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Electronic Conduction Characteristics of Parallel Coupled Triple Quantum Dot System

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Abstract. Electronic conduction characteristics of parallel coupled triple quantum dot system are studied, in which external magnetic field and Rashba spin orbit interaction are considered. Conductance expression of the calculation system is given by using NEGF technology. The effect of Rashba spin orbit interaction on spin transport properties is discussed and the physical explanation is given by total density of states in the systems.

Introduction

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Spin orbit interaction is a very important role in semiconductor spintronics. The coupling between spin freedom and orbit motion is caused by Rashba spin orbit interaction, so the electron spin can be controlled by adjusting external magnetic flux and a gate voltage. Sun Q F, Wang J and Guo H proposed an extra spin-dependent phase factor in the coupling matrix elements between the electrodes and the quantum dot based on the study of Nanostructures with Rashba spin-orbit interaction, as an example, a Aharnov-Bohm ring in which a quantum dot is located in one arm of the ring is investigated. A substantial spin-polarized conductance or current emerges due to a combined effect of a magnetic flux and the Rashba interaction. The direction and strength of the spin-polarization are shown to be controlled by both the magnetic flux and a gate voltage. The theoretical study discussed above promotes the theoretical studies on spin transport properties of coupled quantum dot system, and new vitality is poured to the studies on spintronics. For example, Fano-Rashba Effect in a double quantum dot AB Interferometer is studied by Chi F, Liu J L, and Sun L L. The Fano line shapes of the two spin electrons in the conductance spectra can be tuned either synchronously or individually with the help of the structure parameters relevant to the Rashba spin-orbit coupling strength, magnetic flux, and the structure configuration. The effect of the Rashba spin splitting and a magnetic field on the energy levels of electrons in parabolic quantum dots is investigated by Lee J, Spector H N, Chou W C, and Chu C S. In the presence of a magnetic field, the electrons degeneracy is removed and the energy splitting of the spin states increases with the increase in both the Rashba parameter and the magnetic field.

A triple quantum dot structure is proposed in the paper, in which Rashba spin orbit interaction is considered in every quantum dot and every quantum dot can couple with electrode. The proposed system has more tunnels for electron resonant tunneling and more adjustable parameters. The transport properties of the system electrons and spin transport are more abundant by adjusting external magnetic field and Rashba spin orbit interaction, which provide more significant physical and applications.

Theory Model

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The system framework which consists of triple quantum dot is shown in Fig.1. Every quantum dot can couple with the electrode simultaneously.

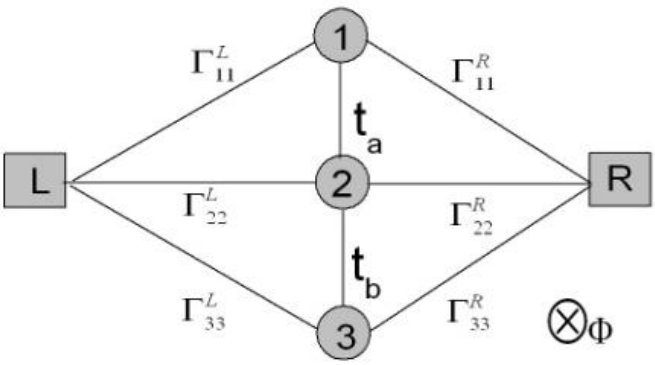

Fig.1 Scheme of parallel coupled triple quantum dot system

The Hamiltonian of the system is expressed as:

$$H_{total} = H_{lead} + H_{dots} + H_T \tag{1}$$

H_{lead} describes the contribution of the two electrodes in the quasi particle approximation with no interaction, and it is given as

$$H_{lead} = \sum_{k,\sigma} \sum_{\beta=L,R} \varepsilon_{k\beta} C_{k\beta\sigma}^{+} C_{k\beta\sigma} \tag{2}$$

Where, $C_{k\beta\sigma}^{+}\left(C_{k\beta\sigma}\right)$ is the operator yielded by electron with wave vector k and spin σ in electrode β; $\varepsilon_{k\beta}$ is the electron energy level with wave vector k in electrode β.

