

# Nonequilibrium transport properties for a three-site quantum wire model

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We derive nonequilibrium electronic transport properties for a three-site quantum wire model within Hartree-Fock approximation making use of Keldysh formalism. Some rigorous formulas are provided for direct calculations when Coulomb repulsion is present. According to numerical calculations using these formulas, we investigate the conductance, transport current, and on site electronic charges of the wire in some special occasions. In noninteracting case, when site-site couplings in the wire are tougher than wire-electrode couplings, the resonant tunneling transport takes place and the phenomenon of conductance quantization can be easily ob-

served. The transport properties of up-spin are identical with those of down-spin. When the Coulomb interaction is present, the line shapes of transport characteristics are changed because of electron-electron repulsions. With the increase of  $U$ , the Coulomb blockade and metal-insulator transition (Mott transition) phenomena are obvious if the self-energies  $\Gamma$  have small values compared with  $U$ . The transport properties of the up-spin also become quite different from those of the down-spin indicating that the spin polarization takes place in the wire.

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**1 Introduction** With advantage of top-down and bottom-up fabrication techniques for nanometer scale structures, it becomes possible to create quantum wire (QW) with the diameter of the order of the Fermi wavelength, and to experimentally study the quantum transport properties through them [1, 2]. In order to understand the experiment results, furthermore, to predict transport properties for applications in the future nanodevice design, theoretical approaches for clarifying QW electronic transport become necessary. In this paper, we present some theoretical formulas and numerical results for nonequilibrium electronic transport, using a simplest model of three-site QW, in which each site has a single level.

In this study, the rigorous formulas of conductance, transport current and charge distributions for the three-site QW model are derived within Hartree-Fock approximation, based on the nonequilibrium transport theory (Keldysh formalism) [3, 4]. From these formulas, the relevance between the transport properties and the temperature or the

parameters in the Hamiltonian is expressed clearly and can be investigated in detail. In noninteracting case ( $U = 0$ ), we focus on the resonant tunneling transport and conductance quantization phenomenon. When Coulomb interaction is present ( $U > 0$ ), we investigate Coulomb blockade and metal-insulator transition, as well as spin transport properties in the QW. It is reasonable to consider that the results of our study are available in the complicated case of actual QWs which are probably longer and thicker containing larger number of atoms (sites) having multiple levels.

The paper is organized as follows, in Sec. 2, we describe the three-site QW model and the concise derivations of transport properties formulas for this model. Sec. 3 is devoted to present numerical results calculated from these formulas and their interpretations. Finally, we summarize our results in Sec. 4.

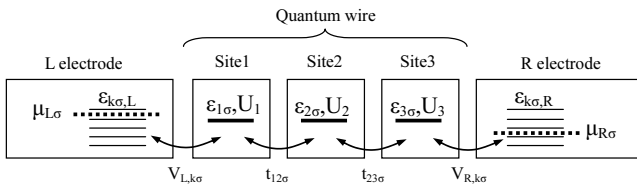
## 2 Model and formulation

**2.1 Model** We consider a one-dimensional QW with three lattice sites which are mutually coupled by tunneling

barriers. They are combined with two external electrodes as shown in Fig. 1.

The tight-binding Hamiltonian of such system is described by Eq. (1). Here  $\hat{c}_{k\sigma,\alpha}^+$  and  $\hat{c}_{k\sigma,\alpha}$  ( $\alpha = L$  or  $R$ ) denote creation and annihilation operators of an electron with wave vector  $k$  and spin  $\sigma$  within  $L$  or  $R$  one-dimension perfect crystalline electrodes. The same operators of an electron within  $i$ -th site of the centre wire are denoted by  $\hat{d}_{i\sigma}^+$  and  $\hat{d}_{i\sigma}$ .  $\varepsilon_{k\sigma,\alpha}$  and  $\varepsilon_{i\sigma}$  are on-site energies in the electrodes and wire region, respectively. The transfer integrals between the nearest-neighbor sites are  $t_{i,j\sigma}$ . The sites labelled by 1 and 3 are connected to the left and right electrode, respectively, and  $v_{\alpha,k\sigma}$  denote the tunnel combination integrals between those boundary sites and the electrodes. The on-site Coulomb repulsion energies are denoted by  $U_i$ . When bias voltage  $V$  is applied to the wire, it can be regarded as electrochemical potentials,  $\mu_L$  and  $\mu_R$ , associate with the left and right electrode, respectively ( $eV = \mu_L - \mu_R$ ). We assume that the electrodes are electric reservoirs, the capacities of which are large enough that  $\mu_L$  and  $\mu_R$  are not perturbed by the transport current. In the case of  $\mu_L > \mu_R$ , electrons will flow from the left electrode to the right electrode.

