1. Introduction

With the ever-increasing minimization of electronic devices, reducing power consumption and dissipation of devices has become vital. This issue can be solved by using spintronic devices, which have the potential advantages of faster data processing speed, lower power consumption, and higher integration densities [1, 2]. In realizing spintronic devices, a major challenge is to control and manipulate spin currents, which are useful for spin injection into semiconductors [3–5] and magnetic reorientation of ferromagnets [6–9].

Traditionally, spin currents can be manipulated using magnetic fields, bias voltages, gate voltages, etc. Besides regular electrical methods, the burgeoning research field of ‘spin caloritronics’ offers a new way to manipulate spin currents, viz. thermal manipulation [10, 11]. Interestingly, experiments performed by Cahill et al have provided evidence that spin transfer torques, which are components of a spin current absorbed at an interface, could be enhanced by the intense and ultrafast heat current created by laser light [12]. Due to the simultaneous variation of the temperature, it is not clear whether there is an intrinsic enhancement of spin currents in the transient regime or not. Although electrically-induced transient phenomena have been well investigated for charge currents [13–17] and spin currents [9, 18, 19], little is known about thermally-induced transient spin currents.
Previously, investigations of transient quantum transport phenomena have mostly focused on electrically-driven ones. For a simplest two-probe transport system, one can assume that the system is in equilibrium before an arbitrary time \( t = t_0 \). Then, the nonequilibrium Hamiltonian is added, and the system is in nonequilibrium afterwards \([13, 20]\). However, when the temperature difference between two leads is involved, one cannot assume a sudden temperature variation of a lead at \( t = t_0 \) because the characteristic time scale for lattice dynamics is at least three orders larger than that of electrons \([12]\). Instead, the temperature difference can be set up before \( t = t_0 \) with leads disconnected from the central region. Therefore, to explore thermally-induced transient spin currents under a temperature difference, one can connect leads at various temperatures with the central part instantaneously at \( t = t_0 \). This operation is called a ‘thermal switch’ \([21, 22]\).

In this work, we use the nonequilibrium Green’s function (NEGF) method to investigate the transient spin current under a thermal switch. A closed-form solution is obtained and formulated in terms of steady-state NEGFs, greatly simplifying the transient problem and facilitating further \textit{ab initio} studies. Our formalism is applicable in the entire nonlinear quantum transport regime. Furthermore, we perform a model calculation for a quantum dot coupled to ferromagnetic leads with Lorentzian linewidths. We find that the transient spin current may vary spatially, causing spin accumulation or depletion in the central region. In addition, the transient spin current is enhanced a lot compared to the steady-state thermoelectric spin current: the in-plane components \((x, z)\) of the spin current increase by several orders of magnitude; while the out-of-plane component of the spin current increases by a few percent. Further analysis reveals the dependence of transient spin currents on the temperature, the QD energy level, and the noncollinear angle. Our studies demonstrate that spin currents can be effectively manipulated by thermal switches.

2. Theory

2.1. Model Hamiltonian

Considering a magnetic tunnel junction (MTJ) consisting of an insulating central part \((C)\) and two ferromagnetic leads \((L, R)\), we can write down the Hamiltonian of the system as \([9, 23]\)

\[ \hat{H}_L = \sum_{k, \sigma = \pm 1} \left\{ \varepsilon_{kL\sigma} + sM_L \cos \theta \right. \hat{c}_{kL\sigma}^\dagger \hat{c}_{kL\sigma} + \left. M_L \sin \theta \hat{c}_{kL\sigma}^\dagger \hat{c}_{kL\sigma} \right\}, \]

\[ \hat{H}_R = \sum_{k \sigma} \left[ \varepsilon_{kR\sigma} + sM_R \right] \hat{c}_{kR\sigma}^\dagger \hat{c}_{kR\sigma}, \]

\[ \hat{H}_C = \sum_{m, \alpha} \varepsilon_m \hat{d}_{m \alpha}^\dagger \hat{d}_{m \alpha}, \]

\[ \hat{V} = \sum_{s, m, k, \alpha \in L, R} t_{k, \alpha, s} \hat{c}_{k \alpha s}^\dagger \hat{d}_{m \alpha} + \text{H.c.}, \]

where \( M(L, R) \) is the total magnetic moment of lead \( L(R) \) with unit magnetization vector \( M_L(M_R), \varepsilon_{kL(R)} \) is an energy level with band index \( k \) and spin \( s \) in lead \( L(R) \), \( s = \pm 1, and \) \( \tilde{s} = -s \). In addition, \( \hat{c}_{k \alpha s}^\dagger(\hat{c}_{k \alpha s}) \) creates (annihilates) an electron labeled by \( k \) and \( \alpha \) in lead \( \alpha \). \( \hat{d}_{m \alpha}^\dagger(\hat{d}_{m \alpha}) \) creates (annihilates) an electron with spin \( s \) and energy \( \varepsilon_m \) in the central region \((C)\), which is spin-degenerate. Hopping between \( C \) and lead \( \alpha \) is described by \( t_{k, \alpha, s} \), which is spin-independent. ‘H.c.’ means Hermitian conjugate. In this model, \( M_L \) aligns with the \( z \)-axis, \( M_L \) lies in the \( x-z \) plane, forming a noncollinear angle of \( \theta \) \((0^\circ \leq \theta < 360^\circ)\) with \( M_R \) (see figure 1). In experiments, the magnetization direction of ferromagnetic leads can be manipulated by applying a magnetic field or using pinning layers \([1, 24]\).

