Effective capacitance of the metallic single electron transistor: a path integral Monte Carlo study

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Abstract. We proposed a method to calculate the effective capacitance of a metallic single-electron transistor using the quantum Monte Carlo method to describe the Coulomb blockade effect. The effective capacitance depended on the induced gate charge, temperature, and conductance of the system. Furthermore, the results can be used to calculate the effective charging energy, which has been characterizing the strength of the Coulomb blockade effect. In the Coulomb blockade regime, the effective charging energy was approximately equal to charging energy. In particularly, the effective charging energy decreased with an increase in the conductance and temperature.

1. Introduction

Single-electron transistors are meanwhile standard tools for nanoscience [1]. One of the basic problems of single-electron transistors is charge fluctuation [2]. Usually, a single electron transistor (SET) consists of two tunneling junctions and a single metallic island as shown in Figure 1. Since the electrostatic potential of the island is tuned by its gate electrode, it allows to control the tunneling currents on the single electron level. In a nanoscale tunneling junction, electron transport is strongly affected by charging effect. It is therefore crucial to include the charging energy into the tunneling processes of electrons in the single electron transistors [3]. The theoretical model of the SET has been verified in great detail also in the low temperature range where simplified quasiclassical concepts fail [4-7]. Experimental data of linear-response conductance for the metallic single electron transistors have been compared with numerical data form quantum Monte Carlo (QMC) simulations [8]. This study confirms a close match between the theoretical model and its experimental realization for the single-electron transistors. However, it is still unclear whether the theoretical calculation would agree with experimental data of a capacitance of the SET.
For vanishing source and drain voltages and a small external gate voltage, the average island charge grows linearly as $e \langle n \rangle = C^* V_g$, where $C^*$ is an effective capacitance of the SET and the elementary charge is denoted by $e$. In the absence of Coulomb blockade effects the effective capacitance is equal to the total capacitance of the metallic island, $C^* = C_\Sigma = C_L + C_R + C_g$. In the other hands, the effective capacitance equals zero $C^* = 0$ for strong Coulomb blockade effects [9]. It is thus natural to determine the strength of the Coulomb blockade effects by the effective capacitance. In this paper we therefore calculate the effective capacitance of the metallic single electron transistor by the QMC technique for strong charge fluctuation regime. The results are not only outside of the range of the perturbation theory but also used to calculate the effective charging energy for characterizing the strength of the Coulomb blockade effect.

2. Model and computational method
Consider the circuit diagram of the metallic single electron transistor consisting of two tunneling junctions shown in Figure 1.

![Circuit diagram of the SET. The region encircled by dashed line is the island containing $n$ excess charge. The relevant parameters in this work were obtained by the sample VII of Wallisser et al. [8].](image)

In the case that $V_L - V_R = 0$, the effective capacitance can be defined by

$$\frac{C^*}{C_g} = \frac{d \langle n \rangle}{dn_g}$$

where the dimensionless gate voltage $n_g = V_g / e$, is the continuous charge induced by the gate voltage coupled to the metallic island via a capacitance $C_g$. The average island charge can be expressed as [10]

$$\langle n \rangle = n_g + \frac{1}{2\beta E_C} \frac{\partial \ln Z}{\partial n_g}.$$  

Where the dimensionless inverse temperature $\beta E_C$ relates $\beta = (k_B T)^{-1}$ to the charging energy $E_C = e^2 / 2C_\Sigma$. Since throughout this work we set $\hbar = 1$. In units of the charging energy $E_C$ the partition function of the single electron transistor can be represented in term of the path integral as [8, 11]

$$Z = \sum_{k \in \mathbb{Z}} \int_{\phi(0) = 0} D\phi e^{-S[\phi,A]},$$
where the partition function is expressed as a path integral over a phase variable \( \phi \) (conjugate to the number of excess charge on the island) where \( k \) stands for winding number. The Euclidian action \( S[\phi,k] \) consists of the Coulomb action

\[
S_c[\phi] = \int_0^{\beta E_C} d\tau \left( \frac{\phi^2}{4} \right) + 2\pi i k n_g
\]

which describes the charging of the island and the tunneling action

\[
S_t[\xi] = -g \int_0^{\beta E_C} d\tau \int_0^{\beta E_C} d\tau' \alpha(\tau - \tau') \cos(\xi(\tau) - \xi(\tau')) ,
\]

which describes the tunneling process. The dimensionless parallel conductance \( g = G_{cl} / G_k \) with \( G_{cl} = G_s + G_d \) denotes the high-temperature parallel conductance and \( G_k = e^2 / h \) is the quantum conductance. The tunneling kernel reads

\[
\alpha(\tau) = \frac{1}{4(\beta E_C)^2 \sin^2 \left( \frac{\pi - \tau}{\beta E_C} \right)} .
\]

Substitution the partition function and the average island charge number into Eq. (2) and Eq. (1), respectively, the effective capacitance can be therefore rewritten as

\[
\frac{C^*}{C_g} = 1 - \frac{2\pi^2}{\beta E_C} \langle k^2 \rangle
\]

where the expectation value of the winding number can be calculated as

\[
\langle k^2 \rangle = \frac{1}{Z} \sum_k e^{\phi(\beta E_C) - 2\pi k} \int D\phi \ k^2 e^{-S[\phi,k]} .
\]

Furthermore, it is clear that for the case of \( V_l = V_g \) the SET behaves as a single electron box.

