Shot noise of the spin inelastic tunneling through a quantum dot with single molecule-magnet

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We have studied the quantum fluctuations of inelastic spin-electron scattering in quantum dot with an embedded biaxial single molecule-magnet and particularly investigated the zero-frequency shot noise and Fano factor in different magnetic fields. It is found that the shot noise and Fano factor exhibit a stepwise behaviour as bias increases in the presence of interaction between the electron and molecule-magnet for a weak magnetic field. As magnetic field becomes strong, a dip is displayed in the shot-noise-bias curve due to the suppression of inelastic shot noise caused by the quantum tunneling of magnetisation. Because of the spontaneous inelastic tunneling at zero bias, a small shot noise occurs, which results in the case of Fano factor $F \gg 1$. Moreover, our results show that the sweeping speed can also influence the shot noise and Fano factor obviously.

Keywords: quantum dot, shot noise, molecular magnet, quantum tunneling of spin

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1. Introduction

Over the past several decades, great interest has been given to the shot noise accompanying electric current through mesoscopic systems.[1−4] Due to the discrete nature of charge carriers, there is the time-dependent fluctuation, which even persists at zero temperature, around the mean value of electrical current. Shot noise defined as the mean-square fluctuations of the current is of great importance, because the spectrum of shot noise is a powerful tool to provide additional information of the interactions beyond the mean-current properties, which can be used to discern different mechanisms resulting in the same mean current. In classical transport, electrons are uncorrelated, so the shot noise $S(0)$ at the zero frequency is given by a typical Poissonian with a power density $S(0) = 2e\langle I\rangle$, where e is the unit charge and $\langle I\rangle$ is the net average current. However, when the size of device reaches nanoscale, the Pauli's exclusion principle and Coulomb interaction will result in a negative correlation between quantum transport events and lead to shot-noise deviation from the Poissonian form, so the shot noise becomes an important aspect of the electron transport in the mesoscopic system. An important parameter for describing the shot noise in the electron transport is Fano factor $F = S(0)/e\langle I\rangle$, by which the shot noise is classified as a sub-Poissonian noise $F < 1$, Poissonian noise $F = 1$ and super-Possonian noise $F > 1$. In general, the Pauli's exclusion principle induces sub-Poissonian noise while the electron–electron interaction can lead to the super-Poissonian noise.

Recently, a great deal of effort has been paid to the study of quantum transport through single molecule-magnet (SMM), such as Fe_8, Mn_{12}, both theoretically and experimentally.[5−20] These molecules are characterised by the large spin and strong anisotropy energy barrier, the quantum tunneling of spins occurs between the states $|-S\rangle$ and the $|S-n\rangle$ whenever the pair levels become degenerate.[21] The experiment of electron transport through the Mn_{12} attached by nonmagnetic electrodes has shown that the quantum tunneling of SMM plays an important role due to breaking symmetry.[5] Moreover, theoretical investigations have predicted many fascinating transport properties as results of the interplay between the quantum tunneling and electron interaction, such as Kondo effect,[10−12] stepwise conductance[20] and Berry phase blockade.[15] In fact, it is expected to utilise the magnetic anisotropy and quantum tunneling of SMM to modulate quantum transport. The obtained unique features have potential applications in nanoelectronics in the future. However, it is still

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a challenging problem in nanoscience about how to make single-molecule junctions and then understand the emergent transport properties resulting from the quantum nature of SMMs.

Until now, most of theoretical studies on transport through SMM have been focused on properties of current and conductance. Recently, the shot noise through the uniaxial SMM is investigated theoretically by Misiorny *et. al.*[18] with consideration of the cotunneling. They have shown that super-Poissonian shot noise could be observed due to the competition between the elastic and inelastic second-order processes. In the present work, we investigate systematically the shot noise of quantum transport through a quantum dot with an embedded biaxial SMM Fe_8 and a driving magnetic-field which is time dependent. This is achieved by employing the mapping of many-body interaction-system onto a one-body problem with the non-equilibrium Green function (NGF) technique.[22−24] In this framework, electron transport is related to the spin-states of the embedded SMM since if the state $|S-n\rangle$ of SMM is populated with an occupation probability $P_{(S-n)}$ due to the quantum tunneling of magnetisation (QTM), new transport channels are opened. The shot noise for zero-field is enhanced by inelastic transport with the increase of the coupling. However, as the magnetic field increases, more transport channels are opened and shot noise could be suppressed by inelastic tunneling from certain channels at a certain bias. Especially, a small shot noise occurs due to the inelastic tunneling. Moreover, sweeping speed of the magnetic field also affects shot noise.

The rest of this work is organised as follows. In Section 2, we introduce an effective Hamiltonian to describe the interaction between electron-spin and embedded SMM, and establish the formulas of current and shot noise by means of the NGF technique. Section 3 is devoted to the corresponding numerical results and discussion. Finally, a brief summary is given in Section 4.

2. Model and method

We consider electron transport through a single quantum dot (QD) in which an SMM is embedded, with an external magnetic field $\boldsymbol{h}=(h_x,0,h_z)$ applied on the SMM, as shown schematically in Fig. 1.

