \) \((s \neq s')\) describes coherency between 

states \(| \uparrow \rangle \) and \(| \downarrow \rangle \). \( W_{ss'} \) stands for transition from state \(| s \rangle \) to \(| s' \rangle \) and is 

computed by Fermi’s golden rule as

\[ W_{ss'} = \sum_{\sigma} \Gamma_{\sigma}^{\alpha} [f_{\alpha}(\varepsilon_{ss'}) \delta_{N_{ss'} N_{ss'}^\alpha + 1} + \bar{f}_{\alpha}(\varepsilon_{ss'}) \delta_{N_{ss'}^\alpha N_{ss''}}] \]  

where \( N_{s} \) denotes the number of electrons in the state \( s \) and \( \varepsilon_{ss'} = \varepsilon_{s} - \varepsilon_{s'} \). 

\( f_{\alpha}(x) = (1 + \exp((x - \mu_{\alpha})/k_{B}T_{\alpha}))^{-1} \) is Fermi distribution function of lead \( \alpha \) 

where \( T_{\alpha} \) and \( \mu_{\alpha} \) are temperature and chemical potential of lead \( \alpha \) and \( f_{\alpha} = 1 - f_{\alpha} \). \( \Gamma_{\sigma} \) is spin-dependent tunneling rate of the lead \( \alpha \) obtained by using 

wide band approximation. As an instance, \( P_{\uparrow \downarrow} \) is obtained from Eq.(2) as

\[ \frac{dP_{\uparrow \downarrow}}{dt} = iR[P_{\uparrow \downarrow} - P_{\downarrow \uparrow}] - \frac{1}{2} \sum_{k \neq \uparrow} W_{\uparrow k} + \sum_{k \neq \downarrow} W_{\downarrow k} P_{\uparrow \downarrow} \]  

and \( P_{\uparrow \uparrow} = P_{\downarrow \downarrow}^* \).

Now, we define \( n_{\sigma} = P_{\sigma \sigma} + P_{22} \). Using Eq.(2) and normalization condition 

\((P_{00} + \sum_{\sigma} P_{\sigma \sigma} + P_{22} = 1)\), it is straightforward to show

\[ \frac{dn_{\sigma}}{dt} = W_{0\sigma}[1 - n_{\sigma} - n_{\bar{\sigma}}] - W_{\sigma 0} n_{\sigma} + W_{\bar{\sigma} 2} n_{\bar{\sigma}} + iR[P_{\sigma \bar{\sigma}} - P_{\bar{\sigma} \sigma}] \]  

(5)
where $\bar{\sigma}$ is opposite of $\sigma$. Solving Eq. (5) in the steady state ($\frac{dn_{\sigma}}{dt} = 0$), the spin-dependent current crossing from the lead $\alpha$ is given as

$$I_{\sigma}^\alpha = W_{\sigma\alpha}^0 [1 - n_{\sigma} - n_{\bar{\sigma}}] - W_{\sigma\alpha}^{0\sigma} n_{\sigma} + W_{\sigma\alpha}^{0\bar{\sigma}} n_{\bar{\sigma}}$$  \hspace{1cm} (6)

In the continue, we consider $\Gamma_0 = 10\mu eV$ as lead-QD tunneling rate and set $\Gamma_{\sigma}^L = \Gamma_0$ and $\Gamma_{\sigma}^R = \Gamma_0 [1 + \sigma \rho]$ where $\sigma = 1(-1)$ for $\uparrow(\downarrow)$, and $\rho$ is the spin polarization degree of the ferromagnetic lead. Note that the left lead is a normal meta thus its tunneling rate is spin-independent whereas, the right lead is a ferromagnet whose majority carriers are assumed to be spin-up electrons. In addition, we assume $\varepsilon_{\sigma} = -2meV$, $U = 5meV$, and $\Delta T = T_L - T_R$. $\Delta T > 0$ means the left lead is warmer ($T_L = T_0 + \Delta T$) while, $\Delta T < 0$ means $T_R = T_0 + \Delta T$ where $T_0 = 0.2meV$ is the base temperature of the system.

