A theoretical extraction scheme of transport information based on exclusion models*

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In order to explore how to extract more transport information from current fluctuation, a theoretical extraction scheme is presented in a single barrier structure based on exclusion models, which include counter-flows model and tunnel model. The first four cumulants of these two exclusion models are computed in a single barrier structure, and their characteristics are obtained. A scheme with the help of the first three cumulants is devised to check a transport process to follow the counter-flows model, the tunnel model or neither of them. Time series generated by Monte Carlo techniques is adopted to validate the abstraction procedure, and the result is reasonable.

Keywords: transport information extraction, higher order cumulant, exclusion model, full counting statistics
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1. Introduction

A broad and relatively thorough research on electron device noise has been performed, and a series of reliability characterization techniques based on noise have been developed.[1−5] Generally speaking, in nanoscale, elastically scattering is dominant and more information is contained in current fluctuation. However, noise is only a kind of second order statistics quantity. Therefore, how to utilize higher order statistics quantities to describe carrier transport becomes a fascinating problem. Full counting statistics (FCS) originating from optics is a natural choice.[6] In the optical FCS, the statistics of the number of photons absorbed by a photodetector in a fixed time interval characterizes the quantum state of the electromagnetic field. Analogy to optical FCS, to study the FCS in nanometer structure is helpful for exploring the theoretical frame to extract information from current fluctuation.

FCS in electronical structure is mainly concerned with the calculation of higher order statistics quantity of a specific structure from cumulant generating function (CGF),[7,8] and different methods are introduced to calculate these quantities, such as semi-classical approach based on the cascade of Langevin equations, semi-classical circuit theory based on Keldysh Green's function technique, and so on. But how to extract transport information is not still reported definitely. Exclusion models widely used in single barrier, double barriers and diffusive medium,[9] define the stochastic process of the counter-flows model, and deduce the tunnel model after a complex and elusive decomposition on the process of the counter-flows model. But these exclusion models introduce a relatively simple physical picture in the view of Monte Carlo method.[10] A theoretical scheme is presented to obtain the relevant information with high order cumulants in Section 2, and the validation is accomplished in Section 3.

2. Fundamentals and information extractation procedure

In Ref. [9] introduced were two relatively simple exclusion models: counter-flows model and tunnel model. In the former, the Pauli principle always holds, and in the latter, the principle also holds when the intensity of either contribution of two independent Poisson processes in the opposite direction is extremely small.[10] The time-normalized cumulant gen-

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erating function (CGF) of a single-barrier structure is given by

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

for the counter-flows model, and

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

for the tunnel model, where

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

are Fermi functions of left lead and right lead, respectively, $\Gamma^{(\rightarrow)}$ is the transmission coefficient from left to right through the barrier, $\Gamma^{(\leftarrow)}$ the transmission coefficient in the inverse direction of $\Gamma^{(\rightarrow)}$, superscript C indicates counter-flows model , superscript T indicates tunnel model, and variable z is called the counting field in Ref. [7]. The CGF, S_t^i, i=T, C is thought to be dimensionaless. The single energy level cumulant can be generated by differential of $S(z)$,

$$C_n = \left.\frac{\partial^n S(z)}{\partial(\ln z)^n}\right|_{z=1}. \quad (2)$$

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

$$K_n = \int C_n(\varepsilon, \rho_{\mathrm{L}}(\varepsilon), \rho_{\mathrm{R}}(\varepsilon))n(\varepsilon)\mathrm{d}\varepsilon. \quad (3)$$

For simplicity, we just assume $n(\varepsilon) = 1$ and count one energy channel in this paper. Before calculation, it is defined that $a = (\varepsilon - \varepsilon_{\mathrm{F}})/k_{\mathrm{B}}T$, $b = eV/k_{\mathrm{B}}T$, and $T_{\mathrm{L/R}} = \Gamma^{(\rightarrow)}/\Gamma^{(\leftarrow)}$. For $a = 3$, $b = 2$, and $\Gamma^{(\rightarrow)} = 0.8$, the first four cumulants of two exclusion models are shown in Fig. 1. When the ratio of $\Gamma^{(\rightarrow)}$ to $\Gamma^{(\leftarrow)}$ is large enough, corresponding to a small enough $\Gamma^{(\leftarrow)}$ value, the first four cumulants for these two exclusion models level off with the ratio increasing. Figure 1(b) reveals that the odd order cumulants are equal and so do the even order cumulants in the tunnel model.

