Counting Statistics of Non-Markovian Quantum Stochastic Processes

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I. Motivation

Full Counting Statistics

Full counting statistics (FCS) has recently attracted intensive theoretical [1] and experimental [2] attention. The interest stems from the usefulness of FCS as a sensitive diagnostic tool of stochastic electron transport through mesoscopic systems. Detectable mechanisms include quantum-mechanical coherence, entanglement, disorder, and dissipation [1]. The study of counting statistics for stochastic processes in general is of broad relevance for a wide class of problems, also outside mesoscopic physics. For example, rare events, whose study has become an important topic within non-equilibrium statistics of stochastic systems in physics, chemistry and biology, are reflected in higher order cumulants. Efficient methods for evaluating the counting statistics of stochastic processes are therefore of urgent need.
Here we present a method [3] which unifies and extends a number of earlier approaches to FCS within a generalized master equation (GME) formulation [4, 5, 6].
The distribution of the current fluctuations can be characterized by the probability that n carriers pass in time t through the contacts: $P(n,t)$. The generating function is

$$P(\chi,t) = e^{\mathcal{S}(\chi,t)} = \sum_n P(n,t)\, e^{in\chi}, \tag{1}$$

where $P(\chi,t)$ is the Generating Function (GF) and $S(\chi,t)$ is the Cumulant Generating Function (CGF). The Fourier variable χ is traditionally called *counting field*. The current and irreducible current moments (cumulants) at zero frequency are simply given by $\langle\langle I\rangle\rangle_k = e^k(-i)^k\partial_\chi^k S(\chi,t)_{\chi=0}/t$ where e is the carrier charge. For k=1, 2 we have respectively the stationary current and the noise spectral density at zero frequency. With k=3 we address the *current induced time reversal asymmetry*, the *skewness*.

II. The non-Markovian GME

Consider a nanoscale transport system governed by a generic non-Markovian GME of the form [7]

$$\frac{d}{dt}\hat\rho(n,t) = \sum_{n'}\int_0^t dt'\mathcal{W}(n-n',t-t')\hat\rho(n',t') + \hat\gamma(n,t). \tag{2}$$

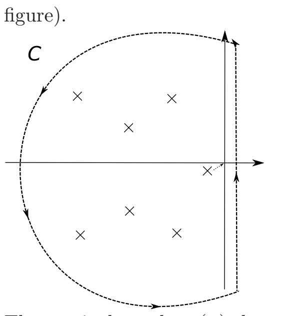
$\hat\rho(t)$ is the reduced density matrix of the system resolved into components $\hat\rho(n,t)$ corresponding to the number of electrons n passing through the nanosystem. $\mathcal{W}(t)$ is the memory kernel and describes the influence of the environment on the dynamics of the system. $\hat\gamma(t)$ is the initial inhomogeneity and accounts for initial correlations between system and environment. Both $\mathcal{W}(t)$ and $\hat\gamma(t)$ decay with time, usually on a comparable timescale, so that $\hat\gamma(t)$ is irrelevant for the long-time limit.
The probability distribution for the number of transferred charges is $P(n,t) = \mathrm{Tr}\{\hat\rho(n,t)\}$.
In Laplace space Eq. (2) leads to the algebraic expression

$$\hat\rho(\chi,z) = \frac{1}{z-\mathcal{W}(\chi,z)}[\hat\rho(\chi,t=0)+\hat\gamma(\chi,z)] = \mathcal{G}(\chi,z)[\hat\rho(\chi,t=0)+\hat\gamma(\chi,z)] \tag{3}$$

where we introduced the counting field χ with the transformation $\hat\rho(\chi,z)\equiv\sum_n\int_0^\infty dt\hat\rho(n,t)e^{in\chi-zt}$ and similarly for $\hat\gamma(\chi,z)$ and $\mathcal{W}(\chi,z)$. Inverting the Laplace transformation, the CGF then becomes

$$e^{\mathcal{S}(\chi,t)} = \frac{1}{2\pi i}\oint_{\mathcal{C}} dz\ \langle\hat\rho(\chi,z)\rangle e^{zt} \tag{4}$$

The structure of poles of $\langle\hat\rho(\chi,z)\rangle \equiv \mathrm{Tr}\{\mathcal{G}(\chi,z)[\hat\rho(\chi,t=0)+\hat\gamma(\chi,z)]\}$. contains all the statistical information about the counting process (see the figure).



