Theory of Nonequilibrium Transport Properties for a Three-site Quantum Wire

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With advantage of fabrication techniques for nanometer scale structures, it becomes possible to create quantum wire with the diameter of the order of the Fermi wavelength, and to experimentally study the quantum transport properties through them.[1,2] We present theoretical and numerical results for nonequilibrium transport properties with a simplest model of three-site quantum wire(Fig.1) making use of Keldysh formalism.[3-5] Some rigorous formulas in noninteracting case are provided for direct calculations.

$$g(\mu) = \frac{e^2}{h}\int_{-\infty}^{+\infty} dy \left\{ \frac{4\gamma^2}{(y_1 y_2 y_3 - \gamma^2 y_2 - y_1 - y_3)^2 + (\gamma y_1 y_2 + \gamma y_2 y_3 - 2\gamma)^2} \left(\frac{1}{4k_B T} \frac{1}{\cosh^2\left(\frac{y-\mu}{2k_B T}\right)} \right) \right\} \tag{1}$$

$$\rho_{1\sigma}(\mu_L, \mu_R) = \frac{e}{\pi}\int_{-\infty}^{+\infty} dy \left\{ \frac{f_{\mu_L}\gamma\left[(y_2 y_3 - 1)^2 + \gamma^2 y_2^2\right] + f_{\mu_R}\gamma}{(y_1 y_2 y_3 - \gamma^2 y_2 - y_1 - y_3)^2 + (\gamma y_1 y_2 + \gamma y_2 y_3 - 2\gamma)^2} \right\} \tag{2}$$

$$\rho_{2\sigma}(\mu_L, \mu_R) = \frac{e}{\pi}\int_{-\infty}^{+\infty} dy \left\{ \frac{f_{\mu_L}\gamma(y_3^2 + \gamma^2) + f_{\mu_R}\gamma(y_1^2 + \gamma^2)}{(y_1 y_2 y_3 - \gamma^2 y_2 - y_1 - y_3)^2 + (\gamma y_1 y_2 + \gamma y_2 y_3 - 2\gamma)^2} \right\} \tag{3}$$

$$f_{\mu_{L(R)}}(\varepsilon) = \frac{1}{1 + \exp\left(\frac{\varepsilon - \mu_{L(R)}}{k_B T}\right)} \tag{4}$$

Where $\gamma = \Gamma / t$, $y = \varepsilon / t$, $y_i = y - (\varepsilon_{i\sigma} / t)$.

According to numerical calculation results obtained from those formulas, we investigate differential conductance, transport current, conductance and site electron charges of the wire in some special occasions. In the case of a uniform ingredient wire, we show that, if site-site couplings in wire are tougher than wire-electrode couplings (γ<1), the resonant tunneling transport takes place and the phenomenon of conductance quantization can be easily observed. Whereas wire-electrode couplings are tougher than site-site couplings in wire (γ>1), these quantum effects in transport will disappear gradually with the increase of strength of the wire-electrode couplings (Fig.2, Fig.3). We also discuss charge distributions in three sites of the wire and the characteristics of charge barrier (Schottky barrier) regardless of Coulomb interaction (Fig.4). When T>0K, line shapes of transport characteristics become not to change so much and become all smoother than those in T=0K due to thermal fluctuations. In the case of a wire containing impurities, line shapes of transport characteristics are changed because of the change of system electronic states.

References

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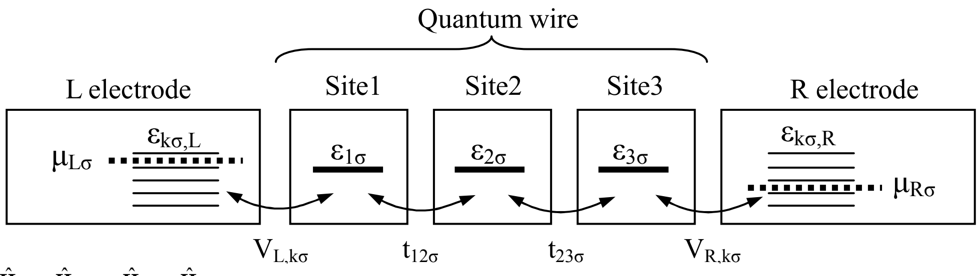

$$\hat{\boldsymbol{H}} = \hat{\boldsymbol{H}}_{ed} + \hat{\boldsymbol{H}}_{wire} + \hat{\boldsymbol{H}}_{wt} + \hat{\boldsymbol{H}}_{ewt}$$

