Quantum Transport Modeling of Current Fluctuations in Semiconductor Quantum Dots

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1. Introduction

Shot noise has attracted a lot of attention in mesoscopic conductors because it gives information on the temporal correlation of the electrons, which is not contained in the conductance [1][2]. The theory of shot noise in single-electron tunneling devices has been developed by Hershfield *et al.* [3], where the electron-electron interaction in the dot has been described by charging energy in terms of a classically defined capacitance. Although the so-called orthodox model of single-electron tunneling seems to be reasonable for metallic quantum dot systems with fine subband spacings, it may be impossible to apply it to a semiconductor quantum dot with larger level spacings. On the other hand, as a quantum transport theory, the Anderson model has been presented to analyze the noise suppression due to Coulomb interactions for a Coulomb staircase [4]. However, even there, only a two-level quantum dot with very narrow level spacings is discussed.

In this paper, we propose a novel approach based on interacting Green's functions on a tight-binding basis to analyze the current fluctuation through a semiconductor quantum dot, where electron-electron interaction is represented by the retarded self-energy.

2. Theory

One-dimensional model

Figure 1 shows the one-dimensional double-barrier structure consisting of two semi-infinite perfect leads, two barriers and a quantum dot. The source-drain voltage U/e is defined as the difference in the electrochemical potentials between the left and right electrodes. The potential in the dot is assumed to drop linearly by the applied voltage. In our tight-binding approximation, spinless electrons with a single basis state per site are assumed (single-band calculation). The Hamiltonian will be represented in second quantized form, where the single-particle basis states are taken to be spatially localized pseudo-Wannier states. Furthermore, only the nearest-neighbor hopping between sites is considered. The effect of barriers is introduced by means of the coupling energy between the dot and the lead. Electron-electron interaction is assumed only in the dot.

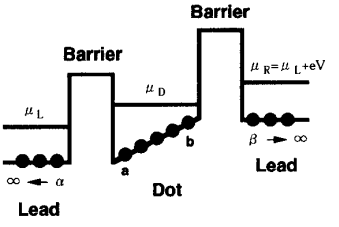

Figure 1: Schematic illustration of a one-dimensional double-barrier quantum dot. Both leads are semi-infinite. μ_L, μ_R and μ_D are the chemical potentials of the left lead, the right lead and the dot, respectively. U is the potential in the right lead due to the applied bias.

The Hamiltonian of the system is written generally as

$$H = \sum_I H_I + H_T + H_{ee} + H_\xi \quad (I = LL, D, RL), \tag{1}$$

where H_I denotes the noninteracting Hamiltonians of the left (right) lead ($I = LL$, RL), and the quantum dot ($I = D$), respectively. H_T denotes the couplings between the dot and the leads, H_{ee}, the electron-electron interaction on the dot, and H_ξ, the external potential.

The term of electron-electron interaction H_{ee} is generally given as

$$H_{ee} = \frac{1}{2}\sum_{ijkl} V_{ijkl} c_i^\dagger c_j^\dagger c_l c_k, \tag{2}$$

where i, j, k and l are indices for sites in our pseudo-Wannier basis. One can immediately see that there is a set of dominant terms corresponding to $i = k$ and $j = l$,

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giving

$$H_{ee} = \frac{1}{2}\sum_{ij} V_{ij}\hat{n}_i\hat{n}_j, \tag{3}$$

where V_{ijij} is rewritten as V_{ij} for simplicity. When the sites i and j are different, the matrix element V_{ij} is estimated as [5]

$$V_{ij} = \frac{V_0}{|\, i-j\,|}, \qquad i \neq j, \tag{4}$$

where V_0 is the strength of the interaction between nearest neighbors. Here, we neglect the $i = j$ interaction term because we are only considering spinless electrons with a single basis state per site. We note that the model is easily extended to account for spin per site.

Noise power spectrum

Keldysh's perturbation theory [6][7] based on nonequilibrium real-time Green's functions is applied to calculate the quantum transport in the quantum dot. In the theory, the electron-electron interaction is well incorporated as a term of self-energy through the perturbation series. Only two Green's functions, $G^<(t-t')$ and $G^R(t-t')$, are used for the quantum transport. The retarded Green's function and the correlation Green's function are defined, respectively, as

$$\mathrm{i}G^R_{ij}(t-t') \equiv \theta(t-t')\left\langle\left\{c_i(t), c_j^\dagger(t')\right\}\right\rangle, \tag{5}$$

and

$$-\,\mathrm{i}G^<_{ij}(t-t') \equiv \left\langle c_j^\dagger(t')c_i(t)\right\rangle, \tag{6}$$

