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Spin current through quantum-dot spin valves

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Abstract

We report a theoretical study of the influence of the Coulomb interaction on the equilibrium spin current in a quantum-dot spin valve, in which the quantum dot described by the Anderson impurity model is coupled to two ferromagnetic leads with noncollinear magnetizations. In the Kondo regime, electrons transmit through the quantum dot via higher-order virtual processes, in which the spin of either lead electrons or a localized electron on the quantum dot may reverse. It is found that the magnitude of the spin current decreases with increasing Coulomb interactions due to spin flip effects on the dot. However, the spatial direction of the spin current remains unchanged; it is determined only by the exchange coupling between two noncollinear magnetizations.

Spin polarized electron transport in microstructures has been one of the most active research fields in recent years not only because it is a fundamental problem in condensed matter physics, but also because it has potential applications in future spin devices such as spin valve transistors, spin selective electron interferometers, and nonvolatile random access memory [1–3]. A prominent example is the spin valve device based on the tunnelling magnetoresistance (TMR) in magnetic tunnel junctions [4]. The tunnelling conductance for moments of two ferromagnetic metallic (FM) electrodes aligned parallel is usually greater than that for the moments aligned antiparallel, giving rise to a TMR effect. The spin polarized tunnelling through nanostructured devices has been extensively studied—such as semiconductor quantum dots (QDs) or metallic single-electron transistors. In a QD spin valve system, the QD coupled to two FM leads, some novel transport characteristics have been identified [5–7]. For example, it was reported that the interplay of the spin-dependent tunnelling and Coulomb interaction gives rise to an exchange field on the QD, which leads in turn to spin precession in a biased QD spin valve [8]. In the same system, for the antiparallel magnetization configuration, a zero-bias anomaly in the cotunnelling transport through the QD was predicted and attributed to the interplay of single-barrier and double-barrier spin flip cotunnelling processes rather than the Kondo effect [9].

For an FM/FM tunnel junction, if two leads' magnetization directions are aligned with a noncollinear angle, an equilibrium spin current (ESC) will flow through the junction without

any bias [10–13]. Within the linear response approximation the ESC in the noncollinear FM/FM junction depends on the exchange coupling $\mathbf{M}_L \times \mathbf{M}_R$ between two magnetic moments, \mathbf{M}_L and \mathbf{M}_R . The dissipationless spin current is quite similar to the dissipationless charge current in the Josephson junctions. The magnetization rotates spins in both FM leads and their macroscopic phase difference drives the spin current through the magnetic junction, while a difference in superconducting phase between two superconducting leads induces a supercurrent through the Josephson junction. The dissipationless spin current has attracted much attention in recent years. For instance, the intrinsic spin Hall current, which was suggested by Sinova *et al* [14] for two-dimensional electron gas and by Murakami *et al* [15] for p-doped semiconductor, is indeed a dissipationless pure spin current. Meier *et al* [16] studied the transport of magnetization by magnons and showed that by using a finite length spin chain between magnetic reservoirs, the pure spin current can be generated without the transport of electron charge.

In this work we investigate the dissipationless ESC in the QD spin valves by taking the strong Coulomb correlation into account. Particular attention is paid to the spin transport in the Kondo regime [17–20], in which either double or empty occupation is mostly prohibited and a localized spin forms so that the electron on the QD cannot tunnel out of it and no electron outside of the QD can tunnel into it due to the strong Coulomb interaction. As a result, the first-order current must be blocked. However, the leakage current could take place in the Coulomb blockage valley by virtual higher-order cotunnelling events, e.g., the electron on the QD tunnels out of it followed by an electron with opposite spin tunnelling from a lead into the QD. In this cotunnelling process, the local spin is flipped. The coherent superposition of all possible cotunnelling events gives rise to the Kondo effect, the logarithmic divergence of the leakage current at the Fermi level [21]. The Coulomb interaction can lead to a spin flip effect for both tunnelling electrons and localized electrons on the QD, forming an exchange field on the QD. An interesting question is how the exchange field or the Coulomb interaction affects the ESC. By comparatively studying the two cases in the presence and absence of Coulomb interactions on the QD, we find that the spatial direction of the ESC stays the same and is determined only by the exchange coupling between two noncollinear magnetizations. This indicates that the spin symmetry on the QD is not broken by the Coulomb interaction. On the other hand, the magnitude of the ESC decreases with increasing Coulomb interaction due to the spin flip effects in higher-order virtual processes.

