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RAPID COMMUNICATION

Electrically tunable spin diode effect in a tunneling junction of quantum dot*

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Control over the tunneling current in spintronic devices by electrical methods is an interesting topic, which is experiencing a burst of activity. In this paper, we theoretically investigate the transport property of electrons in a spin-diode structure consisting of a single quantum dot (QD) weakly coupled to one nonmagnetic (NM) and one half-metallic ferromagnet (HFM) leads, in which the QD has an artificial atomic nature. By modulating the gate voltage applied on the dot, we observe a pronounced decrease in the current for one bias direction. We show that this rectification is spin-dependent, which stems from the interplay between the spin accumulation and the Coulomb blockade on the quantum dot. The degree of such spin diode behavior is fully and precisely tunable using the gate and bias voltages. The present device can be realized within current technologies and has potential application in molecular spintronics and quantum information processing.

Keywords: half-metallic ferromagnet, quantum dots, spin blockade, spin dependent electron tunneling

PACS: 72.25.–b, 72.15.Jf, 85.80.Lp **DOI:** 10.1088/1674-1056/ab53d0

1. Introduction

A key challenging problem in modern physics is understanding and controlling electronic transport properties of low-dimensional systems, such as molecules, graphene, and nanowires.[1–3] A quantum dot (QD) is an artificial nanoscale structure that can be filled with electrons or holes.[4] Two or more QDs can be coupled together to form multiple-QD systems, such as artificial molecules.[5–7] Because the degrees of freedom of the QDs are well controlled, it is possible to add or remove the electrons in the QDs, and the QD system can be coupled via tunneling barriers to electrodes, with which electrons can be exchanged. If a quantum dot is connected to two ferromagnetic leads with different polarizations, it can be operated as a spin-diode or a spin-valve, as predicted recently.[8–10] In this system, the spin dependent asymmetry in the tunneling rates between the two junctions is predicted to lead to spin accumulation, current rectification, and spin-polarized currents. If a quantum dot is attached to one ferromagnetic and one normal leads, the effect is even more pronounced[11,12] and can potentially be used for spin injection.[13] The current polarization in such a system can be controlled entirely by the gate and bias voltages.

Owing to the development of material science, half-metallic ferromagnet (HFM) has been considered as one of the most promising candidates for high-spin-polarized materials due to its distinctive band structure, where one of the two spin channels is metallic and the other behaves with semiconductor or insulator characteristics.[14] It can produce completely-polarized electrons around the Fermi level. Up to date, different classes of HMFs have been predicted theoretically and realized experimentally,[15] and spintronic devices based on HMFs have been designed and found to exhibit high magnetoresistances, spin diode effects, and spin filtering effects.[16–18]

In this paper, we consider an HFM–QD–NM system which consists of a QD weakly coupled to an HFM lead and a nonmagnetic (NM) lead, as shown in Fig. 1. We focus on the regime where sequential tunneling dominates the transport and the system can be described in terms of the generalized master equation with transition rates obtained via a real-time diagrammatic approach. We find that the charge current shows asymmetric I–V characteristics. In the single-electron tunneling regime, an anomalous suppression of the charge current from the HMF lead to the NM lead is observed. In the double-electron tunneling regime, the diode-like effect is reversed and the current can not flow from the NM lead to HMF lead. This asymmetry in the current profile suggests a diode-like behavior with respect to the bias voltage. Such diode like behavior can be tuned, and even reversed, by changing the energy level of the quantum dot via the gate voltage. We discuss the physics of the anomalous current suppression in terms of spin blockade for electron transport in our system.