where $\theta(t-t')$ denotes the step function. $\{AB\} = AB+BA$ is the anticommutator, and $\langle\ldots\rangle$ represents statistical expectation values over all available states. In the steady-state transport, the Green's functions are Fourier transformed with respect to the relative time $\tau = t-t'$, and denoted by $G^R(E)$ and $G^<(E)$. They satisfy the following steady-state transport equations derived from Dyson's equation

$$G^R = G^{R0} + G^{R0}\Sigma^R G^R, \tag{7}$$

$$\begin{aligned} G^< &= \left(1+G^R\Sigma^R\right)G^{<0}\left(1+G^R\Sigma^R\right)^\dagger \\ &\quad +G^R\Sigma^< G^{R\dagger}, \end{aligned} \tag{8}$$

where Green's functions and the self-energies (Σ^R and $\Sigma^<$) are matrices in site space and functions of energy E. The G^{R0} and $G^{<0}$ terms are the Green's function associated with a noninteracting system. They are determined exactly. The self-energies Σ^R_{lm} are comprised of a sum of the single-particle part $\Sigma^{R(1)}_{lm}$ and the electron-electron interaction part $\Sigma^{R(2)}_{lm}$. $\Sigma^{R(1)}_{lm}$ is given by the nearest-neighbor hopping term t_{lm} in the dot, and the coupling term t^{LD} (t^{RD}) at the left (right) lead-dot interface. The two-particle interaction term $\Sigma^{R(2)}_{lm}$ is obtained using the established rules of the perturbation theory. The lowest-order terms are represented by [5]

$$\begin{aligned} \Sigma^{R(2)}_{lm} &= \delta_{lm}\sum_{k\in D} V_{lk}\int\frac{-\mathrm{i}dE}{2\pi}G^<_{kk}(E) \\ &\quad +V_{lm}\int\frac{\mathrm{i}dE}{2\pi}G^<_{lm}(E), \end{aligned} \tag{9}$$

where $l, m \in D$. On the other hand, $\Sigma^<_{lm}$ is always found to be zero. The nonequilibrium Green's functions $G^R(E)$ and $G^<(E)$ will be obtained numerically by solving eqs. (7)-(9) self-consistently.

Once the nonequilibrium Green's functions have been calculated, the expectation values of the steady-state current $\langle I\rangle$ and the total electron number on the dot $\langle N\rangle$ are obtained directly from $G^<(E)$.

$$\begin{aligned} \langle I_{\alpha a}\rangle &= \frac{et^{LD}}{\hbar}\int_{-\infty}^{\infty}\frac{dE}{2\pi}\left[G^<_{\alpha a}(E) - G^<_{a\alpha}(E)\right] \\ &\quad (\alpha \in LL;\ a \in D;\ \alpha, a = \mathrm{nn}), \end{aligned} \tag{10}$$

$$\langle N\rangle = \int\frac{-\mathrm{i}dE}{2\pi}\sum_{l\in D}G^<_{ll}(E). \tag{11}$$

The noise power spectrum is related to the Fourier transform of the current correlation function as [8]

$$\begin{aligned} S_{\alpha a}(E) &= \int_{-\infty}^{\infty}d\tau e^{\mathrm{i}E\tau/\hbar}\langle\Delta I_{\alpha a}(\tau)\Delta I_{\alpha a}(0) \\ &\quad +\Delta I_{\alpha a}(0)\Delta I_{\alpha a}(\tau)\rangle \\ &\quad (\alpha \in LL;\ a \in D;\ \alpha, a = \mathrm{nn}), \end{aligned} \tag{12}$$

where $\Delta I_{\alpha a} = I_{\alpha a} - \langle I_{\alpha a}\rangle$. The noise power spectrum derived from eq. (12) is expressed in the form of the two-electron Green's function, which will be approximated as the sum of products of two one-electron Green's functions using Wick's theorem. Since the noise power is constant over a very wide frequency range, we only investigate the zero-frequency shot noise. Then, the noise power is represented as

$$\begin{aligned} S_{\alpha a}(0) &= -\frac{2e^2(t^{LD})^2}{h}\int_{-\infty}^{\infty}dE[G^<_{a\alpha}(E)G^>_{a\alpha}(E) \\ &\quad +G^<_{\alpha a}(E)G^>_{\alpha a}(E) - G^<_{aa}(E)G^>_{\alpha\alpha}(E) \\ &\quad -G^<_{\alpha\alpha}(E)G^>_{aa}(E)], \end{aligned} \tag{13}$$

where $G^>_{ij}(E) = G^<_{ij}(E) + G^R_{ij}(E) - (G^R_{ji})^*(E)$, and i, $j = \alpha$, a. Here, it should be pointed out that eq. (13) is completely satisfied when the interaction between electrons is neglected.