Consider a QD spin valve system consisting of a QD coupled through tunnel barriers to two identical FM leads, with current flowing along the x direction, as shown in figure 1. The QD with Coulomb interaction U is described by the single-level Anderson impurity model [22, 23], and two FM leads are described by the Stoner model [24] with magnetic moments \mathbf{M}_L and \mathbf{M}_R at an angle of θ . Taking the quantum spin axis along the direction of \mathbf{M}_L , we have $\mathbf{M}_L = M(0, 0, 1)$ and $\mathbf{M}_R = M(\sin \theta, 0, \cos \theta)$. The model Hamiltonian is given by

$$\mathcal{H} = \mathcal{H}_L + \mathcal{H}_R + \mathcal{H}_{\text{QD}} + \mathcal{H}_{TL} + \mathcal{H}_{TR} \quad (1a)$$

$$\mathcal{H}_\alpha = \sum_{k\sigma} \varepsilon_{k\alpha\sigma} C_{k\alpha\sigma}^\dagger C_{k\alpha\sigma}, \quad \alpha = L, R \quad (1b)$$

$$\mathcal{H}_{\text{QD}} = \sum_{\sigma} \varepsilon_d d_{\sigma}^\dagger d_{\sigma} + U d_{\uparrow}^\dagger d_{\uparrow} d_{\downarrow}^\dagger d_{\downarrow}, \quad (1c)$$

$$\mathcal{H}_{T\alpha} = \sum_{k\alpha\sigma} (t_{k\alpha} C_{k\alpha\sigma}^\dagger d_{\sigma} + \text{c.c.}). \quad (1d)$$

Here \mathcal{H}_α is the Hamiltonian of the α th FM lead with operator $C_{k\alpha\sigma}^\dagger$ ($C_{k\alpha\sigma}$) creating (annihilating) a conduction electron with spin σ ($\sigma = \pm = \uparrow, \downarrow$) and $\varepsilon_{k\alpha\sigma}$ denoting the energy dispersion of spin polarized conducting electrons within the Stoner model. \mathcal{H}_{QD} is

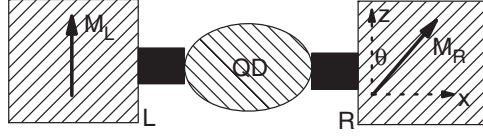


Figure 1. Schematic diagram of a QD spin valve with two noncollinear magnetizations in left and right FM. The left and right tunnelling barrier connect them with the dot. The right FM has an angle θ with the common spin axis z in the x - z plane.

the Hamiltonian of the QD with d_σ^\dagger (d_σ) creating (annihilating) an electron with spin σ and ε_d as the single energy level. $\mathcal{H}_{T\alpha}$ describes the electron tunnelling between the QD and FM leads, where hopping matrix element $t_{k\alpha}$ is independent of spin. Due to the noncollinearity of \mathbf{M}_L and \mathbf{M}_R , we need either to transform \mathcal{H}_R into the common σ_z representation or to transform \mathcal{H}_{TR} into the local eigenspin space of the right FM lead. The latter is chosen here, yielding

$$\mathcal{H}_{TR} = \sum_{kR\bar{\sigma}} \left[t_{kR} \left(\cos \frac{\theta}{2} C_{kR\sigma}^\dagger - \sigma \sin \frac{\theta}{2} C_{kR\bar{\sigma}}^\dagger \right) d_\sigma + \text{c.c.} \right], \quad (2)$$

where subscript $\bar{\sigma}$ stands for the spin opposite to σ .