$$\begin{aligned} \hat{H} = & \sum_{k\sigma} (\varepsilon_{k\sigma,L} \hat{c}_{k\sigma,L}^+ \hat{c}_{k\sigma,L} + \varepsilon_{k\sigma,R} \hat{c}_{k\sigma,R}^+ \hat{c}_{k\sigma,R}) + \varepsilon_{1\sigma} \hat{d}_{1\sigma}^+ \hat{d}_{1\sigma} + \varepsilon_{2\sigma} \hat{d}_{2\sigma}^+ \hat{d}_{2\sigma} + \varepsilon_{3\sigma} \hat{d}_{3\sigma}^+ \hat{d}_{3\sigma} \\ & + \sum_{\sigma} (t_{12\sigma} \hat{d}_{1\sigma}^+ \hat{d}_{2\sigma} + t_{12\sigma}^* \hat{d}_{2\sigma}^+ \hat{d}_{1\sigma} + t_{23\sigma} \hat{d}_{2\sigma}^+ \hat{d}_{3\sigma} + t_{23\sigma}^* \hat{d}_{3\sigma}^+ \hat{d}_{2\sigma}) \\ & + \sum_{k\sigma} (v_{L,k\sigma} \hat{c}_{k\sigma,L}^+ \hat{d}_{1\sigma} + v_{L,k\sigma}^* \hat{d}_{1\sigma}^+ \hat{c}_{k\sigma,L}) + \sum_{k\sigma} (v_{R,k\sigma} \hat{c}_{k\sigma,R}^+ \hat{d}_{3\sigma} + v_{R,k\sigma}^* \hat{d}_{3\sigma}^+ \hat{c}_{k\sigma,R}) \\ & + U_1 \hat{d}_{1\uparrow}^+ \hat{d}_{1\uparrow} \hat{d}_{1\downarrow}^+ \hat{d}_{1\downarrow} + U_2 \hat{d}_{2\uparrow}^+ \hat{d}_{2\uparrow} \hat{d}_{2\downarrow}^+ \hat{d}_{2\downarrow} + U_3 \hat{d}_{3\uparrow}^+ \hat{d}_{3\uparrow} \hat{d}_{3\downarrow}^+ \hat{d}_{3\downarrow} \end{aligned} \quad (1)$$



**Figure 1** Model of three-site quantum wire combined with two external electrodes.

**2.2 Formulation** We consider a system consisting of three regions, a left electrode, a right electrode and a intermediate wire, they uncouple and each one maintains its noninteracting thermal equilibrium when  $t = -\infty$ , then turn on the perturbation coupling between the wire and electrodes adiabatically with a route of  $t = -\infty \rightarrow 0 \rightarrow +\infty \rightarrow -\infty$  (Keldysh contour). According to the quantum statistical theory (perturbation expansion), any nonequilibrium observable physical quantity at time  $t$  can be expressed exactly by Keldysh Green's functions (GF), such as correlation function  $G_{ij}^r(t, t_0) = i \langle \hat{c}_i^+(t) \hat{c}_j(t_0) \rangle$  and retarded/advanced GF

$G_{ij}^{r(a)}(t, t_0) = \mp i \theta[\pm(t - t_0)] \langle \hat{c}_i(t) \hat{c}_j^+(t_0) + \hat{c}_j^+(t_0) \hat{c}_i(t) \rangle$  (Keldysh formalism) [3, 4]. These GFs can be solved from Dyson-equation.