2.2. Transient spin currents at \( t > 0 \) under an instantaneous switching-on of connection at \( t = 0 \)

When the connection of leads to the central region is suddenly switched on at \( t = 0 \), the spin current flowing from the central region to lead \( l \) after \( t > 0 \) is

\[ J_{\alpha \in \sigma}^{\text{spin}}(t) = - \int_0^t dt_1 \text{TrRe} \left\{ G'_{\alpha \in \sigma}(t, t_1) \hat{\Sigma}_l^{\in}(t_1, t) \sigma_\alpha \right\} \]

\[ + \hat{G}_{\alpha \in \sigma}(t, t_1) \hat{\Sigma}_l^{\in}(t_1, t) \sigma_\alpha \]

according to equation (A.6). Here, \( \sigma_\alpha \) is a Pauli matrix, \( G'^{(\in)}(t, t_1) \) is the retarded (lesser) Green’s function of the system, and \( \hat{\Sigma}_l^{(\in)} \) is the lesser (advanced) self-energy of lead \( l \). To obtain \( J_{\alpha \in \sigma}^{\text{spin}}(t) \), one needs to obtain the Green’s functions \( G'^{(<)} \) and self-energies \( \hat{\Sigma}_l^{(<)} \).

Self-energies for lead \( l \) are
\[
\sum_{\lambda,\nu',\nu''} g_{\lambda,\nu',\nu''}^{s} (t_{1}, t) = \theta (t_{1}) \theta (t) \sum_{k' \nu'' \lambda, \lambda 
\sum_{k, k' \nu'' \lambda \lambda} t_{k, k' \nu'' \lambda} g_{k, k' \nu'' \lambda}^{s} (t_{1}, t), \tag{6}
\]

where \( \theta (t) \) is the Heaviside step function and \( \gamma = r, a, >, < \). When both time variables are larger than 0, we can also obtain the Fourier transform of the self-energies for the connected system as \( \gamma = 0, t_{1} > 0 \):

\[
\sum_{\lambda, \nu', \nu''} g_{\lambda, \nu', \nu''}^{s} (t_{1}, t) = \int \frac{d \varepsilon}{2 \pi} \sum_{\lambda, \nu', \nu''} g_{\lambda, \nu', \nu''}^{s} (\varepsilon) e^{-i \varepsilon (t - t_{1})}, \tag{7}
\]

where

\[
\sum_{\lambda, \nu', \nu''} g_{\lambda, \nu', \nu''}^{s} (\varepsilon) = \sum_{k, k' \nu'' \lambda \lambda} t_{k, k' \nu'' \lambda} g_{k, k' \nu'' \lambda}^{s} (\varepsilon) \tag{8}
\]

Thus, self-energies actually depend on time difference when both time variables \( t, t' \) are later than 0 \( (t, t_{1} > 0), i.e.,

\[
\Sigma_{\lambda}^{s} (t_{1}, t) = \Sigma_{\lambda}^{s} (t_{1} - t). \tag{9}
\]

After obtaining the steady-state self-energies in equation (8), the double-time self-energies can be determined using equation (7).

For the lesser and retarded Green’s function of the central system, we note the Keldysh formula: \( \text{[25–27]} \)

\[
G^{<} = (1 + G^{r} \Sigma^{r}) G_{0}^{0} (1 + \Sigma^{<} G^{a}) + G^{r} \Sigma^{<} G^{a}, \tag{10}
\]

where a product of two terms is interpreted as a matrix product in the internal variable time. With the first term on the right-hand side rewritten, this equation can be further simplified to \( \text{[28]} \)

\[
G^{<} (t, t') = G^{r} (t, 0) G^{<} (0, 0) G^{a} (0, t') + \int_{0}^{+\infty} dt_{1} dt_{2} G^{r} (t, t_{1}) \Sigma^{<} (t_{1}, t_{2}) G^{a} (t_{2}, t'), \tag{11}
\]

where \( G^{<} (0, 0) \) is the initial population of the central region at \( t = 0 \). From this equation, \( G^{<} \) can be obtained once \( G^{r} \) and the initial population are known. For using a thermal switch at \( t = 0 \), we have \( \text{[26]} \)

\[
G^{<} (t, t') = G^{r} (t, 0) G^{<} (0, 0) G^{a} (0, t') + \int_{0}^{+\infty} dt_{1} dt_{2} G^{r} (t, t_{1}) \Sigma^{<} (t_{1}, t_{2}) G^{a} (t_{2}, t'), \tag{12}
\]

And then, for the retarded Green’s function of the central region, we may utilize the Dyson equation:

\[
G^{r} (t, t') = G_{0}^{r} (t, t') + \int_{0}^{+\infty} dt_{1} dt_{2} G^{r} (t, t_{1}) \Sigma^{<} (t_{1}, t_{2}) G^{a} (t_{2}, t'), \tag{13}
\]

where \( G_{0}^{r} (t, t') \) is the retarded Green’s function of the disconnected central region and depends on \( t - t' \):

\[
G_{0}^{r} (t, t') = G_{0}^{r} (t - t') = \int \frac{d \varepsilon}{2 \pi} G_{0}^{r} (\varepsilon) e^{-i \varepsilon (t - t')}. \tag{14}
\]

By introducing a double-time Fourier transformation of Green’s functions, we can prove that (see appendix B)

\[
G^{r} (t, t') = G^{r} (t - t'), \quad t, t' > 0, \tag{15}
\]

where \( G^{r} (t, t') \) is the retarded Green’s function in the steady-state limit. Its Fourier component \( G^{r} (\varepsilon) \) can be calculated using

\[
G^{r} (\varepsilon) = [\varepsilon + i \eta - H_{0} - \Sigma^{r}]^{-1}. \tag{16}
\]

where \( \eta \) is an infinitesimal positive number. Although the system undergoes a sudden change at \( t = 0 \), the retarded Green’s function \( G^{r} (t, t') \), strikingly, has time-translational invariance when \( t, t' > 0 \). This result is key to our formulas, because it means that the double-time Green’s function \( G^{r} (t, t') \) can be obtained through Fourier transform of \( G^{r} (\varepsilon) \). Then, the double-time lesser Green’s function can be acquired using equation (12), which is in a closed form and does not need iterative calculation.