Figure 2: Spin accumulation versus temperature bias. $S = 0$ and $\rho = 0.4$ (solid), $S = 0$ and $\rho = 0.8$ (dashed), $S = 0.5$ and $\rho = 0.4$ (dotted) and $S = 0.5$ and $\rho = 0.8$ (dash-dotted). Inset shows $\alpha$ (solid), $\beta$ (dashed), and $\alpha + \beta$ (dotted).

3 Results and discussions

In order to analyze the spin accumulation and the current, we have assumed that $f_R(\varepsilon_{\sigma}) = 1$, $f_R(\varepsilon_{\sigma} + U) = 0$, $f_L(\varepsilon_{\sigma}) = \alpha$ and $f_L(\varepsilon_{\sigma} + U) = \beta$ for $\Delta T > 0$ whereas, $f_L(\varepsilon_{\sigma}) = 1$, $f_L(\varepsilon_{\sigma} + U) = 0$, $f_R(\varepsilon_{\sigma}) = \alpha$ and $f_R(\varepsilon_{\sigma} + U) = \beta$ in $\Delta T < 0$. Note that $\alpha$ and $\beta$ are temperature-dependent and their dependence on
the temperature is shown in inset of fig. 2. Fig. 2 shows the spin accumulation \( m = n_\uparrow - n_\downarrow \) as a function of temperature bias. Results show that the most change in \( m \) is happened when the temperature difference is very low. As one can see in inset of fig. 2, \( \alpha \to 1 \) and \( \beta \to 0 \) in low temperature, so that there is only one electron in the QD and as a result, the ferromagnetic electrode affects the spin properties of the system significantly. By increase of temperature, the second electron enters the QD thus the spin characteristics of the system are vanished. By solving Eq. (5) in the steady state we obtain blow equation for the spin accumulation as a function of temperature, polarization, and spin-flip rate.

\[
m = \frac{2\rho[\alpha - 1]}{4S^2[3 + \alpha - \beta] + y[4 - (\alpha + 1 - \beta)^2]} \quad \Delta T > 0 \tag{7a}
\]

\[
m = \frac{2\rho[\alpha + \beta - 1]}{\rho y[(\alpha - \beta)^2 - 1] + 4S^2[3 + \alpha - \beta] - y[(\alpha - \beta + 1)^2 - 4]} \quad \Delta T < 0 \tag{7b}
\]

where \( y = 1 + \beta - \alpha \).

From Eq. (7), it is obvious that increase of temperature difference results in \( m = 0 \) because of \( \alpha, \beta \to 1/2 \). Physically, by warming an electrode, electrons near the Fermi surface occupy states above the chemical potential, see fig. 1, so that there will be some holes below the chemical potential. The excited electrons have the necessary energy to overcome the charging energy so that the QD will have two electrons and as a consequence, \( m = 0 \). Eq. (7) also shows that the dependence of \( m \) on \( \rho \) and \( S \) is different in positive and negative temperature bias and this difference results in an asymmetry in spin accumulation-temperature bias characteristic of the system. As one can see in fig. 2. In positive and low temperature difference, \( m \) is positive because the ferromagnetic lead acts as an emitter and due to \( \Gamma_\Upsilon^R > \Gamma_\Upsilon^L \), the probability of being in the spin-up state is more. Note that \( \alpha + \beta < 1 \), see dotted line in the inset, and as a result \( (\alpha - 1)^2 - \beta^2 \) becomes positive in Eq. (7). In negative and low temperature difference, the left lead acts as the emitter and as a result, \( m \) becomes negative because the spin-down electron has to stay in the QD for a longer time.

The dependence of the spin accumulation on the spin-flip rate and the polarization is plotted in fig. 3. Aspect from Eq. (7), \( m \) is significantly reduced by increase of \( R \). The dependence of \( m \) on \( \rho \) is much more interesting. In positive temperature bias, the spin accumulation is linearly increased by increase of \( \rho \) whereas, its behavior is completely different in negative temperature difference. The main result is risen due to the change of the emitter. In \( \Delta T > 0 \) where the right lead is emitter, the linear relation is dominant while, in the condition that the left lead is emitter, the dependence is more complicated. We reported the same behavior for the spin accumulation in a spin-diode under influence of voltage bias [32].