The self-energies resulting from wire-electrode coupling and Coulomb repulsion are derived in Hartree-Fock approximation and shown in Eqs. (2) and (3), respectively:

$$\begin{aligned} \begin{bmatrix} \Sigma_{pq}^{(i)-}(\varepsilon) & \Sigma_{pq}^{(i)<}(\varepsilon) \\ \Sigma_{pq}^{(i)>}(\varepsilon) & \Sigma_{pq}^{(i)+}(\varepsilon) \end{bmatrix} = & \sum_{k\sigma} v_{L,k\sigma}^* \delta_{p,L} \delta_{q,k\sigma-L} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} + \sum_{k\sigma} v_{L,k\sigma} \delta_{p,k\sigma-L} \delta_{q,L} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \\ & + \sum_{k\sigma} v_{R,k\sigma}^* \delta_{p,N\sigma} \delta_{q,k\sigma-R} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} + \sum_{k\sigma} v_{R,k\sigma} \delta_{p,k\sigma-R} \delta_{q,N\sigma} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \end{aligned} \quad (2)$$

$$\Sigma_{n\sigma,n'\sigma'}^{(i)-}(\varepsilon) = \delta(n\sigma, n'\sigma') U_n \rho_{n\sigma,n\sigma'}(\varepsilon)/e \quad \Sigma_{pq}^{(i)>}(\varepsilon) = 0, \quad (3)$$

$$\Sigma_{n\sigma,n'\sigma'}^{(i)+}(\varepsilon) = \delta(n\sigma, n'\sigma') (-U_n) \rho_{n\sigma,n\sigma'}(\varepsilon)/e \quad \Sigma_{pq}^{(i)<}(\varepsilon) = 0. \quad (3)$$

Corresponding retarded / advanced Self-energies are given by Eq. (4):

$$i\Gamma_{\alpha\sigma}^r(\varepsilon) = -i\pi v_{\alpha,\sigma}(\varepsilon) |V_{\alpha,k\sigma}|^2 \quad i\Gamma_{\alpha\sigma}^a(\varepsilon) = i\pi v_{\alpha,\sigma}(\varepsilon) |V_{\alpha,k\sigma}|^2, \quad (4)$$

where  $v_{\alpha,\sigma}(\varepsilon)$  is the density-of-states (DOS) in the electrodes,  $\alpha = L, R$ .

The single spin current flowing in the wire and the spin electron charge on the site  $n$  are given by Eq. (5) and Eq. (6), respectively [5]:

$$I_\sigma = \frac{e}{h} \sum_{k\sigma,n} \int_{-\infty}^{+\infty} \frac{d\varepsilon}{2\pi} [V_{k\sigma-L,n\sigma} G_{n\sigma,n\sigma}^<(\varepsilon) - V_{k\sigma-L,n\sigma}^* G_{k\sigma-L,n}^<(\varepsilon)] \quad (5)$$

$$\rho_{n\sigma} = e(-i) \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\varepsilon G_{n\sigma,n\sigma}^<(\varepsilon) \quad (6)$$

From Eqs. (5) and (6), the following transport formulas can be obtained by correlation functions calculations straightforwardly ( $f_{\mu\sigma}$  is the Fermi distribution function):

The spin current:

$$I_\sigma(\mu_{L\sigma}, \mu_{R\sigma}) = \frac{e}{h} \int_{-\infty}^{+\infty} d\varepsilon (f_{\mu_{L\sigma}} - f_{\mu_{R\sigma}}) \frac{4\Gamma_{L\sigma}^r \Gamma_{R\sigma}^r |t_{12\sigma} t_{23\sigma}|^2}{|B_\sigma^r|^2}. \quad (7)$$

The spin conductance:

$$G_\sigma(\mu_{L(R)\sigma}) = \frac{e^2}{h} \int_{-\infty}^{+\infty} d\varepsilon \left\{ \frac{4\Gamma_{L\sigma}^r \Gamma_{R\sigma}^r |t_{12\sigma} t_{23\sigma}|^2}{|B_\sigma^r|^2} \left[ \frac{1}{4k_B T} \frac{1}{\cosh^2\left(\frac{\varepsilon - \mu_{L(R)\sigma}}{2k_B T}\right)} \right] \right\} \quad (8)$$

