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Quantum coherence effect in spin-polarized transport through nano-magnets

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Abstract

Using a simplified toy model, we study the quantum coherence effect in the spin-polarized transport of nano-magnets. A density matrix master equation is used to describe the correlation in the magnet. Through comparison with the classical rate equation, the coherence effect is clearly demonstrated. We find that the interaction between the spin-polarized current and the nano-magnet can be tuned by changing the bias voltage. At small bias voltage, the ferromagnetic lead will induce an antiferromagnetic exchange field. This exchange field is raised from the dynamics of the nondiagonal reduced density matrix elements of the nano-magnet. It is an obvious coherence effect and is beyond the scope of the classical rate equation. When bias voltage increases, tunneling becomes important and the dominating spin control mechanism is the spin accumulation which has been well studied in recent works (Timm and Elste 2006 *Phys. Rev. B* **73** 235304, Timm 2007 *Phys. Rev. B* **76** 014421, Misiorny and Barnas 2007 *Phys. Rev. B* **76** 054448, Barnas *et al* 2000 *Phys. Rev. B* **62** 12363). Our results obviously imply that the coherence effect in the spin-polarized transport of the nano-magnet cannot be ignored even in the collinear structure. This phenomenon is quite different from the case of the quantum dot (QD) spin valve which means that the classical rate equation, which is widely used in the study of the QD spin valve, is invalid for the nano-magnet-based spin valve. A density matrix description becomes essential. Our results are helpful for future investigations of nano-magnet devices.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Due to recent fascinating progress in experiments [5–7], magnetic nanostructures and electronic transport through them have attracted great attention [1–11]. This is not only because of their potential technological applications in quantum computing or information storage [12, 13], but also because of fundamental interest in their intriguing properties [14, 15].

From the point of view of application, using spin-polarized electronic current to manipulate and read the spin information of magnetic nanostructures seems to be the most promising practical scheme for scalable quantum computation and non-volatile memory devices, since it can combine the spin-based devices with conventional semiconductor technology. The study of the transport can also reveal inner information about

nano-magnets because the transport current depends greatly on their internal structures.

Two kinds of nano-magnets have been intensively studied recently. One is the single molecular magnet (SMM). The most famous SMM is the Mn_{12} [5, 6, 9, 10]. It is based on a $\text{Mn}_{12}\text{O}_{12}$ core coupled with organic ligands. In the neutral states, Mn_{12} has a large spin with $S = 10$. Due to the strong easy-axis magnetic anisotropy, there is an energy barrier for a change of spin direction. Hence, without an external magnetic field, the spin information in SMMs can persist for a long time. That is crucial for non-volatile memory devices. Charge transport through SMMs has been studied both theoretically [1–4, 9, 10] and experimentally [5, 6]. The other is the II–VI semiconductor quantum dot (QD) doped with a single Mn atom, which can be considered as an artificial

molecular magnet [7, 8, 16]. In this case, the single Mn atom behaves as a local spin $S = 5/2$ and is coupled with the carriers (electrons or holes) through exchange interaction. The magnetic anisotropy and spin configuration of the single Mn atom are quite different depending on the charge state of the QD. Therefore, we can reversibly manipulate the magnetic properties through electrical or optical control of the charge state of the QD. Conversely, the charge transport through the QD is not only determined by the gate and bias voltages, but also by the quantum state of the local spin.

The theoretical methods to study the transport of the above two systems are similar to the ones used for normal QD systems. The only difference is that the internal structure becomes more complex. As pointed out in the QD system, if the charge number is not the only quantum number of the QD, electrons will not tunnel into an eigenstate but a coherent superposition of states, or entangled states, with the same charge number [17–20]. In this case, the quantum coherence, which is essentially the influence of the dynamics of off-diagonal QD density matrix elements, has to be considered. In order to include the quantum coherence effect, the density matrix master equation should be used instead of the classical rate equation. Quantum coherence manifests itself through the coupling between nondiagonal density matrix elements (coherences) and diagonal ones (occupation probabilities). Without this coupling, the master equation reduces to the classical rate equation. As for transport, in the absence of coupling, the quantum coherence has nothing to do with the tunneling.