Finally, the \( \alpha \)-component of the transient spin current flowing into lead \( l \) (equation (5)) can be computed as

\[
J_{\alpha l}^{\text{spin}} = - \int_{-\infty}^{+\infty} d \omega \frac{e^{i (\omega - \varepsilon) t}}{2 \pi \varepsilon} \text{ReTr} \left[ A (\varepsilon, t) \Sigma_{\alpha}^{<} (\varepsilon) \sigma_{\alpha} + B (\varepsilon, t) \Sigma_{\alpha}^{<} (\varepsilon) B_{l} (\varepsilon, t) \sigma_{\alpha} + G^{r} (t, 0) G^{<} (0, 0) G^{a} (\varepsilon) C_{l} (\varepsilon, t) \sigma_{\alpha} \right], \tag{17}
\]

where

\[
A (\varepsilon, t) = G_{l}^{r} (\varepsilon) + \int_{-\infty}^{+\infty} \frac{d \omega}{2 \pi} e^{-i (\omega - \varepsilon) t} G_{l}^{a} (\omega), \tag{18}
\]

\[
B_{l} (\varepsilon, t) = G_{l}^{a} \Sigma_{l}^{<} - \int \frac{d \omega}{2 \pi} e^{i (\omega - \varepsilon) t} G_{l}^{a} (\omega) \Sigma_{l}^{<} (\omega), \tag{19}
\]

\[
C_{l} (\varepsilon, t) = \int \frac{d \omega}{2 \pi} e^{i \omega t} (\varepsilon) e^{-i (\omega - \varepsilon) t}, \tag{20}
\]

respectively. In particular, when the central part is initially unpopulated, the third term in equation (17) is zero. This closed-form formula for the transient spin current greatly simplifies numerical calculations, which would be rather complicated and time-consuming using the perturbation theory \( \text{[21]} \). So far, we have solved for the transient spin current, and the final expression (equation (17)) requires only the steady-state quantities. We shall apply equations (17)–(20) to the simplest spin-degenerate single-level quantum dot model to investigate the transient spin current under a thermal switch.

3. Spin-degenerate single-level QD with Lorentzian bandwidth functions

In the above section, the transient spin current under a thermal switch is expressed as a single integral over energy. In some cases where self-energies of leads are in simple analytic forms, the retarded Green’s function of the central region and even the \( A (\varepsilon, t) \) and \( B_{l} (\varepsilon, t) \) functions can be acquired analytically.
We consider a system which consists of two ferromagnetic (FM) leads and a single-level quantum dot (QD) between the leads. Similar FM/QD/FM systems have been widely studied previously [23, 29–31]. When \( t < 0 \), the three parts are disconnected and in individual thermal equilibrium. When \( t = 0 \), the QD is instantaneously connected to both leads. (See figure 1) Coulomb blockade effects are usually found in single-level quantum dots where the single-electron charging energy \( U_0 \) exceeds the thermal energy \( k_B T \) and the level broadening (\( \gamma_{\uparrow, \downarrow} \)) in below). Therefore, we assume that the bandwidth function oflead \( l \) is well-delocalized, having \( U_0 \) small enough, so that the Coulomb blockade effects can be neglected. The bandwidth function of lead \( l \) (\( \Gamma_l \)), defined as

\[
\Gamma_l = -2\text{Im}\Sigma_l^r,
\]

is also a key factor for transport properties. To obtain analytical results, the bandwidth function is usually supposed to be constant (wide-band limit) [17, 20, 23]. In our work, we go beyond the wide-band limit and introduce the Lorentzian linewidths. We suppose that the bandwidth function of lead \( l \) in parallel configuration (\( \theta = 0 \)) is in Lorentzian line-shape as \([13, 26]\) (see the inset of figure 2(a))

\[
\Gamma_{\sigma}(\epsilon) = \frac{\gamma_{\sigma} W^2}{\epsilon^2 + W^2},
\]

where \( \sigma (= \uparrow, \downarrow) \) labels spin (\( |z \uparrow \rangle, |z \downarrow \rangle \)) states, \( \gamma_{\sigma} \) is the linewidth amplitude of spin-\( \sigma \) channels in lead \( l \), and \( W \) is the bandwidth. Lorentzian linewidths are mathematically convenient, and are widely used to introduce finite-bandwidth effects. The retarded self-energies of leads \( L \) and \( R \) can then be obtained by utilizing the spectral representation of Green’s functions as \([13]\)

\[
\Sigma_{\sigma L}^r(\epsilon) = \int \frac{d\omega}{2\pi} \frac{\Gamma_{\sigma L}(\omega)}{\epsilon - \omega + i0^+} = \frac{1}{2} \frac{\gamma_{\sigma L} W}{\epsilon \pm iW},
\]

\[
\Sigma_{\sigma R}^r(\epsilon) = \frac{W}{2 \epsilon + iW} \left( \gamma_{\sigma R} \right),
\]

\[
\Sigma_{\sigma 0}^r(\epsilon) = \frac{1}{2} \frac{W}{\epsilon + iW} \left( \gamma_{\sigma L} \right)
\]

\[
\Sigma_{\sigma 0}^r(\epsilon) = \frac{1}{2} \frac{W}{\epsilon + iW} \left( \gamma_{\sigma R} \right)
\]

For a general noncollinear angle \( \theta \), the retarded self-energy of the left lead can be written as

\[
\Sigma_{\sigma L}^r = R^\dagger \Sigma_{\sigma L}^0 R
\]

with the rotation matrix \([23]\)

\[
\begin{aligned}
R &= diag \left( \cos \frac{\theta}{2}, -\sin \frac{\theta}{2}, \cos \frac{\theta}{2} \right).
\end{aligned}
\]

With well-defined self-energies, the transient spin current can then be obtained. Analytical results of the auxiliary functions \( A(\epsilon, t) \) and \( B_l(\epsilon, t) \) for this single-level QD model can be found in appendix D.