The second term in the right of eq.(1) describes the contribution of triple quantum dot system, and is given as:

$$H_{dots} = \sum_{j\sigma} \varepsilon_{j\sigma} d_{j\sigma}^{+} d_{j\sigma} - \sum_{\sigma} (t_a d_{1\sigma}^{+} d_{2\sigma} + t_b d_{2\sigma}^{+} d_{3\sigma} + H.C.) \tag{3}$$

Where: $d_{j\sigma}^{+}\left(d_{j\sigma}\right)$ is the operator yielded by electron with spin σ in quantum $j(=1,2,3)$;

$\varepsilon_{j\sigma}$ is the electron energy level with spin σ in quantum j;

$t_a\left(t_b\right)$ is the coupling strength of tunneling between quantum $1(2)$ and $2(3)$.

The last term H_T in eq. (1) describes the electron tunneling between quantum dot and electrode, and the expression is

$$H_T = \sum_{j} \sum_{k,\sigma} \sum_{\beta=L,R} (t_{\beta j\sigma} C_{k\beta\sigma}^{+} d_{j\sigma} + H.C.) \tag{4}$$

Where $t_{\beta j\sigma}$ describes tunneling couple between quantum dot and electrode, which is assumed that it is irrelevant with k. $t_{\beta j\sigma}$ has the following form,

$$\begin{aligned}
t_{L1\sigma} &= |t_{L1}| e^{i\varphi/4} e^{-i\sigma\phi_{R1}/2} \\
t_{L2\sigma} &= |t_{L2}| e^{-i\sigma\phi_{R2}/2} \\
t_{L3\sigma} &= |t_{L3}| e^{-i\varphi/4} e^{-i\sigma\phi_{R3}/2} \\
t_{R1\sigma} &= |t_{R1}| e^{-i\varphi/4} e^{i\sigma\phi_{R1}/2} \\
t_{R2\sigma} &= |t_{R2}| e^{i\sigma\phi_{R2}/2} \\
t_{R3\sigma} &= |t_{R3}| e^{i\varphi/4} e^{i\sigma\phi_{R3}/2}
\end{aligned} \tag{5}$$

Where, φ is phase factor induced by flux; ϕ_{R_j} is phase factor induced by Rashba spin orbit interaction in quantum dot j.

Linewidth matrix element $\Gamma_{ij\sigma}^{\beta}=2\pi\sum_k t_{\beta i\sigma}t_{\beta j\sigma}^{*}\delta(\varepsilon-\varepsilon_{k\beta})$ is defined as the following calculation and matrix Γ_{σ}^{α} can be wrote as

$$\Gamma_{\sigma}^{L}=\begin{pmatrix}\Gamma_1^L & \sqrt{\Gamma_1^L\Gamma_2^L}e^{i\varphi/4}e^{-i\sigma(\phi_{R1}-\phi_{R2})/2} & \sqrt{\Gamma_1^L\Gamma_3^L}e^{i\varphi/2}e^{-i\sigma(\phi_{R1}-\phi_{R3})/2}\\ \sqrt{\Gamma_1^L\Gamma_2^L}e^{-i\varphi/4}e^{i\sigma(\phi_{R1}-\phi_{R2})/2} & \Gamma_2^L & \sqrt{\Gamma_2^L\Gamma_3^L}e^{i\varphi/4}e^{-i\sigma(\phi_{R2}-\phi_{R3})/2}\\ \sqrt{\Gamma_1^L\Gamma_3^L}e^{-i\varphi/2}e^{i\sigma(\phi_{R1}-\phi_{R3})/2} & \sqrt{\Gamma_2^L\Gamma_3^L}e^{-i\varphi/4}e^{i\sigma(\phi_{R2}-\phi_{R3})/2} & \Gamma_3^L\end{pmatrix} \tag{6a}$$