The up-spin electron charge on each site of the wire:

$$\begin{aligned} \rho_{1\uparrow,1\uparrow}(\mu_{L\uparrow}, \mu_{R\uparrow}) = & \frac{e}{\pi} \int_{-\infty}^{+\infty} d\varepsilon \left\{ \frac{f_{\mu_{L\uparrow}} \Gamma_{L\uparrow}^r \left[ \left( (x_{1\uparrow} - U_2 \rho_{2\uparrow,2\uparrow}/e)(x_{1\uparrow} - U_3 \rho_{3\uparrow,3\uparrow}/e) - |t_{12\uparrow}|^2 \right) + (\Gamma_{R\uparrow}^r)^2 (x_{1\uparrow} - U_2 \rho_{2\uparrow,2\uparrow}/e)^2 \right] + f_{\mu_{R\uparrow}} \Gamma_{R\uparrow}^r |t_{12\uparrow} t_{23\uparrow}|^2}{|B_{1\uparrow}^r|^2} \right\} \\ \rho_{2\uparrow,2\uparrow}(\mu_{L\uparrow}, \mu_{R\uparrow}) = & \frac{e}{\pi} \int_{-\infty}^{+\infty} d\varepsilon \left\{ \frac{f_{\mu_{L\uparrow}} \Gamma_{L\uparrow}^r \left[ (x_{2\uparrow} - U_3 \rho_{3\uparrow,3\uparrow}/e)^2 + (\Gamma_{R\uparrow}^r)^2 |t_{12\uparrow}|^2 \right] + f_{\mu_{R\uparrow}} \Gamma_{R\uparrow}^r \left[ (x_{2\uparrow} - U_1 \rho_{1\uparrow,1\uparrow}/e)^2 + (\Gamma_{L\uparrow}^r)^2 |t_{23\uparrow}|^2 \right]}{|B_{2\uparrow}^r|^2} \right\} \\ \rho_{3\uparrow,3\uparrow}(\mu_{L\uparrow}, \mu_{R\uparrow}) = & \frac{e}{\pi} \int_{-\infty}^{+\infty} d\varepsilon \left\{ \frac{f_{\mu_{L\uparrow}} \Gamma_{L\uparrow}^r |t_{12\uparrow} t_{23\uparrow}|^2 + f_{\mu_{R\uparrow}} \Gamma_{R\uparrow}^r \left[ (x_{3\uparrow} - U_1 \rho_{1\uparrow,1\uparrow}/e)(x_{3\uparrow} - U_2 \rho_{2\uparrow,2\uparrow}/e) - |t_{23\uparrow}|^2 \right] + (\Gamma_{L\uparrow}^r)^2 (x_{3\uparrow} - U_2 \rho_{2\uparrow,2\uparrow}/e)^2}{|B_{3\uparrow}^r|^2} \right\} \end{aligned} \quad (9)$$

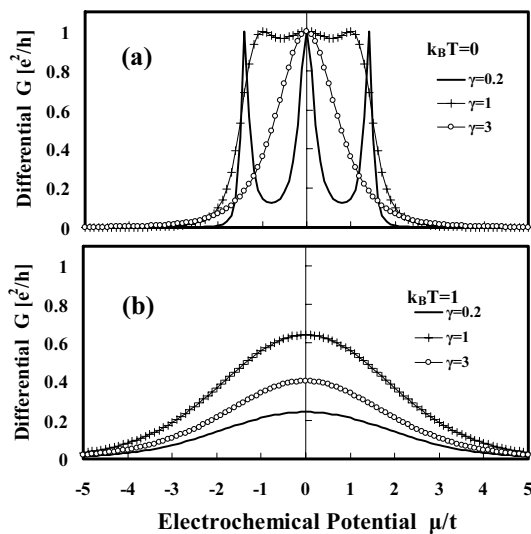
Where  $x_{1\sigma} = \varepsilon - \varepsilon_{1\sigma}$ ,  $x_{2\sigma} = \varepsilon - \varepsilon_{2\sigma}$ ,  $x_{3\sigma} = \varepsilon - \varepsilon_{3\sigma}$ , value B is given by Eq. (10). The electron charge formulas for down-spin can be obtained by exchanging the subscript  $\uparrow$  and  $\downarrow$  in the up-spin formulas above.