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2. Model and method

We consider a QD weakly coupled to an HFM and an NM lead as shown in Fig. 1(a). The total Hamiltonian of the system is written as

$$H = H_{\rm dot} + \sum_{\alpha={\rm L,R}} (H_\alpha + H_{t,\alpha}), \tag{1}$$

where the lead label $\alpha = {\rm L,R}$ corresponds to the left and right leads. The Hamiltonians for the leads are written as

$$H_\alpha = \sum_{\alpha,k,\sigma} \varepsilon_{\alpha,k,\sigma} c^\dagger_{\alpha,k,\sigma} c_{\alpha,k,\sigma}. \tag{2}$$

And the tunneling Hamiltonian between the leads and the QD is expressed as

$$H_{t,\alpha} = (t_\alpha c^\dagger_{\alpha k\sigma} d_\sigma + {\rm h.c}), \tag{3}$$

where $c^\dagger_{\alpha k\sigma}$ ($c_{\alpha k\sigma}$) is the creation (annihilation) operator of an electron with momentum k and spin σ in lead α, and $\varepsilon_{\alpha k\sigma}$ denotes the corresponding single-particle energy. Considering the Coulomb interaction, the Hamiltonian of the QD is given as

$$H_{\rm dot} = \sum_\sigma \varepsilon_\sigma d^\dagger_\sigma d_\sigma + U d^\dagger_\uparrow d_\uparrow d^\dagger_\downarrow d_\downarrow, \tag{4}$$

where $d^\dagger_\sigma$ (d_σ) denotes the relevant electron creation (annihilation) operator. $\varepsilon_\sigma = \varepsilon_0 + \sigma\Delta B - eV_{\rm g}$ is the single energy level in the QD, which is spin dependent due to a field-induced Zeeman splitting ΔB and can be shifted by gate voltage $V_{\rm g}$. U represents the strength of the Coulomb interaction in the QD.

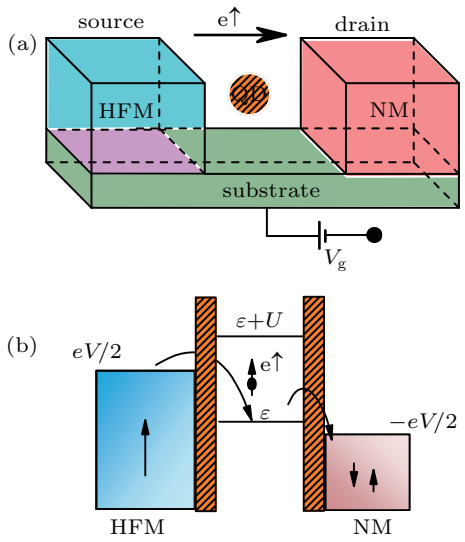


Fig. 1. The model setup. (a) Illustration showing a possible realization of a QD-based current diode device employing one half-metallic ferromagnetic lead and one nonmagnetic lead. (b) Schematic energy diagram of spin-dependent electron tunneling in this nano-junction.

We investigate the electronic transport in the sequential tunneling regime by the generalized master equation, where only four diagonal terms of the density matrix describing the charge occupation probability of the QD have been taken into account. Namely, we consider the occupation probability of four states $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, $|\uparrow\downarrow\rangle$, which correspond to the dot being empty, singly occupied with spin up or down, and doubly occupied, respectively. By using the master equations,[19,20] we obtain the evolution of the occupation probabilities of different states in the QD as

$$\frac{{\rm d}P_i}{{\rm d}t} = \Sigma(P_j W_{ji} - P_i W_{ij}). \tag{5}$$

Here, P_i is the probability of finding electrons in the state $|i\rangle$ of the dot, and $W_{ij} = \Sigma_{\alpha\sigma}(W^{\alpha\sigma+}_{ij} + W^{\alpha\sigma-}_{ij})$ describing the transition rate between state $|i\rangle$ and state $|j\rangle$ with Fermi golden law can be written as

$$\begin{aligned} W^{\alpha\sigma+}_{ij} &= \Gamma_{\alpha\sigma} f_\alpha(\varepsilon_j - \varepsilon_i - \mu_\alpha) |\langle j|d^\dagger_\sigma|i\rangle|^2, \\ W^{\alpha\sigma-}_{ij} &= \Gamma_{\alpha\sigma} f_\alpha(\varepsilon_i - \varepsilon_j + \mu_\alpha) |\langle i|d_\sigma|j\rangle|^2, \end{aligned} \tag{6}$$