We now derive the ESC formula in the QD spin valve. The total spin in the left lead is $\mathbf{S}_L = (\hbar/2) \sum_{k\gamma\beta} C_{kL\gamma}^\dagger \boldsymbol{\sigma}_{\gamma\beta} C_{kL\beta}$ where $\boldsymbol{\sigma}$ is the Pauli spin operator, and γ and β are spin indices. The time evolution of \mathbf{S}_L in the Heisenberg picture is equal to $\dot{\mathbf{S}}_L = (1/i\hbar)[\mathbf{S}_L, H_T]$; thus the spin current in a steady state is given by

$$\mathbf{J}_s = \frac{-1}{2} \int \frac{d\omega}{2\pi} \sum_k \text{Tr} [t_{kL} \boldsymbol{\sigma} G_{dk}^<(\omega) - t_{kL}^* \boldsymbol{\sigma} G_{kd}^<(\omega)]. \quad (3)$$

Here the trace Tr is over the spin space, $G_{kd}^<(dk)$ is the 2×2 lesser Green's function in spin space and its matrix elements are defined as $G_{k\beta, d\gamma}^<(t, t') = i \langle d_\gamma^\dagger(t') C_{kL\beta}(t) \rangle$. The Fourier transform of the Green's function is given by $G_{kd}^<(t - t') = \int \frac{d\omega}{2\pi} G_{kd}^<(\omega) e^{-i\omega(t-t')}$. Since the spin current is a tensor quantity and the current direction in our study is along the x direction in figure 1, \mathbf{J}_s is a vector whose Cartesian components are related to three Pauli matrices. To simplify the equation above, we employ the equation-of-motion approach of the nonequilibrium Green's function (Langreth theorem) [25] to decouple $G_{kd}^<(dk)$ as a product of the Green's function of the FM lead and that of the QD. In the equilibrium case under consideration, i.e., zero bias applied on the junction, it is convenient to calculate the Green's functions in equation (3) by use of relation $G^< = (G^a - G^r)f(\omega)$, [26] where $f(\omega)$ is the Fermi distribution function, $G^{r(a)}$ is the retarded (advanced) Green's function and can be calculated from the usual Dyson equation. With a little algebra, we obtain the ESC as

$$\mathbf{J}_s = \frac{-1}{2} \int \frac{d\omega}{2\pi} f(\omega) \sum_k |t_{kL}|^2 \text{Tr} [\boldsymbol{\sigma} (g_L^r G_d^r - G_d^r g_L^r + \text{h.c.})]. \quad (4)$$

Here g_L^r is the retarded Green's function of the free electron in the left FM lead and G_d^r is that of the QD, both of them being 2×2 matrices in spin space. It is worthy of note that the electrons not only near the Fermi energy but also in the full band contribute to the ESC, quite different from the usual charge transport case. From the equation above, the off-diagonal term of G_d^r is vital for forming the ESC in the system, since g_L^r itself is diagonal in spin space, $g_L^r(\omega) = \delta_{\sigma\sigma'}/(\omega - \varepsilon_{kL\sigma})$. The off-diagonal term of G_d^r appears as \mathbf{M}_L and \mathbf{M}_R are not collinear, and so a nonzero ESC can flow through the junction according to equation (4).

We proceed to derive the Green's function of the QD, which is given by in a general form

$$G_d^r(\omega) = \frac{1}{\omega I - \mathcal{H}_{\text{QD}} - \Sigma^r}, \quad (5)$$

where I is a unit matrix and Σ^r is a 2×2 self-energy in spin space coming from both FM leads and from strong e–e Coulomb interactions on the QD. In the absence of U , G_d^r can be readily worked out, $\Sigma^r = \Sigma_L^r + \Sigma_R^r$ describing the coupling of the QD to the left and right FM leads. As the Coulomb interaction is turned on, there is an additional self-energy contribution from U apart from Σ_L^r and Σ_R^r . In order to qualitatively study the influence of U on the ESC, we consider the dot–lead coupling to be weak enough so that $\mathcal{H}_{TL(R)}$ may be regarded as a perturbation. This permits us to derive the effective self-energy Σ_{eff} by the Schrieffer–Wolff transformation [27], which is equivalent to the effective Hamiltonian from the second-order $\mathcal{H}_{TL(R)}$ on replacing ε_d with energy argument ω . Within the lowest-order perturbation, the left and right tunnelling Hamiltonians \mathcal{H}_{TL} and \mathcal{H}_{TR} contribute independently to the effective self-energy. Following the standard procedure of transformation, we arrive at Σ_{eff} from the right dot–lead coupling as