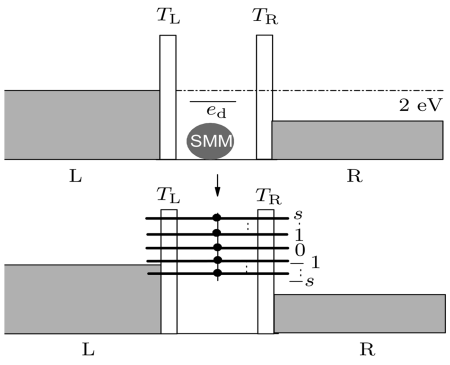


Fig. 1. The schematic illustration of the system consisting of a quantum well (QD) coupled to electrodes with a SMM embedded in the well. The easy axis of the SMM is directed in the Z axis. Each state of the SMM can be visualised as a pseudo-channel, which is connected to the two leads by the hopping parameters $\Gamma_{L/R}$. A symmetric bias-voltage is applied on the leads such that $\mu_{\rm L}=-\mu_{\rm R}=eV$.

The model can be decomposed into three parts $H=H_{\rm QD}+H_{\rm T}+H_{\rm l}$. The Hamiltonian of the QD with an embedded SMM is

$$H_{\rm QD}=\sum_{\sigma}\epsilon_{\sigma}d_{\sigma}^{\dagger}d_{\sigma}+J\widehat{\boldsymbol{s}}\cdot\widehat{\boldsymbol{S}}-g\mu_{\rm B}\boldsymbol{h}\cdot\widehat{\boldsymbol{s}}+H_{\rm SMM}, \quad (1)$$

with the Hamiltonian of SMM

$$\begin{aligned}H_{\rm SMM} =& -K_2(\widehat{S}_z)^2+E((\widehat{S}_x)^2-(\widehat{S}_y)^2)\\ &+C((\widehat{S}_+)^4+(\widehat{S}_-)^4)\\ &-g\mu_{\rm B}(h_z\widehat{S}_x+h_x\widehat{S}_x),\end{aligned}$$

where ϵ_{σ} is the energy level of electron with spin-index σ ($\sigma=\uparrow,\downarrow$), J denotes the exchange-interaction constant between electron-spin $\widehat{\boldsymbol{s}}$ and the total-spin $\widehat{\boldsymbol{S}}$ of SMM; $d_{\sigma}^{\dagger}$ (d_{σ}) is the electron (of spin-σ) creation (annihilation) operator in the QD. The parameters K_2, E, and C with $K_2\gg E\gg C$ describe the anisotropy of SMM, $\mu_{\rm B}$ is Bohr magneton, and the last term of the SMM Hamiltonian is Zeeman energy induced by the applied magnetic field $\boldsymbol{h}$. For simplicity, we assume that the g -factor is identical for both the electron and SMM spins $\boldsymbol{s}$ and $\boldsymbol{S}$. $\widehat{S}_x$, $\widehat{S}_y$, and $\widehat{S}_z$ are three components of the total-spin operator of SMM, and $\widehat{S}_{\pm}=\widehat{S}_x\pm{\rm i}\widehat{S}_y$ are the corresponding raising and lowering operators. $H_{\rm l}$ is the Hamiltonian of the two electrodes denoted by $\alpha=$L,R

$$H_{\rm l}=\sum_{\alpha,k,\sigma}\epsilon_{\alpha k\sigma}c_{\alpha k\sigma}^{\dagger}c_{\alpha k\sigma}, \quad (2)$$

with $\epsilon_{\alpha k\sigma}=\epsilon_{k\sigma}+eV_{\alpha}$, where eV_{α} is the potential bias applied on the α-th electrode, $\epsilon_{k\sigma}$ is the energy of the conduction electrons with spin-$\sigma(\sigma=\uparrow,\downarrow)$ characterised by the wave vector k, and $c_{\alpha k\sigma}^{\dagger}(c_{\alpha k\sigma})$ creates

(annihilates) an conduction electron with spin-σ on the α-th electrode. $H_{\rm T}$ models the coupling between the electrodes and the QD,

$$H_{\rm T} = \sum_{\alpha,k,\sigma} V_{k\alpha} c^{\dagger}_{\alpha k\sigma} d_{\sigma} + {\rm H.C.}, \tag{3}$$

where $V_{k\alpha}$ is the hopping matrix-element between the QD and the electrode-α.

The problem we are facing is to solve the many-body problem involving spin-flip for the electron-spin and the SMM when the electron tunnels through the QD. Following the works of Dong *et al.*,[22,23] we take the direct-product states of electron-spin $|\sigma\rangle$ in QD and the eigenstates of $\widehat{S}_z$ ($\widehat{S}_z|m\rangle = m|m\rangle$)

$$\begin{aligned} &|\, m,\sigma\rangle \\ &= \frac{(S^{\dagger})^m}{\sqrt{(S-m)(S-m+1)}\cdot\ldots\cdot\sqrt{S(S+1)}} c^{\dagger}_{\sigma}\,|0,0\rangle \end{aligned}$$

as the basic state. Similarly, $|m,\alpha k\sigma\rangle$ is the state of conduction electron of spin-σ in the electrode-α along with the SMM in the state $|m\rangle$. Furthermore, we define pseudo-Fermi operators as

$$d^{\dagger}_{m\sigma} = |m,\sigma\rangle\langle 0|\,, \quad c^{\dagger}_{m\alpha k\sigma} = |m,\alpha k\sigma\rangle\langle 0|\,;$$

they satisfy the anti-commutation relation

$$\begin{aligned} &\{d_{m\sigma}, d^{\dagger}_{n\sigma'}\} = \delta_{mn}\delta_{\sigma\sigma'}, \\ &\{c_{m\alpha k\sigma}, c^{\dagger}_{n\alpha' k'\sigma'}\} = \delta_{mn}\delta_{\alpha\alpha'}\delta_{kk'}\delta_{\sigma\sigma'}. \end{aligned} \tag{4}$$

