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Spin-flip transport through an interacting quantum dot

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Abstract

The spin-flip associated transport based on the Anderson model is studied. It is found that the electrons are scattered due to spin-flip effect via the normal, mixed and Kondo channels. The spin-flip scattering via Kondo channel enhances the Kondo resonance peak and causes a slight blue shift. The conductance is suppressed by the spin-flip scattering. This is attributed to the reason that electrons with energy near Fermi level are scattered by Kondo channel.

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It is already evident that Anderson model, which describes the conduction electron in the Fermi sea coupled with the local spin-electron in the magnetic impurity, describes quantum dots also. The quantum dot described by the Anderson Hamiltonian can be treated as a single impurity. The Kondo behavior was also found in quantum dot system [1]. In Anderson model, the Kondo resonance peak near Fermi level can be described by the strong coupling between the local electron in magnetic impurity and the conduction electron. It is known that a system of magnetic impurity embedded in bulk metal may be considered as an equilibrium situation, however, it was pointed out that the quantum dot system can be considered as a system in a non-equilibrium situation [2,3].

Due to the advances in material and nanofabrication techniques, the spin-electronic device may be realized very soon. Thus, the study of the relation between the electron transport and the spin-flip process might become very important. The intradot spin-flip effect which shifts the resonant energy ε_0 of the quantum dot to $\varepsilon_0 \pm R$, where R is the spin-flip scattering amplitude, has been studied previously, [4]. Sergueev et al.[5] studied the spin-flip associated tunneling through a quantum dot and described the spin valve effect by neglecting the current contributed by the off-diagonal process. Chu and Balatsky [6] studied a local nuclear spin processing in a magnetic field to investigate the spin-flip associated tunneling. They found the inclusion of the off-diagonal process indeed modifies the conductance of system. In this communication, the spin-flip associated transport through a quantum dot is studied. Both cases are considered, i.e. the magnetic impurity (the equilibrium situation) and the quantum dot (the non-equilibrium situation), coupled with the leads in which the magnetic impurity is embedded and thus the spin-flip effect may occur. As shown in Ref. [6], the conductance may be modified by the spin-flip process (i.e. the off-diagonal term) and may cause some interesting result. We model the spin associated tunneling between the lead and dot as the model proposed by Ref. [5], however, the off-diagonal part of conductance will be included in our study. The variation of spectrum function (or the local density of state, LDOS) and the conductance with respect to the strength of the spin-flip coupling are studied in this work. As shown in Ref. [7], the coupling constant between QD and the lead can be described by $\Gamma^{\alpha}_{\sigma'\sigma} = 2\pi \sum_{k,s,\alpha\in \mathrm{L,R}} V^{*'}_{k_\alpha s,\sigma'} V_{k_\alpha s,\sigma}\delta(\omega-\varepsilon_{k_\alpha s})$ and the spin-

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flip coupling constant is set to be symmetric for the state $\sigma(\sigma')$ flipped into the state $\sigma'(\sigma)$, i.e. $\Gamma^{\alpha}_{\sigma'\sigma}=\Gamma^{\alpha}_{\sigma\sigma'}=\Gamma^{s}_{\sigma}$. In this communication, we will use the non-equilibrium transport equation which was developed by Antti-Pekka Jauho [8] et al. to calculate the non-equilibrium conductance. The related Green functions are evaluated by the equation of motion method and used the decoupling approximations:

$$\langle c^{+}_{k_\alpha s}(t)c_{k_\beta s'}(t)d_{\sigma'}(t)d^{+}_{\sigma}(t)\rangle = \delta_{k_\alpha,k_\beta}\delta_{s,s'}f(\varepsilon_{k_\alpha s})\langle d_{\sigma'}(t)d^{+}_{\sigma}(t)\rangle \tag{1}$$

$$\langle c^{+}_{k_\alpha s}(t)c_{k_\beta s'}(t)d_{\sigma}(t)d^{+}_{\sigma}(t)\rangle = \delta_{k_\alpha,k_\beta}\delta_{s,s'}f(\varepsilon_{k_\alpha s})\langle d_{\sigma}(t)d^{+}_{\sigma}(t)\rangle \tag{2}$$

$$\langle c_{k_\alpha s}(t)c_{k_\beta s'}(t)d^{+}_{\sigma'}(t)d^{+}_{\sigma}(t)\rangle \simeq 0 \tag{3}$$

$$\langle d^{+}_{\sigma}(t)c_{k_\alpha s}(t)\rangle = \langle c^{+}_{k_\alpha s}(t)d_{\sigma}(t)\rangle \simeq 0 \tag{4}$$