We can proceed for system described by time dependent kernel $\mathcal{W}(t)$ with no power-law tails.
For $\chi\to 0$ the system in the long times tends exponentially to a unique stationary state determined by the $1/z$ pole of the resolvent. The stationary state is given by the eigenvector corresponding to the zero-eigenvalue of $\mathcal{W}(0,0)$.
With finite values of χ, an eigenvalue $\lambda_0(\chi,z)$ develops adiabatically from the zero-eigenvalue, such that $\lambda_0(0,z)=0$.
The particular pole $z_0(\chi)$ that solves the self-consistent equation

$$z_0 - \lambda_0(\chi,z_0) = 0 \tag{5}$$

and goes to zero with χ going to zero, i.e., $z_0(0)=0$. Consequently the CGF is $\mathcal{S}(\chi,t) = z_0(\chi)t$ in agreement to Eq. (4). The solution of this equation it is a difficult task and there are the methods developed:

- Non-Markovian expansion introduced in Ref. [6]
- Recursive approach introduced in Ref. [3]

Note that FCS does not depend on the initial correlations encoded in $\hat\gamma(\chi,z)$

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IV. Non-Markovian expansion

Let's start to iteratively solve Eq.(3) in terms of the expansion $\hat\rho(\chi,z) = \sum_{n=0}^\infty[\mathcal{W}(\chi,z)]^n/z^{n+1}\hat\rho(\chi,t=0)$. Using the kernel properties and by performing the inverse Laplace transformation in the long-time limit one has

$$e^{\mathcal{S}(\chi,t)} = \sum_{n=0}^\infty \frac{\partial_z^n\left([\mathcal{W}(\chi,z)]^n e^{\mathcal{W}(\chi,z)t}\right)}{n!}\Big|_{z=0^+}\hat\rho(\chi,t=0) \tag{6}$$

By making use of simple algebra it is possible to show that $\mathcal{S}(\chi,t) = z_0(\chi)t$ is linear with counting time t, demonstrating that FCS is meaningful also for this class of non-Markovian problems. The CGF is obtained from the serie

$$z_0(\chi) = -\sum_j S_j(\chi) \tag{7}$$

called *non-Markovian expansion* because the memory effects of Eq.(2) are fully included in *non-Markovian terms* $S_j(\chi)$ with $j>0$. The Markovian term $S_0(\chi)$ is obtained by the dominant eigenvalues $\lambda_0(\chi,0)$ of the memory kernel $\mathcal{W}(\chi,z\to 0)$ in agreement with previous theory [4]. The analytical formula of the non-Markovian corrections are known and they are given by a recursive formula [6]

$$S_n(\chi) = \left[\frac{\partial_z^n[\lambda_0^{n+1}(\chi,z)]}{n!} - \sum_{i=0}^{n-1}S_i\,\frac{\partial_z^{n-i}[\lambda_0^{n-i}(\chi,z)]}{(n-i)!}\right]_{z=0} \tag{8}$$

where we see the important dependence from the z-derivatives of eigenvalues. An important result was to establish that *the n-th order of current cumulants requires only the knowledge of non-Markovian terms until to $(n-1)$-th* and not all the terms of Eq.(8).

Unfortunately the approach requires the knowledge analytical formula of the eigenvalue as a function of χ and z variables around their zero values. So we are restricted to consider only simple systems where the eigenvalue problem is analytical solvable and that means a strong limitation to the number of degrees of freedom of the system.
Can we find a method to calculate the current cumulants without solving the eigenvalue equation? The answer is YES!
Here we show how to do it using an algebraical approach.