The quantum coherence effect has been demonstrated clearly in the QD system. It will play an important role in the double QD system [17, 18] and the single QD system coupled with noncollinear polarized leads [19, 20]. For the QD spin valve (single QD coupled with collinear ferromagnetic leads), the coherence effect is zero and the classical rate equation is exact. However, in the more complicated nano-magnet system, the quantum coherence effect has not been studied much. Recently, one work started to address this issue [21], but detailed calculations to determine the coherence effect in the nano-magnet system are still absent thus far.

In this work, we use a simplified model to elaborate the quantum coherence effect in the spin-polarized transport through a nano-magnet. A detail comparison between the result of the master equation (with the coherences) and that of the rate equation (without the coherences) is given. Our result shows that the coherence effect is essential when the leads are spin polarized, either collinear or noncollinear. This implies that when we study the nano-magnet-based spin valve, the quantum coherence effect becomes a factor that cannot be neglected. The classical rate equation is invalid in this case. We find that the spin control (or manipulation) mechanism via spin-polarized current will change greatly with the bias voltage. When the bias voltage is large, the spin manipulation mechanism is primarily the spin accumulation caused by the asymmetry of the polarizations of the leads. If the bias voltage is small, the manipulation mechanism is quite different from the one with spin accumulation. The ferromagnetic leads will induce an antiferromagnetic exchange field. This completely

results from the quantum coherence and obviously exceeds the scope of the classical rate equation. When the bias voltage is varied, due to the change of the spin manipulation mechanism, the spin state of the nano-magnet can be greatly changed. This phenomenon is useful for further investigation of the spin control of nano-magnets.

Our model and analyses are suitable for both systems mentioned above, namely, either SMM or QD doped with a single Mn atom.

The paper is organized as follows. In section 2, we set up the model Hamiltonian and describe the method employed. Then the numerical result is discussed in section 3. Finally, in section 4, we summarize our work.

2. Model and method

We consider a nano-magnet weakly coupled to two ferromagnetic electrodes. The total Hamiltonian is

$$H = H_c + H_l + H_t. \quad (1)$$

Here, H_c is the central region Hamiltonian of the nano-magnet. For the SMM,

$$H_c = \sum_{\sigma=\{\uparrow,\downarrow\}} \epsilon_0 n_\sigma + U n_\uparrow n_\downarrow - J \mathbf{s} \cdot \mathbf{S}_l - K_2 (\mathbf{S}_l^z)^2 - \mathbf{B} \cdot (\mathbf{S}_l + \mathbf{s}), \quad (2)$$

where $n_\sigma = d_\sigma^\dagger d_\sigma$ is the occupation of the lowest unoccupied molecular orbital (LUMO), d_σ^\dagger (d_σ) is the creation (annihilation) operator of the LUMO electron with spin σ ($\sigma' = \{\uparrow, \downarrow\}$). We also define the LUMO electron spin operator $\mathbf{s} \equiv \sum_{\sigma\sigma'} d_\sigma^\dagger (\boldsymbol{\sigma}_{\sigma\sigma'}/2) d_\sigma$. \mathbf{S}_l is the spin operator of the local spin. ϵ_0 is the onsite energy of the LUMO electron. U is the Coulomb repulsion between two electrons in the LUMO orbital and J is the exchange interaction between the LUMO electron and the local spin. K_2 is the easy-axis magnetic anisotropy.