In the new representation, the model Hamiltonian (1)–(3) can be rewritten as an effective Hamiltonian in which transverse terms of SMM are neglected[19]

$$\begin{aligned} \widetilde{H} &= \widetilde{H}_{\rm QD} + \widetilde{H}_{\rm l} + \widetilde{H}_{\rm T} \\ &= \sum_{\sigma,\sigma',m,n} [\epsilon_{m\sigma} d^{\dagger}_{m\sigma} d_{m\sigma} - \lambda_m (d^{\dagger}_{m-1\uparrow} d_{m\downarrow} + d^{\dagger}_{m\downarrow} d_{m-1\uparrow}) + r_x (d^{\dagger}_{m\downarrow} d_{m\uparrow} + d^{\dagger}_{m\uparrow} d_{m\downarrow})] \\ &\quad + \sum_{\alpha,k,\sigma,m} \epsilon_{n\alpha k\sigma} c^{\dagger}_{n\alpha k\sigma} c_{m\alpha k\sigma} + \sum_{m,\alpha,k,\sigma} V_{m\alpha k} c^{\dagger}_{m\alpha k\sigma} d_{m\sigma} + V^{*}_{m\alpha k} d^{\dagger}_{m\sigma} c_{m\alpha k\sigma}, \end{aligned} \tag{5}$$

with $\epsilon_{m\sigma} = \epsilon_d - K_2 m^2 - g\mu_{\rm B} h_z(\sigma/2+m) - J\sigma m/2$, $\lambda_m = (J\sqrt{(S+m)(S-m+1)}\ )/2$, $r_x = g\mu_{\rm B} h_x$ and $\epsilon_{m\alpha k\sigma} = \epsilon_{\alpha k\sigma} - K_2 m^2 - g\mu_{\rm B} h_z(\sigma/2+m)$. $V_{m\alpha k}$ is the hopping matrix element between the m-th pseudo-channel in the electrode-α, which is independent of the spin-σ. The transverse terms of SMM in the $H_{\rm SMM}$ are considered to affect only the probability of states as follows.

With the model Hamiltonian of Eq. (5), the total current flowing from the left electrode can be given by means of NGF technique[22,23,25]

$$I_{\rm L} = \frac{e}{\hbar} \sum_{m,n,\sigma,\sigma'} \int \frac{{\rm d}\omega}{2\pi} \Gamma^{\rm L}_{\sigma} \Gamma^{\rm R}_{\sigma'} \{P(n) f^{\rm L}_n(\omega)(1 - f^{\rm R}_m(\omega)) - P(m) f^{\rm R}_m(\omega)(1 - f^{\rm L}_n(\omega))\} |G^r_{n\sigma,m\sigma'}(\omega)|^2, \tag{6}$$

where $P(n)$ is the probability of the n-th pseudo-channels of the left electrode, $\Gamma^{\alpha}_{\sigma}(\alpha = {\rm L},{\rm R}; \sigma = \uparrow,\downarrow)$ is the linewidth function which is assumed to be independent of the n,

$$\Gamma^{\alpha}_{\sigma} = 2\pi \rho^{\alpha}_{\sigma} |V_{\alpha k}|^2.$$

$G^r_{n\sigma,m\sigma'}(\omega)$ is the Fourier transformation of the retarded Green function of the electron in the dot

$$G^r_{n\sigma,m\sigma'}(t,t') = -{\rm i}\theta(t-t') \left\langle \{d_{n\sigma}, d^{\dagger}_{m\sigma'}\} \right\rangle, \tag{7}$$

and $f^{\eta}_n(\omega) = (1 + {\rm e}^{\omega + K_2 n^2 + g\mu_{\rm B} h_z n - \mu_{\eta}})^{-1}$ is the Fermi–Dirac function of the n-th pseudo-channel in the η lead, which is independent of electron spin. The elastic contribution of the current is given by imposing the constrain elastic tunneling $m = n$

$$I^e_{\rm L} = \frac{e}{\hbar} \sum_{n,\sigma,\sigma'} \int \frac{{\rm d}\omega}{2\pi} \Gamma^{\rm L}_{\sigma} \Gamma^{\rm R}_{\sigma'} P(n) (f^{\rm L}_n(\omega) - f^{\rm R}_n(\omega)) |G^r_{n\sigma,n\sigma'}(\omega)|^2. \tag{8}$$