The terms $\langle d^{+}_{\sigma}(t)c_{k_\alpha s}(t)\rangle$, $\langle c^{+}_{k_\alpha s}(t)d_{\sigma}(t)\rangle$ and $\langle c_{k_\alpha s}(t)c_{k_\beta s'}(t)d^{+}_{\sigma'}(t)d^{+}_{\sigma}(t)\rangle$ are the higher order correlation Green function which can be approximated as zero when the temperature is higher than the Kondo temperature [9,10]. This decoupling approximation has been known to give qualitatively correct Kondo physics for $T\leq T_K$ and quantitatively reasonable result for $T>T_K$ [2]. In order to ensure the validity of the decoupling approximation, we will consider the temperature at $T=10T_K$.

The system we consider is the Anderson model with spin-flip associated tunneling which could be caused by the magnetic impurity in the lead or contact (or a magnetic impurity adulterated electron reservoir). The Hamiltonian of the system can be written as:

$$H_d = \sum_{\sigma}\varepsilon_\sigma d^{+}_{\sigma}d_\sigma + U d^{+}_{\sigma}d^{+}_{\sigma'}d_\sigma d_{\sigma'}$$

$$H_C = \sum_{\substack{k_\alpha s\\ \alpha\in L,R}}\varepsilon_{k_\alpha s}c^{+}_{k_\alpha s}c_{k_\alpha s}$$

$$H_T = \sum_{k_\alpha s}V^{*}_{k_\alpha s,\sigma}d^{+}_{\sigma}c_{k_\alpha s} + V_{k_\alpha s,\sigma}c^{+}_{k_\alpha s}d_\sigma$$

where d^{+}_{σ} (d_σ) is the creation (annihilation) operator of the electron with spin σ in the dot, $c^{+}_{k_\alpha s}(c_{k_\alpha s})$ is the creation (annihilation) operator of an electron with momentum k and spin s at α lead (where $\alpha\in L,R$). The $\varepsilon_{k_\alpha s}$ is the single particle energy of the conduction electron in the α lead. The electron tunneling between the lead and the dot is described by the tunneling matrix $V_{k_\alpha s,\sigma}$.

By using the equation of motion method and employing the decoupling approximations Eqs. (1–4). We obtain the Green functions for infinite U limit by taking $U\to\infty$ [11]:

$$G_{\sigma\sigma} = \frac{1-\langle n_{\sigma'}\rangle}{(g^0_\sigma)^{-1} - \left(\sum^{s}_{\sigma} - Y^{(2)}_{\sigma}\right)g^0_{\sigma'}\left(\sum^{s}_{\sigma'} - Y^{(2)}_{\sigma'}\right)} \tag{5}$$

$$G_{\sigma'\sigma} = g^0_{\sigma'}\left[\sum^{s}_{\sigma} - Y^{(2)}_{\sigma'}\right]G_{\sigma\sigma} \tag{6}$$

where

$$g^0_\sigma = \frac{1}{\omega-\varepsilon_\sigma-\sum^{n}_{\sigma}+X^{(2)}_{\sigma}}$$

$$\Sigma^{n}_{\sigma} = \sum_{k_\alpha s}\frac{|V_{k_\alpha s,\sigma}|^2}{\omega-\varepsilon_{k_\alpha s}};\quad \Sigma^{s}_{\sigma} = \sum_{k_\alpha s}\frac{V^{*}_{k_\alpha s,\sigma}V_{k_\alpha s,\sigma'}}{\omega-\varepsilon_{k_\alpha s}}$$

$$X^{(2)}_{\sigma} = -\Sigma^{1c}_{\sigma'\sigma'}$$

$$Y^{(2)}_{\sigma} = -2\langle d^{+}_{\sigma'}d_\sigma\rangle\Sigma^{n}_{\sigma} + (1-\langle n_{\sigma'}\rangle)\Sigma^{3a}_{\sigma\sigma'} - \Sigma^{2a}_{\sigma\sigma'}$$