The main aim of this work is to investigate the quantum coherence effect. In order to make the physics more transparent, we only consider a nano-magnet with local spin $S_l = 1/2$ and do not consider the external magnetic field \mathbf{B} . In this case, $K_2 (\mathbf{S}_l^z)^2$ becomes a constant and the associated term can be neglected. The simplified model is

$$H_c = \sum_{\sigma=\{\uparrow,\downarrow\}} \epsilon_0 n_\sigma + U n_\uparrow n_\downarrow - J \mathbf{s} \cdot \mathbf{S}_l, \quad (3)$$

where $S_l = 1/2$.

The Hamiltonian (3) is a simplified Hamiltonian for the semiconductor quantum dot doped with a single Mn atom if we consider only one electronic orbital in the QD. U is the Coulomb repulsion between electrons in the same orbital and J is the exchange coupling between the carriers and the local spin of the Mn atom. In the self-assembled CdTe QD, the local spin of the doped Mn atom is $S_l = 5/2$. For the same reason mentioned above, in the simplified toy model, we set $S_l = 1/2$.

The Hamiltonian of the ferromagnetic leads is

$$H_l = \sum_{\alpha=\{L,R\}} \sum_{k,\sigma=\{\uparrow,\downarrow\}} \epsilon_{\alpha k \sigma} c_{\alpha k \sigma}^\dagger c_{\alpha k \sigma}, \quad (4)$$

where $\alpha = \{R, L\}$ is the lead index. $c_{\alpha k \sigma}^+$ ($c_{\alpha k \sigma}$) is the create (annihilation) operator of the noninteracting electron in lead α with wavevector k and spin σ (σ'). Here, we use the wide band approximation, i.e. the density of states of each lead $\rho_{\alpha \sigma}$ is independent of the wavevector k . The ferromagnetism of the lead is described by the polarization parameter $P_{\alpha} = (\rho_{\alpha \uparrow} - \rho_{\alpha \downarrow}) / (\rho_{\alpha \uparrow} + \rho_{\alpha \downarrow})$ and we assume the magnetization directions of the leads are collinear.

The tunneling Hamiltonian is

$$H_t = \sum_{\alpha=\{L,R\}} \sum_{k,\sigma=\{\uparrow,\downarrow\}} (t d_{\sigma}^+ c_{\alpha k \sigma} + \text{h.c.}). \quad (5)$$

The tunneling induced broadening is $\Gamma_{\alpha} = \sum_{\sigma} 2\pi |t|^2 \rho_{\alpha \sigma} = \sum_{\sigma} \Gamma_{\alpha \sigma}$.

The eigenstates of Hamiltonian (3) are easy to obtain. For simplicity, we restrict ourselves to the large U limit with $U = \infty$, which is a quite good approximation when the bias voltage is not too large. Thereafter, the double occupation of the LUMO orbital is forbidden. The states of the orbital are $|0\rangle$ (no electron on it), $|\uparrow\rangle$ (one electron with up spin) and $|\downarrow\rangle$ (one electron with down spin). The quantum states of the local spin are $|\uparrow\rangle$ ($m = 1/2$), $|\downarrow\rangle$ ($m = -1/2$), where m is the eigenvalue of S_z^1 . Hence, the entire Hilbert space of the central region is spanned by the states $|0 \uparrow\rangle$, $|0 \downarrow\rangle$, $|\uparrow \uparrow\rangle$, $|\downarrow \uparrow\rangle$, $|\uparrow \downarrow\rangle$, $|\downarrow \downarrow\rangle$, where the first index indicates the state of the orbital and the second one is the state index of the local spin. However, due to the exchange interaction, not all the six states are eigenstates. After diagonalization, the eigenstates are $|0 \uparrow\rangle$, $|0 \downarrow\rangle$, $|\uparrow \uparrow\rangle$, $|+\rangle$, $|-\rangle$, $|\downarrow \downarrow\rangle$. Here

$$|+\rangle = \frac{\sqrt{2}}{2} |\uparrow \downarrow\rangle + \frac{\sqrt{2}}{2} |\downarrow \uparrow\rangle \quad (6)$$

$$|-\rangle = \frac{\sqrt{2}}{2} |\uparrow \downarrow\rangle - \frac{\sqrt{2}}{2} |\downarrow \uparrow\rangle. \quad (7)$$