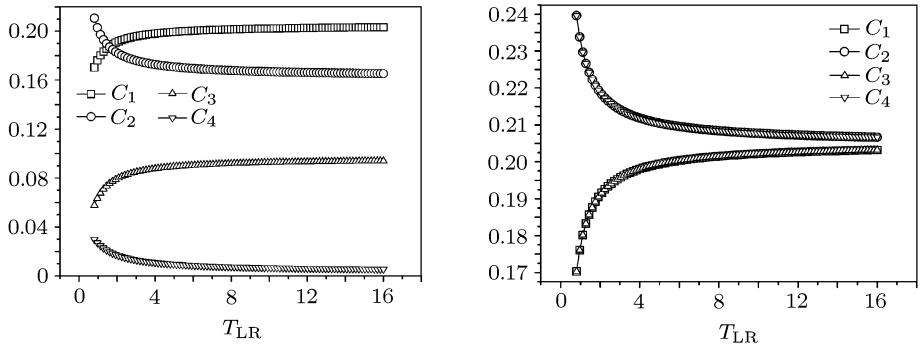


Fig. 1. First four order cumulants of exclusion models including (a) counter-flows model and (b) tunnel model.

It becomes very clear through the cumulant computation with Eqs. (1b) and (2), in the from of

$$C_k = \begin{cases} N_{\mathrm{L}\rightarrow\mathrm{R}} - N_{\mathrm{R}\rightarrow\mathrm{L}}, & k \text{ is odd}, \\ N_{\mathrm{L}\rightarrow\mathrm{R}} + N_{\mathrm{R}\rightarrow\mathrm{L}}, & k \text{ is even}, \end{cases} \quad (4)$$

where $N_{\mathrm{L}\rightarrow\mathrm{R}} = f_{\mathrm{L}}(1-f_{\mathrm{R}})\Gamma_{\mathrm{L}\rightarrow\mathrm{R}}$, and $N_{\mathrm{R}\rightarrow\mathrm{L}} = f_{\mathrm{R}}(1-f_{\mathrm{L}})\Gamma_{\mathrm{R}\rightarrow\mathrm{L}}$. All cumulants are known only if any one even order cumulant and any one odd order cumulant are obtained. It is the characteristic of the tunnel model in single barrier structure, in agreement with that in Ref. [11].

Similar to the tunnel model, the first four cumulants of counter-flows model are listed as follows:

$$C_1 = N_{\mathrm{L}\rightarrow\mathrm{R}} - N_{\mathrm{R}\rightarrow\mathrm{L}}, \quad (5a)$$

$$C_2 = N_{\mathrm{L}\rightarrow\mathrm{R}} + N_{\mathrm{R}\rightarrow\mathrm{L}} - (N_{\mathrm{L}\rightarrow\mathrm{R}} - N_{\mathrm{R}\rightarrow\mathrm{L}})^2, \quad (5b)$$

$$C_3 = N_{\mathrm{L}\rightarrow\mathrm{R}} - N_{\mathrm{R}\rightarrow\mathrm{L}} - 6N_{\mathrm{R}\rightarrow\mathrm{L}}(N_{\mathrm{L}\rightarrow\mathrm{R}} - N_{\mathrm{R}\rightarrow\mathrm{L}}) + 2(N_{\mathrm{L}\rightarrow\mathrm{R}} - N_{\mathrm{R}\rightarrow\mathrm{L}})^3 - 3(N_{\mathrm{L}\rightarrow\mathrm{R}} - N_{\mathrm{R}\rightarrow\mathrm{L}})^2, \quad (5c)$$

$$C_4 = N_{\mathrm{L}\rightarrow\mathrm{R}} + N_{\mathrm{R}\rightarrow\mathrm{L}} - 12N_{\mathrm{R}\rightarrow\mathrm{L}}(N_{\mathrm{L}\rightarrow\mathrm{R}} - N_{\mathrm{R}\rightarrow\mathrm{L}}) + 24N_{\mathrm{R}\rightarrow\mathrm{L}}(N_{\mathrm{L}\rightarrow\mathrm{R}} - N_{\mathrm{R}\rightarrow\mathrm{L}})^2 - 12N_{\mathrm{R}\rightarrow\mathrm{L}}^2 - 6(N_{\mathrm{L}\rightarrow\mathrm{R}} - N_{\mathrm{R}\rightarrow\mathrm{L}})^4 + 12(N_{\mathrm{L}\rightarrow\mathrm{R}} - N_{\mathrm{R}\rightarrow\mathrm{L}})^3$$

$$-7(N_{\mathrm{L}\to\mathrm{R}}-N_{\mathrm{R}\to\mathrm{L}})^2. \tag{5d}$$

All cumulants are the binary polynomials of $N_{\mathrm{L}\to\mathrm{R}}$ and $N_{\mathrm{R}\to\mathrm{L}}$. From Eq. (5a) to Eq. (5d), if we know any two order cumulants, $N_{\mathrm{L}\to\mathrm{R}}$ and $N_{\mathrm{R}\to\mathrm{L}}$ could be determined, and further all the other cumulants could be obtained.