$$\Sigma_{\text{eff}}(\omega) = S_1(\omega) + S_2(\omega) + S_3(\omega) \quad (6a)$$

$$S_1(\omega) = \sum_{k\sigma} A_{k\sigma} \left[n_{d\sigma} \cos^2 \frac{\theta}{2} + n_{d\bar{\sigma}} \sin^2 \frac{\theta}{2} - \frac{\bar{\sigma}}{2} \sin \theta (d_{\sigma}^{\dagger} d_{\sigma} + d_{\sigma}^{\dagger} d_{\bar{\sigma}}) \right] - \sum_{kk'\sigma} A_{k\sigma} [C_{k'\sigma}^{\dagger} C_{k\sigma} + \text{c.c.}], \quad (6b)$$

$$S_2(\omega) = \frac{1}{2} \sum_{kk'\sigma} \{ \cos \theta (t_{kR} F_{k\sigma} C_{k\sigma}^{\dagger} d_{\sigma} C_{k'\bar{\sigma}}^{\dagger} d_{\bar{\sigma}} - \text{c.c.}) + \sigma \sin \theta (t_{kR} F_{k\sigma} C_{k\sigma}^{\dagger} d_{\sigma} C_{k'\sigma}^{\dagger} d_{\bar{\sigma}} - \text{c.c.}) \} + \sum_{k\sigma} D_{k\sigma} n_{\sigma} n_{\bar{\sigma}}, \quad (6c)$$

$$S_3(\omega) = \frac{1}{2} \sum_{kk'\sigma} D_{k\sigma} \left\{ \cos^2 \frac{\theta}{2} C_{k'\bar{\sigma}}^{\dagger} C_{k\sigma} d_{\sigma}^{\dagger} d_{\bar{\sigma}} - \sin^2 \frac{\theta}{2} C_{k'\bar{\sigma}}^{\dagger} C_{k\sigma} d_{\bar{\sigma}}^{\dagger} d_{\sigma} + \frac{\sigma}{2} \sin \theta \times (C_{k'\bar{\sigma}}^{\dagger} C_{k\sigma} n_{d\bar{\sigma}} - C_{k'\bar{\sigma}}^{\dagger} C_{k\sigma} n_{d\sigma}) + \text{c.c.} \right\} - \frac{1}{2} \sum_{kk'\sigma} D_{k\sigma} \left\{ \left(\cos^2 \frac{\theta}{2} n_{d\bar{\sigma}} + \sin^2 \frac{\theta}{2} n_{d\sigma} \right) \times (C_{k'\sigma}^{\dagger} C_{k\sigma} + \text{c.c.}) + \frac{\sigma}{2} \sin \theta (d_{\sigma}^{\dagger} d_{\sigma} + d_{\sigma}^{\dagger} d_{\bar{\sigma}}) (C_{k\sigma} C_{k'\sigma}^{\dagger} - C_{k\sigma}^{\dagger} C_{k'\sigma} - 1) \right\}, \quad (6d)$$

with

$$A_{k\sigma} = \frac{|t_{kR}|^2}{\omega - \varepsilon_{k\sigma}}; \quad F_{k\sigma} = t_{kR} \left(\frac{1}{\omega + U - \varepsilon_{k\sigma}} - \frac{1}{\omega - \varepsilon_{k\sigma}} \right); \quad (7)$$

$$D_{k\sigma} = |t_{kR}|^2 \left(\frac{1}{\omega + U - \varepsilon_{k\sigma}} - \frac{1}{\omega - \varepsilon_{k\sigma}} \right).$$

Here $S_1(\omega)$ is the second-order self-energy modification from \mathcal{H}_{TR} , including decoupling terms for both the QD and leads. $S_2(\omega)$ and $S_3(\omega)$ result from the Coulomb interaction and will vanish at $U = 0$. $S_2(\omega)$ includes the electron pair exchange terms [28] such as $C_{k\sigma}^{\dagger} d_{\sigma} C_{k'\bar{\sigma}}^{\dagger} d_{\bar{\sigma}}$, which are related to the double occupancy on the QD and can be disregarded in the Kondo regime under consideration. $S_3(\omega)$ represents the Kondo-type spin exchange processes between the QD and leads.