where the Fermi distribution of lead α reads $f_\alpha = [{\rm e}^{(\varepsilon-\mu_\alpha)/k_{\rm B}T_\alpha} + 1]^{-1}$ with the chemical potential μ_α and the lead temperature T_α. $\Gamma_{\alpha\sigma} = 2\pi\rho_{\alpha\sigma}|t_\alpha|^2$ characterizes the linewidth function as being the density of states of the spin species σ in lead α. The spin polarization of the HFM lead α is defined as $\mathcal{P}_\alpha = (\rho_{\alpha\uparrow} - \rho_{\alpha\downarrow})/(\rho_{\alpha\uparrow} + \rho_{\alpha\downarrow})$. In the stationary state, the probabilities are obtained through $\sum_i P_i = 0$ and ${\rm d}P_i/{\rm d}t = 0$. We obtain the following spin-resolved current through lead α:

$$I_{\alpha,\sigma} = -(e/h)\sum_{i,j}(n_i - n_j) W^{\alpha\sigma}_{ji} P_j, \tag{7}$$

by which the charge current can be evaluated as $I_{\alpha{\rm c}} = I_{\alpha\uparrow} + I_{\alpha\downarrow}$. In the following numerical calculations, we choose the intra-dot Coulomb interaction $U = 1$ as the energy unit and fix the lead temperatures at the same $T_{\rm L} = T_{\rm R} = T$. We also set $\hbar = e = k_{\rm B} = 1$ (unless noted otherwise), and then the bias (gate) voltages as well as temperature T are all in units of energy.

3. Results and discussion

First, we demonstrate how the gate voltage controls the diode effect of the charge current in this QD junction without a magnetic field ($\Delta B = 0$ and $\varepsilon_\uparrow = \varepsilon_\downarrow = \varepsilon_d$). We study the tunneling current I as a function of bias voltage V and gate voltage, i.e., a Coulomb stability diamond (CD), in the few-electron QD regime. In Fig. 2(a), we present maps as calculated for a symmetric tunneling junction of NM–QD–NM structure, i.e., a single-level QD attached between a pair of nonmagnetic electrodes with $P_{\rm L} = P_{\rm R} = 0$. The regions labeled by the numbers 0, 1, and 2 indicate the Coulomb blockade regions. The symmetries of the charge current changes can be seen with respect to the direction of bias voltage V. In this case, the device does not have diode features. But if the QD

is sandwiched between one half-metallic ferromagnetic electrode and one nonmagnetic one ($P_{\rm L}=1$ and $P_{\rm R}=0$), an asymmetry in tunneling current I with respect to the bias direction is typically observed (see Fig . 2(b)), and a negative differential conductance (NDC) phenomenon is markedly exhibited in the reverse bias regime. To further examine this anomalous suppression of the charge current, we display representative I–V characteristics at two gate resonance voltages $\varepsilon_d=0$ and $-U$ in Figs. 2(c) and 2(d). It is obvious that if we tune gate voltage $\varepsilon_d=0$ (see Fig. 2(c)), the current can flow easily from the HMF lead to the nonmagnetic one ($V<0$), while it is suppressed for the opposite direction ($V>0$). More interestingly, this situation becomes significantly different when the QD's level is tuned at $\varepsilon_d=-U$ in Fig. 2(d). The behavior of charge current is reversed compared to the case of $\varepsilon_d=0$, since the current is suppressed for $V<0$, i.e., for electrons tunneling from the magnetic lead.