The three eigenstates $|\uparrow \uparrow\rangle$, $|\downarrow \downarrow\rangle$ and $|+\rangle$ are energy degenerate, $\epsilon_{\uparrow \uparrow} = \epsilon_{\downarrow \downarrow} = \epsilon_+ = \epsilon_0 - \frac{1}{4}J$. Here, ϵ_0 is the onsite energy of the LUMO electron. The eigenenergies of $|0 \uparrow\rangle$ and $|0 \downarrow\rangle$ are degenerate. Actually, it is a constant and we can choose it as zero. The eigenenergy of $|-\rangle$ is $\epsilon_- = \epsilon_0 + \frac{3}{4}J$.

We used the real-time diagram formalism [22] to compute the stationary density matrix and the current. The main idea of this method is to integrate out the electronic degrees of freedom in the leads in order to get the reduced density matrix of the nano-magnet. The starting point is the generalized master equation:

$$\frac{d}{dt} P_{\chi_2}^{\chi_1} + i(\epsilon_{\chi_1} - \epsilon_{\chi_2}) P_{\chi_2}^{\chi_1} = \sum_{\chi_1' \chi_2'} P_{\chi_2'}^{\chi_1'} \Sigma_{\chi_2' \chi_2}^{\chi_1' \chi_1}, \quad (8)$$

where $P_{\chi_2}^{\chi_1} = \langle \chi_2 | \rho | \chi_1 \rangle$ is the element of the reduce density matrix of the nano-magnet. χ_i is the i th eigenstate and ϵ_{χ_i} is the corresponding eigenenergy of the nano-magnet. $\Sigma_{\chi_2' \chi_2}^{\chi_1' \chi_1}$ is the general transition rate from $P_{\chi_2'}^{\chi_1'}$ to $P_{\chi_2}^{\chi_1}$. The transition rate $\Sigma_{\chi_2' \chi_2}^{\chi_1' \chi_1}$ is defined as the sum of all the irreducible self-energy blocked diagrams, which are enclosed by a Keldysh contour. The irreducible self-energy diagram can be expanded in powers of the hybridization Γ_{α} . In the limit of interest of this paper,

i.e. in the sequential tunneling region, only the terms linear in Γ_{α} are retained. A good description of the technical derivation of the transition rate can be found in [25].

Normally, the dynamic equations of the diagonal density matrix elements are decoupled from those of the nondiagonal ones. That gives rise to the classical rate equations

$$\frac{d}{dt} P_{\chi} = \sum_{\chi'} P_{\chi'} \Sigma_{\chi' \chi}, \quad (9)$$

where $P_{\chi} \equiv P_{\chi}^{\chi}$ is the occupation of eigenstate χ and $\Sigma_{\chi \chi'} \equiv \Sigma_{\chi \chi'}^{\chi \chi'}$ is just the normal transition rate. However, if the coupling is nonzero, the density matrix description should be used and we have to consider the quantum coherence effect. In our case, obviously, the quantum coherence effect should be included when the leads are spin polarized. For example, $\Sigma_{+-}^{++} = \sum_{\alpha} \frac{i(\Gamma_{\alpha \uparrow} - \Gamma_{\alpha \downarrow})}{2\pi} \cdot \int d\omega \frac{f_{\alpha}^{-}(\omega)}{\epsilon_- - \omega - \epsilon_0 - i\eta}$, where $f_{\alpha}^{-}(\epsilon) = 1 - f_{\alpha}^{+}(\epsilon)$ and $f_{\alpha}^{+}(\epsilon)$ is the Fermi distribution function of lead α . It means that when the leads are spin polarized, i.e. $\Gamma_{\alpha \uparrow} \neq \Gamma_{\alpha \downarrow}$, P_{+}^{+} is coupled to P_{+}^{-} . For the same reason, we will find that P_{-}^{+} is also coupled to P_{-}^{-} . The case of P_{+}^{-} is similar. P_{+}^{+} and P_{+}^{-} are the only two off-diagonal elements which are connected with the occupation of the SMM in our case. This is essentially the result of the charge and spin conservation laws in the diagrammatic method [25]. Hence, with the master equation description, in total eight equations have to be considered, including the dynamics of P_{+}^{+} and P_{+}^{-} . Meanwhile, for the rate equation, we only need to calculate the six occupation dynamics equations.