The left tunnelling Hamiltonian \mathcal{H}_{TL} contributes also to the effective self-energy, and it can be obtained from equation (6) by replacing the right lead's parameters with those for the left lead and by setting $\theta = 0$ in it. Having the self-energy, the QD Green's function in equation (5) as well as the ESC in equation (4) can be directly worked out. We first consider the case of

$U = 0$, in which neither $S_2(\omega)$ nor $S_3(\omega)$ makes a contribution to the self-energy, and the contribution of $S_1(\omega)$ to the dot self-energy is given by

$$\Sigma_0^r = \begin{pmatrix} \Sigma_{L\uparrow}^r + \Sigma_{R\uparrow}^r \cos^2 \frac{\theta}{2} + \Sigma_{R\downarrow}^r \sin^2 \frac{\theta}{2} & \frac{1}{2}(\Sigma_{R\uparrow}^r - \Sigma_{R\downarrow}^r) \sin \theta \\ \frac{1}{2}(\Sigma_{R\uparrow}^r - \Sigma_{R\downarrow}^r) \sin \theta & \Sigma_{L\downarrow}^r + \Sigma_{R\uparrow}^r \sin^2 \frac{\theta}{2} + \Sigma_{R\downarrow}^r \cos^2 \frac{\theta}{2} \end{pmatrix}. \quad (8)$$

For the identical FM leads, we have $\Sigma_{L\sigma}^r = \Sigma_{R\sigma}^r = \sum_k A_{k\sigma}$. They are approximately equal to $-i\Gamma_\sigma/2$ with $\Gamma_\sigma = 2\pi\rho_\sigma(\omega)|t|^2$ in the wide band approximation, where $\rho_\sigma(\omega)$ is the spin polarized density of states in FM leads and the weak hopping element t is a constant independent of k . In this case, we obtain the ESC as $J_z = J_x = 0$ and

$$J_y = \frac{-\sin \theta}{4} \int \frac{d\omega}{2\pi} f(\omega) (\Gamma_\uparrow - \Gamma_\downarrow)^2 \text{Im}(1/Z_0), \quad (9)$$

where

$$Z_0 = \left\{ \omega - \varepsilon_d + \frac{i}{2} \left(\Gamma_\uparrow + \Gamma_\downarrow - (\Gamma_\uparrow - \Gamma_\downarrow) \cos^2 \frac{\theta}{2} \right) \right\} \\ \times \left\{ \omega - \varepsilon_d + \frac{i}{2} \left(\Gamma_\uparrow + \Gamma_\downarrow + (\Gamma_\uparrow - \Gamma_\downarrow) \cos^2 \frac{\theta}{2} \right) \right\} + \sin^2 \frac{\theta}{2} (\Gamma_\uparrow - \Gamma_\downarrow)^2 / 16. \quad (10)$$

This indicates that the ESC comes from the exchange coupling between two magnetizations, $\mathbf{M}_L \times \mathbf{M}_R$, which is consistent with the result obtained by other methods [11, 12, 29].

In the finite U case, the Kondo-type spin exchange term $S_3(\omega)$ in equation (6) contributes also to the self-energy. In this step, we employ a mean-field approximation for the lead electron states by using $\langle C_{k\alpha\sigma}^\dagger C_{k'\alpha\sigma'} \rangle = f(\varepsilon_{k\alpha\sigma}) \delta_{\sigma\sigma'} \delta_{kk'}$ and $\langle C_{k'\alpha\sigma'} C_{k\alpha\sigma}^\dagger \rangle = (1 - f(\varepsilon_{k\alpha\sigma})) \delta_{\sigma\sigma'} \delta_{kk'}$. Then the resulting effective self-energy from the Coulomb interaction reads