$$\Sigma^{ia}_{\sigma'\sigma} = \sum_{k_\alpha s}\frac{V^{*}_{k_\alpha s,\sigma'}V_{k_\alpha s,\sigma}}{\omega-\varepsilon_{k_\alpha s}}A_{(i)}(\varepsilon_{k_\alpha s})$$

$$\Sigma^{ic}_{\sigma'\sigma} = \sum_{k_\alpha s}\frac{V^{*}_{k_\alpha s,\sigma'}V_{k_\alpha s,\sigma}}{\omega-\varepsilon_{k_\alpha s}-\varepsilon_\sigma+\varepsilon_{\sigma'}}A_{(i)}(\varepsilon_{k_\alpha s})$$

$$A_{(1)} = f(\varepsilon_{k_\alpha s});\quad A_{(2)} = 1-f(\varepsilon_{k_\alpha s});\quad A_{(3)} = 1$$

Note that the Eq. (5) is a form of standard Green function with the quasiparticle energy $(g^0_\sigma)^{-1}$ where g^0_σ is the Green function of the quasiparticle of Anderson Hamiltonian without spin-flip effect, i.e. it is the Green function as shown in Eq. (3) of Ref. [7]. The term $X^{(2)}_{\sigma}$ and $Y^{(2)}_{\sigma}$ are the self-energies related to the electron–electron correlation, i.e. the Kondo effect. The term $X^{(2)}_{\sigma}$ is related to non-spin-flip process and $Y^{(2)}_{\sigma}$ to spin-flip process. The physical picture of the Green function Eq. (5) can be interpreted as follows. Eq. (5) can be understood as the σ state quasiparticle of Anderson Hamiltonian. It is scattered between σ and σ' states via three channels, i.e. the normal channel which causes the self-energy $\sum^{s}_{\sigma} g^0_{\sigma'}\sum^{s}_{\sigma'}$, the Kondo effect channel which causes the self-energy $Y^{(2)}_{\sigma}g^0_{\sigma}Y^{(2)}_{\sigma'}$ and the mixed channel which causes the self-energy $-\sum^{s}_{\sigma}g^0_{\sigma'}Y^{(2)}_{\sigma'}$ and $-Y^{(2)}_{\sigma}g^0_{\sigma'}\sum^{s}_{\sigma'}$. Furthermore, if one considers the high temperature with infinite U limit, the Kondo channel will disappear i.e. $X^{(2)}_{\sigma}=0$ and $Y^{(2)}_{\sigma}=0$ and the Green functions Eqs. (5) and (6) will reduce to the Green functions Eqs. (6) and (7) in Ref. [5] but without interaction with local spin. The corresponding retarded Green function of Eq. (5) can be obtained by setting $\omega\to\omega+i\delta$ [11] and is found to obey the fluctuation-dissipation theorem $\sum_\sigma\int_{-\infty}^{\infty}(d\omega/2\pi)(-2\,\mathrm{Im}\,G^{r}_{\sigma\sigma})=1$.

In the following discussion, all of the energy scale will be normalized to the bandwidth of the virtual bound state $\Gamma=((\Gamma^{L}_{n}/2)+(\Gamma^{R}_{n}/2))=2\Gamma^{\alpha}_{n}=1$. The resonant energy of quantum dot is set as $\epsilon_0=-5$. The Fermi level of the lead E_F is set to be zero for the equilibrium situation. The Kondo temperature is estimated by the equation $T_K\approx\sqrt{\Gamma D}\exp(\pi(\varepsilon_0-E_F)/(2\Gamma))\approx 0.004$ with a half-width $D=100$ and $E_F=0$. [12]. The temperature of the system is set to be $T=10T_K$.