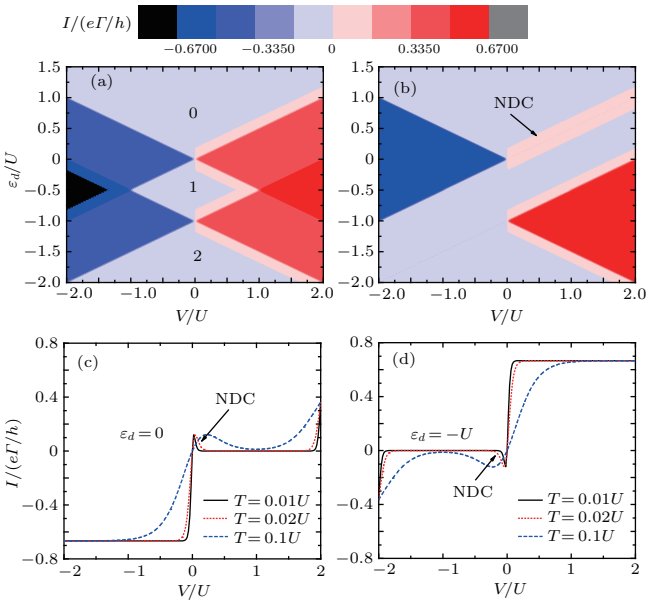


Fig. 2. The tunneling current I as a function of bias voltage V and gate voltage (QD's level) ε_d for(a) NM–QD–NM structure and (b) HMF–QD–NM structure at temperature $T=0.01$. For the HMF–QD–NM structure, the I–V curves exhibit diode features and can be tuned or even reversed by different gate voltages (c) $\varepsilon_d=0$ and (d) $\varepsilon_d=-U$.

In order to clarify the underlying physics, we plot the probabilities of the QD's states as functions of bias voltage at temperature $T=0.05$ (see Fig. 3). It is plotted with a fixed gate voltage $\varepsilon_d=0$ in Fig. 3(a). If a negative bias voltage is applied across the junction, only spin-up electrons can tunnel from the left HMF lead to the right NM one as shown in Fig. 3(c). In Fig. 3(a), we can see when the system reaches equilibrium in the $V<-0.2$ regime, the sum of two states $P_{|0\rangle}+P_{|\uparrow\rangle}\approx 1$, showing that the QD's electron current is dominated by the transmission between states $|0\rangle$ and $|\uparrow\rangle$ and the current $I=-e(P_{|\uparrow\rangle}W^{\rm R\uparrow}_{|\uparrow\rangle\to|0\rangle}+P_{|0\rangle}W^{\rm L,\uparrow}_{|0\rangle\to|\uparrow\rangle})\approx -0.67$. If a positive bias voltage is applied, all state probabilities reduce to zero quickly except $P_{|\downarrow\rangle}\to 1$, which means that there is a spin-down electron transport from the NM lead to the QD, but the electrons can not hop into the half-metallic ferromagnetic electrode (see Fig. 3(d)). For the case of high gate voltage $\varepsilon_d=0$, the occupation of spin-up electrons will cost a high energy due to the Coulomb interaction, which means that spin-up electrons cannot occupy the QD simultaneously. As a result, the electron current from the NM lead to the HFM one is totally blocked in the regime of single-electron tunneling, and the diode-like current reads as

$$I_{\rm c}\simeq\begin{cases}-0.67e\Gamma/\hbar, & (V<-0.2U),\\ 0, & (V>0.2U).\end{cases}\tag{8}$$

Second, we tune gate voltage $\varepsilon_d=-U$ in Fig. 3(b). For the case of the relatively low bias voltage, if a large enough ($V<-0.2U$) nagative bias voltage is applied across the junction, only $P_{|\uparrow\rangle}\approx 1$, while other state probabilities reduce to zero quickly, which means that a spin-up electron is trapped at the QD's level and can not hop into the NM lead as shown in Fig. 3(e). If a large enough (for example,$V>0.2$) positive bias voltage is applied, the sum of two states $P_{|\uparrow\downarrow\rangle}+P_{|\downarrow\rangle}\approx 1$, which means that the electron tunneling process is dominated by the transition between the doubly-occupied state $|\uparrow\downarrow\rangle$ and the single down spin state $|\downarrow\rangle$ (see Fig. 3(f)) with current $I=e(P_{|\uparrow\downarrow\rangle}W^{\rm L\uparrow}_{|\uparrow\downarrow\rangle\to|\downarrow\rangle}+P_{|\downarrow\rangle}W^{\rm R\uparrow}_{|\downarrow\rangle\to|\uparrow\downarrow\rangle})\approx 0.67$. As a result, in this double-electron tunneling regime the charge current can be summarized as