Shot noise is the time-dependent fluctuation of the electrical current due to the discreteness of the charge of current carriers and can be obtained from Fourier transformation of the correlation $S_{\rm LL}(t)$ between electronic

currents in leads L

$$S_{\rm LL}(t) = \frac{1}{2}\int_{-\infty}^{\infty}[\langle I_{\rm L}(t)I_{\rm L}(0)\rangle + \langle I_{\rm L}(0)I_{\rm L}(t)\rangle - 2\langle I_{\rm L}(t)\rangle\langle I_{\rm L}(0)\rangle], \tag{9}$$

where $\langle\ldots\rangle$ represents the quantum statistical average. Following the works of Dong *et al.*[22,23] and Walczak,[24] the expression for the total spectral density of shot noise in the zero-frequency limit is

$$\begin{aligned} S_{\rm LL}(0) = \frac{e^2}{\hbar}\int\frac{{\rm d}\omega}{\pi}\sum_{m,n,\sigma,\sigma'}\{&[P(m)f_{\rm L}^m(1-f_{\rm L}^n)+P(n)f_{\rm R}^n(1-f_{\rm R}^m)](A_{m,n}^{\sigma,\sigma'})^2 \\ &+[P(m)f_{\rm L}^m(1-f_{\rm R}^n)+P(n)f_{\rm R}^n(1-f_{\rm L}^m)](1-A_{m,n}^{\sigma,\sigma'})A_{m,n}^{\sigma,\sigma'}\} \end{aligned} \tag{10}$$

with $A_{m,n}^{\sigma,\sigma'} = \Gamma_{\sigma}^{\rm L}\Gamma_{\sigma'}^{\rm R}|G^r_{n\sigma,m\sigma'}(\omega)|^2$.

We can also determine the elastic contribution to shot noise by imposing the constraint of elastic tunneling $m = n$

$$\begin{aligned} S_{\rm LL}^{\rm el}(0) = \frac{e^2}{\hbar}\int\frac{{\rm d}\omega}{\pi}\sum_{n,\sigma,\sigma'}P(n)\{&[f_{\rm L}^n(1-f_{\rm L}^n)+f_{\rm R}^n(1-f_{\rm R}^n)](A_{n,n}^{\sigma,\sigma'})^2 \\ &+[f_{\rm L}^n(1-f_{\rm R}^n)+f_{\rm R}^n(1-f_{\rm L}^n)](1-A_{n,n}^{\sigma,\sigma'})A_{n,n}^{\sigma,\sigma'}\}. \end{aligned} \tag{11}$$

The Fano factor, which describes the deviation of current noise from its Poissonian value, is defined as

$$F = \frac{S_{\rm LL}(0)}{2e\langle I_{\rm L}\rangle}, \tag{12}$$

where $\langle I_{\rm L}\rangle$ is the average current. Equations (10), (11), and (12) are the main results of the present paper.

Following our previous paper,[19] we can have the matrix-form of the retarded (advanced) Green function $\boldsymbol{G}^{r(a)}$ in the wide band approximation in terms of the equation-of-motion technique

$$((\omega \pm {\rm i}\Gamma)\boldsymbol{I} - \boldsymbol{M})\boldsymbol{G}^{r(a)} = \boldsymbol{I}, \tag{13}$$

where $\boldsymbol{I}$ is the unit matrix, $\Gamma = \sum_{\sigma}(\Gamma_{\sigma}^{\rm L} + \Gamma_{\sigma}^{\rm R})$ is the linewidth function and $\boldsymbol{M}$ is the $(2S+1)\times(2S+1)$ symmetrical tridiagonal matrix:

$$\boldsymbol{M} = \begin{pmatrix} \epsilon_{s\uparrow} & r_x & 0 & 0 & . & . & . & . & . & 0 \\ r_x & \epsilon_{s\downarrow} & \lambda_s & 0 & . & . & . & . & . & . \\ 0 & \lambda_s & \epsilon_{(s-1)\uparrow} & r_x & . & . & . & . & . & . \\ 0 & 0 & r_x & ... & . & . & . & . & . & . \\ . & . & . & . & \epsilon_{m\uparrow} & r_x & 0 & 0 & . & . \\ . & . & . & . & r_x & \epsilon_{m\downarrow} & \lambda_m & 0 & . & . \\ . & . & . & . & . & \lambda_m & ... & r_x & 0 & 0 \\ . & . & . & . & . & 0 & r_x & \epsilon_{-(s-1)\downarrow} & \lambda_{-(s-1)} & 0 \\ . & . & . & . & . & . & 0 & \lambda_{-(s-1)} & \epsilon_{-s\uparrow} & r_x \\ 0 & . & . & . & . & . & 0 & 0 & r_x & \epsilon_{-s\downarrow} \end{pmatrix}.$$