For any type of exclusion model in a single barrier structure, there are at most two cumulants to supply independent equation for obtaining the transmission coefficient. To establish the relation between two unknown quantities f_{L} and f_{R} in cumulant equation, f_{L} and f_{R} could be written as

$$f_{\mathrm{L}}=\frac{B}{A+B}, \tag{6a}$$

and

$$f_{\mathrm{R}}=\frac{1}{A+1}, \tag{6b}$$

where $A=\mathrm{e}^{\frac{\varepsilon-E_{\mathrm{F}}}{k_{\mathrm{B}}T}}$, and $B=\mathrm{e}^{\frac{eV}{k_{\mathrm{B}}T}}$ with B being the known quantity determined by bias and conductor temperatures. With Eqs. (4)–(6), the ratio between two transmission coefficients could be expressed as

$$T_{\mathrm{L/R}}=\frac{C_1^2+C_1+C_2}{B(C_1^2-C_1+C_2)}$$

for the counter-flows model, (7a)

and

$$T_{\mathrm{L/R}}=\frac{C_1+C_2}{B(-C_1+C_2)} \quad \text{for the tunnel model.} \tag{7b}$$

In terms of the analysis above, aiming at time series, we could do a mechanism identification and parameter extraction by following the procedure listed in Fig. 2.

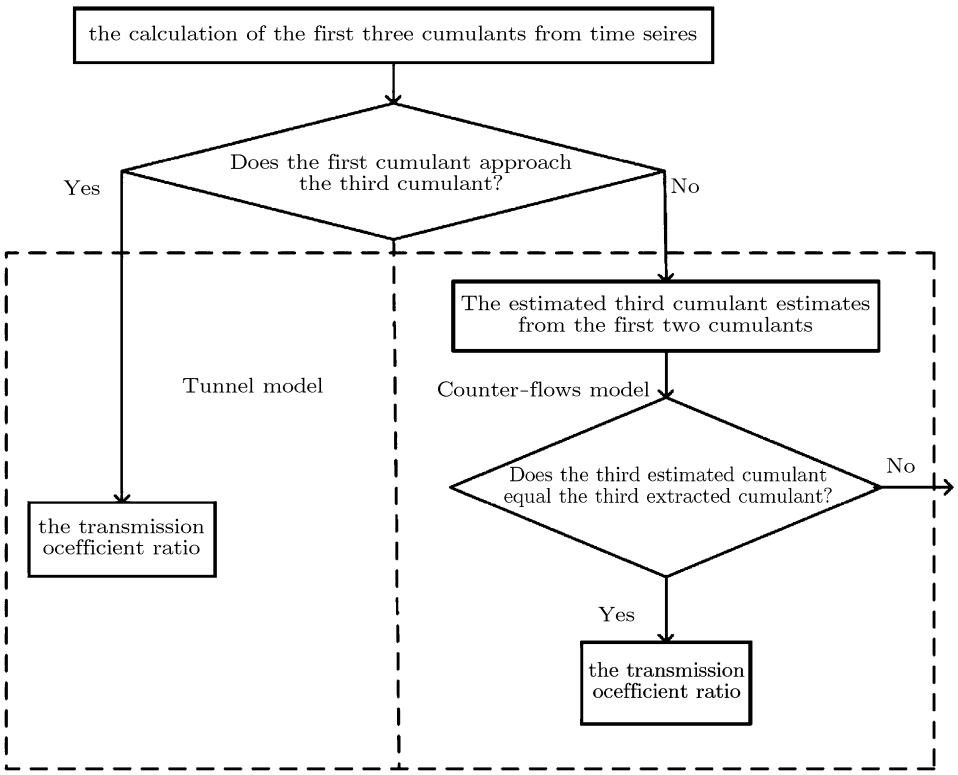


Fig. 2. Procedure of extracting information.

3. Discussion

Time series are simulated with Monte Carlo techniques by the guide of the definition and CGF of these two exclusion models.[9] The tool to extract the first four order cumulants from time series, is provided by Matlab high-order spectrum analysis toolbox.[10] From Tables 1 to 4, the analytical results of the first four order cumulants from CGF are written in the first row, in order to compare the extracted results and validate the method in Fig. 2. In the second row and the third column of Tables 1 and 3, the figures

before skew line are extraction results from time series and the figures after skew line are the calculated results from Eq. (5c).