$$B_{\uparrow}^{\sigma} = \left[ \varepsilon - (\varepsilon_{1\uparrow} + U_1 \rho_{1\downarrow,1\downarrow}/e) + i\Gamma_{L\uparrow}^{\sigma} \right] \left[ \varepsilon - (\varepsilon_{2\uparrow} + U_2 \rho_{2\downarrow,2\downarrow}/e) \right] \left[ \varepsilon - (\varepsilon_{3\uparrow} + U_3 \rho_{3\downarrow,3\downarrow}/e) + i\Gamma_{R\uparrow}^{\sigma} \right] - \left[ \varepsilon - (\varepsilon_{1\uparrow} + U_1 \rho_{1\downarrow,1\downarrow}/e) + i\Gamma_{L\uparrow}^{\sigma} \right] t_{23\uparrow}^{\downarrow} \left[ \varepsilon - (\varepsilon_{2\uparrow} + U_2 \rho_{2\downarrow,2\downarrow}/e) \right] - \left[ \varepsilon - (\varepsilon_{2\uparrow} + U_2 \rho_{2\downarrow,2\downarrow}/e) \right] t_{12\uparrow}^{\downarrow} \left[ \varepsilon - (\varepsilon_{3\uparrow} + U_3 \rho_{3\downarrow,3\downarrow}/e) + i\Gamma_{R\uparrow}^{\sigma} \right] t_{12\uparrow}^{\downarrow} \quad (10)$$

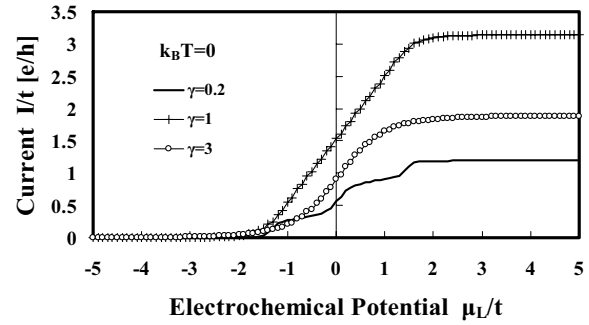
**3 Numerical results and interpretations** In this section, we calculate the transport properties of the three-site QW in some special cases applying the formulas in previous section. We assume that  $\varepsilon_{i\sigma} = 0$ ,  $t_{12\uparrow\downarrow} = t_{23\uparrow\downarrow} = t$ ,  $V_{L,k\uparrow\downarrow} = V_{R,k\uparrow\downarrow} = V$ ,  $\Gamma_{L\uparrow\downarrow}(\varepsilon) = \Gamma_{R\uparrow\downarrow}(\varepsilon) = \Gamma$  and  $U_1 = U_2 = U_3 = U$ . All of the energies are normalized by the transfer integral  $t$ . Especially, the normalized self-energy is defined as  $\gamma = \Gamma/t$  in the following numerical calculations.

**3.1 Case of  $U = 0$**  The numerical results of conductance, current and electron charges in the three sites of the wire as a function of electrochemical potential  $\mu$  for several values of  $\gamma$  are illustrated in Fig. 2, Fig. 3 and Fig. 4.

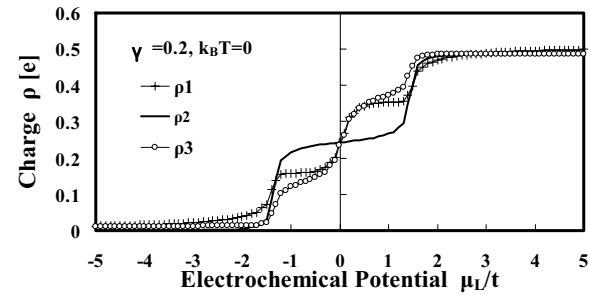
The behavior of conductance and transport current changes dramatically when the value of  $\gamma$  crosses unity. When  $\gamma < 1$ , the conductance has three maximums at  $y = 0$  and  $y = \pm\sqrt{2}$ , and the corresponding current increases intermittently with a step shape. These phenomena imply that resonant tunneling and conductance quantization take place easily in this case. Whereas when  $\gamma \geq 1$ , these quantum effects in transport will disappear gradually with the increase of  $\gamma$ . In the case of  $T > 0$  K, the line shapes of the transport characteristics become not to change so much and become all smoother than those in  $T = 0$  K due to the



**Figure 2** Conductance as a function of electrochemical potential  $\mu$  for self-energy  $\gamma = 0.2, 1$  and  $3$  (normalized by transfer energy  $t$ ), (a) when  $k_B T = 0$  ( $T = 0$  K), (b) when  $k_B T = 1$  ( $T > 0$  K).