The effective charging energy of a single electron box is defined by the gradient of the average island charge number at \( n_g = 0 \) [11], analogously, the effective charging energy of the SET can be defined as

\[
\frac{E_{c}^*}{E_C} = 1 - \frac{\partial \langle n \rangle}{\partial n_g} \bigg|_{n_g=0} = 1 - \frac{\partial C}{C_g} \bigg|_{n_g=0} .
\]

The effective charging energy is well known as the strength of the Coulomb blockade effect.

Before we present the results for the effective capacitance of the SET, we first give the relevant Monte Carlo parameters obtained by the the sample VII of Wallisser et al. [8]. The high-temperature parallel conductance \( G_{cl} = 23.0 (k\Omega) \), the total capacitance of the metallic island \( C_x = 497.0 (aF) \), and the charging energy \( 1.87 (k_B K) \). In order to obtain accurate numerical results for temperatures corresponding to the Coulomb blockade regime, we did the Monte Carlo simulation to calculate the expectation values of the winding number. For the application of the Metropolis algorithm [12-13], we need a positive definite action. Therefore the imaginary part of the Coulomb action was reduced to be measured. Additionally, importance sampling was applied to reduce the influence of the fermionic sign problem [14], which is arising from the imaginary part of the Coulomb action and impedes the
convergence of the Monte Carlo calculation. Since the action is independent of $n_g$, we can obtain the expectation values of the winding number over the whole range of the dimensionless gate voltages for a single Monte Carlo simulation. Additionally, the error bars shown in Figures 2, 3, and 4 denote one standard deviation and are smaller than the symbol size.

3. Result and discussion
In this section we present the Monte Carlo results for the effective capacitance as a function of the dimensionless gate voltage. Figure 2 shows the effective capacitance of the SET $^\ast C$ is normalized to the gate capacitance $C_g$ for the dimensionless inverse temperatures.

![Figure 2](image)

Figure 2. The dimensionless effective capacitance of the single electron transistor as a function of the dimensionless gate voltage with $\beta E_c = 1, 5, 10, 15, \text{and } 20$ for the dimensionless parallel conductance $g = 4.75$ and the gate capacitance $C_g = 19.0 \text{ aF}$.

We find that for the non-Coulomb blockade regime ($\beta E_c = 1$) the dimensionless effective capacitance of the SET is equal to the gate capacitance, i.e., $^\ast C = C_g$ and independent of the dimensionless gate voltage. However, for larger inverse temperature ($\beta E_c \gg 1$) Coulomb oscillation of the normalized effective capacitance can be observed. The magnitude of the normalized effective capacitances depend on the dimensionless gate voltage and get the maximum values (or minimum values) at $n_g = 1/2, 3/2$ and $5/2$ (0, 1, 2, and 3), respectively. The Coulomb blockade effect exhibited in the SET can be reflected by the positions of the maximum and minimum values of the normalized effective capacitance as the study of the Coulomb oscillation of the linear response conductance in Ref. [8].

![Figure 3](image)

Figure 3. The normalized effective capacitance of the SET as a function of the dimensionless gate voltage with the dimensionless parallel conductance (from bottom to top) $g = 0, 1, 5, 10, 15, \text{and } 20$ for $\beta E_c = 20$ and the gate capacitance $C_g = 19.0 \text{ aF}$.
In Figure 3 we show the Coulomb oscillation of the normalized effective capacitance for the dimensionless parallel conductance, which are beyond the perturbative regime. For two smallest \( g \) the normalized effective capacitances equal unity. Moreover, In the case that the normalized effective capacitance in the limit of the dimensionless gate voltage approach to zero, one can use the results to determine the effective charging energy as defined in Eq. (9). As an example from the Monte Carlo data of the normalized effective capacitance in Figure 3, one can obtain the effective charging energy as shown in Figure 4.

![Figure 4](image)

Figure 4. The effective charging energy as a function of the dimensionless parallel conductance for \( \beta E_c = 20 \).

As shown in Figure 4, in the limit of strong quantum fluctuation the effective charging energy vanishes and become unit in the opposite limit. In the Coulomb blockade regime, the effective charging energies are exponentially suppressed by the increasing of the dimensionless parallel conductance. In other words the Coulomb blockade effect is smeared when the dimensionless parallel conductance is very larger than unity.

4. Conclusion

The effective capacitances of the metallic single-electron transistor were calculated for describing of the Coulomb blockade effect outside of the range of the perturbative region. The results show that the effective capacitance depended on the gate voltage, temperature, and the parallel conductance of the system. Moreover, the results were also used to calculate the effective charging energy to indicate the strength of the Coulomb blockade effect. In particularly, the effective charging energy decreased with an increase in the dimensionless parallel conductance. Our results confirmed that Coulomb blockade effect are governed by two dimensionless parameters, i.e., \( g \) and \( \beta E_c \). Since the effective capacitance can be directly calculated by the quantum Monte Carlo technique and related to the effective charging energy, we therefore proposed that the effective capacitance would be one of relevant quantities to investigate the charge fluctuation in the single electron transistors and next more complicated single electron devices. The proposed calculation should be of conceptual interest and can future stimulate experimental work.

5. References

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