The results in Tables 1 and 2 are obtained in the case of $a = 3$, $b = 2$, $\Gamma^{(\rightarrow)} = 1$ and $\Gamma^{(\leftarrow)} = 0.5$, for counter-flows model and tunnel model, respectively. The difference between the first order cumulant and the third order cumulant in Table1 is quite large, so the emerging possibility of tunnel model is very small. Next, whether it obeys counter-flows model depends on the agreement degree between the extracted third order cumulant and the calculated value from Eq. (5c). The consistent value in the second row and the third column of Table1 from these two different methods demonstrates the establishment of counter-flows model, indeed. Thus, Eq. (7a) is adopted to estimate $T_{\mathrm{L/R}}$, and the value approaches 2.0000. The similarity between the first order cumulant and the third order cumulant in Table 2 indicates that tunnel model is followed. The value of $T_{\mathrm{L/R}}$ obtained from Eq. (7b) also nearly equals 2.0000. From the analysis of Tables 1 and 2 it follows that the theoretical sketch in Fig. 2 could distinguish whether the generating mechanism of a time series is described by one or neither of the two exclusion models, and that $T_{\mathrm{L/R}}$ could be obtained if either of the two models is suitable.

Table 1. Validation of the counter-flows model.

	first order cumulant	second order cumulant	third order cumulant	$T_{\mathrm{L/R}}$
analytical results	0.2389	0.2165	0.0701	2.0000
extracted results	0.2376	0.2165	0.0702/0.0702	1.9813

Table 2. Validation of the tunnel model.

	first order cumulant	second order cumulant	third order cumulant	$T_{\mathrm{L/R}}$
analytical results	0.2389	0.2735	0.2389	2.0000
extracted results	0.2393	0.2723	0.2379	2.0969

Tables 3 and 4 are obtained in the case of $a = 3$, $b = 2$, $\Gamma^{(\rightarrow)} = 0.01$ and $\Gamma^{(\leftarrow)} = 0.005$, for counter-flows model and tunnel model, respectively. When $\Gamma^{(\rightarrow)}$ and $\Gamma^{(\leftarrow)}$ are small enough, S^{C} and S^{T} are nearly equal, cumulants from CGF and from time series also nearly equal for two exclusion models, shown in Tables 3 and 4. So, which exclusion model is chosen has little effect on the results. A comparison between the expressions of S^{C} and S^{T} in Eqs. (1a) and (1b) shows that there are six other cases for a single barrier structure, where S^{C} and S^{T} are equivalent, and two exclusion models are consistent, such as f_{L} and either of f_{R} and $\Gamma^{(\leftarrow)}$ are far less than one, $1 - f_{\mathrm{R}}$ and either of $1 - f_{\mathrm{L}}$ and $\Gamma^{(\leftarrow)}$ far less than one, and so are $\Gamma^{(\rightarrow)}$ and any one of f_{R}, $1 - f_{\mathrm{L}}$ and $\Gamma^{(\leftarrow)}$.[10]

Table 3. Counter-flows model for small enough $\Gamma^{(\rightarrow)}$ and $\Gamma^{(\leftarrow)}$.

	first order cumulant	second order cumulant	third order cumulant	$T_{\mathrm{L/R}}$
analytical results	0.0024	0.0027	0.0024	2.0000
extracted results	0.0023	0.0027	0.0022/0.0022	1.5916/1.6097

Table 4. Tunnel model for small enough $\Gamma^{(\rightarrow)}$ and $\Gamma^{(\leftarrow)}$.

	first order cumulant	second order cumulant	third order cumulant	$T_{\mathrm{L/R}}$
analytical results	0.0024	0.0027	0.0024	2.0000
extracted results	0.0024	0.0027	0.0024/0.0024	2.0789/2.0460

4. Summary

In the case of single-barrier and single-energy-level structure, the expressions of the first four order cumulants based on exclusion models are given and their variations with the transmission coefficient ratio at a fixed $\Gamma^{(\rightarrow)}$ are computed and shown in Fig. 1. From these equations and figures about cumulants, it follows that the tunnel model is characterized by the phenomenon that all odd cumulants are equal, and all even cumulants are also equal. According to the traits of the first three cumulants of these two models, the procedure contained in Fig.2, is presented to decide whether a transport process is characterized by counter-flows model, tunnel model or neither of them. No matter whether counter-flows model or tunnel model is suitable, the ratio of transmission coefficient from left to that from right can be denoted by two cumulants. The validation is completed by the extracted cumulants from time series generated with Monte Carlo techniques.

The theoretical extraction scheme of information about transport in this paper is a simple but pioneering job. In Landauer's picture, the sum of different energy channels could extend the assumption of uniform energy levels or single energy level, whose information extraction may need high order nonzero frequency cumulants and higher-than-four order zero frequency cumulants.

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