The particle number n_σ and the expectation value of $\langle d_\sigma^+ d_{\sigma'}\rangle$ are determined by self-consistent method which can be calculated by the following identities:

$$\langle n_\sigma\rangle = -\mathrm{i}\int \frac{\mathrm{d}\omega}{2\pi} G^<_{\sigma\sigma}(\omega) \quad (7)$$

$$\langle d_{\sigma'}^+ d_\sigma\rangle = -\mathrm{i}\int \frac{\mathrm{d}\omega}{2\pi} G^<_{\sigma'\sigma}(\omega) \quad (8)$$

In Eqs. (7) and (8) the lesser Green function can be obtained by Keldysh equation $G^< = G^r\sum^< G^a$. In general, the lesser self-energy $\sum^<$ is difficult to be solved for the interacting case, i.e. $U\neq 0$, thus, we will follow the generalized Ng′s ansatz and express the lesser self-energy in term of the non-interacting retarded (advanced) and lesser self-energies, $\sum_0^{r(a)}$ and $\sum_0^<$ [4,5,13]. The expression of the lesser self-energy is $\sum^< = (\sum^r - \sum^a)/(\sum_0^r - \sum_0^a)\sum_0^<$ which can be solved analytically.

The spectrum function (or local density of state, LDOS, for $\sigma'=\sigma$) $A_{\sigma'\sigma}(\omega) = -2\ \mathrm{Im}\ G^r_{\sigma'\sigma}$ in equilibrium situation is calculated in terms of the strength of spin-flip tunneling coupling constant Γ^s_α. According to Eq. (5), the quasiparticle of Anderson Hamiltonian is scattered by the normal channel, the mixed channel and the Kondo effect channel. The self-energy $\sum_\sigma^s$ in the normal channel is energy independent, thus any electron with arbitrary energy will be scattered by the normal channel. On the contrary, the Kondo effect channel is energy dependent and the strength is increased logarithmly near Fermi level. Therefore, the Kondo channel and the mixed channel dominate the spin-flip scattering near Fermi level and the normal channel dominates the spin-flip scattering for electrons with energies far away from the Fermi level. Fig. 1 shows the equilibrium spectrum functions with various Γ_s^α. Since the temperature of system is higher than the Kondo temperature, the Kondo resonance peak is very small when $\Gamma^s_\alpha = 0$. It is noticeable that the Kondo resonance peak is enhanced due to the spin-flip effect. The LDOS of σ electron is shown in Fig. 1(a). It shows that the spin-flip scattering accumulates the electron at the vicinity via the Kondo channel and enhances the Kondo resonance peak. In the inset, it shows that the spin-flip effect also causes a slight blue shift of Kondo resonant peak. The electron with energy far away from Fermi level is scattered via the normal channel and causes the peak shifts toward the resonant energy of quantum dot. The spectrum function of off-diagonal process which reflects the spin-flip scattering process is shown in Fig. 1(b). The positive (negative) value of off-diagonal spectrum function $A_{\sigma'\sigma}$ indicates that the $\sigma(\sigma')$ electron is scattered to $\sigma'(\sigma)$ state. Noted that the spectrum function $A_{\sigma'\sigma}$ near the Fermi level is negative and the strength is increased as the spin-flip coupling Γ^s_α is increased that causes the decrease of the equilibrium conductance.

The conductance for the equilibrium case is calculated by Eq. (3) of Ref. [6]. Fig. 2 shows the equilibrium conductance versus the spin-flip coulping constant Γ^s. Since