Before investigating transient behaviors, we would like to present transport properties of the steady-state limit at \( t \to \infty \), where the spin current is driven by the thermal gradient. The steady-state limit restrains the long-time tail, which is necessary for us to get a full picture of the transient behavior. Due to the retarded nature of Green’s functions, all time-related quantities in \( A(\epsilon, t) \) and \( B_l(\epsilon, t) \) vanish when \( t \to \infty \), which means that only the dc component persists to infinite time. Assuming that the initial population on the central QD is zero, we can prove that \([9]\)

\[
J_{Lz}^{dc, spin} = -\frac{1}{2} \int_{-\infty}^{+\infty} \frac{dx}{2\pi} \left( f_L - f_R \right) \text{Tr} \left[ G^r_l G^\dagger_R \Gamma_{Lz} \sigma_{z} \right]
\]

\[
J_{Rz}^{dc, spin} = -\frac{1}{2} \int_{-\infty}^{+\infty} \frac{dx}{2\pi} \left( f_L - f_R \right) \left[ \Gamma_{Rz} (\epsilon) - \Gamma_{Lz} (\epsilon) \right].
\]

Actually, the dc spin current is proportional to the dc charge current \([32]\). This connection can be attributed to the fact that the investigated spin angular momentum is carried by electrons. Under a thermal voltage, the dc spin current is the thermoelectric spin current, which within linear response theory can be expressed as \([33]\)

\[
J_{Lz}^{dc, spin} = \frac{\hbar}{2e} (G_{S\uparrow} S_{\uparrow} - G_{S\downarrow} S_{\downarrow}) \Delta T,
\]

where \( \Delta T = T_L - T_R \), and \( G_{\sigma} (S_{\sigma}) \) is the electrical conductance (Seebeck coefficient) of spin-\( \sigma \) electrons.
4. Results and discussion

To begin with, we choose a particular set of parameters to investigate the transient spin current in detail and focus on the parallel configuration, i.e. $\theta = 0$, where only spin-$z$ current exists. Considering that the bandwidth function in a Phenyldithiol molecular junction could be $\Gamma = 0.11$ eV or $0.0042$ eV \cite{34}, we choose $\gamma_{L}\uparrow = 0.2, \gamma_{L}\downarrow = 0.05, \gamma_{R}\uparrow = 0.02$, and $\gamma_{R}\downarrow = 0.01$ eV, corresponding to leads $L$ and $R$ with spin polarization $60\%$ and $33\%$ respectively. The energy level of QD is $\varepsilon_0 = 0.03$ eV for a better thermoelectric performance, as we shall see below. Also, we assume that the energy level of the QD is initially unoccupied.

In figure 2(a), spin-resolved transmission coefficients are plotted as a function of energy. It shows that transmission spectra of spin-up and down electrons exhibit resonant tunneling peaks near $\varepsilon_0$. Both transmission peaks are in the typical Lorentzian line shape. In particular, the transmission of spin-up electrons has a wider peak than that of spin-down electrons. This phenomenon is due to the stronger coupling between the leads and the central region of the spin-up electrons in our model \cite{25, 35, 36}. Heights of resonant peaks are between the leads and the central region of the spin-up electrons. This phenomenon is due to the stronger coupling of spin-up electrons with the central region estimated as a function of time, corresponding to (a)–(c) respectively. Solid blue lines indicate results obtained using the accumulated number of electrons, and red dots indicate results for conservation of spin angular momentum. The other parameters are set as: $W = 1$ eV, $\varepsilon_0 = 0.03$ eV, $\gamma = 1 \times 10^{-11}$ eV, $T_L = 300$ K, and $T_R = 270$ K.

![Figure 3](image_url)

**Figure 3.** (a)–(c) Transient spin currents at lead $L$ (thin dashed orange line) and $R$ (thick light-blue line) as a function of time at the parallel configuration ($\theta = 0^\circ$) during $t = 0$ to $20$ fs. (a) Leads $L$ and $R$ are different: $\gamma_{L}\uparrow = 0.2, \gamma_{L}\downarrow = 0.05, \gamma_{R}\uparrow = 0.02, \gamma_{R}\downarrow = 0.01$ eV. (b), (c) Leads $L$ and $R$ are identical, where $\gamma_{L}\uparrow = \gamma_{L}\downarrow = \gamma_{R}\uparrow = \gamma_{R}\downarrow$ are set to be (b) $0.2, 0.1$ eV and (c) $0.02, 0.01$ eV respectively. (d)–(f) Accumulated spin angular momentum at the central region estimated as a function of time, corresponding to (a)–(c) respectively. Solid blue lines indicate results obtained using the accumulated number of electrons, and red dots indicate results for conservation of spin angular momentum. The other parameters are set as: $W = 1$ eV, $\varepsilon_0 = 0.03$ eV, $\gamma = 1 \times 10^{-11}$ eV, $T_L = 300$ K, and $T_R = 270$ K.

In figure 2(c), dc spin current $J_{L/R}^{\text{spin}}$ is shown as a function of temperature difference. It is clearly demonstrated that $J_{L}^{\text{spin}} = -J_{R}^{\text{spin}}$, indicative of the steady-state condition and conservation of spin angular momentum. Noting that $J_{L}^{\text{spin}} > 0$, $T_L > T_R$, and that the system is in the electron-like regime, one knows that spin current $J_{L}^{\text{spin}}$ is dominated by hot spin-down electrons transporting from $L$ to $R$. When no temperature difference is present, the spin current should be zero, since no driving force is involved. Then, as the temperature difference $\Delta T = T_L - T_R$ increases within the linear-response regime, the steady-state thermoelectric spin current increases linearly, which is in good agreement with equation (30). It is worth noting that the thermoelectric spin current is about $2.41 \times 10^{-5}$ eV when $\Delta T = 30$ K and $T_R = 270$ K.

