Monte Carlo study of single-barrier structure based on exclusion model full counting statistics*

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Different from the usual full counting statistics theoretical work that focuses on the higher order cumulants computation by using cumulant generating function in electrical structures, Monte Carlo simulation of single-barrier structure is performed to obtain time series for two types of widely applicable exclusion models, counter-flows model, and tunnel model. With high-order spectrum analysis of Matlab, the validation of Monte Carlo methods is shown through the extracted first four cumulants from the time series, which are in agreement with those from cumulant generating function. After the comparison between the counter-flows model and the tunnel model in a single barrier structure, it is found that the essential difference between them consists in the strictly holding of Pauli principle in the former and in the statistical consideration of Pauli principle in the latter.

Keywords: Monte Carlo simulation, higher order cumulant, exclusion model, full counting statistics
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1. Introduction

Since the 1970s, scholars and engineers all over the world have performed a broad and relatively thorough research on electron device noise, and developed a series of reliable characterisation techniques based on noise.[1−4] In nanoscale, elastically scattering is dominant and nonelastically scattering cannot equalise the contribution of non-equilibrium states to carrier transport, resulting in more information contained in current fluctuation. However, noise is only a kind of second-order statistical quantities. Therefore, how to utilise higher order statistical quantities to describe carrier transport, becomes an important task. Full counting statistics (FCS) originating from optics is a natural choice.[5] In optical FCS, the statistics of the number of photons absorbed by a photodetector in a fixed time interval characterises the quantum state of the electromagnetic field. Analogous to optical FCS, study of the FCS in nanometer structure is helpful for exploring the theoretical frame to extract information from current fluctuations.

At present, FCS in electronic structure mainly focuses on how to obtain higher order statistical quantities of a specific structure,[6,7] and different methods are introduced to calculate these quantities, which include semi-classical approach based on the cascade of Langevin equations, semi-classical circuit theory based on Keldysh Green's function technique, semi-classical stochastic path integral method, and exclusion models based on stochastic process. Reference [8] defines the stochastic process of the counter-flows model, deduces the tunnel model after a complex and elusive decomposition of the process in terms of the counter-flows model, and for these two types of exclusion models, the procedure is devised to acquire the cumulant generating function(CGF). Although introduction of the tunnel model is difficult to give a clear physical picture, the job still deserves to carry out, because it can be used in many typical structures, such as the single barrier, double barriers, and diffusive medium, etc. But, in practical measurements, CGF is not attainable directly, and time series is generally available only if the electrical signal detected by testing apparatus can distinguish the relatively slow carrier speed. This paper will propose a Monte Carlo scheme to obtain time series, the abstraction of its higher order cumulants will be achieved, and the simulation of exclusion models will give a clear and simple physical picture.

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2. Monte Carlo models and their validation

2.1. Monte Carlo models

Following the general procedure for the exclusion models, including the counter-flows model and the tunnel model,[8] the normalised CGF of a single-barrier structure is given by, for the counter-flows model,

$$S_t^{\mathrm{C}}(z)/t = \ln[f_{\mathrm{L}}(1-f_{\mathrm{R}})\Gamma^{(\rightarrow)}(z-1) + f_{\mathrm{R}}(1-f_{\mathrm{L}})\Gamma^{(\leftarrow)}(z^{-1}-1)+1], \quad (1a)$$

and for the tunnel model,

$$S_t^{\mathrm{T}}(z)/t = f_{\mathrm{L}}(1-f_{\mathrm{R}})\Gamma^{(\rightarrow)}(z-1) + f_{\mathrm{R}}(1-f_{\mathrm{L}})\Gamma^{(\leftarrow)}(z^{-1}-1), \quad (1b)$$

where

$$f_{\mathrm{L}} = \frac{1}{1+\mathrm{e}^{\frac{\varepsilon-E_F-eV}{k_{\mathrm{B}}T}}} \quad \text{and} \quad f_{\mathrm{R}} = \frac{1}{1+\mathrm{e}^{\frac{\varepsilon-E_F}{k_{\mathrm{B}}T}}}$$

are Fermi functions of the left lead and the right lead, respectively, $\Gamma^{(\rightarrow)}$ is the transmission coefficient from left to right through the barrier, $\Gamma^{(\leftarrow)}$ the transmission coefficient in the reverse direction of $\Gamma^{(\rightarrow)}$, superscript C indicates counter-flows model, superscript T indicates tunnel model, and the variable z was called the counting field in Ref. [6]. And t is the long time corresponding to the lower bound time of usual measurement in electronic apparatus, and most often is decades times larger than all the physical times experienced by carriers, such as diffusion time, dwell time, coherence time, and so on. We assume $t = 1$, and ignore variable t in the rest of this paper. Therefore, S_t^i $(i = \mathrm{T}, \mathrm{C})$ is nondimensional.

From the viewpoint of the stochastic process, Eq. (1b) reveals that the tunnel model of a single-barrier structure contains two independent Poisson processes in two opposite directions with parameters of $f_{\mathrm{L}}(1-f_{\mathrm{R}})\Gamma^{(\rightarrow)}$ and $f_{\mathrm{R}}(1-f_{\mathrm{L}})\Gamma^{(\leftarrow)}$, respectively. Thus, the clear conception suggests a way to simulate the time series of the tunnel model of a single barrier, by mixing two Poisson processes using Monte Carlo methods.