Spin-resolved currents as a function of temperature bias, spin-flip rate, and polarization are shown in figs. 4 and 5, respectively. First, we estimate the
current in the presence of positive temperature bias. By solving Eq. (5) and with respect to Eq. (6), spin-dependent currents are obtained as:

\[ I_{L}^{\uparrow} = \Gamma_{0}[\alpha - n_{\uparrow} - (\alpha - \beta)n_{\downarrow}] \]  
\[ I_{L}^{\downarrow} = \Gamma_{0}[\alpha - (\alpha - \beta)n_{\uparrow} - n_{\downarrow}] \]  

where \( n_{\sigma} \) is given as

\[ n_{\sigma} = \frac{\rho[1 - (1 - \alpha)^2 - \beta^2] + 4S^2(1 + \alpha) + (\beta + 1)^2 + \alpha[(\alpha - \beta)^2 - (1 + \alpha)]}{4S^2[\beta + \alpha - \beta] + y[4 - (1 + \alpha - \beta)^2]} \]  

where \( \sigma = 1(-1) \) for \( \uparrow(\downarrow) \). In positive bias, the current crossing from the left lead is negative because the right lead acts as the emitter, as explained before. From Eq. (9), it is clear that \( n_{\uparrow} \) is reduced by increase of \( R \) whereas, increase of \( R \) gives rise to increasing \( n_{\downarrow} \). This effect results in reduction of \( I_{L}^{\uparrow} \) and increase of \( I_{L}^{\downarrow} \), as it is seen in Eq. (8). Note that the probability of finding the QD in spin-up state is more in positive temperature bias if spin-flip process is absent. In the presence of spin-flip, the spin-up electron may rotate and change to a spin-down electron. Therefore, the spin-flip increases the probability of being in the spin-down while, the probability of being in spin-up state is reduced. With respect to Eq. (9), although the existence of \( R \) influences significantly on the current, the magnitude of it does not have significant role in the curvature of the current due to existence of a large term in denominator. Furthermore, \( I_{L}^{\uparrow} \) will be equal to \( I_{L}^{\downarrow} \) if \( R >> \Gamma_{0} \) because of \( n_{\uparrow} = n_{\downarrow} \), see Eq. (9). From Eqs. (8,9),

Figure 3: (a) \( \rho \) versus \( S \) for \( \Delta T = 3 \) (solid) and \( \Delta T = -3 \) (dashed). (b) \( \rho \) versus \( S \) for \( \Delta T = 0 \) (solid) and \( \Delta T = 0.3 \) (dashed). \( \Delta T = -3 \) is shown in gray.
it is obvious that the current is related to \( \rho \) linearly. This dependence is well observed in fig. 5b. It is very interesting to note that unlike \( R \), increase of \( \rho \) results in increase of \( I^\uparrow \) and decrease of \( I^\downarrow \). Indeed, with increase of \( \rho \) the spin-up electron is injected into the QD faster and as a result \( I^\uparrow > I^\downarrow \).

Now, we analyze the current when the ferromagnetic lead is warmer. In this case, \( I^\uparrow \) is equal to \( I^\downarrow \) and given as

\[
I^\sigma = \Gamma_0 [1 - n^\uparrow - n^\downarrow]
\]

where \( n^\sigma \) is obtained from

\[
n^\sigma = \frac{\rho \sigma y [\alpha + \beta - 1] - \alpha y^2 \rho^2 + 4 S^2 [1 + \alpha] + y^2 [1 + \alpha]}{\rho^2 y^2 (\alpha - \beta)^2 - 1] + 4 S^2 (3 + \alpha - \beta) - y((1 + \alpha - \beta)^2 - 4)}
\]

The first result observed in fig. 4 is the current is positive i.e. the left lead acts as the emitter. It comes from the fact that electrons below the Fermi level in the right lead are lesser than electrons in the left lead. On the other hand, increase of \( R \) results in increase of both \( I^\uparrow \) and \( I^\downarrow \). From inset of fig. 4, it is clear that increase of \( R \) gives rise to reduction of \( n^\downarrow \) and increase of \( n^\uparrow \). Note that the probability of being in the spin-down state is more if \( R = 0 \) because the spin-up electron injected from the left lead leaves the QD faster than the