and

$$\Gamma_{\sigma}^{R}=\begin{pmatrix}\Gamma_1^R & \sqrt{\Gamma_1^R\Gamma_2^R}e^{-i\varphi/4}e^{i\sigma(\phi_{R1}-\phi_{R2})/2} & \sqrt{\Gamma_1^R\Gamma_3^R}e^{-i\varphi/2}e^{i\sigma(\phi_{R1}-\phi_{R3})/2}\\ \sqrt{\Gamma_1^R\Gamma_2^R}e^{i\varphi/4}e^{-i\sigma(\phi_{R1}-\phi_{R2})/2} & \Gamma_2^R & \sqrt{\Gamma_2^R\Gamma_3^R}e^{-i\varphi/4}e^{i\sigma(\phi_{R2}-\phi_{R3})/2}\\ \sqrt{\Gamma_1^R\Gamma_3^R}e^{i\varphi/2}e^{-i\sigma(\phi_{R1}-\phi_{R3})/2} & \sqrt{\Gamma_2^R\Gamma_3^R}e^{i\varphi/4}e^{-i\sigma(\phi_{R2}-\phi_{R3})/2} & \Gamma_3^R\end{pmatrix} \tag{6b}$$

Where Γ_j^{β} is the reduced form of $\Gamma_{jj}^{\beta}\left(j=1,2,3\right)$.

In recent studies, the transport properties of the system can be determined by NEGF $G_{jj}(\varepsilon)(j=1,2,3)$.The Dyson equation and the motion equation of every NEGF are used simultaneously to calculate those. Retarded (advanced) Green function can be expresses as the following by adopting Hartree-Fock high order approximation.

$$\boldsymbol{G}_{\sigma}^{r}(\varepsilon)=\left(\boldsymbol{G}_{\sigma}^{a}(\varepsilon)\right)^{+}=\begin{pmatrix}\varepsilon-\varepsilon_{1\sigma}+\frac{i}{2}(\Gamma_{11\sigma}^{L}+\Gamma_{11\sigma}^{R}) & t_a+\frac{i}{2}(\Gamma_{12\sigma}^{L}+\Gamma_{12\sigma}^{R}) & \frac{i}{2}(\Gamma_{13\sigma}^{L}+\Gamma_{13\sigma}^{R})\\ t_a+\frac{i}{2}(\Gamma_{21\sigma}^{L}+\Gamma_{21\sigma}^{R}) & \varepsilon-\varepsilon_{2\sigma}+\frac{i}{2}(\Gamma_{22\sigma}^{L}+\Gamma_{22\sigma}^{R}) & t_b+\frac{i}{2}(\Gamma_{23\sigma}^{L}+\Gamma_{23\sigma}^{R})\\ \frac{i}{2}(\Gamma_{31\sigma}^{L}+\Gamma_{31\sigma}^{R}) & t_b+\frac{i}{2}(\Gamma_{32\sigma}^{L}+\Gamma_{32\sigma}^{R}) & \varepsilon-\varepsilon_{3\sigma}+\frac{i}{2}(\Gamma_{33\sigma}^{L}+\Gamma_{33\sigma}^{R})\end{pmatrix}^{-1} \tag{7}$$

The current expression passed through the systems can be got by using NEGF technology.

$$J_{\sigma}=\frac{e}{\hbar}\int\frac{d\varepsilon}{2\pi}\left[f_L(\varepsilon)-f_R(\varepsilon)\right]\mathrm{Tr}\left[\boldsymbol{G}_{\sigma}^{a}(\varepsilon)\Gamma_{\sigma}^{R}\boldsymbol{G}_{\sigma}^{r}(\varepsilon)\Gamma_{\sigma}^{L}\right], \tag{8}$$

Where

$$f_{\beta}(\varepsilon)=\left\{1+\exp\left[\left(\varepsilon-u_{\beta}\right)/k_BT\right]\right\}^{-1} \tag{9}$$

is the electron Fermi distribution function at electrode. u_{β} is the corresponding chemical potential at electrode β.