$$= \sum_{k\sigma}\left(\varepsilon_{k\sigma,L}\hat{c}^{+}_{k\sigma,L}\hat{c}_{k\sigma,L} + \varepsilon_{k\sigma,R}\hat{c}^{+}_{k\sigma,R}\hat{c}_{k\sigma,R}\right) + \varepsilon_{1\sigma}\hat{d}^{+}_{1\sigma}\hat{d}_{1\sigma} + \varepsilon_{2\sigma}\hat{d}^{+}_{2\sigma}\hat{d}_{2\sigma} + \varepsilon_{3\sigma}\hat{d}^{+}_{3\sigma}\hat{d}_{3\sigma} + t_{12\sigma}\hat{d}^{+}_{1\sigma}\hat{d}_{2\sigma} + t^{*}_{12\sigma}\hat{d}^{+}_{2\sigma}\hat{d}_{1\sigma} + t_{23\sigma}\hat{d}^{+}_{2\sigma}\hat{d}_{3\sigma} + t^{*}_{23\sigma}\hat{d}^{+}_{3\sigma}\hat{d}_{2\sigma}$$

$$+ \sum_{k\sigma}\left(V_{L,k\sigma}\hat{c}^{+}_{k\sigma,L}\hat{d}_{1\sigma} + V^{*}_{L,k\sigma}\hat{d}^{+}_{1\sigma}\hat{c}_{k\sigma,L}\right) + \sum_{k\sigma}\left(V_{R,k\sigma}\hat{c}^{+}_{k\sigma,R}\hat{d}_{3\sigma} + V^{*}_{R,k\sigma}\hat{d}^{+}_{3\sigma}\hat{c}_{k\sigma,R}\right)$$

Fig.1. Model of three-site quantum wire combined with two external electrodes. $\varepsilon_{k\sigma,\alpha}$ (α=L or R) and $\varepsilon_{i\sigma}$ are on-site energies in the electrodes and the wire region, respectively. Transfer integrals between nearest-neighbor sites are $t_{i,j\sigma}$, and tunnel combination integrals between the wire and the electrodes are $V_{\alpha,k\sigma}$. μ_L and μ_R denote electrochemical potentials of the left and right electrodes, respectively.

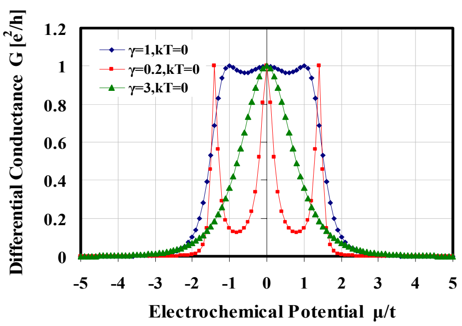

Fig.2. Differential conductance as a function of electrochemical potential μ for self energies γ= 1, 0.2 and 3 (normalized by t), when T=0K. t is transfer energy between nearest- neighbor sites.

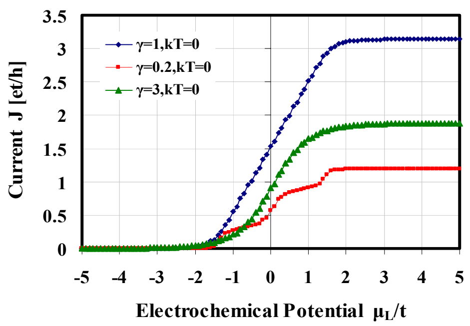

Fig.3. Transport current as a function of electrochemical potential of left electrode μ_L (μ_R=-5) for self energies γ= 1, 0.2 and 3, when T=0K.

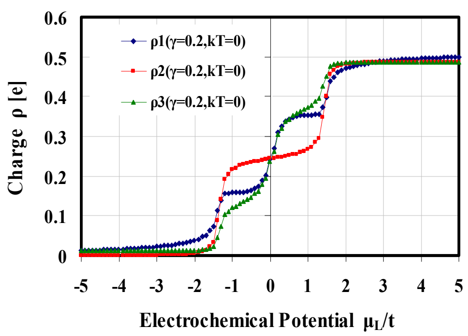

Fig.4. Charges in the three sites as a function of electrochemical potential of the left electrode μ_L (μ_R=-5) for self energy γ= 0.2, when T=0K.