Through the comparison of the results of the master equation and the rate equation, we can distinguish the quantum coherence effect in this system. Also, it is meaningful to clarify the condition under which the rate equations is still applicable.

Here, we use $k_B T$ as the energy unit, i.e. $k_B T = 1$ and we only concentrate on the sequential tunneling case, $k_B T \gg \Gamma_{\alpha}$. So, we assume $\Gamma_{\alpha} = 0.1$ hereafter.

3. Results and discussion

In the following, we discuss the numerical results of this simplified model. Due to the simplification, this model allows us to exhibit the physics clearly. Only the stationary case is being considered here, hence, $\frac{d}{dt} P_{\chi_2}^{\chi_1} = 0$.

When the leads are nonmagnetic, i.e. $P_L = P_R = 0$, as expected, the results of the master equation are nearly the same as that of the rate equation. It means that the nondiagonal density matrix elements have nothing to do with the stationary properties. In this case, rate equations are sufficient.

If the leads are ferromagnetic, differences appear. Consider first the case of $P_L = P_R$. With the rate equation, as shown in figure 1, the central region is always nonmagnetic. The expected value of the z component of the molecule's total spin S_z , including the LUMO electron and the local spin, is independent of the polarization and bias voltage. That is to say that for $P_L = P_R$, neglecting the quantum coherence effect in the nano-magnet, the spin-polarized current will not influence the spin state of the molecule.

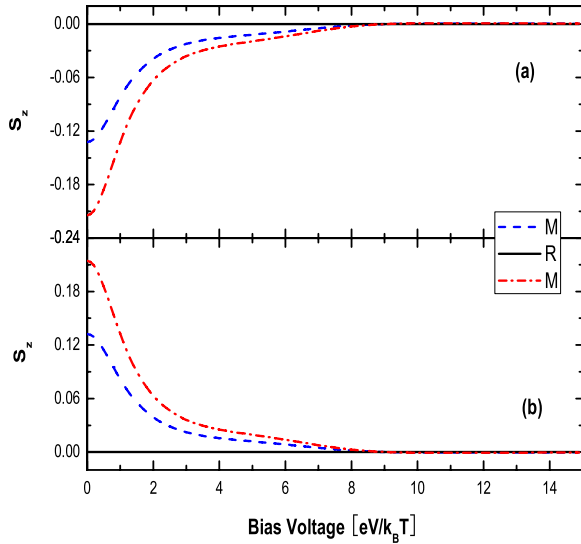


Figure 1. Bias dependence of S_z of the molecule. (a) The red dotted-dashed line is for $P_L = P_R = 0.8$ with the master equations. The blue dashed line is for $P_L = P_R = 0.5$ with the master equations. The black solid line is for $P_L = P_R = 0.8$ with the rate equations. With the rate equation, both the case $P_L = P_R = 0.8$ and 0.5 will give the same result and we only show one of them. (b) The red dotted-dashed line is for $P_L = P_R = -0.8$ with the master equations. The blue dashed line is for $P_L = P_R = -0.5$ with the master equations. The black solid line is for $P_L = P_R = -0.5$ with the rate equations. With the rate equations, both the cases $P_L = P_R = -0.8$ and -0.5 will give the same result and we only show one of them. The M (R) in the legend indicates that the result is calculated with master equation (rate equation). Here, the parameters are $k_B T = 1.0$, $J = 4.0$, $\Gamma_\alpha = 0.1$, $\epsilon_0 = 5.0$.