V. Recursive Scheme

As we said it may be non-trivial to determine the eigenvalue $\lambda_0(\chi,z)$, and thereafter solve Eq.(5). The recursive scheme is an efficient implementation of the Rayleigh-Schrödinger perturbative approach to solve in two steps the problem:

1. Calculate the eigenvalue expansion $\lambda_0(\chi,z) = \sum_{k,l=0}^\infty\frac{(i\chi)^k}{k!}\frac{z^l}{l!}c^{(k,l)}$
2. Solution of the self-consistent equation Eq.(5) at a given order in χ

For the first step we have the equations [3]:

$$\begin{aligned} c^{(K,L)} &= \sum_{k=0}^K\binom{K}{k}\sum_{l=0}^L\binom{L}{l}\langle\langle\tilde 0|\overline{\mathcal{W}}^{(k,l)}|0^{(K-k,L-l)}\rangle\rangle,\\ |0^{(K,L)}\rangle\rangle &= \sum_{k=0}^K\binom{K}{k}\sum_{l=0}^L\binom{L}{l}\\ &\quad\times\mathcal{R}\left[c^{(k,l)}-\overline{\mathcal{W}}^{(k,l)}\right]|0^{(K-k,L-l)}\rangle\rangle, \end{aligned} \tag{9}$$

with $K,L = 0,1,2,\dots$ and $c^{(0,L)}\equiv 0$. Here, $\langle\langle\tilde 0|$ solves $\langle\langle\tilde 0|\mathcal{W}=0$, while $|0^{(0,0)}\rangle\rangle$ is the stationary state the right eigenvector of $\mathcal{W}$. Moreover, $\overline{\mathcal{W}}(\chi,z)\equiv\mathcal{W}(\chi,z)-\mathcal{W}$ has been expanded as $\overline{\mathcal{W}}(\chi,z) = \sum_{k,l=0}^\infty\frac{(i\chi)^k}{k!}\frac{z^l}{l!}\overline{\mathcal{W}}^{(k,l)}$ with $\overline{\mathcal{W}}^{(0,0)}\equiv 0$. Finally, the pseudoinverse of the kernel is $\mathcal{R}\equiv\mathcal{Q}\mathcal{W}^{-1}\mathcal{Q}$ with $\mathcal{Q}\equiv 1-|0^{(0,0)}\rangle\rangle\langle\langle\tilde 0|$.
With the $c^{(k,l)}$'s at hand we can do the second step to calculate $z_0(\chi)$ at a given order in χ and the the zero-frequency cumulants $\langle\langle I^n\rangle\rangle$. We have

$$\begin{aligned} \langle\langle I^N\rangle\rangle &= N!\sum_{k,l=0}^N\frac{1}{k!}\frac{1}{l!}P^{(N-k,l)}c^{(k,l)},\\ P^{(K,L)} &= \sum_{n=1}^K\frac{\langle\langle I^n\rangle\rangle}{n!}P^{(K-n,L-1)} \end{aligned} \tag{10}$$

with $L=0,1,2,\dots$, and $K,N=1,2,3,\dots$. For the auxiliary quantity $P^{(K,L)}$, we have $P^{(K,0)}=\delta_{K,0}$, $P^{(0,L)}=\delta_{0,L}$, and $P^{(K,-1)}\equiv 0$. This algebraical scheme is convenient both in *analitycal* calculations both in *numerical* evaluations. Here we show only the first three cumulants of the current but higher order cumulants can be obtained in a similar manner:

$$\begin{aligned} \langle\langle I^1\rangle\rangle &= c^{(1,0)}, \qquad \langle\langle I^2\rangle\rangle = c^{(2,0)}+2c^{(1,0)}c^{(1,1)},\\ \langle\langle I^3\rangle\rangle &= c^{(3,0)}+3c^{(2,0)}c^{(1,1)}+3c^{(1,0)}\left[c^{(1,0)}c^{(1,2)}+2(c^{(1,1)})^2+c^{(2,1)}\right]. \end{aligned} \tag{11}$$

Coefficients of the form $c^{(L,0)}$ are purely Markovian quantities, and the mean current is thus not sensitive to non-Markovian effects, whereas higher order cumulants are [6]. From Eq. (9) we find the coefficients $c^{(K,L)}$. The computational bottle-neck is the valuation of the pseudoinverse $\mathcal{R}$ but it is feasible even with very large matrices. Numerically, the recursive scheme is stable for very high orders of cumulants (>20) as we have tested on simple models.