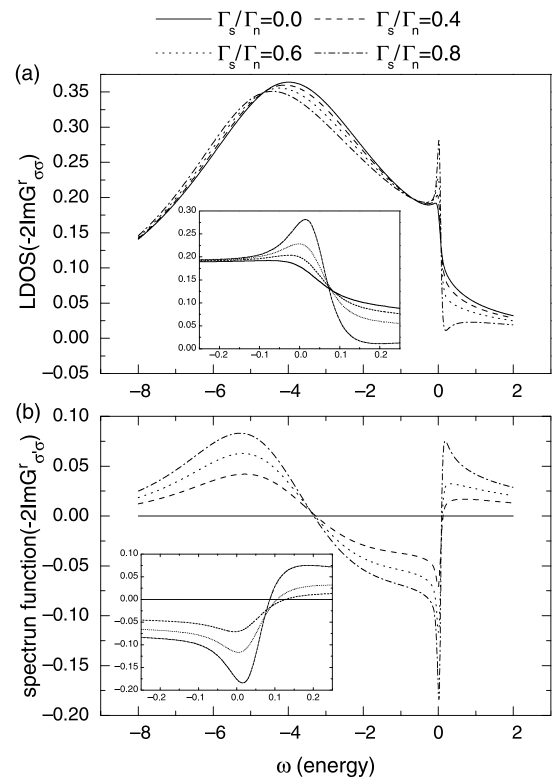

Fig. 1. The LDOS (or spectrum function) $A_{\sigma'\sigma} = 2\ \ \mathrm{Im}\ G^r_{\sigma'\sigma}$ versus the ratio Γ_s/Γ_n. (a) The diagonal process, $\sigma'=\sigma$. (b) The off-diagonal process, $\sigma\neq\sigma'$. The inset is the detail plot of $A_{\sigma'\sigma}$ near Fermi level.

the spin-flip associated tunneling effect accumulates the electron at vicinity of Fermi energy, the conductance due to diagonal process $g^c_{\sigma\sigma}$ increases as the spin-flip associated tunneling coupling constant Γ^s is increased. The off-diagonal part $g^c_{\sigma'\sigma}$ decreases (more negative) since the

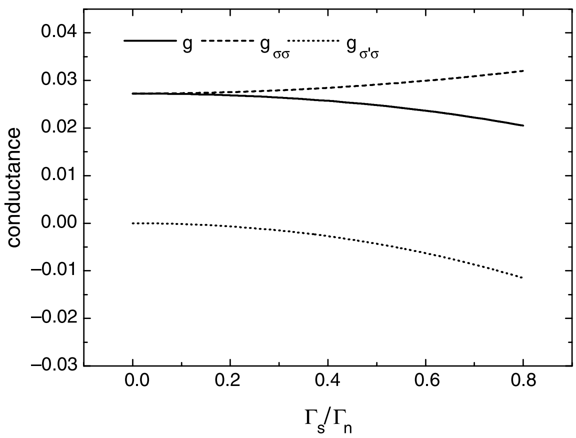

Fig. 2. The equilibrium conductance versus the strength of spin-flip associated tunneling.

spectrum function of the off-diagonal process at the vicinity of the Fermi level is negative and the strength is increased as Γ^s is increased. Since the off-diagonal term decreases faster than the increase of the diagonal term as Γ^s is increased, as a result the total conductance is suppressed by the spin-flip associated tunneling effect.

For the non-equilibrium case, we consider a quantum dot connected to the leads in which the Fermi level of the right lead E_F^R is set as zero, the Fermi level of left lead is E_F^L and the bias voltage is set as $V_b = E_F^L - E_F^R$. In the following, we focus our discussion on the case with a bias voltage $|V_{bias}| \leq 1$. The non-equilibrium differential conductance is defined as $g^c_{noneq} = \Delta J/\Delta V_b$ and shown in Fig. 3 where current J is calculated by the method of Ref. ([8]). In the first, as the description in Ref. ([7]), g^c_{noneq} will reflect the profile of the equilibrium spectrum function, hence the non-equilibrium differential conductance will decrease as the bias voltage is increased. Secondly, as same as the equilibrium situation, g^c_{noneq} is suppressed by spin-flip effect. Thirdly, one can find that there is a valley at $V_{bias} \sim 0$ 0 i.e. the Kondo channel dominates the region when $\Gamma^s >$ 0.4. This phenomenon is ascribed by the spin-flip scattering via the Kondo channel which enhances the peak height and causes a slight blue shift of Kondo peak as Fig. 4 shows. As the bias voltage is close to zero, the peak height of diagonal and off-diagonal spectrum function is enhanced. As the description of the equilibrium case, the peak height enhancement of the off-diagonal spectrum is stronger than diagonal part, hence the total conductance is decreased. Besides, there are more LDOS with an energy larger than the Fermi energy of right lead where the Fermi-Dirac distribution of lead is small and contributes lesser current when $V_{bias} \sim 0$. Hence the current is decreased as the bias voltage is close to zero and causes a valley of non-equilibrium differential conductance near the zero bias voltage.