Conductance can be wrote as eq. (10) under zero temperature condition.

$$\mathrm{G}_{\sigma}(\varepsilon_{\mathrm{F}})=\frac{e^2}{\hbar}\mathrm{Tr}\left[\boldsymbol{G}_{\sigma}^{a}(\varepsilon)\Gamma_{\sigma}^{R}\boldsymbol{G}_{\sigma}^{r}(\varepsilon)\Gamma_{\sigma}^{L}\right]\Big|_{\varepsilon=\varepsilon_F} \tag{10}$$

Where ε_F is the Fermi energy of electrons at electrode.

Calculation Results

The basic spin transport properties can be calculated by the above equations. Assumed that energy levels of all quantum dots are the same and dot-electrode coupling strength $\Gamma_1^{\beta}=\Gamma_2^{\beta}=\Gamma(\beta\in L,R)$, and Γ is energy unit. Supposed $\phi_{R_2}=\phi_{R_3}$, so $\Gamma_{\sigma}^{L,R}$ is only dependent on $\phi_{R_{12}}=\phi_{R_{13}}=\phi_{R_1}-\phi_{R_{2(3)}}=\phi_R$, where ϕ_R is difference between ϕ_{R_1} and $\phi_{R_2}(or\ \phi_{R_3})$.

The effects that for conductance under zero flux are shown in Fig.2 to Fig.4. The relative parameters are chosen as: $t_a=t_b=t=1.0$, $\varphi=0$, $\varepsilon_0=0$ and $\Gamma_3^{L,R}=1.0$. For comparison, when Rashba spin orbit interaction is not considered, the system conductance is shown in Fig. 2(a). Quantum dot 1 and quantum dot 3 is equivalent completely, when the flux is zero and Rashba spin orbit interaction is

not considered. So the shape of the system conductance spectrum is like the one in the parallel coupled double quantum dot system. And a Breit-Winger resonance peak can be observed at energy level $\varepsilon_0 - \sqrt{2}t$ and a Fano anti-resonance peak can be observed at energy level $\varepsilon_0 + \sqrt{2}t$ in the conductance spectrum. Compare with the system conductance spectrum of the parallel coupled double quantum dot system, the positions of these resonance peaks moved. When Rashba spin orbit interaction is considered and the phase factor $\phi_R = \pi/50$(shown as Fig. 2(b)), compare with Fig. 2(a), a steep Fano resonance peak appears at $\varepsilon = 0$, the other resonance peaks are the same as the one in the conductance spectrum when Rashba spin orbit interaction is not considered. Phase factor induced by Rashba spin orbit interaction results in the steep Fano resonance peak. The corresponding total density of states which has the same parameters with Fig.2 is shown in Fig.3. When Rashba spin orbit interaction is not considered, total density of states in the system is shown in Fig.3(a), and a δ function appears at $\varepsilon = 0$, which means there is a bound state here. When $\phi_R = \pi/50$, total density of states in the system is shown in Fig.3(b). There is a narrow peak appears at $\varepsilon = 0$, which is corresponding with the steep Fano resonance peak in Fig.2(b).

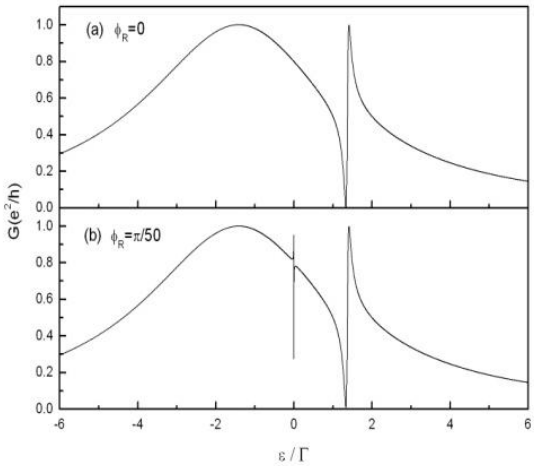

Fig.2 Conductance versus electron energy. The parameters are given by $t = 1.0$, $\varphi = 0$, $\varepsilon_0 = 0$, $\Gamma_3^{L,R} = 1.0$, and $\varphi = 0$, $\varepsilon_0 = 0$, $\Gamma_3^{L,R} = 1.0$, and (a) $\phi_R = 0$; (b) $\phi_R = \pi/50$.