Now we move on to obtain the transient spin current as a function of time. Results with three different parameter sets are demonstrated in figure 3. Various coupling strength parameters are chosen to compute the transient spin current in the two leads. As illustrated in figure 3(a), the transient spin current $J_{L(R)}^{\text{spin}}$ starts from zero at $t = 0$, showing reasonable consistency in time domain. Also, the transient spin current flows out of both leads immediately after $t = 0$. In particular, lead $L$, which has higher spin polarization, has a larger transient spin current. Remarkably, the transient spin current of lead $L$ reaches $-0.0248$ eV, which is three orders of magnitude larger than that of the steady-state dc spin current shown in the long-time limit of spin currents when $\Delta T = 30$ K (figure 2(c)). The enhancement factor, 

$$ P(X) = \frac{|X|_{\text{max}}}{|X(t \rightarrow \infty)|}, $$

(31)

is $P(J_{L}^{\text{spin}}) = 1.0 \times 10^3$. Compared with normal enhancement of 1–6 times in electrically-induced transient charge or spin currents \cite{14, 19}, this result demonstrates that the transient spin current can be anomalously larger than the corresponding steady-state thermoelectric spin current.

When the two leads have the same coupling strength with the central QD, the transient spin current has nearly the same magnitude in both leads, as shown in figures 3(b) and (c). This
overlap of the transient spin current in both leads also implies negligible influence of the thermoelectric spin current near $t=0$. Also, when the coupling strength is weakened (figure 3(c) compared to figure 3(b)), the enhancement factor $P$ significantly decreases from $4.9 \times 10^2$ to $1.2 \times 10^2$.

As reflected in figure 2, $J_{L,z}^{\text{spin}} + J_{R,z}^{\text{spin}} = 0$ should be satisfied for steady-state transport. For the transient spin current, $J_{L,z}^{\text{spin}} + J_{R,z}^{\text{spin}} \neq 0$ as made evident in figures 3(a)–(c). Conservation of spin angular momentum implies that there is accumulation or depletion of spins in the central QD:

$$\int_0^t \left( J_{L,z}^{\text{spin}} + J_{R,z}^{\text{spin}} \right) \, dt + \langle S_z(t) \rangle = 0,$$

where $\langle S_z(t) \rangle$ is the expected value of spin angular momentum in the QD at time $t$. Therefore, we may estimate the accumulation of spins using

$$\langle S_z(t) \rangle = -\int_0^t \left( J_{L,z}^{\text{spin}} + J_{R,z}^{\text{spin}} \right) \, dt.$$

Alternatively, the accumulation of spins can be calculated using the number of accumulated electrons:

$$\langle n_\sigma \rangle = \frac{\hbar}{2} \left( \langle n_1 \rangle - \langle n_{-1} \rangle \right),$$

where $\langle n_\sigma \rangle$ is the number of spin-$\sigma$ electrons in the QD:

$$\langle n_\sigma \rangle = -iG_{\sigma \sigma}^{\text{spin}}(t,t).$$

As demonstrated in figures 3(d)–(f), two methods lead to the same results. From figures 3(d)–(f), one can see that after $t=0$ spin angular momentum accumulates quickly to a maximum and then decreases. The accumulation of spins in the central region is in accordance with the time variation of the transient spin current.

As demonstrated above, transient spin currents can be much larger than the steady-state thermoelectric spin currents. To examine the influence of temperature, transient spin currents at different times $t$ as a function of $T_R$ are plotted in figures 4(a)–(d). For $t=0.1, 1$ and 10 fs, the transient spin current in both leads show nearly no dependence on $T_R$. And when $t=1000$ fs, it displays the steady-state signature, where $J_{L,z}^{\text{spin}} = -J_{R,z}^{\text{spin}}$. From figure 4(d), variation of the spin current is up to $3 \times 10^{-5}$ eV. Therefore, the temperature mainly changes the dc thermoelectric spin current, and has little effect on the fast transient region near $t=0$. Interestingly, the independence of the transient spin current near $t=0$ and the quasi-linear dependence of dc thermoelectric spin currents near $t \gg 0$ on $\Delta T$ lead to a rough estimation that the enhancement factor varies with $\Delta T$ in a fashion $\propto 1/\Delta T$.

Thus, the enhancement of $J_{R,z}^{\text{spin}}$ when $\Delta T = 3$ K is about ten times larger than that of $J_{L,z}^{\text{spin}}$ when $\Delta T = 30$ K. By contrast, the transient spin current significantly depends on the quantum dot energy level $\varepsilon_0$, as plotted in figures 4(e)–(h). Although the transient spin current has only a little dependence on $\varepsilon_0$ when $t=0.1$ fs, it changes a lot when $t=1$ fs. Strong dependence is also shown at $t=10$ fs and $t=1000$ fs. For $t=10$ fs, variation is contributed by the transient component. While, for $t=1000$ fs, variation is caused by the steady-state thermoelectric component [33].

Finally, we shall have a short discussion about the dependence of transient spin current on the noncollinear angle $\theta$. In our model, the magnetization direction of lead $R$ is along $z$, thus the $x(y)$ component of the spin current actually corresponds to the in-plane (out-of-plane) spin transfer torque (STT), respectively [9]. For simplicity, we choose identical leads, i.e. the same coupling parameters for leads $L$ and $R$, $\gamma_{\Delta x} = \gamma_{\Delta y}$, and focus on the transient spin current in lead $R$. Results are demonstrated in figure 5. As mentioned above, when $\theta = 0$, both $x$ and $y$ components of the spin current are zero (figure 5). As $\theta$ increases from $0^\circ$ to $90^\circ$, the absolute values of both $J_{R,x}^{\text{spin}}$ and $J_{R,y}^{\text{spin}}$ increase from 0 to their respective maxima.