Unlike the tunnel model, no idea of the simulation of the counter-flows model is obtained from CGF. However, we could be illumined by the definition sketch map of the counter-flows model shown in Fig. 1. The procedure of Monte Carlo simulation consists of (I) generate a uniformly distributed array P_{L} with a length of M. (II) compare $P_{\mathrm{L}}(i)$ with f_{L}, $i = 1, 2, 3 \ldots, M$. If $P_{\mathrm{L}}(i) \leq f_{\mathrm{L}}$,$P_{\mathrm{L}}(i) = 1$, or the incident state in the left lead is occupied. If $P_{\mathrm{L}}(i) > f_{\mathrm{L}}$, $P_{\mathrm{L}}(i) = 0$, or the incident state in the left lead is empty. (III) repeat procedures I and II three times. When repeating the procedure II, f_{L} is replaced by f_{R}, $\Gamma^{(\rightarrow)}$, and $\Gamma^{(\leftarrow)}$, respectively, and correspondingly, P_{R}, T_{LR} and T_{RL} are obtained, with a length of M. Different from $P_{\mathrm{L}}(i)$ and $P_{\mathrm{R}}(i)$, $T_{\mathrm{LR}}(i) = 1$(or $T_{\mathrm{RL}}(i) = 1$) means tunnelling successfully, and $T_{\mathrm{LR}}(i) = 0$(or $T_{\mathrm{RL}}(i) = 0$) denotes the occurrence of reflection. (IV) for each i, $(i = 1, 2, 3 \ldots, M)$,

$$\mathrm{Num}(i) = [P_{\mathrm{L}}(i)(1-P_{\mathrm{R}}(i)) + (1-P_{\mathrm{L}}(i))P_{\mathrm{R}}(i)] \times [P_{\mathrm{L}}(i)T_{\mathrm{LR}}(i) - P_{\mathrm{R}}(i)T_{\mathrm{RL}}(i)], \quad (2)$$

where Num denotes the number of carriers. If both sides of a single barrier are empty or occupied, the term in the first square bracket of Eq. (2) equals zero, leading to the zero value of Num(i), or no net transport of charge carriers. The situation describes the top evolution and the bottom evolution of Fig. 1, and the Pauli principle is satisfied by the simultaneous occurrence of tunnel or reflection for states in both sides of a single barrier. If one side is occupied and the other is empty, the term in the first square bracket equals one, and therefore, the term in the second square bracket plays a role in carriers transport, which is depicted by the middle two evolution of Fig. 1.

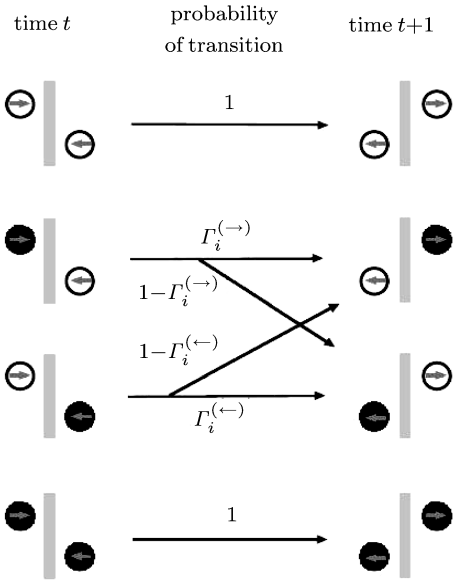


Fig. 1. Counter-flows model.[8] Probability of evolution for the various configurations of electrons reaching the ith barrier at time t.

2.2. Validation of Monte Carlo models

Time series of exclusion process could be obtained with the procedure stated in Section 2.1, and the computation codes of the first four cumulants from Matlab high-order spectrum analysis, could be used to analyse the time series. The n order cumulant can be generated by the n order differential of CGF,

$$C_n(\varepsilon) = \left.\frac{\partial^n S(\varepsilon, z)}{\partial(\ln z)^n}\right|_{z=1}. \quad (3)$$

Before simulation, we define $a = (\varepsilon - \varepsilon_{\rm F})/k_{\rm B}T$ and $b = eV/k_{\rm B}T$. For $a = 3$, $b = 2$, $\Gamma^{(\rightarrow)} = 1$ and $\Gamma^{(\leftarrow)} = 0.5$, the simulation of time series and the computation of the first four cumulants are performed for two types of exclusion processes, and the results are recorded in Table 1. From Table 1, we conclude that whether for the counter-flows model or for the tunnel model, the first four order cumulants of numerical simulation with Monte Carlo techniques are in a good agreement with those by analytical calculation with CGF.