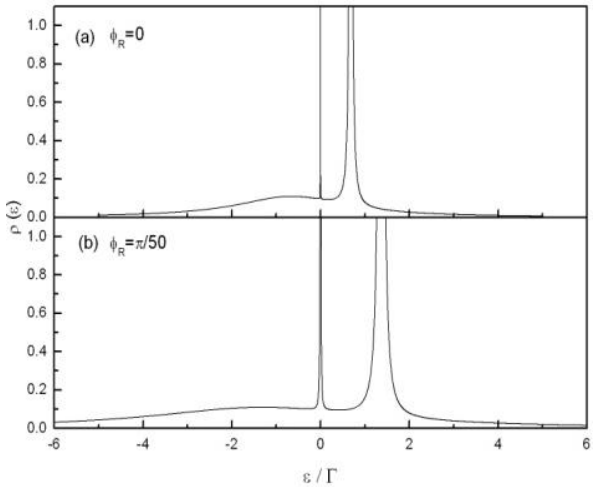

Fig.3 Density of state versus electron energy The parameters are the same as in Fig.2.

The system conductance spectrum at $\phi_R = \pi/10$ is illustrated in Fig.4(a), when the strength of Rashba spin orbit interaction is increased. Compare with the conductance spectrum at $\phi_R = \pi/50$, there is a steep Fano resonance peak changed into Fano anti-resonance peak, and the Fano resonance peak at $\varepsilon_0 + \sqrt{2}T$ becomes smaller, the position of anti-resonance point is increased. The system conductance spectrum at $\phi_R = \pi/4$ is illustrated in Fig.4(b), when the strength of Rashba spin orbit interaction is increased further. The Fano resonance peak at $\varepsilon_0 + \sqrt{2}T$ is changed into resonance peak.

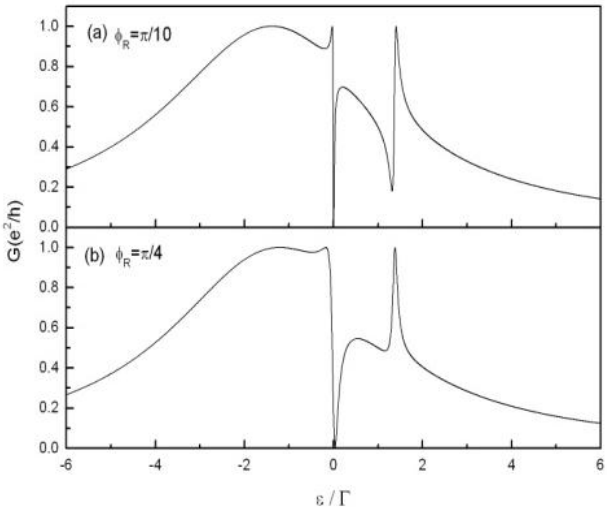

Fig.4 Conductance versus electron energy. The parameters are given by $t=1.0$, $\varphi=0$, $\varepsilon_0=0$, $\Gamma_3^{L,R}=1.0$, and (a) $\phi_R=0$; (b) $\phi_R=\pi/50$.