However, when we take into account the coherence terms, the behaviors are quite different. The SMM can be magnetized by the spin-polarized current even when $P_L = P_R$. Coherence induces an antiferromagnetic interaction between the SMM and the conduction electrons in the leads. It is shown that the larger the polarization of the leads is, the stronger the molecular magnetism is. And when we increase the voltage, S_z decreases monotonically until it reaches zero. This is extremely different from the normal QD spin valve system [23, 24] in which as long as $P_L = P_R$ (symmetrical junction), the QD is always nonmagnetic. The reason for this is that in the single level QD, the charge number is the only quantum number (collinear case) for the tunneling. Hence, coherence is naturally decoupled from the occupations of the QD and there is no exchange field. But in SMMs, due to the more complex inner structure, charge number is no longer the only quantum number of the molecule. Therefore, the exchange field occurs naturally. This exchange field surely can be used to control the spin states of the SMM. We call this spin manipulation mechanism ‘spin torque’, distinguishing it from another magnetization mechanism called ‘spin accumulation’ which we shall discuss later.

Through the comparison in figure 1, we can see that this exchange interaction is clearly absent in the framework of rate equations and is completely a quantum coherence effect, caused by the dynamics of the nondiagonal density matrix elements. It means that, when the bias voltage is small, the

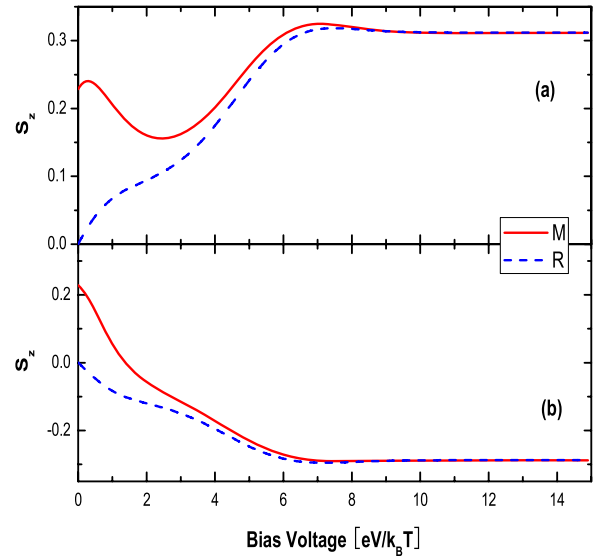


Figure 2. Bias dependence of the S_z of the molecule. (a) The red solid line is for $P_L = -0.8$ and $P_R = -0.9$ with the master equation. The blue dashed line is for $P_L = -0.8$ and $P_R = -0.9$ with rate equation. (b) The red solid line is for $P_L = -0.9$ and $P_R = -0.8$ with the master equation. The blue dashed line is for $P_L = -0.9$ and $P_R = -0.8$ with the rate equation. Other parameters are the same as in figure 1.

classical rate equations are not sufficient for the spin dynamics of the molecule. The full master equation needs to be used.

The spin accumulation mechanism, intensively studied in previous investigations [23, 24], is considered as an effective way to control the spin state of the molecule. It results from the asymmetry of the polarizations of the leads. For example, as shown in figure 2(a), the density of states of the up spin of the left lead is larger than that of the right lead. Hence, if the bias is positive, electrons with up spin will be accumulated in the molecule with increasing bias voltage. Conversely, the electrons with down spin will be accumulated as shown in figure 2(b). Actually, the spin is accumulated on the LUMO and, through the exchange coupling J , changes the spin state of the SMM. However, if bias voltage is small, tunneling is blocked and the spin accumulation will not occur. In this case, the dominating spin control mechanism is just the spin torque mentioned above. In the intermediate bias voltage regime, it will be a combination of (or competition between) the two. From the comparison in figure 2, obviously in order to describe the spin manipulation correctly in all bias voltage regimes, the quantum coherence effect has to be considered, i.e. the master equation is necessary.