$$I_{\rm c}\simeq\begin{cases}0, & (V<-0.2U),\\ +0.67e\Gamma/\hbar, & (V>0.2U).\end{cases}\tag{9}$$

Similar effects have also been reported in other molecular MTJ structures,[21] which are called spin-diode effects and experimentally proven in a Ni/QD/Au sandwich structure.[12]

In Fig. 3(a), we also observe at bias $V=0$, $P_{|\uparrow\downarrow\rangle}=0$, and the other three states $|\uparrow\rangle$, $|\downarrow\rangle$, $|0\rangle$ have equal probabilities and both transitions between $|\downarrow\rangle\rightleftharpoons|0\rangle$ and $|\uparrow\rangle\rightleftharpoons|0\rangle$ can occur according to the bias direction. But the transitions between $|\downarrow\rangle\rightleftharpoons|0\rangle$ in the $V>0$ regime will be suppressed quickly because $P_{|\downarrow\rangle}\to 1$, which results in a small peak in current $I_{V\to 0+}>0$ and negative differential conductance (NDC) is markedly exhibited in the reverse bias regime $V\to V(0+)$ (see Fig. 2(c)). Similarly, in Fig. 3(b), we tune the gate voltage in the double-electron tunneling regime $\varepsilon_d=-U$, the probabilities of $|\uparrow\rangle$, $|\downarrow\rangle$, and $|\uparrow\downarrow\rangle$ are almost equal and $P_{|0\rangle}$ reduces to zero at bias $V=0$. By choosing different bias directions, both transitions between $|\downarrow\rangle\rightleftharpoons|\uparrow\downarrow\rangle$ and $|\uparrow\rangle\rightleftharpoons|\uparrow\downarrow\rangle$ can occur near the $V=0$ point. But the electron tunneling process between $|\uparrow\rangle\rightleftharpoons|\uparrow\downarrow\rangle$ in the $V<0$ regime will decrease quickly due to the rapid increase of $P_{|\uparrow\rangle}\to 1$, which means that a spin-up electron is trapped in the QD's level and the tunneling current is blocked. As a consequence, a small peak in current $I_{V\to 0-}<0$ and NDC take place in the bias regime $V\to V(0-)$ as shown in Fig. 2(d).

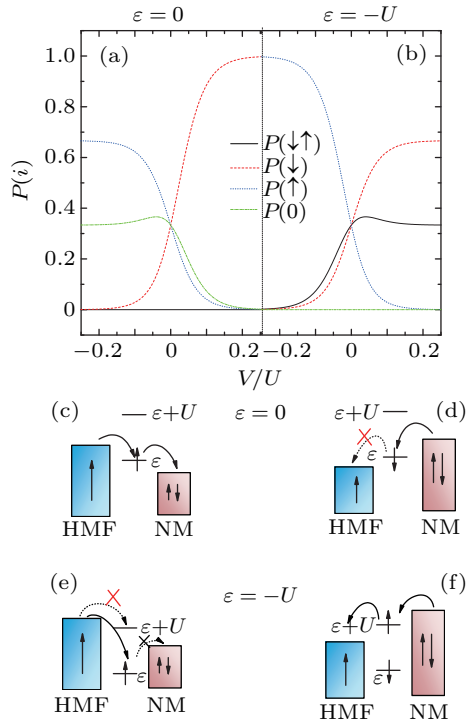


Fig. 3. The probabilities of the QD's states at the gate voltage (a) $\varepsilon_d = 0$ and (b) $\varepsilon_d = -U$. For the single-electron tunneling regime, the electron current can transport from HMF lead to NM lead direction (c) and block in the backward direction (d). For the double-electron tunneling regime, the electron can hop from NM lead to HMF lead direction (f) and block in the backward direction (e).