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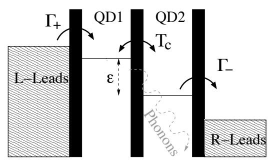
V. FCS and Noise in dissipative qbit

We consider the model of transport through a charge qubit in a dissipative environment previously studied in Refs. [8]. With the Hamiltonian $\hat H = \frac{\varepsilon}{2}\hat\sigma_z + T_c\hat\sigma_x + V_B\hat\sigma_z + H_B + \hat H_T + \hat H_{\rm res}$



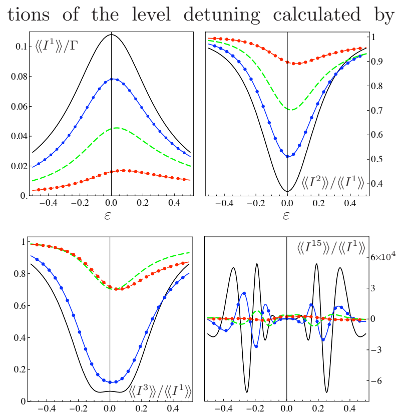
$$\begin{aligned} V_B &= \frac{g}{2}\sum_j(\hat a_j^\dagger+\hat a_j) &(12)\\ H_B &= \sum_j\hbar\omega_j\hat a_j^\dagger\hat a_j &(13)\\ \hat H_{\rm res} &= \sum_{k,\alpha=\pm}\epsilon_{k,\alpha}\hat c_{k,\alpha}^\dagger\hat c_{k,\alpha} &(14)\\ \hat H_T &= \sum_{k,\alpha=\pm}(t_\alpha\hat c_{k_\alpha}^\dagger|0\rangle\langle\alpha|+\mathrm{h.c.}) &(15) \end{aligned}$$

The dynamics is described by the EOM method of Gurvitz & Prager for the reduced density matrix $\hat\sigma^{(N)}$ of the electronic system + the phonon bath and N-resolved with respect to the tunnelled electrons [9]. Charges are assumed to enter/leave the quantum dots via the energy-independent rates $\Gamma_{L/R} = 2\pi\varrho_{L/R}|t_{L/R}|^2$. For electronic occupation probabilities tracing out the bosonic bath $\rho_i = \mathrm{Tr}_B\{\hat\sigma_{ii}\}$, $i=0,L,R$. A closed system of equations is obtained by assuming that the boson bath at any time is in local equilibrium corresponding to the given charge state [10]. The approximation is valid if the bath-assisted hopping rates $\Gamma_B^{(\pm)}(z)$ (proportional to T_c^2, see below) are much smaller than $\Gamma_{L/R}$. The counting field dependent memory kernel for this model then reads

$$\mathcal{W}(\chi,z) = \begin{pmatrix}-\Gamma_L & 0 & \Gamma_R e^{i\chi}\\ \Gamma_L & -\Gamma_B^{(+)}(z) & \Gamma_B^{(-)}(z)\\ 0 & \Gamma_B^{(+)}(z) & -\Gamma_B^{(-)}(z)-\Gamma_R\end{pmatrix}. \tag{16}$$

The bath-assisted hopping rates entering the kernel are $\Gamma_B^{(\pm)}(z) = T_c^2[\tilde g^{(+)}(z_\pm)+\tilde g^{(-)}(z_\mp)]$ with $\tilde g^{(+)}(z)$ the Laplace transform of $g^{(\pm)}(t) = e^{-W(\mp t)}$, $W(t) = \int_0^\infty d\omega J(\omega)\{[1-\cos(\omega t)]\coth(\beta\omega/2)+i\sin(\omega t)\}/\omega^2$, and $z_\pm = z\pm i\varepsilon+\Gamma_R/2$. The spectral function of the heat bath is taken Ohmic $J_\Omega(\omega) = 2\alpha\omega e^{-\omega/\omega_c}$, then the rates can be evaluated either analytically (for $\beta\omega_c\gg 1$) or numerically.