The spin accumulation depends on the relative magnitude of the spin polarizations of the leads. But the spin torque is determined by the total polarization of the leads. In figure 2, the total polarization of (a) and (b) are the same. So at small voltage, due to the antiferromagnetic interaction, $S_z > 0$ in both (a) and (b). However, due to the difference in the spin accumulation, different behaviors appear in the transition regime (middle bias voltage). An interesting spin state reversal is realized in figure 2(b). If the total polarization is zero, i.e. $P_L + P_R = 0$, the spin torque disappears because in this

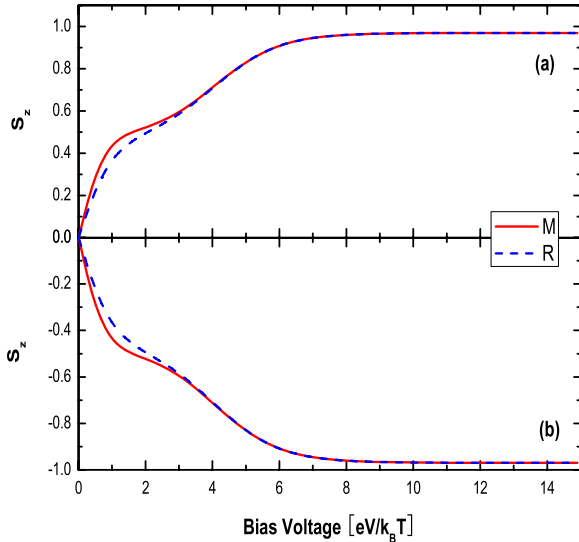


Figure 3. Bias dependence of the S_z of the molecule. (a) The red solid line is for $P_L = 0.9$ and $P_R = -0.9$ with the master equation. The blue dashed line is for $P_L = 0.9$ and $P_R = -0.9$ with the rate equation. (b) The red solid line is for $P_L = -0.9$ and $P_R = 0.9$ with the master equation. The blue dashed line is for $P_L = -0.9$ and $P_R = 0.9$ with the rate equation. Other parameters are the same as in figure 1.

case, the exchange fields of the two leads cancel each other (see figure 3).

In practice, the exchange coupling J can be deduced from the energy levels through experiments. In our model, $J = \epsilon_- - \epsilon_+$. In the single molecule system, normally the energy space is several meV. That is to say that the temperature here is about 10 K.

Although our simple model accounts fairly well for the quantum coherence effect in the spin manipulation, it is not sufficient to describe the influence of the dynamics of nondiagonal density matrix elements on the electronic transport, such as the current. As shown in figure 4, the coherence effect is absent in the current. The reason for this is that in this simple model, we ignore the magnetic anisotropy in the nano-magnet. Hence, due to the energy degeneracy of the spin states, the spin rotation will not influence the transport current. Moreover, this model is too limited and several of the characteristics of a nano-magnet have been neglected. Meanwhile, the interaction between the molecule and the environment, which can surely influence the quantum correlation in the SMM, has also not been considered here. Further theory needs to be developed to study the quantum coherence effect on electronic transport in realistic nano-magnet systems. Such a theory should include the large local spin, easy-axis, transverse magnetic anisotropy and the interaction with the environment. The results presented here can be considered as a first attempt in this direction.