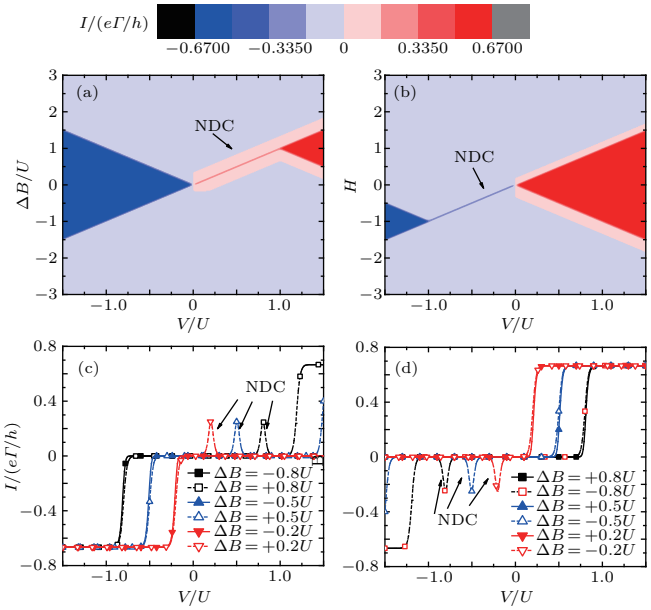


Fig. 4. The tunneling current I as a function of bias voltage V and Zeeman splitting energy ΔB in HMF–QD–NM structure with equal temperatures $T = 0.01$ and different gate voltages (a) $\varepsilon_d = 0$ and (b) $\varepsilon_d = -U$. The NDC can be shifted to a higher bias regime by the positive or negative external magnetic field's direction, with respect to different tunneling regimes at (c) $\varepsilon_d = 0$ and (d) $\varepsilon_d = -U$.

In Fig. 4, we show the currents as a function of the external magnetic field ΔB and bias voltage, where gate voltage V_g is fixed at the single-electron tunneling regime (see Figs. 4(a) and 4(c)) or the double-electron tunneling regime (see Figs. 4(b) and 4(d)). If the magnetic field is large enough, for example, $\Delta B > U$ in Fig. 4(a) or $\Delta B < -U$ in Fig. 4(b), the symmetries of the current can be observed with respect to the direction of bias voltage V, which means that the device's diode features are destroyed by the large Zeeman splitting. In Fig. 4, we also observe that the series of NDC regimes is shifted with the external magnetic field. In Figs. 4(c) and 4(d), the I–V spectra with different magnetic fields are demonstrated at gate voltages $\varepsilon_d = 0$ and $\varepsilon_d = -U$. It is clear to see that the NDC phenomena originating from the transitions between $|\downarrow\rangle \rightleftharpoons |0\rangle$ in the $V > 0$ regime will be shifted to a higher bias regime in Fig. 4(c), while the NDC current from the transition between $|\uparrow\rangle \rightleftharpoons |\uparrow\downarrow\rangle$ in the $V < 0$ direction will be pulled back to a lower bias regime. But no matter how an external magnetic field is applied, the electron suppression effect still exists. In a word, our numerical results show large asymmetries of the charge current changes with respect to the direction of bias voltage V in the small external magnetic field regime, which means that the device will robustly keep its the diode features.