Current cumulants: The first three cumulants of the current as functions of the level detuning calculated by using the recursive scheme



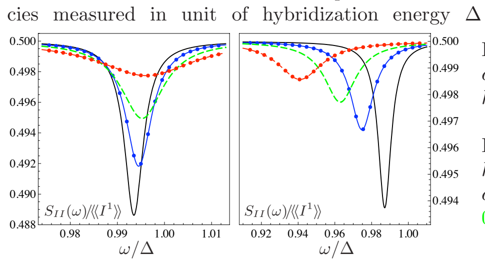
The fourth picture is an illustrative example for the 15'th cumulant
Parameters:
$T=0$ $\Gamma=\Gamma_L=\Gamma_R=0.5$
$T_c=0.1$ $\omega_c=500$
$2\pi\alpha = 0, 0.2, 0.5, 1$

As the dissipation strength is increased, a clear suppression of the coherent features (with $\alpha=0$) is seen. The heat bath tends to localize the electron to one of the two quantum dots suppressing the coherent effects.

Finite-frequency noise. The expression for the CGF, Eq. (4), allows us also to study the finite-frequency spectrum of the second cumulant of the current, the (symmetrized) current noise expressed by MacDonald's formula as $S_{II}(\omega) = \omega\int_0^\infty dt\sin(\omega t)\langle\langle I^2\rangle\rangle(t)$ [11], where $\langle\langle I^2\rangle\rangle(t) = \frac{d}{dt}\frac{\partial^2\mathcal{S}(\chi,t)}{\partial(i\chi)^2}|_{\chi\to 0}$. We find that

$$S_{II}(\omega) = -\frac{\omega^2}{2}\frac{\partial^2}{\partial(i\chi)^2}\left[\langle\hat\rho(\chi,z=i\omega)\rangle+(\omega\to-\omega)\right]|_{\chi\to 0}. \tag{17}$$

In order to evaluate this expression, we need to choose $\hat\rho(\chi,t=0)$ appropriately and find the inhomogeneity $\hat\gamma(\chi,z)$ as they enter the definition of $\langle\hat\rho(\chi,z)\rangle$. Following Ruskov and Korotkov [12] we assume that the system evolves from $t_0=-\infty$, such that the electronic occupation probabilities at $t=0$, where electron counting begins, have reached the stationary state, i.e., $\hat\rho(n,t=0) = \delta_{n,0}|O^{(0,0)}\rangle\rangle$. For this model [?] the inhomogeneity is independent of the counting field $\hat\gamma(z) = [\mathcal{W}-\mathcal{W}(\chi=0,z)]|O^{(0,0)}\rangle\rangle/z$. We see that the effects of the initial correlations accounted for by $\hat\gamma(z)$ vanish in the long-time limit. Moreover, since $\mathcal{W}|O^{(0,0)}\rangle\rangle = 0$, we find $\langle\hat\rho(\chi,z)\rangle = \mathrm{Tr}\{\mathcal{G}(\chi,z)\mathcal{G}^{-1}(\chi=0,z)|O^{(0,0)}\rangle\rangle\}/z$ from which we can calculate the finite-frequency current noise. We note that only the proper inclusion of the inhomogeneity ensures a correct finite-time behavior, such as proper normalization of $\langle\hat\rho(\chi=0,t)\rangle = \mathrm{Tr}\{\hat\rho^{\rm stat}\}=1$ at all times. Taking appropriately in account the displacement currents we can calculate the noise spectrum as a function of frequencies measured in unit of hybridization energy $\Delta = \sqrt{\varepsilon^2+(2T_c)^2}$.



Left figure:
$\alpha = 0.005$
$k_BT = 0, 1, 2, 5$

Right figure:
$k_BT = 0$
$\alpha = 0.01, 0.02, 0.03, 0.05$

Other parameters are $\Gamma_L=\Gamma_R=0.01$, $T_c=3$, $\varepsilon=10$, $\Delta=\sqrt{\varepsilon^2+(2T_c)^2}$, and $\omega_c=500$. The junction right/left capacitances are the same. A large bias is applied across the system.

Resonances are not observed exactly at the 'bare' value $\omega=\Delta$, but are shifted towards lower frequencies because the renormalization occurs due to coupling to the heat bath. The left figure shows how the signatures due to the coherent coupling between the two quantum dots are washed out with increasing temperature. In the right figure, we show how the frequency shift increases with increasing dissipation strength, which simultaneously reduces the effect of the coherent coupling.