Now, the effect of Rashba spin orbit interaction on spin transport properties is investigated. The relative parameters are chosen as: $t=1.0$, $\varphi=\pi/2$, $\varepsilon_0=0$ and $\Gamma_3^{L,R}=0.01$. For comparing, the condition at $\phi_R=0$ that Rashba spin orbit interaction is not considered is shown in Fig.5. The conductance spectrum showed that conductance spectrum of spin up electrons is consistent with the conductance spectrum of spin up electrons. When $\phi_R=0$, phase factors related to these different spin electrons are equal, namely $\phi_\uparrow=\phi_\downarrow$, so the conductance has no relation to spin. Conductance spectrum in Fig.5 consists of two resonance peaks and a Fano peak.

When Rashba spin orbit interaction is considered, phase factors related to these different spin electrons are not equal, namely $\phi_\uparrow\neq\phi_\downarrow$, and the conductance will be spin-polarized. The conductance spectrum at $\phi_R=\pi/2$ is shown in Fig.6. The conductance curve of spin up electrons and the curve of spin down electrons are quite different, which means that conductance is spin-polarized. In addition, the conductance curve of spin up electrons is like the one shown in Fig.5. Conductance spectrum of spin down electrons has three resonance peaks which are different completely with the one on the conductance spectrum of spin up electrons.

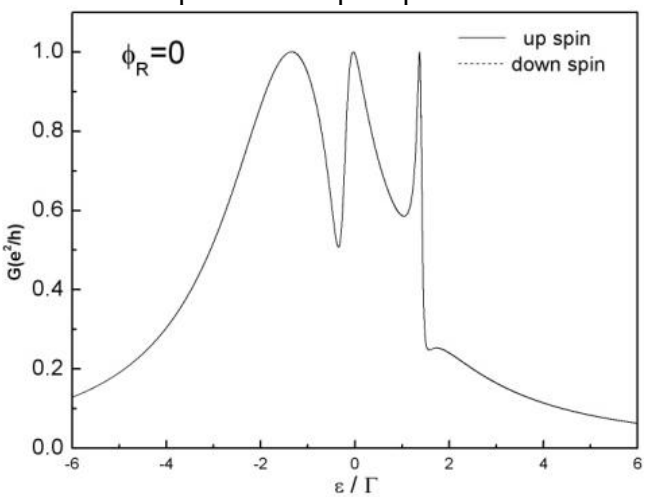

Fig.5 Conductance versus electron energy. The parameters are given by $t=1.0$, $\varphi=\pi/2$, $\varepsilon_0=0$, $\Gamma_3^{L,R}=0.01$ and $\phi_R=0$.

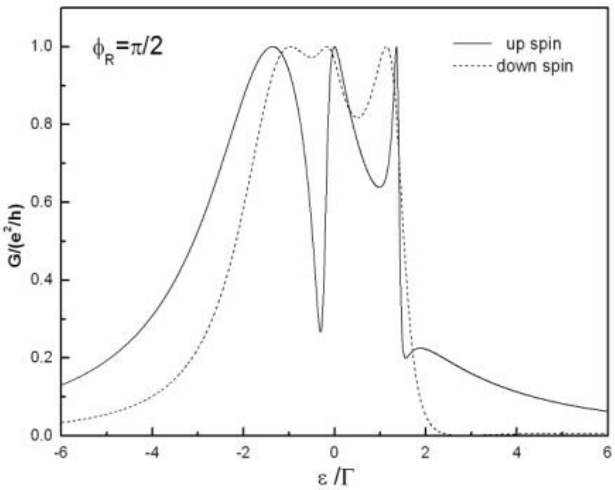

Fig.6 Conductance versus electron energy. The parameters are given by $t=1.0$, $\varphi=\pi/2$, $\varepsilon_0=0$, $\Gamma_3^{L,R}=0.01$ and $\phi_R=\pi/2$.

Conclusion

Electronic conduction characteristics of parallel coupled triple quantum dot system are studied in the paper. The electronic transport properties are discussed and the physical explanations for the transport results are given by total density of states. Rashba spin orbit interaction is very important to the spin transport of the system. When Rashba spin orbit interaction is considered, the system conductance is spin polarized. The Fano resonance peak is changed into resonance peak by controlling the spin orbit interaction phase factor ϕ_R.

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