**Figure 3** Transport current as a function of electrochemical potential of left electrode  $\mu_L$  ( $\mu_R = -5$ ) for self-energy  $\gamma = 0.2, 1$  and  $3$ , when  $T = 0$  K.



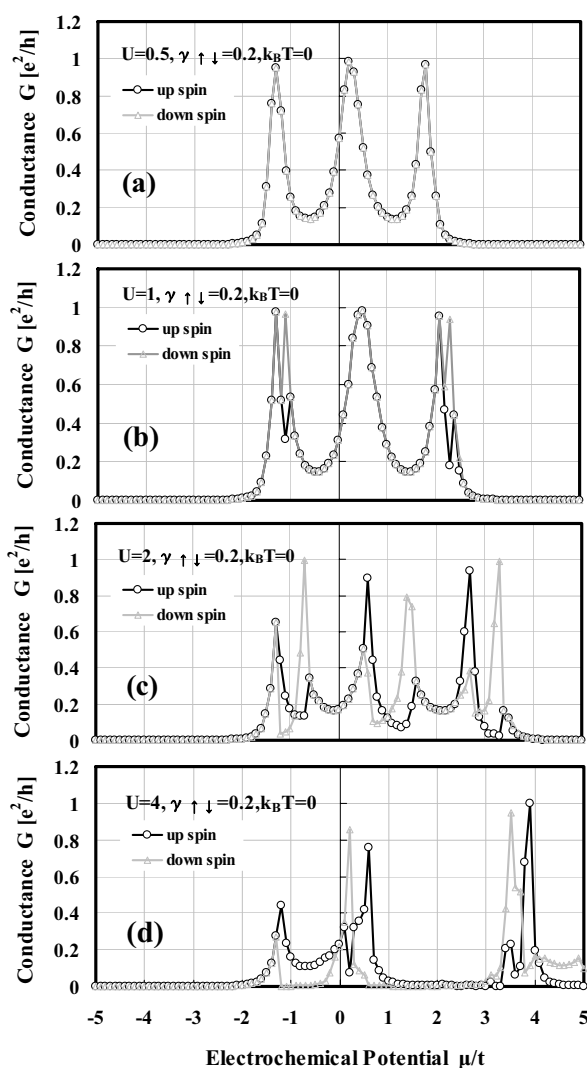
**Figure 4** Electronic charges in the three sites as a function of electrochemical potential of left electrode  $\mu_L$  ( $\mu_R = -5$ ) for self-energy  $\gamma = 0.2$ , when  $T = 0$  K.

thermal fluctuations. The charge distributions shown in Fig. 4 result in the fact that in the area of  $\mu_L < 0$ , a minus charge barrier will be formed at the boundary of the wire, whereas in the area of  $\mu_L > 0$ , a plus charge barrier will be formed.

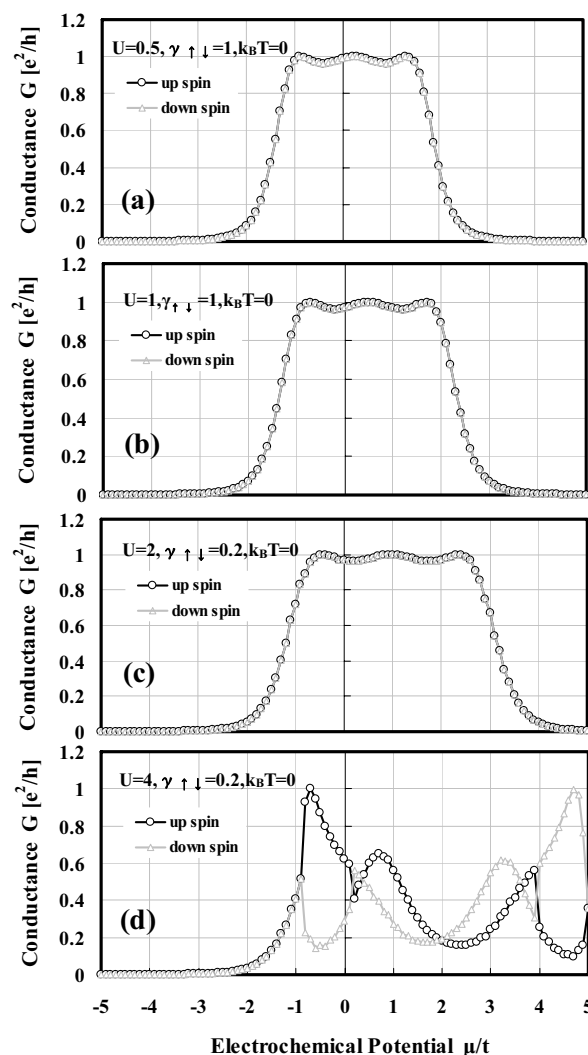
**3.2 Case of  $U > 0$**  We select comparative small value of  $U$  ( $U < 5$ ) to investigate Coulomb interaction effects in transport due to the limits of Hartree-Fock approximation. The transport properties are computed by self-consistent calculations concern with site charges  $\rho_{n\uparrow\downarrow}$ . The initial site charges are decided by the ground state of the three-site QW with half-filling ( $N = 3$ ) assumption, which is an anti-ferromagnet state with total spin of  $+1/2$ .