Table 1. Results of numerical simulation (in front of skew line) and analytical calculation (in back of skew line) for two types of exclusion models.

	first order cumulant	second order cumulant	third order cumulant	fourth order cumulant
counter-flows model	0.2393/0.2389	0.2168/0.2165	0.0700/0.0701	–0.0117/–0.0114
tunnel model	0.2389/0.2389	0.2735/0.2732	0.2388/0.2389	0.2739/0.2735

3. Discussion

If the density of energy levels and the energy range are considered, a complete n order cumulant is obtained through integrating cumulant of a single energy level over energy,

$$K_n = \int C_n(\varepsilon, \rho_{\rm L}(\varepsilon), \rho_{\rm R}(\varepsilon)) n(\varepsilon) {\rm d}\varepsilon. \quad (4)$$

For simplification, we just assume $n(\varepsilon) = 1$ and count one energy channel in this paper. The sum of single energy cumulant C_n for all energy channels as the full cumulant K_n, could be done easily with the methods described in Ref. [9].

The column of the first order cumulant in Table 1, indicates that the two types of exclusion models have the same first order cumulant or mean value, which is characterised as

$$\begin{aligned} C_1^{\rm T} &= z\left.\frac{\partial S^{\rm T}}{\partial z}\right|_{z=1} = \left.\frac{z}{S^{\rm T}+1}\frac{\partial S^{\rm T}}{\partial z}\right|_{z=1} \\ &= z\left.\frac{\partial S^{\rm C}}{\partial z}\right|_{z=1} = C_1^{\rm C}, \end{aligned} \quad (5)$$

where $S^{\rm T}\big|_{z=1} = 0$. The holding of Eq. (5) denotes that for one specific structure with a determinate transmission coefficient the two types of exclusion models always have the same mean value under the same bias and at the same temperature.

Equation (2) from the counter-flows model guarantees the application of Pauli principle in the simulation process. However, for the tunnel model, only the intensities of Poisson statistics $f_{\rm L}(1-f_{\rm R})\Gamma^{(\rightarrow)}$ and $f_{\rm R}(1-f_{\rm L})\Gamma^{(\leftarrow)}$ take Pauli principle into account, statistically. These two models are equivalent in the following cases: if $f_{\rm L}$ and either of $f_{\rm R}$ and $\Gamma^{(\leftarrow)}$ are far less than one; if $1-f_{\rm R}$ and either of $1-f_{\rm L}$ and $\Gamma^{(\leftarrow)}$ are far less than one; and so for $\Gamma^{(\rightarrow)}$ and any one of $f_{\rm R}$, $1-f_{\rm L}$ and $\Gamma^{(\leftarrow)}$; thus we have seven cases in all. In any one of these cases, even though the tunnel model does not inhibit two carriers from occupying one state in one procedure, the probability of two carriers in one state is extremely small after reflection or transmission, and thus, the CGF follows,

$$S^{\rm T} = S^{\rm C}. \quad (6)$$

To clarify this point, the ratios of the first four order cumulants of the counter-flows model to the tunnel model is calculated by Monte Carlo techniques and CGF method for two specific cases. One is for $\Gamma^{(\rightarrow)} << 1$ and $\Gamma^{(\leftarrow)} << 1$, the results are listed in Table 2, and the other for $f_{\rm L} << 1$ and $f_{\rm R} << 1$, the results are in Table 3. In terms of Tables 2 and 3, the worst conformity is 7.35%, and we could think that Eq. (6) holds. It is thus concluded that the essential difference between the counter-flows model and the tunnel model is the strictly holding of Pauli principle in the former.

Table 2. Ratio of the first four order cumulants of the counter-flows model to the tunnel model, for $a = 3$, $b = 2$, $\Gamma^{(\rightarrow)} = 0.02$ and $\Gamma^{(\rightarrow)} = 0.005$.

	first order cumulant ratio	second order cumulant ratio	third order cumulant ratio	fourth order cumulant ratio
Monte Carlo model	0.9942	1.0091	0.9825	0.9873
CGF	1.0000	0.9954	0.9842	0.9659

Table 3. Ratio of the first four order cumulants of the counter-flows model to the tunnel model for $a = 6$, $b = 1$, $\Gamma^{(\rightarrow)} = 1$ and $\Gamma^{(\rightarrow)} = 0.5$.

	first order cumulant ratio	second order cumulant ratio	third order cumulant ratio	fourth order cumulant ratio
Monte Carlo model	0.9709	0.9680	0.9609	0.9265
CGF	1.0000	0.9962	0.9763	0.9616

4. Conclusion

For a single barrier, the tunnel model constitutes of two independent Poisson processes in opposite directions, and Monte Carlo model of the counter-flows model is realised by the four steps listed in Section 2.1 after a deep understanding of definition map. Matlab high-order spectrum analysis toolbox is used to compute the first four cumulants of time series produced by Monte Carlo techniques, and the cumulants are consistent with those from CGF. Thus, we obtain a clear physical picture. From another different point of view, the satisfying validation shows that Matlab high-order spectrum analysis toolbox is useful for cumulant extraction of experimental data. The most important difference between the counter-flows model and the tunnel model consists in whether Pauli principle is always effective, and it always holds in the counter-flows model but not in the tunnel model. The most evident similarity of both types of exclusion models is that the mean values are always equal for the similar structures under the same bias and at the same temperature.

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