Figure 4. (a)–(d) Temperature and (e)–(h) $\varepsilon_0$ dependence of the transient spin current at lead $L$ (thin black line) and $R$ (thick red line) at different times: (a) and (e) $t=0.1$ fs; (b) and (f) $t=1$ fs; (c) and (g) $t=10$ fs; (d) and (h) $t=1000$ fs. In (a)–(d), $T_L = T_R + 30$ K; while in (e)–(h), $T_L = 300$ K, $T_R = 270$ K. The other constant parameters are set to be the same as those in figure 3(a).
In addition, the angular dependence of transient \( J_{\text{spin}}^{\text{Ry}} \) and \( J_{\text{spin}}^{\text{Ry}} \) roughly follow the \( \sin \theta \) function, similarly to transient STTs realized using traditional electrical approaches \[19\]. For the in-plane \( J_{\text{Rx}} \), its maximum value in the transient region far exceeds the steady-state limit, which is dominated by the thermoelectric spin current. By contrast, the out-of-plane \( J_{\text{Ry}}^{\text{spin}} \) has a rather large steady-state zero-field STT, and the transient enhancement is very small. The enhancement factor (equation (31)) for the \( x \) and \( y \) components of the spin current are biggest at \( \theta = \pi/2 \), for which we have

\[
P(J_{\text{Lx}}^{\text{spin}}) = 3.9 \times 10^2 \tag{36}
\]

and

\[
P(J_{\text{Ly}}^{\text{spin}}) = 1.16 \tag{37}
\]

respectively. As for the spin-\( z \) current, it is well known that the spin-\( z \) current has its biggest and smallest values at \( \theta = 0^\circ \) and \( \theta = 180^\circ \) respectively. As a result, the noncollinearity angle has a much smaller impact on \( J_{\text{Ry}}^{\text{spin}} \) than on other components.

In summary, we have investigated the transient spin current under a thermal switch using the NEGF method. A closed-form solution has been obtained and formulated in terms of steady-state nonequilibrium Green’s functions. This solution is applicable across the entire nonlinear quantum transport regime, and can be used for further \textit{ab initio} studies\[^8\]. As a model application of the general solution, we perform a model calculation on an FM/QD/FM system, where the connection between the single-level QD and the leads is described by a Lorentzian linewidth function. Interestingly, it shows that the transient spin current may vary spatially, causing spin accumulation or depletion in the central region.Remarkably, the transient spin current is greatly enhanced compared to the dc limit of thermoelectric spin current: the in-plane components \((x, z)\) of the spin current increase by two–three orders of magnitude for a temperature difference of 30 K, while the out-of-plane component of the spin current increases by a few percent. Further analysis shows that the transient spin current near \( t = 0 \) has negligible dependence on temperature, but strongly relies on the QD energy level and the noncollinear angle. The key factor in the transient enhancement of the spin current is the transient nature instead of the temperature gradient. Our studies demonstrate that spin currents can be effectively amplified by thermal switches.

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\[\text{Appendix A. General expression for time-dependent spin currents}\]

The general form of a spin current flowing from the central region to lead \( l \) is \((\hbar = 1)\) \[9\]

\[
J_l^{\text{spin}}(t) = - \sum_{l',i,j} \text{Re} \left[ \sigma_{l',l}^\dagger k_{i\alpha l}^\dagger m \sigma_{n s} G_{n s l}^{<}(t,t') \right],
\tag{A.1}
\]

where \( J_{n s}^{\text{spin}} = (J_{n x}^{\text{spin}}, J_{n y}^{\text{spin}}, J_{n z}^{\text{spin}}) \), \( \sigma = (\sigma_x, \sigma_y, \sigma_z) \), \( \sigma_{s x/s y/s z} \) are Pauli matrices, and the lesser Green’s function is defined as \[20\]

\[
G_{n s l}^{<}(t,t') = i(\epsilon_{l s l}^\dagger(t')d_{n s}(t)).
\tag{A.2}
\]

Assuming that the hopping between lead \( l \) and the central region does not cause spin-flipping, i.e. \( t_{l,i,l',j} = t_{j,l,i,l'} \delta_{\alpha l'} \) is spin-independent, we have

\[
J_l^{\text{spin}}(t) = - \sum_{l',i} \text{Re} \left[ \sigma_{l',l}^\dagger k_{i\alpha l}^\dagger m \sigma_{n s} G_{n s l}^{<}(t,t') \right].
\tag{A.3}
\]

By analytic continuation rules \[20\], the lesser Green’s function \( G_{n s l}^{<}(t,t) \) can be written in terms of Green’s functions of leads in the uncoupled system \( G_{n s l l'}^{\gamma}(t,t') \) and Green’s functions of the central region in the coupled systems \( G_{n s l}^\gamma(t,t') \). Then, the spin current in lead \( l \) turns to be

\[
J_l^{\text{spin}}(t) = \sum_{l',i,j} \int dt' \text{Re} \left\{ \sigma_{l',l}^\dagger \left[ G_{n s l l'}^{\gamma}(t,t') \right] \right\} .
\tag{A.4}
\]

\[^8\] Besides the multi-level QD system investigated, our formulas (equations (17)–(20)) are also applicable for multi-site systems.
where the time-dependent self-energies of lead $l$ are defined as ($\gamma = \sigma, r, a$)

$$
\Sigma_{l}^{\gamma}(t_1, t_2) = \sum_{k', \alpha', k, \alpha} \Gamma_{l}^{\gamma}(k', \alpha', k, \alpha)(t_1, t_2).
$$

Written in matrix form, the $\alpha$-component of the spin-current flowing through lead $l$ (equation (A.4)) is ($\alpha = x, y, z$)

$$
J_{\alpha}^{\text{flow}}(t) = -\int dt \text{Tr} \{ G'_{\alpha}(t, t_1) \Sigma_{l}^{\alpha}(t_1, t) + G_{\alpha}(t, t_1) \Sigma_{l}^{\alpha}(t_1, t) \}
= -\int dt \text{Tr} \{ G'_{\alpha}(t, t_1) \Sigma_{l}^{\alpha}(t_1, t) \sigma_{\alpha} + G_{\alpha}(t, t_1) \Sigma_{l}^{\alpha}(t_1, t) \sigma_{\alpha} \},
$$

where the trace goes over both the spin and orbital degrees of freedom. Here and hereinafter, bold-face quantities are defined in the central region.