The numerical results of spin conductance in the case of  $\gamma = 0.2$  and  $1$  as a function of  $\mu$  for several values of  $U$  are illustrated in the Fig. 5 and Fig. 6, respectively. Compared with the case of  $U = 0$ , the conductance curves shift to right and peaks are broadened with the increase of  $U$ . When  $U > 2\gamma$ , the peaks of conductance start to split into two corresponding to up or down spin conductance. These phenomena all result from the changes of spin orbits in the

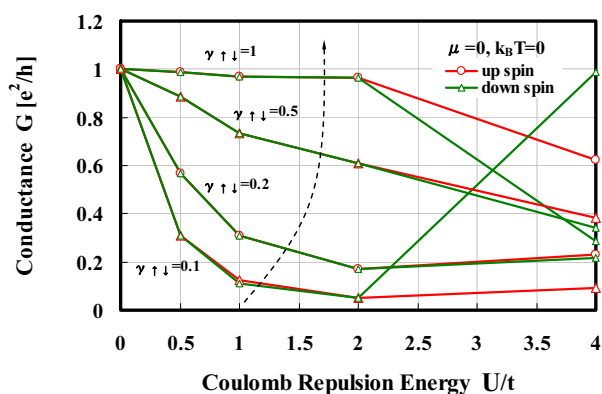
wire due to the Coulomb repulsion between the up and down spin electrons on sites. The series of peaks and valleys in the conductance characteristics can be considered a synthetic effect of resonant tunneling and Coulomb blockade. One of the valley happens to shift on the Fermi-level of the wire ( $\mu = 0$ ), the metal-insulator transition (Mott transition) will take place. We show the spin conductance as a function of  $U$  for several values of  $\gamma$  when  $\mu = 0$  in the Fig. 7. This result indicates that, if the self-energy  $\gamma$  has small value compared with  $U$ , generally the spin conductance will rapidly decrease with the increase of  $U$ , and the wire becomes an insulator from a metal (Mott transition).



**Figure 5** Up-spin and down-spin conductance as a function of electrochemical potential  $\mu$  for self-energy  $\gamma = 0.2$  when  $T = 0$  K. (a)  $U = 0.5$ , (b)  $U = 1$ , (c)  $U = 2$ , (d)  $U = 4$ .

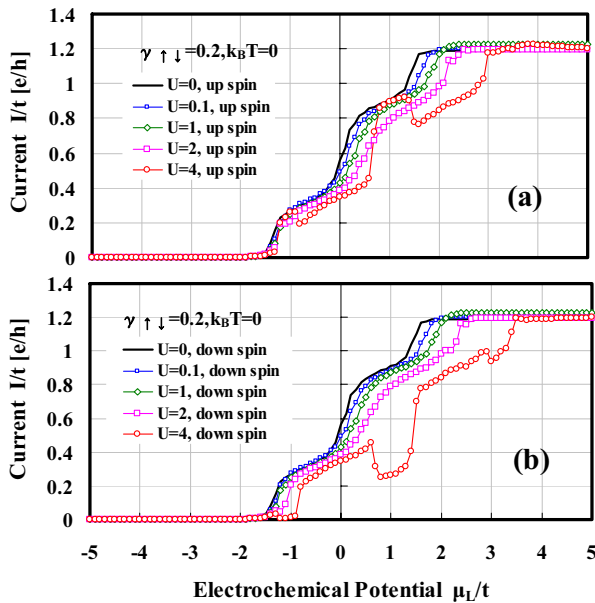


**Figure 6** Up-spin and down-spin conductance as a function of electrochemical potential  $\mu$  for self-energy  $\gamma = 1$  when  $T = 0$  K. (a)  $U = 0.5$ , (b)  $U = 1$ , (c)  $U = 2$ , (d)  $U = 4$ .