3. Numerical Results

In this study, the unit of energy is taken to be $|t|$, where t is the hopping energy. Unless otherwise noted, the following parameters will be used throughout the paper; the temperature is zero, and the frequency is zero. In two leads and the dot, the on-site energy is set to be $2[|t|]$ and

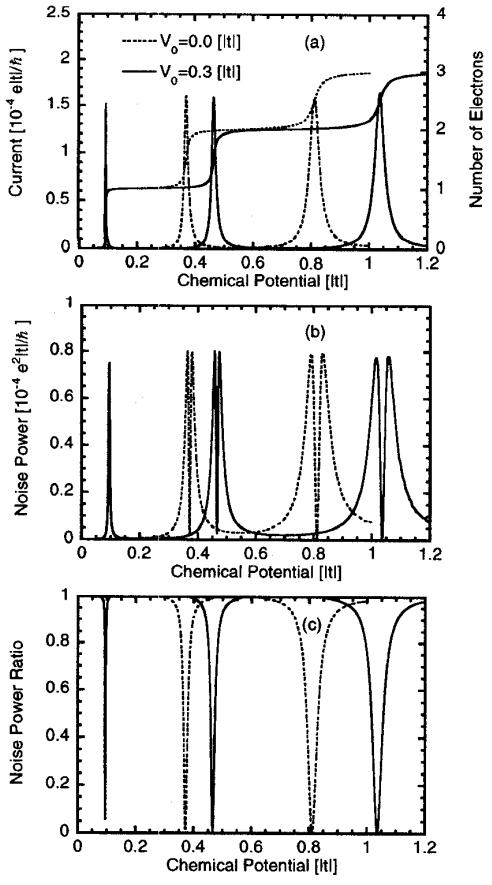

Figure 2: Coulomb oscillation characteristics (a), shot-noise power (b), and noise power ratio (c) as a function of the chemical potential of the dot with equal barriers ($t^{LD} = t^{RD} = -0.3[|t|]$). Coulomb interaction between electrons V_0 is $0.3[|t|]$ for solid-line curves and zero for dashed-line curves. The source-drain voltage is $0.001[|t|/e]$. The number of sites on the dot is 9.

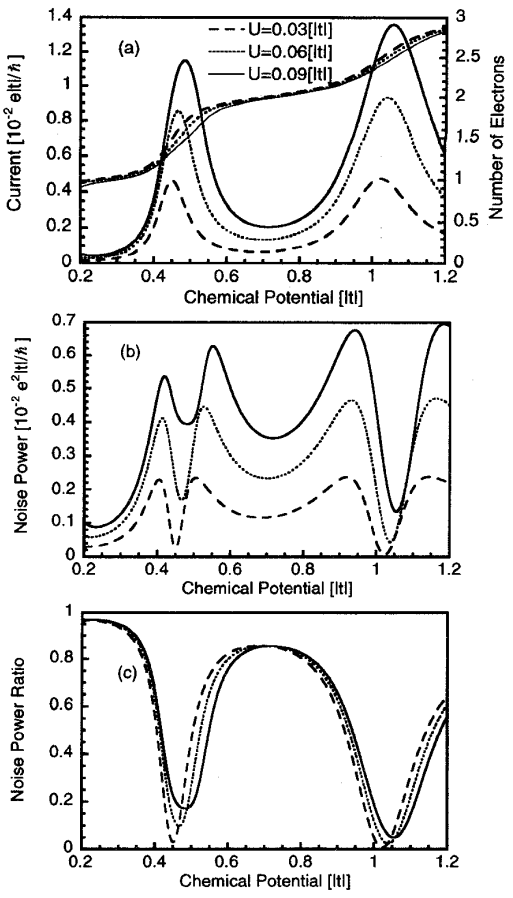

Figure 3: Coulomb oscillation characteristics (a), shot-noise power (b), and noise power ratio (c) as a function of the chemical potential of the dot with equal barriers ($t^{LD} = t^{RD} = -0.6[|t|]$). Coulomb interaction between electrons V_0 is $0.3[t]$. The source-drain voltage is varied from $0.03[|t|/e]$ to $0.09[|t|/e]$ in a $0.03[|t|/e]$ step. The number of sites on the dot is 9.

the hopping energy is -1[|t|]. The number of sites on the dot is set as 9 for the Coulomb oscillation, and 21 for the Coulomb staircase.