$$\Sigma_U^r = \begin{pmatrix} X_\downarrow + X_\downarrow \cos^2 \frac{\theta}{2} + X_\uparrow \sin^2 \frac{\theta}{2} & \frac{1}{2}(X_\downarrow - X_\uparrow) \sin \theta \\ \frac{1}{2}(X_\downarrow - X_\uparrow) \sin \theta & X_\uparrow + X_\downarrow \sin^2 \frac{\theta}{2} + X_\uparrow \cos^2 \frac{\theta}{2} \end{pmatrix}, \quad (11)$$

where $X_\sigma = -\sum_k D_{k\sigma} f(\varepsilon_{k\alpha\sigma})$. This self-energy induced by U represents actually the second-order virtual process in which both conducting and localized electrons reverse their spins. Comparing equation (11) with (8), one finds that Σ_U^r and Σ_0^r have the same θ dependence. From consideration of both Σ_U^r and Σ_0^r , we obtain the ESC as

$$J_y = \frac{-\sin \theta}{2} \int \frac{d\omega}{2\pi} f(\omega) \left[\frac{1}{2} (\Gamma_\uparrow - \Gamma_\downarrow)^2 \text{Im}(1/Z_U) - (\Gamma_\uparrow - \Gamma_\downarrow) \text{Re}[(X_\uparrow - X_\downarrow)/Z_U] \right], \quad (12)$$

where

$$Z_U = \left[\omega - \varepsilon_d + \frac{i}{2} \left(\Gamma_\uparrow + \Gamma_\downarrow - (\Gamma_\uparrow - \Gamma_\downarrow) \cos^2 \frac{\theta}{2} \right) - \left(X_\downarrow + X_\downarrow \cos^2 \frac{\theta}{2} + X_\uparrow \sin^2 \frac{\theta}{2} \right) \right] \\ \times \left[\omega - \varepsilon_d + \frac{i}{2} \left(\Gamma_\uparrow + \Gamma_\downarrow + (\Gamma_\uparrow - \Gamma_\downarrow) \cos^2 \frac{\theta}{2} \right) \right. \\ \left. - \left(X_\uparrow + X_\uparrow \cos^2 \frac{\theta}{2} + X_\downarrow \sin^2 \frac{\theta}{2} \right) \right] \\ - \left[\frac{i}{4} \sin \theta (\Gamma_\uparrow - \Gamma_\downarrow) - \frac{1}{2} \sin \theta (X_\downarrow - X_\uparrow) \right]^2. \quad (13)$$

In the presence of U , the J_z and J_x components still vanish and J_y is proportional to $\sin \theta$. It then follows that the Coulomb interaction does not rotate the ESC, i.e., $\mathbf{J}_s \sim \mathbf{M}_L \times \mathbf{M}_R$; while its magnitude decreases with increasing U . The latter stems from the fact that in the second-order virtual process the appearance of nondiagonal terms in equation (11) leads to spin flip effects

on the QD. Although there exists a spin flip on the QD, the Coulomb interaction itself does not result in spin polarization on the QD, nor does the ESC change its direction. In reality, the Coulomb interaction does not break spin symmetry of the QD. In the Kondo regime, the single spin on the QD and lead spins form a spin singlet state, whereas the time-averaged spin on the QD is zero and the QD remains unpolarized. The second term in equation (12) comes from nonzero U , and the expression for the ESC will reduce to equation (9) in the limit of $U = 0$. In the present mean-field approach, we have made the lowest-order perturbation approximation to obtain the self-energy from both U and FM leads on an equal footing. It is expected that if the higher-order processes of Coulomb interactions are taken into account, the direction of the ESC will remain unchanged.

In summary we have investigated the Coulomb interaction influence on the ESC in a quantum-dot spin valve system. In the Kondo regime, although electrons tunnel through the QD by the higher-order virtual processes accompanied by spin flip effect, the ESC direction (spatial spin direction rather than current direction) is given by $\mathbf{J}_s \sim \mathbf{M}_L \times \mathbf{M}_R$, staying unchanged no matter whether nonzero U is present or absent. The physical origin is that the Coulomb interaction itself does not result in the spin polarization on the QD or break its spin symmetry.

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