**Figure 7** Up-spin and down-spin Conductance as a function of  $U$  for self-energy  $\gamma = 0.1, 0.2, 0.5$  and  $1$ , when electrochemical potential  $\mu = 0$  and  $T = 0$  K.

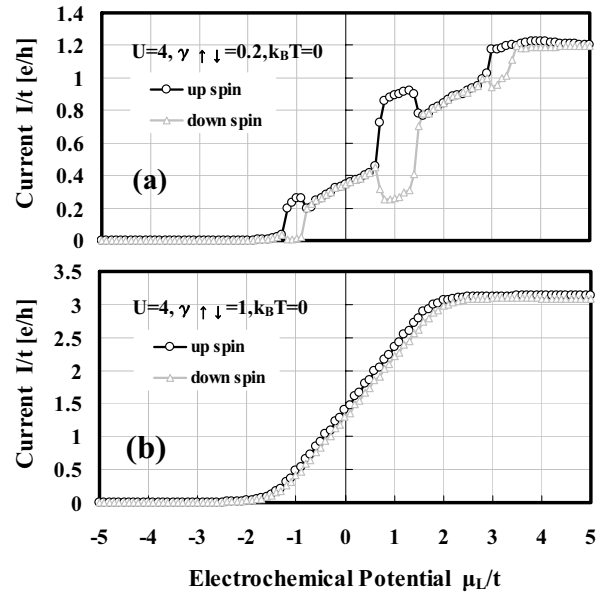
We illustrate the spin current as a function of left electrode potential  $\mu_L$  ( $\mu_R = -5$ ) for several values of  $U$  in the Fig. 8 when  $\gamma = 0.2$ . Because the self-energy  $\gamma$  has a small value, the nonequilibrium spin current gradually decreases with the increase of  $U$ . Meanwhile, the line shape of the up spin current separates from that of the down spin current.



**Figure 8** Spin transport current as a function of electrochemical potential of left electrode  $\mu_L$  ( $\mu_R = -5$ ) for  $U = 0, 0.5, 1, 2$ , and  $4$ , when self-energies  $\gamma = 0.2$  and  $T = 0$  K. (a) Up-spin, (b) down-spin.

In Fig. 9, we demonstrate the up and down spin current as a function of  $\mu_L$  ( $\mu_R = -5$ ) for  $\gamma = 0.2$  and  $1$  when  $U$  has a large value of  $4$ . Especially, in the case of  $\gamma = 0.2$ , when  $\mu_L$  approaches some positions where the conductance has peak values in the Fig. 5, the up-spin current increases while the down-spin current decreases, indicating that the spin polarization takes place in the wire.

**4 Summary** Based on the Keldysh formalism, we derived some rigorous formulas of nonequilibrium electronic transport for a three-site QW model within Hartree-Fock approximation when Coulomb repulsion is present. According to numerical calculations, we investigate the conductance, transport current and electronic charge distribution of the three-site QW in some special occasions. In noninteracting case, when self-energy  $\gamma < 0$ , the resonant tunneling transport and the conductance quantization can be easily observed. The transport properties of up-spin are identical with those of down-spin. While if the Coulomb interaction is present, the conductance curves shift to right and the peaks are broadened with the increase of  $U$  because of electron-electron repulsions. When  $U > 2\gamma$ , the peaks of conductance split into two. The Coulomb block-



**Figure 9** Up-spin and down-spin transport current as a function of electrochemical potential of left electrode  $\mu_L$  ( $\mu_R = -5$ ) for  $U = 4$ , when  $T = 0$  K. (a)  $\gamma = 0.2$ , (b)  $\gamma = 1$ .

ade and metal-insulator transition (Mott transition) phenomena are obvious if  $\gamma$  has a small value compared with  $U$ . The conductance and transport current of the up-spin also become quite different from those of the down-spin indicating that the spin polarization takes place in the wire.

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