The remaining task is to derive the probability $P(n)$ of channel n (or state of SMM $|n\rangle$), which appears in Eqs. (6), (10), and (11). In the absence of the transverse terms of $H_{\rm SMM}$, $E_n = -K_2n^2 - g\mu_{\rm B}h_zn$ is the the energy level of the state $|n\rangle$ with $h_z = ct$, where c is the field sweeping speed. When the initial state is the saturated state $|-S\rangle$, the quantum tunneling occurs between the degenerate states $|-S\rangle$ and $|S-n\rangle$ in the resonant fields $h_z = h_n = nK_2/g\mu_{\rm B}$. As pointed out by Rastelli and Tassi,[26] $H_{\rm SMM}$ can be reduced to an effective time-dependent Hamiltonian $\widetilde{H}_{\rm SMM}$ by utilising the two-level approximation

$$\widetilde{H}_{\rm SMM} = \begin{pmatrix} -(S-n)g\mu_{\rm B}ct & \Delta_n/2 \\ \Delta_n/2 & Sg\mu_{\rm B}ct \end{pmatrix},$$

where Δ_n is the tunneling splitting between $|-S\rangle$ and $|S-n\rangle$. The transition probabilities

$$P_{(S-n)} = (1-F_n)\left(\prod_{j=0}^{n-1} F_j\right),\ P_{(-S)} = \prod_{j=0}^{n-1} F_j, \quad (14)$$

are written as an analytical form by Kim and Kim,[20] where $F_j = \exp(-2\pi\lambda'_j)$ with $\lambda'_n = 1/(8\alpha_n\gamma_n^2)$, $\alpha_n = (2S-n)/(2\gamma_n)$, and $\gamma_n = \hbar g\mu_{\rm B}c/\Delta_n^2$.

3. Numerical result

In this section, we present the numerical result of zero-frequency shot noise through QD with SMM. In our calculation, we have made use of the parameters of Fe_8[26] as follows: $K_2 = 0.292$ K, $E = 0.046$ K, $C = -0.000064$ K and the total spin is $S = 10$. The tunneling splits Δ_n are adopted as listed in Table 1 in Ref. [22] for $h_x = 0.1h_z$. For simplicity, we set $e = \hbar = g\mu_{\rm B} = 1$ in the rest of the paper. Other parameters for the QD are $\Gamma = 0.04$, $k_{\rm B}T = 0.025$. In Figs. 2(a) and 2(b), respectively, we plot both total current and shot noise as functions of bias in a vanishing external-field $h = 0$ T. It is obvious that the current and shot noise have similar stepwise characteristics as the bias increases. When the electron does not couple to the SMM i.e. $J = 0$, the behaviour of the system is reduced to the normal single-level QD, only one-step structure appears when the bias matches the Fermi surface of electrode with the energy level of the QD, $\epsilon_{\rm d}$. In the presence of coupling J, more steps are present. This means that more channels have involved in the transport. With the increase of coupling J, the main step shifts with suppressed height, simultaneously new steps appear at higher voltages and the step-height is enhanced obviously. The only difference between the behaviours of current and shot noise is that inelastic noise can exceed the shot noise for non-SMM case at higher bias. Moreover, the value of elastic noise becomes higher with the increase of the coupling J as well as the total noise.

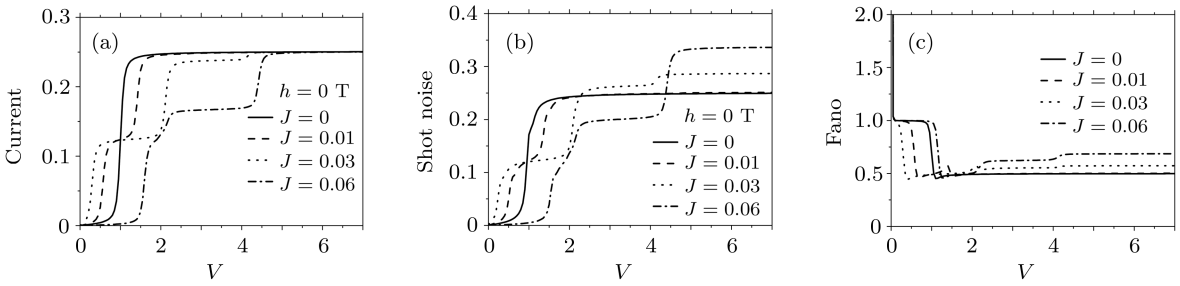


Fig. 2. The bias dependence of the current (a), shot noise (b) and Fano factor (c) in a magnetic field $h = 0$ T for different exchanging coupling $J = 0$ (solid line), $J = 0.01$ (dashed line), $J = 0.03$ (dot line) and $J = 0.06$ (dot-dashed line).

The Fano factor plot is depicted in Fig. 2(c) as a function of the bias at $h = 0$ T for different J. At very low bias i.e. $eV < k_{\rm B}T$, noise is mainly contributed by the thermal noise and the Fano factor is divergent at $V = 0$. As the bias increases and becomes larger than the thermal energy, shot noise dominates. The Fano factor is equal to $F = 1$ in the region below the single-level resonance where the tunneling events are uncorrelated. In contrast, the Fano factor have a tendency to become $F = 1/2$ in high-bias for $J = 0$. The crossover from the Poissonian($F = 1$) to the sub-Poissonian ($F < 1$) is a step, which appears when the bias matches the Fermi surface of the -10-th pseudo channel with energy level of the states $|-10, \downarrow\rangle$. In addition, more fine structures can be observed in the plot. At the coupling $J = 0.01$, a peak occurs for the Fermi surface equals the pseudo energy levels. However, when the interaction between the SMM and electron is strong, steps are exhibited at the resonant energy levels instead of peaks. Moreover, we can observe that the Fano factor is obviously enhanced by the interaction with SMM.

In the region of $h \leq 0.429$ T, the quantitative behaviour is similar to the case of $h = 0$ T except for a little shift of the step-position due to the Zeeman effect. This is because the probabilities $P(n)$ have not

transferred almost from the initial state $|-10\rangle$ at the resonant field for different sweeping speed.