**Appendix B.** $G'(t, t') = G'(t - t') \ (t, t' > 0)$ under a sudden thermal switch

To solve out the retarded Green’s function, we introduce a double-time Fourier transform of a function $F(t, t')$ as

$$
F(\epsilon, \epsilon') = \int_{0}^{+\infty} dt \int_{0}^{+\infty} dt' F(t, t') e^{i\epsilon t - i\epsilon' t'},
$$

Note that the integral over time goes from 0 to $+\infty$, differently from the traditional form that goes from $-\infty$ to $+\infty$ [23]. Due to this difference, its inverse transformation is $F(t, t')$ only when both time variables are later than 0:

$$
\int_{-\infty}^{+\infty} \frac{d\epsilon}{2\pi} \int_{-\infty}^{+\infty} \frac{d\epsilon'}{2\pi} F(\epsilon, \epsilon') e^{-i\epsilon t - i\epsilon' t'} = \int \frac{d\epsilon}{2\pi} \int \frac{d\epsilon'}{2\pi} \int_{0}^{+\infty} dt \int_{0}^{+\infty} dt' \epsilon F(u, u') e^{-i\epsilon u - i\epsilon' u'}
= \int \frac{d\epsilon}{2\pi} \int \frac{d\epsilon'}{2\pi} \int_{0}^{+\infty} dt \int_{0}^{+\infty} dt' \epsilon F(u, u') e^{-i\epsilon u - i\epsilon' u'}
= \int_{0}^{+\infty} dt \int_{0}^{+\infty} dt' F(u, u') \delta(u - t) \delta(u' - t')
= F(t, t') \ qquad t, t' > 0.
$$

Under this transform, we may write

$$
G'_{\alpha}(\epsilon, \epsilon') = \int_{0}^{+\infty} dt \int_{0}^{+\infty} dt' G'_{\alpha}(t, t') e^{i\epsilon t - i\epsilon' t'},
$$

$$
G'_{\alpha}(\epsilon, \epsilon') = \int_{-\infty}^{+\infty} \frac{d\epsilon}{2\pi} \int_{-\infty}^{+\infty} \frac{d\epsilon'}{2\pi} G'_{\alpha}(\epsilon, \epsilon') e^{-i\epsilon t - i\epsilon' t'} \ (t, t' > 0).
$$

To work out $G'$ from the Dyson equation (equation (13)), we replace $G'$ in the r.h.s. of equation (13) by the r.h.s. of equation (13) iteratively, obtaining

$$
G'(t, t') = G_{0}'(t, t') + X_1(t, t') + X_2(t, t') + \cdots
$$

where

$$
X_1(t, t') = \int_{0}^{+\infty} dt_1 \int_{0}^{+\infty} dt_2 \Gamma_{0}(t_1, t_2) G_{0}'(t_2, t'),
$$

$$
X_{n+1}(t, t') = \int_{0}^{+\infty} dt_1 \int_{0}^{+\infty} dt_2 X_n(t_1, t_2) G_{0}'(t_2, t').
$$

By utilizing equations (7) and (14), $X_1(t, t')$ can be transformed to

$$
X_1(t, t')
= \int_{-\infty}^{+\infty} \frac{d\epsilon}{2\pi} \int_{-\infty}^{+\infty} \frac{d\epsilon'}{2\pi} G_{0}'(\epsilon, \epsilon') e^{-i\epsilon t - i\epsilon' t'}
= \int_{-\infty}^{+\infty} \frac{d\epsilon}{2\pi} \int_{-\infty}^{+\infty} \frac{d\epsilon'}{2\pi} G_{0}'(\epsilon, \epsilon') e^{-i\epsilon t - i\epsilon' t'}
= \int \frac{d\epsilon}{2\pi} \int \frac{d\epsilon'}{2\pi} \int_{-\infty}^{+\infty} \frac{d\epsilon_1}{2\pi} \int_{-\infty}^{+\infty} \frac{d\epsilon_2}{2\pi} \Sigma'_{\epsilon}(\epsilon_2, \epsilon_1) G_{0}'(\epsilon_2, \epsilon_1)
= \int \frac{d\epsilon}{2\pi} \int \frac{d\epsilon'}{2\pi} \int \frac{d\epsilon_1}{2\pi} \int \frac{d\epsilon_2}{2\pi} \Sigma'_{\epsilon}(\epsilon_2, \epsilon_1) G_{0}'(\epsilon_2, \epsilon_1)
= \int \frac{d\epsilon}{2\pi} \int \frac{d\epsilon'}{2\pi} \int \frac{d\epsilon_1}{2\pi} \int \frac{d\epsilon_2}{2\pi} \Sigma'_{\epsilon}(\epsilon_2, \epsilon_1) G_{0}'(\epsilon_2, \epsilon_1)
= \int \frac{d\epsilon}{2\pi} \int \frac{d\epsilon'}{2\pi} \int \frac{d\epsilon_1}{2\pi} \int \frac{d\epsilon_2}{2\pi} \Sigma'_{\epsilon}(\epsilon_2, \epsilon_1) G_{0}'(\epsilon_2, \epsilon_1)
$$

where

$$
\int_{0}^{+\infty} e^{i\omega t} dt = \frac{i}{\omega + i0^+}
$$

is used, and the integrals over $\epsilon_1$ and $\epsilon_2$ are carried out in the upper half complex plane as shown in figure B1, using residue
theorem. From this result, we know that $X(t, t')$ actually depends on time difference when $t, t' > 0$:

$$X(t, t') = X(t - t') \quad (t, t' > 0) \tag{B.10}$$

with Fourier components

$$X(f) = G_0^\ast (f) \Sigma (f) G_0^\ast (f). \tag{B.11}$$

Similarly,

$$X(t, t') = \int_0^{+\infty} e^{-t} dt \int_0^{+\infty} e^{-t} dt X(t - t') \Sigma (t, t) G_0^\ast (t, t') \tag{B.12}$$

$$= \int_{-\infty}^{+\infty} \frac{e^{-i\omega(t-t')}}{2\pi} X(f) \Sigma (f) G_0^\ast (f) e^{-i\omega(t-t')} \tag{B.13}$$

$$= X(t, t') \tag{B.14}$$

with Fourier components

$$X_2(f) = X_0(f) \Sigma (f) G_0^\ast (f). \tag{B.15}$$

Consequently, for arbitrary integer $n > 0$ and time $t, t' > 0$, we have

$$X_n(t, t') = X(t - t') \tag{B.16}$$

for convenience.

Therefore, the Dyson equation for the retarded Green’s function in equation (13) becomes

$$G(t, t') = G_0(t - t') + X_1(t - t') + X_2(t - t') + \cdots$$

$$= \int \frac{d\omega}{2\pi} \sum_{n=0}^{+\infty} G_0^\ast (\omega) \left( \Sigma (\omega) G_0^\ast (\omega) \right)^n e^{-i\omega(t-t')} \tag{B.17}$$

where $G_0^\ast (\omega)$ is the retarded Green’s function for the disconnected central region,

$$G_0^\ast (\omega) = \left[ \omega + i\eta - H_0 - \Sigma \right]^{-1}, \tag{B.18}$$

and $G'(\omega)$ is the retarded Green’s function for the connected system in steady state [23]

$$G'(\omega) = [\omega + i\eta - H_0 - \Sigma]^{-1}$$

$$= G_0^\ast (\omega) \sum_{n=0}^{+\infty} \left( \Sigma (\omega) G_0^\ast (\omega) \right)^n. \tag{B.19}$$

**Appendix C. $A(f, t)$**

For simplifying the expression for spin currents, we introduce the $A(f, t)$ function as [26]

$$A(f, t) = \int_0^{t} dt' G' (t, t') e^{i\omega(t-t')} \tag{C.1}$$

Its Fourier transform is

$$G'(t, t') = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} A(f, t) e^{-i\omega(t-t')} \quad t, t' > 0. \tag{C.2}$$

Using equation (15), $A(f, t)$ can be rewritten as [13, 26]

$$A(f, t) = G'(f, t) + \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} G' (f, \omega). \tag{C.3}$$

This equation offers a simpler way to calculate the $A(f, t)$. Replacing $\Sigma$ by its Fourier transform, one finds that equation (12) can also be rewritten in terms of $A(f, t)$ as

$$G'(f, t') = G'(t, 0) G^{\ast} (0, 0) G'(0, t')$$

$$+ \int \frac{d\omega}{2\pi} A(f, t) \Sigma (f) A^\dagger (f, t') e^{-i\omega(t-t')} \tag{C.4}$$

This is advantageous over the original form in that the double integral is eliminated, to be replaced by a single integral.

**Appendix D. Analytical formulas for the spin-degenerate single-level QD with Lorentzian bandwidth functions**

The retarded Green’s function of the FM/QD/FM system in the steady-state limit when $\theta = 0$ is

$$G'(\omega)$$

$$= \left[ \omega + i\eta - \omega_0 - \Sigma \right]^{-1}$$

$$= \text{diag} \left( \begin{bmatrix} \omega + i\eta - \omega_1 & \omega + i\eta - \omega_2 \\ \omega - \omega_1 & \omega - \omega_2 \end{bmatrix} \right) \tag{D.1}$$

where $\omega_\sigma (n = 1, 2; \sigma = \uparrow, \downarrow)$ are defined to be poles of the retarded Green’s function through factorization of the denominators as

$$(\omega - \omega_1) (\omega - \omega_2) = (\omega + iW) (\omega + i\eta - \omega_0) - \gamma_\uparrow W/2,$$

$$(\omega - \omega_1) (\omega - \omega_2) = (\omega + iW) (\omega + i\eta - \omega_0) - \gamma_\downarrow W/2$$

with $\gamma_\uparrow = \gamma_{L\uparrow} + \gamma_{R\uparrow}$, $\gamma_\downarrow = \gamma_{L\downarrow} + \gamma_{R\downarrow}$. Note that due to the retarded nature of $G'$, $\{\omega_\sigma\}$ must distribute in the lower half of the complex plane. Bearing this property in mind, we can go forward to get the key functions $A(f, t)$ and $B(f, t)$.

By applying the residue theorem, we can obtain analytical expressions for $A(f, t)$:

$$A(f, t) = \hat{G}'(f)$$

$$+ \text{diag} \left( \begin{bmatrix} \sum_{n=1,2} (-1)^n e^{-i(\omega_\sigma + \varepsilon)t} (\omega_\sigma + iW) \\ \sum_{n=1,2} (-1)^n e^{-i(\omega_\sigma + \varepsilon)t} (\omega_\sigma + iW) \end{bmatrix} \right) \tag{D.3}$$

and $B(f, t)$:
\[
B_t(\epsilon, t) = G^e \Sigma^e + \text{diag}\left(\sum_{n=1,2} \frac{\gamma n W}{2} e^{i (\omega_n^e - \epsilon)} \left(-1\right)^n \left(\omega_n^e - \omega_n^t\right)\right)
\]

In the above, we have acquired explicit analytical expressions for \(A(\epsilon, t)\) and \(B_t(\epsilon, t)\). The transient spin current under a sudden thermal switch can then be calculated by numerically carrying out a single integration over energy in equation (17). For cases with \(\theta \neq 0\), the above procedures can be performed similarly, except that the number of poles doubles when \(\theta \neq 0\) and 180°.

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