Shot noise for Coulomb oscillation

First, the shot noise characteristics for Coulomb oscillation, are calculated for a dot with equal barriers as a function of the chemical potential of the dot. In Fig. 2, the current and the number of electrons on the dot, the noise power, and the noise power ratio defined by $S/2eI$ are plotted in (a), (b) and (c), respectively, for the two interacting strengths of electrons between nearest neighbors ($V_0 = 0.3[|t|]$ for solid line curves and zero for dashed line curves). In the calculation, the external source-drain voltage is set to be very small. Figure 2(a) shows the Coulomb oscillation properties of the dot. At the peaks of the Coulomb oscillations, the current noise is strongly suppressed as shown in Fig. 2(b). The variation of the noise power ratio is shown in Fig. 2(c), as a function of chemical potential. It takes a value of one when no current flows through the quantum dot, and is close to zero at the peaks of Coulomb oscillations. On the other hand, the influence of the Coulomb interaction between electrons on the shot noise is illustrated by dashed lines in Fig. 2. We found that although the periods of Coulomb oscillations change due to the Coulomb interaction, the noise characteristics themselves hardly change. This suggests that the correlation due to Coulomb interaction between the electrons in the current-carrying state and the bound state is extremely weak in Coulomb oscillations. When the source-drain voltage U/e is increased from $0.03[|t|/e]$ to $0.09[|t|/e]$ in a $0.03[|t|/e]$ step, the Coulomb oscillation characteristics change greatly as

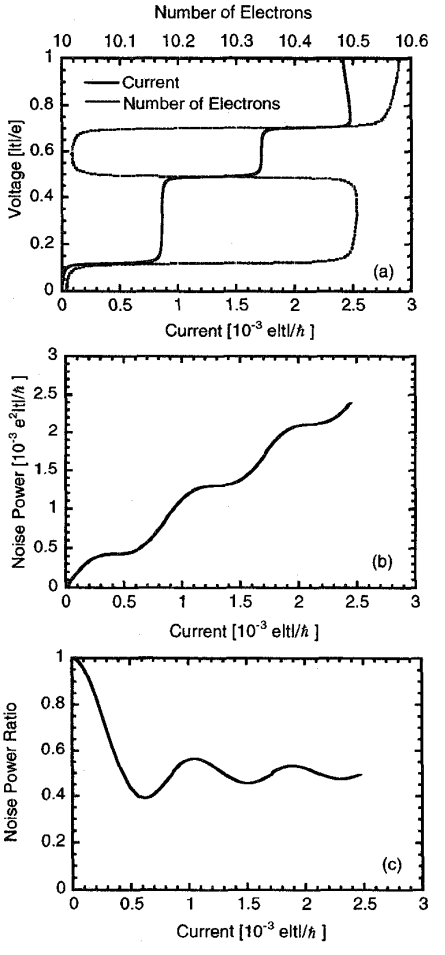

Figure 4: Coulomb staircase characteristics (a), shot-noise power (b), and noise power ratio (c) as a function of the tunneling current for the dot with equal barriers ($t^{LD} = t^{RD} = -0.1[|t|]$). $V_0 = 0.1[|t|]$ and $\mu_L = 2.2[|t|]$. The number of sites on the dot is 21.

shown in Fig. 3. At the peaks of the Coulomb oscillations, as the source-drain voltage increases, the current noise is less suppressed and accordingly the noise power ratio goes up. The wider conductance peaks compared to Fig. 2 are due to the stronger dot-lead coupling.

Shot noise for Coulomb staircase

Next, we study the shot-noise characteristics for the Coulomb staircase. Figure 4 shows the Coulomb staircase characteristics (a), the shot-noise power (b), and the noise power ratio (c) for a dot with equal barriers as functions of tunneling current. The averaged I-V characteristics have steplike increases of current with voltage. At each subsequent step in the current, the number of current-carrying electrons increases by one. It is found, from Fig. 4(a), that the expectation value of the electron number on the dot is not an integer but changes roughly to one half for each opening, which is a reasonable value for the dot with equal barriers. It is found, from Fig. 4(b), that the shot-noise power does not increase linearly with current but is suppressed over each current step. Consequently, the noise power ratio changes periodically with the current as shown in Fig. 4(c). It has a minimum value of about 0.4 and is 0.5 on average.

In Coulomb oscillation where the external source-drain voltage is set to be extremely small, only one level contributes to the transmission. On the other hand, in the Coulomb staircase, all the states which is broadened by the self-energy due to the external coupling and interactions, participate in the transport. Therefore, the strong correlation induced by the Pauli principle is expected in Coulomb oscillation rather than in Coulomb staircase.

4. Conclusion

We have studied the shot-noise characteristics of semiconductor quantum dots using Keldysh's perturbation theory based on nonequilibrium Green's function techniques, where the electron-electron interaction is well described in terms of self-energy. We have found that the shot noise at peaks of Coulomb oscillations decreases sharply to almost zero when the two barriers are equal. We have also found that the Coulomb interaction between the electrons in the current-carrying state and the bound state hardly affect the noise characteristics in Coulomb oscillations. As for the Coulomb staircase, we have found that the shot noise is suppressed over each current step and the noise power ratio changes periodically with the current. However, the noise power ratio has a minimum value of about 0.4 and is 0.5 on average for a dot with equal barriers.

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