Figure 3 is the plot of calculated shot noise and Fano factor as functions of bias V with the field $h = 0.6$ T. In Fig. 3(b), the shot noise is shown for different coupling J with scanning speed 0.14 T/s. For the case of $J = 0$, two steps appear due to the Zeeman effect. With increasing coupling J, more steps are displayed in the plot due to more pseudo-channels in the transport. Moreover, the shot noise in $h = 0.6$ T displays a different behaviour from the case of $h = 0$ T. From Figs. 3(b) and 3(c), we can observe that a small shot noise S_0 exists at $V = 0$. When J is strong, S_0 is strengthened obviously and a dip is seen in the $S - V$ curve, which corresponds to the negative differential shot noise. To understand these phenomena, we consider a simple model with negligibly small h_x, so the pseudo energy levels of QD can be calculated approximately by diagonalising the following matrix

$$\begin{pmatrix} \epsilon_{m\downarrow} & \lambda_m \\ \lambda_m & \epsilon_{(m-1)\uparrow} \end{pmatrix}$$

with corresponding states

$$\left|\Phi^-_{m,m-1}\right\rangle = \frac{1}{2\lambda_m}[2\lambda_m \left|(m-1)\uparrow\right\rangle - c^{(-)}_{m,m-1}\left|m\downarrow\right\rangle],$$
$$\left|\Phi^+_{m,m-1}\right\rangle = \frac{1}{2\lambda_m}[2\lambda_m \left|(m-1)\uparrow\right\rangle - c^{+}_{m,m-1}\left|m\downarrow\right\rangle],$$

where

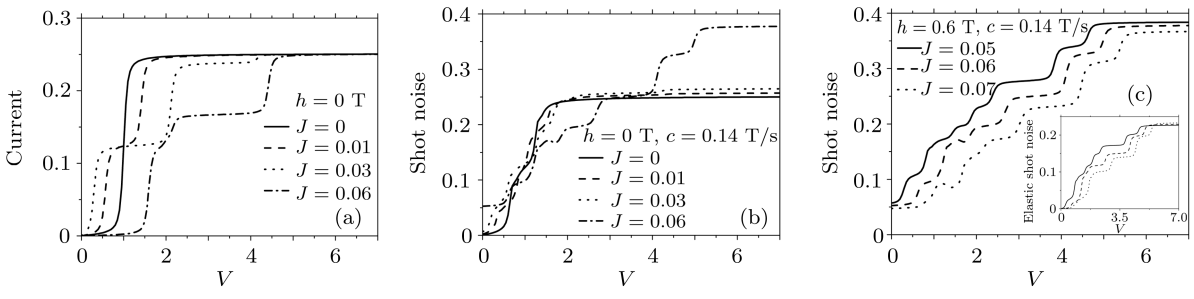
$$c^{(-)}_{m,m-1} = (\epsilon_{(m-1)\uparrow} - \epsilon_{m\downarrow} + \sqrt{4\lambda_m^2 + (\epsilon_{(m-1)\uparrow} - \epsilon_{m\downarrow})^2}),$$

and

$$c^{(+)}_{m,m-1} = (\epsilon_{(m-1)\uparrow} - \epsilon_{m\downarrow} - \sqrt{4\lambda_m^2 + (\epsilon_{(m-1)\uparrow} - \epsilon_{m\downarrow})^2}).$$

The pseudo energy levels and inelastic shot noise from the 8-th channel are shown in Figs. 3(d) and 3(e). The Fermi surface of the 8-th pseudo channel is higher than the pseudo level of $\left|\Phi^-_{9,8}\right\rangle$ which is higher than the Fermi surface of 9-th channel at zero bias, so the inelastic transport from the 8-th channel to the 9-th channel occurs spontaneously through the state $\left|\Phi^-_{9,8}\right\rangle$ of QD without bias (as schematically depicted in the Fig. 3(d)). Because of the symmetric configuration for normal electrodes, currents from the left and right electrodes cancel out each other and total current is zero at the zero bias, but the shot noise S_0 is nonzero due to fluctuation of the spontaneous inelastic tunneling. In the Fig. 3(e), we plot the inelastic contributions from the 8-th pseudo-channel for $J = 0.05$ and $J = 0.07$. For the component from the 8-th to the 9-th pseudo channel, an inelastic shot noise is displayed at zero bias. Once the tunneling from the 8-th pseudo channel to the level of $\left|\Phi^+_{9,8}\right\rangle$ becomes energetically allowed, the components of shot noise from the 8-th channel increases to the plateau. When bias is further increased to allow the level of $\left|\Phi^-_{9,8}\right\rangle$ to be lower than the Fermi surfaces of the 9-th left channel and the 8-th right channel at $V = 1.9$ and $V = 4.6$ respectively, the shot noise is suppressed. Further suppression can be also observed at $V = 2.4$ for the component from the 8-th to 9-th pseudo channel, when the bias-voltage matches the Fermi energy of the left 9-th channel with the level of $\left|\Phi^+_{9,8}\right\rangle$. Furthermore, the plateau becomes narrower and the elastic shot noise is enhanced as coupling J becomes strong.