To discuss the rectification ability of the QD junction, we refer to the forward (reverse) charge current as I_f (I_r). We define the rectification coefficient

$$\eta = 1 - |I_r/I_f|. \tag{10}$$

Note that $\eta = 0$ when there is no rectification and $\eta = 1$ for a perfect diode.[22] It is obvious that as the lead's polarization decreases, the forward current remains the same but the reverse current I_r increases rapidly (see Fig. 5(a)). Following the experimental work on CNT–QD junctions by Merchant and Markovic,[11] the rectification coefficient η can be obtained as

$$\eta = \frac{2\mathcal{P}^2_{\mathrm{L(F)}}}{3 - \mathcal{P}^2_{\mathrm{L(F)}}}. \tag{11}$$

If we use low-dimensional HMF materials such as Co, MoS_2-like MoN_2, graphene, and graphene-like monolayers, η can reach up to 100%, and this extremely high rectification coefficient will not be affected by the temperature. In Fig. 5(b), we plot $\eta = 1 - \left|\frac{I_{(V=0.5U)}}{I_{(V=-0.5U)}}\right|$ as a function of the spin polarization of the HFM lead in the single electron tunneling regime $\varepsilon_d = 0$ for different temperatures T. The characteristics of the η–$\mathcal{P}_L$ curves are stable and the rectification coefficient can reach up to 100% with the spin polarization of HFM $\mathcal{P}_{HMF} = 1$, which leads to a perfect diode.

Finally, it is worthwhile to discuss the experimental realization of the present proposal. Let us now estimate the required bias and gate voltage as well as the temperatures in this QD diode. In the experiment, the intradot Coulomb interaction can reach about $U = 10$ meV. For $T = 1$ K, $k_B T$ is then about 0.1 meV, which corresponds to $T = 0.01$ in units of U. Then the bias V is about $100 k_B T \approx 10$ meV and the

gate $\varepsilon_d \approx -10$ meV. As a result, our proposed scheme can be implemented with current technologies and is particularly feasible for experimental realization.

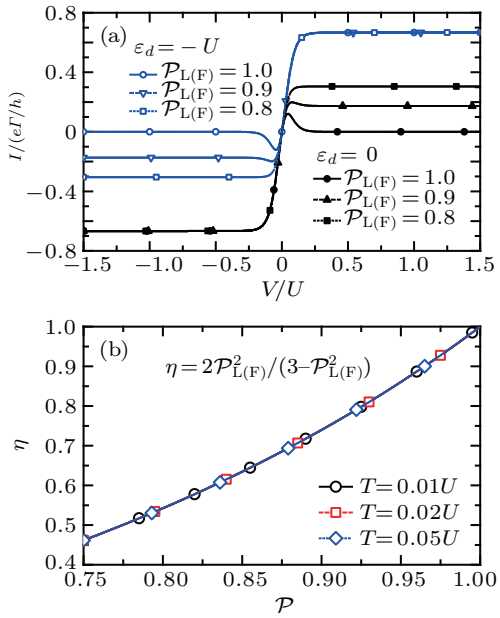


Fig. 5. (a) Tunneling current as a function of bias voltage at different lead spin polarizations with gate voltage $\varepsilon_d = 0$ and $\varepsilon_d = -U$. (b) Rectification coefficient η as function of lead spin polarization $\mathcal{P}$ under different equilibrium temperatures T, with $\varepsilon_d = 0$ and $|V| = 0.5$.

4. Conclusion

We have proposed an electron diode device based on a single quantum dot weakly coupled to one HFM and one NM leads. We have observed a clear asymmetry in the electron current I as a function of bias voltage V. Our analysis shows that this rectification occurs because of the asymmetric tunneling rates between the ferromagnetic lead and the QD for the majority and minority occupations of electrons. Moreover, we have demonstrated that the transport characteristics of such diode-like phenomena strongly depend on the number of electrons occupying the QD's level, which can be tuned by the gate voltage. By increasing the polarization of the ferromagnet, the diode's rectification effect can be increased up to $\eta = 100\%$. The present spin diode scheme is fully electrically controlled, and it will not be easily affected by the external magnetic field or temperature. The results in this work offer a starting point to study multi-layer structures combined with QDs, such as nano-spin diode structures. However, our numerical results also show that the device's functional ability widely depends on the spin polarization of the ferromagnetic electrode, e.g., a half-metallic ferromagnetic lead.

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