Figure 4: Spin-resolved currents versus temperature bias.
Figure 5: (a) $I^\sigma$ as a function of spin-flip rate. We set $\rho = 0.8$ and $\Delta T = \pm 3$. Solid line is $I^\uparrow$ and dashed line is $I^\downarrow$. $\Delta T = -3$ is plotted in gray. (b) spin-dependent current versus $\rho$. We set $R = 0$. Inset shows $n^\uparrow$ (solid) and $n^\downarrow$ (dashed) for $\Delta T = -3$. 

spin-down electron. As it is obvious in inset and Eq.(11), the rate of reducing $n^\downarrow$ is faster than the rate of increase of $n^\uparrow$. This fact leads to increase of $I^\sigma$ in the presence of spin-flip. Increase of $I^\sigma$ due to spin-flip is clearly seen in fig. 5a. Like $\Delta T > 0$, the spin-resolved currents saturate for $R > 0.5Γ_0$. Unlike $\Delta T > 0$, the dependence of $I^\sigma$ on the polarization is not linear anymore. This dependence is plotted in fig. 5b. The behavior of $I^\sigma$ is very interesting in $\rho = 1$. In positive temperature bias, $I^\downarrow$ becomes zero because there are no spin-down electrons in ferromagnetic lead to enter the QD, but $I^\uparrow = I^\downarrow = 0$ if $\Delta T < 0$. It is straightforward to show that $n^\uparrow + n^\downarrow = 1$ if $S = 0$ and $\rho = 1$ and with respect to Eq.(11), $I^\sigma$ becomes zero. Indeed, the electron inside the QD cannot tunnel to the right lead so, other electron cannot enter the QD. In addition, increase of $\rho$ results in decrease of $I^\sigma$.

The current polarization, $\zeta = \frac{I^\uparrow - I^\downarrow}{I^\uparrow + I^\downarrow}$, is plotted in fig. 6a. With respect to
Eqs. (8,10), it is straightforward to show that

\[
\zeta = \frac{y^2}{y^2 + 4S^2 \rho} \quad \text{for} \quad \Delta T > 0 \quad (12a)
\]

\[
\zeta = 0 \quad \text{for} \quad \Delta T < 0 \quad (12b)
\]

Note that our results are identical results given in Ref. [27] if \( S = 0 \) and \( \alpha = \beta = 1/2 \). Presence of spin-flip causes that the current polarization becomes not only a function of spin-flip rate but also a function of temperature because of presence of \( \alpha \) and \( \beta \) in Eq. (12). As expected, spin-flip gives rise to reduction of \( \zeta \) because this process tries to destroy the spin characteristics of the system. If spin-flip rate becomes equal to tunneling rate, \( \zeta \) is reduced up to 90%. However, the system can still work as a rectifier although its performance is weak. The dependence of \( \zeta \) on polarization and \( R \) is shown in figs. 6b and 6c, respectively. Linear behavior of \( \zeta \) versus \( \rho \) is well seen. \( \zeta = 1 \) if \( R = 0 \) and \( \rho = 1 \) because there is no spin-down current through the system but, \( \zeta \) is significantly reduced in the presence of spin-flip because the spin-up electron into the QD can change...
4 Conclusion

In this article, we study spin-dependent transport through a quantum dot coupled to a normal metal and a ferromagnetic electrode. Analytical expressions for spin accumulation and current polarization are obtained in the presence of spin-flip, using master equations. Results show that the dependence of the system on the polarization is linear when the metallic lead is warmer whereas, its behavior is more complicated when ferromagnet is warmer. On the other hand, the spin-flip affects significantly the current polarization so that it is reduced up to 90% if the spin-flip time is equal to tunneling time. The effects of temperature, polarization, and spin-flip rate on the spin-resolved currents are also estimated. When the metallic electrode is warmer, spin-flip results in the increase of spin-down current while, spin-up current is decreased.

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