The resulting Fano factor is plotted as a function of bias for $h = 0.6$ T in Fig. 3(f). At higher bias, the shot noise is dominated by the sub-Poissonion process, i.e., Fano factor $F < 1$, the Fano factor is enhanced by the interaction with SMM as in the case of $h = 0$ T. In the region of low bias, i.e., below the level resonance, spontaneously inelastic tunneling processes from the 8-th channel will enhance the shot noise S_0, which results in $F \gg 1$.



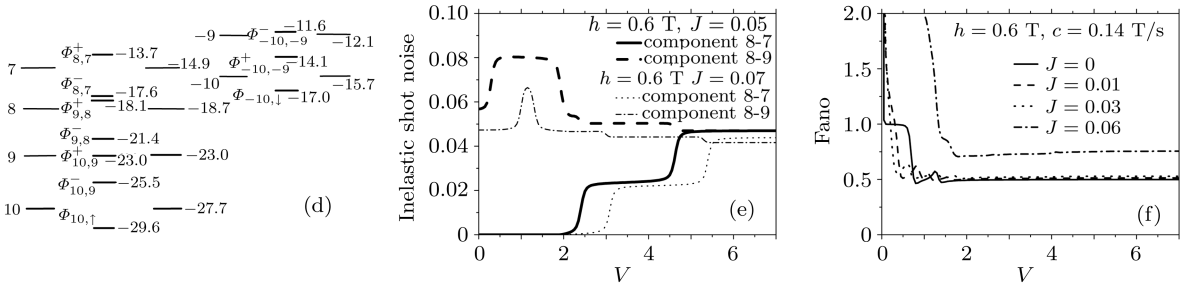


Fig. 3. The shot noise and Fano factor in a magnetic field $h = 0.6$ T as functions of bias V: current (a) and total shot noise (b) versus V for different exchanging coupling $J = 0$ (solid line), $J = 0.01$ (dashed line), $J = 0.03$ (dotted line) and $J = 0.06$ (dot-dashed line); (c) the elastic total noise versus V with strong couplings $J = 0.05$ (solid line), $J = 0.06$ (dashed line) and $J = 0.07$ (dotted line); (d) The pseudo-energy spectrum of the dot and electrodes with coupling $J = 0.06$. (e) Inelastic shot noise versus V from the 8-th channel with different couplings $J = 0.05$ (thick lines) and $J = 0.07$ (thin lines). (f) the Fano factor as a function of V with $h = 0.6$ T for different coupling $J = 0$ (solid line), $J = 0.01$ (dashed line), $J = 0.03$ (dotted line) and $J = 0.06$ (dot-dashed line). The inset in (c) is the elastic shot noise versus bias V.

The influence of sweeping speed on the shot noise is shown in Fig. 4. When the sweeping speed is modulated to $c = 0.014$ T/s, the transition probability of SMM states almost transfers from the state $|-10\rangle$ to the state $|8\rangle$ according to Eq. (14), and the transport is mainly contributed by the component coming from the 8-th pseudo-channel. Thus some steps related to the 8-th pseudo channel are enhanced. In contrast, steps related to the –10-th pseudo-channel are suppressed and even vanish in the plots of $I - V$ and $S - V$, as shown in Figs. 4(a) and 4(b). When the coupling is strong, a basin is exhibited instead of the dips in $S - V$ diagram due to inelastic shot noise from the 8-th channel. As the coupling increases, the basin becomes wider with the suppression of noise. For comparison between different sweeping speeds, we plot the shot noise and Fano factor with $J = 0.06$ and 0.07 in Figs. 4(e) and 4(f), and observe that the shot noise and Fano factor at $c = 0.014$ T/s are larger than those at $c = 0.14$ T/s. In addition, in the case of $c = 0.014$ T/s, steps are observed obviously in $F - V$ diagram at lower bias for $J = 0.03$ and 0.06, as shown in Fig. 4(d).