However, we believe that the quantum coherence effect, especially the coherent spin torque mechanism, will play an important role in actual SMM systems. Essentially, there are two main differences between our toy model and an actual

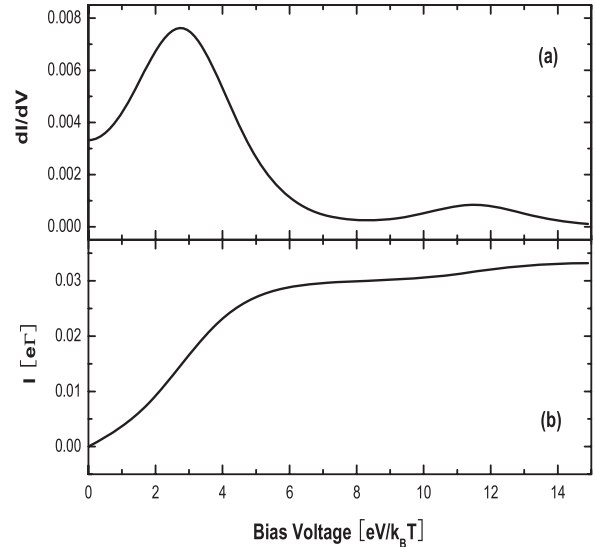


Figure 4. (a) The dI/dV curve. (b) The current through the nano-magnet. With master or rate equations, the currents are exactly the same. $P_L = P_R = -0.5$, $\epsilon_0 = 5.0$ and $J = 8.0$. Other parameters are the same as in figure 1.

SMM system. One is that the local spin of an actual SMM is normally larger than $1/2$, which is used in our toy model. The other is that in an actual SMM system interaction with the environment cannot be avoided. According to a previous work [26], when the spin quantum number increases, the spin-flipping rate of the SMM with spin-polarized current will become lower. That is to say the spin manipulation time τ_m of an actual SMM is longer than that of our toy model. Meanwhile, the influence of the environment on the SMM can be described by the phase coherence time T_2 . Therefore, whether our analysis is suitable for an actual system depends on whether the manipulation time τ_m is much shorter than the phase coherence time T_2 of the SMM. It has been shown that the T_2 of SMMs is of the order of μs at low temperature [27]. As far as we know, there are no experimental data about the manipulation time of SMM with spin-polarized current, but we can deduce it from the domain wall systems. The cycle time for the writing and shifting of the domain walls with spin-polarized current is a few tens of nanoseconds [28]. It is reasonable to suppose that the manipulation time of one SMM with spin-polarized current should not be longer than that of the domain wall system. Therefore, at least for some actual SMM systems, the phase coherence time T_2 is at least ten times larger than the manipulation time τ_m . Thus, in these systems the influence of environment will not overwhelm the coherent spin torque of the spin-polarized current. Our results are suitable for these SMM systems.

4. Conclusion

In summary, we use a simplified model to study the quantum coherence effect, arising from the dynamics of the nondiagonal reduced density matrix elements, in transport through nano-magnets. With the quantum master equation, we find that in

the sequential tunneling case, the current will not only interact with the nano-magnet via an antiferromagnetic exchange field, but also can change the charge states of the nano-magnet. As a result, there are two ways to control the spin states of the nano-magnet by the spin-polarized current, depending on the applied bias voltage. At small bias voltage, the tunneling is weak and the dominating control mechanism is the spin torque due to the antiferromagnetic exchange field between the conduction electrons in the leads and the local molecular spin. Its magnitude depends on the total polarization of the leads. At large bias voltage, tunneling begins to play an important role. In this case, the primary mechanism of the spin control is through spin accumulation, which results from the asymmetry of the polarizations of the leads. In the intermediate bias region, the actual interaction is just the combination of the two mechanisms mentioned above; an intriguing crossover of the spin states can be realized in this region. Through the comparison between the master equation and the classical rate equation, we note that the spin torque results completely from the quantum coherence, which is beyond the framework of the classical rate equations. It means that if we want to understand the spin manipulation of the nano-magnet with a spin-polarized current, the master equation description is essential. Our results demonstrate that the quantum coherence has to be considered carefully in the future study of the nano-magnet-based devices in both spintronics and quantum computing.

Acknowledgments

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