In summary, we study the spin-flip associated tunneling in Anderson model at $T = 10T_K$. The total effect can be

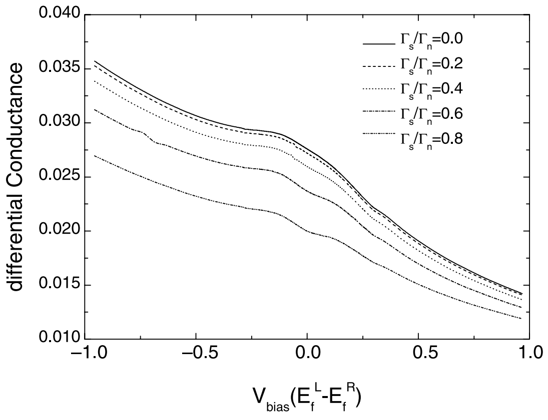

Fig. 3. The non-equilibrium conductance versus the strength of spin-flip associated tunneling.

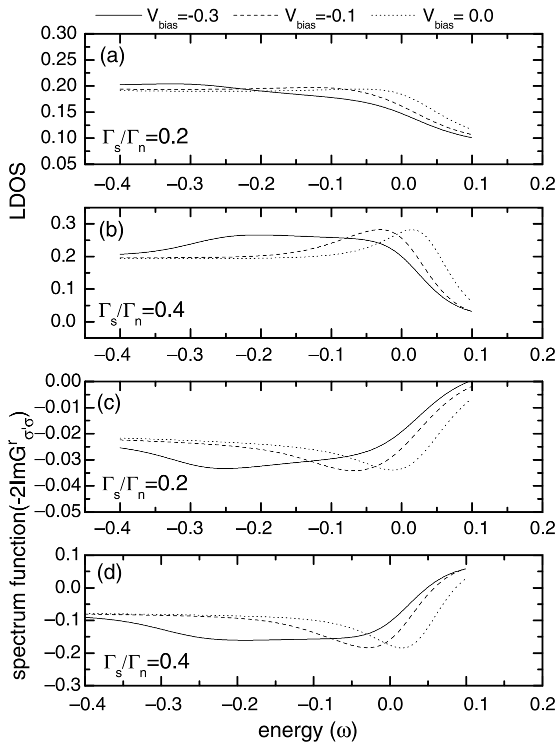

Fig. 4. The non-equilibrium spectrum function versus bias voltage for $\Gamma_s/\Gamma_n = 0.2$ ((a), (c)) and 0.8((b), (d)). The figures (a) and (b) are the diagonal spectrum functions (LDOS). The figures (c) and (d) are the off-diagonal spectrum functions.

interpreted as follows. The Anderson Hamiltonian quasi-particle (the solution of Anderson Hamiltonian without spin-flip effect) is scattered by the normal channel, mixed channel and the Kondo channel. As the plot of diagonal process spectrum function $A_{\sigma\sigma}$, Fig. 1(a), shows the normal channel dominates the scattering of the electrons with energies far away from the Fermi level of the leads and the electrons are scattered into the resonant state of the dot or the impurity. The electron near the Fermi level of the leads is mainly scattered by the Kondo channel. The spin-flip via the Kondo channel enhances the peak height and causes a slight blue shift of Kondo resonant peak. The off-diagonal spectrum function which describes the scattering process $\sigma \rightarrow \sigma'$ and with the negative value at the vicinity of the Fermi level which contributes the negative conductance. Since the decrease of conductance due to off-diagonal process is stronger than the increase of the conductance due to the diagonal process, the total conductance is suppressed by the spin-flip associated tunneling process. The conductance due to the off-diagonal process is negative and cannot be neglected. In the non-equilibrium situation case, we also find that the differential conductance is suppressed by the spin-flip associated tunneling effect. In this communication, we used the decoupling approximation which is qualitatively correct for $T \leq T_K$ and quantitative reasonable for $T > T_K$ to find the Green function. In order to keep a quantitatively correct result, the temperature of the system is set as $10T_K$. Although the decoupling approximation is not quantitatively correct for $T \leq T_K$, it still could give a qualitatively result of Kondo physics for $T \leq T_K$. Our result could hopefully give at least a qualitatively reference for the case of temperature below the Kondo temperature.

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