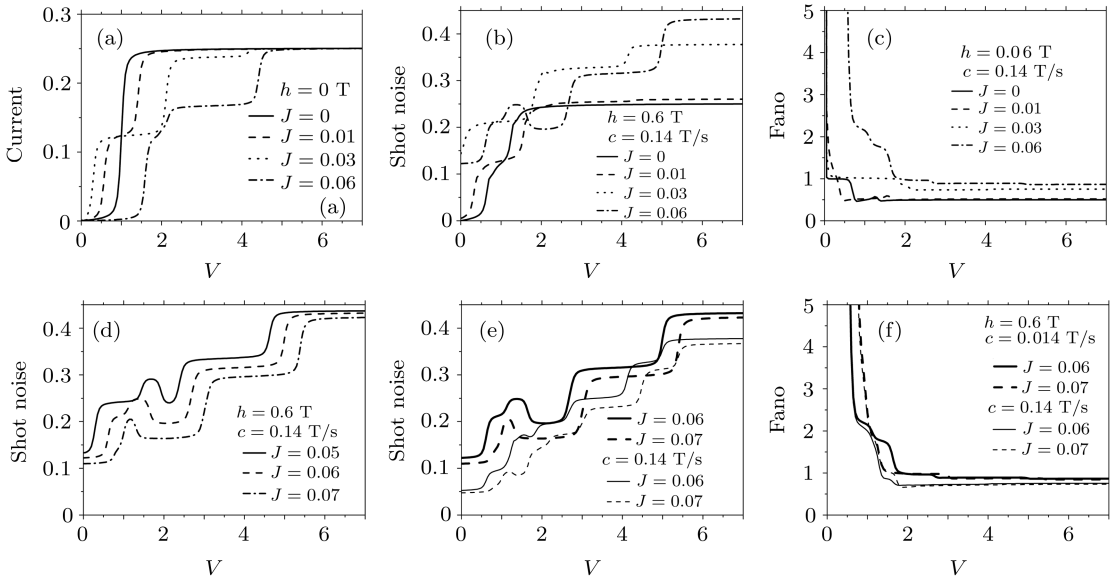


Fig. 4. The shot noise and Fano factor with magnetic field $h = 0.6$ T and $c = 0.014$ T/s as functions of bias V: (a) total current and (b) shot noise versus V for different exchanging couplings $J = 0$ (solid line), $J = 0.01$ (dashed line), $J = 0.03$ (dotted line) and $J = 0.06$ (dot-dashed line); (c) Fano factor versus bias V for different couplings; (d) the shot noise for strong couplings versus bias V; (e) and (f) the comparison of shot noise and Fano factor between the case of $c = 0.014$ T/s and $c = 0.14$ T/s with strong coupling, respectively.

4. Summary

Using the nonequilibrium Green function technique, we have systematically investigated the shot noise properties of a single-level QD with an embedded SMM of saturated state $|-10\rangle$. We find that the shot noise and the Fano factor strongly depend on the magnetic field h and coupling J. In the absence of magnetic field, stair-like shapes are observed in $S-V$ diagram, and Fano factor is enhanced with the increase of coupling J. At the magnetic field value $h = 0.6$ T, other states are populated due to the quantum tunneling, a small shot noise S_0 is generated below level resonance which leads to the case of $F \gg 1$ at the lower bias. When coupling J is strong, we also observe that a dip is exhibited in the $S-V$ diagram due to the suppression of inelastic tunneling. When the sweeping speed is modulated to $c = 0.014$ T/s, a basin is exhibited instead of the dip in the plot of $S-V$, because the transition probability of SMM states almost transfers from the state $|-10\rangle$ to the state $|8\rangle$. Meanwhile, the shot noise and Fano factor are enhanced.

References

[1] Blanter Ya M and Büttiker M 2000 *Phys. Rep.* **336** 1
[2] Ou-Yang S H, Lam C H and You J Q 2010 *Chin. Phys.* B **19** 050519
[3] An X T, Li Y X and Liu J J 2007 *Acta Phys. Sin.* **56** 4105 (in Chinese)
[4] Liang J Q, Wang R and Wang J M 2007 *Chin. Phys.* **16** 2075
[5] Heersche H B, Groot Z, der Folk J A, van der Zant H S J, Romeike C, Wegewijs M R, Zobbi L, Barreca D, Tondello E and Cornia A 2006 *Phys. Rev. Lett.* **96** 206801
[6] Romeike C, Wegewijs M R, Ruben M, Wenzel W and Schoeller H 2007 *Phys. Rev.* B **75** 064404
[7] Elste F and Timm C 2007 *Phys. Rev.* B **75** 195341
[8] Timm C 2007 *Phys. Rev.* B **76** 014421
[9] Elste F and Timm C 2006 *Phys. Rev.* B **73** 235305
[10] Romeike C, Wegewijs M R, Ruben M, Wenzel W and Schoeller H 2006 *Phys. Rev. Lett.* **96** 196601
[11] Romeike C, Wegewijs M R, Ruben M, Wenzel W and Schoeller H 2006 *Phys. Rev. Lett.* **97** 206601
[12] Leuenberger M N and Mucciolo E R 2006 *Phys. Rev. Lett.* **97** 126601
[13] Misiorny M and Barnaś J 2007 *Phys. Rev.* B **75** 134425
[14] Misiorny M and Barnaś J 2007 *Phys. Rev.* B **76** 054448
[15] Gonzalez G and Leuenberger M N 2007 *Phys. Rev. Lett.* **98** 256804
[16] Timm C and Elste F 2006 *Phys. Rev.* B **73** 235304
[17] Lu H Z, Zhou B and Shen S Q 2009 *Phys. Rev.* B **79** 174419
[18] Misiorny M, Weymann I and Barnaś J 2009 *Phys. Rev.* B **79** 224420
[19] Chang B and Liang J Q 2010 *Phys. Lett.* A **373** 2985
[20] Kim G H and Kim T S 2004 *Phys. Rev. Lett.* **92** 137203
[21] Wernsdorfer W and Sessoli R 1999 *Science* **284** 133
[22] Dong B, Cui H L and Lei X L 2004 *Phys. Rev.* B **69** 205315
[23] Dong B, Cui H L, Lei X L and Horing N J M 2005 *Phys. Rev.* B **71** 045331
[24] Walczak K 2006 *J. Magn. Magn. Mater.* **305** 475
[25] Jauho A P, Wingreen N S and Meir Y 1994 *Phys. Rev.* B **50** 5528
[26] Rastelli E and Tassi A 2001 *Phys. Rev.* B **64** 064410