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Shot Noise of a Quantum Shuttle

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We formulate a theory for shot noise in quantum nanoelectromechanical systems. As a specific example, the theory is applied to a quantum shuttle, and the zero-frequency noise, measured by the Fano factor F, is computed. F reaches very low values ($F \simeq 10^{-2}$) in the shuttling regime even in the quantum limit, confirming that shuttling is universally a low noise phenomenon. In approaching the semiclassical limit, the Fano factor shows a giant enhancement ($F \simeq 10^2$) at the shuttling threshold, consistent with predictions based on phase-space representations of the density matrix.

Nanoelectromecanical systems (NEMS) are presently a topic of intense research activity [1]. These devices combine electronic and mechanical degrees of freedom to display new physical phenomena and potentially may lead to new functionalities. An archetypal example of such a new phenomenon is the charge shuttling transition exhibited by the device proposed by Gorelik et al. [2]: here a movable nanoscopic object begins to transport electrons one by one beyond a certain threshold bias. Recent work has extended the original ideas to the quantum regime (the motion of the movable part is also quantized) and has shown that the shuttling transition occurs even in this limit, albeit in a smeared-out form [3–6].

An unequivocal experimental observation of the shuttling transition has not yet been achieved. The *IV* curve measured in the recent experiments on a C_{60} single-electron transistor can be interpreted in terms of shuttling [7], but also alternative explanations have been promoted [8–10]. It is therefore natural to look for more refined experimental tools than just the average current through the device. An obvious candidate is the current noise spectrum [11,12]. The measurement of the noise spectrum or even higher moments (full counting statistics) reveals more information about the transport through the device than just the mean current. The theoretical studies of the noise have attracted much attention recently in NEMS in general [13–15], as well as for the shuttling setup [16–18] in the (semi)classical limit. More specifically, Pistolesi [16] reports a vanishing Fano factor in the large amplitude limit of a driven shuttle. On the other hand, a study by Isacsson and Nord [17] of a classical system exhibiting shuttling instability found, somewhat surprisingly, a higher Fano factor in the shuttling regime than in the tunneling regime. This result is attributed to a different confining potential used in [17] compared to the other studies in this area.

The aim of this Letter is to develop a quantum mechanical theory for the shot noise spectrum for quantum NEMS and apply it to the model introduced by Gorelik et al. [2]. Our method combines the classical nature of the charge transfer processes in the high bias limit [19] with an operator version of a generating function technique [20]. While the present work considers only Markovian master equations, we believe that the method can be generalized to the case where the dynamics of the mechanical degrees of freedom is non-Markovian. For systems where the current noise can be expressed in terms of *system* operators (using the quantum optics language), such as the quantum dot array of Ref. [3], an alternative evaluation of noise, based on the quantum regression theorem (QRT) is possible, and we have verified that the two methods give identical results in this case [21]. We stress that the converse is not true: QRT is not applicable to the single-dot case.

Our previous quantum calculation [4] of the mean current relied on a generalized master equation (GME) for the system density matrices $\rho_{ii}(t)$ (ρ_{11} and ρ_{00} describe the occupied and empty dot, respectively, and the off-diagonal components decouple from their dynamics and can be neglected). In order to compute the noise spectrum, we follow the ideas of Gurvitz and Prager [22] and introduce number-resolved density matrices $\rho_{ii}^{(n)}$, where $n = 0, 1 \ldots$ is the number of electrons tunneled into the right lead by time t. Obviously, $\rho_{ii}(t) = \sum_n \rho_{ii}^{(n)}(t)$. The $\rho_{ii}^{(n)}$ obey

$$
\dot{\rho}_{00}^{(n)}(t) = \frac{1}{i\hbar}[H_{\text{osc}}, \rho_{00}^{(n)}(t)] + \mathcal{L}_{\text{damp}}\rho_{00}^{(n)}(t)
$$
$$
- \frac{\Gamma_L}{2}\{e^{-2x/\lambda}, \rho_{00}^{(n)}(t)\} + \Gamma_R e^{x/\lambda}\rho_{11}^{(n-1)}(t)e^{x/\lambda},
$$

$$
\dot{\rho}_{11}^{(n)}(t) = \frac{1}{i\hbar}[H_{\text{osc}} - eEx, \rho_{11}^{(n)}(t)] + \mathcal{L}_{\text{damp}}\rho_{11}^{(n)}(t)
$$
$$
- \frac{\Gamma_R}{2}\{e^{2x/\lambda}, \rho_{11}^{(n)}(t)\} + \Gamma_L e^{-x/\lambda}\rho_{00}^{(n)}(t)e^{-x/\lambda},
$$

$$
(1)
$$

with $\rho_{11}^{(-1)}(t) \equiv 0$. In (1), the commutators describe coherent evolution of discharged or charged harmonic oscillator of mass m and frequency ω in electric field E, respectively. The terms involving $\Gamma_{L,R}$ describe the charge transfer processes from/to leads while the mechanical damping with the damping coefficient γ is determined by the kernel (at $T = 0$) [4]

$$\mathcal{L}_{\text{damp}}\rho = -\frac{i\gamma}{2\hbar}[x, \{p, \rho\}] - \frac{\gamma m\omega}{2\hbar}[x, [x, \rho]]. \quad (2)$$

The mean current and the zero-frequency shot noise are given by [19]

$$I = e\frac{d}{dt}\sum_n nP_n(t)\bigg|_{t\to\infty} = e\sum_n n\dot{P}_n(t)\bigg|_{t\to\infty}, \quad (3)$$

$$S(0) = 2e^2\frac{d}{dt}\left[\sum_n n^2 P_n(t) - \left(\sum_n nP_n(t)\right)^2\right]\bigg|_{t\to\infty}, \quad (4)$$

where $P_n(t) = \text{Tr}_{\text{osc}}[\rho_{00}^{(n)}(t) + \rho_{11}^{(n)}(t)]$ are the probabilities of finding n electrons in the right lead by time t. Using Eq. (1) we find $I = \sum_n n\dot{P}_n(t) = \Gamma_R\text{Tr}_{\text{osc}}[e^{2x/\lambda}\rho_{11}(t)]$; i.e., one recovers the stationary current used previ-

ously [4]. In a similar fashion, $\sum_n n^2\dot{P}_n(t) = \Gamma_R\text{Tr}_{\text{osc}}\{e^{2x/\lambda}[2\sum_n n\rho_{11}^{(n)}(t) + \rho_{11}(t)]\}$, whose large-time asymptotics determines the shot noise according to (4). This can be computed using an operator-valued generalization of the generating function concept. We introduce the generating functions $F_{ii}(t;z) = \sum_n \rho_{ii}^{(n)}(t)z^n$ with the properties $F_{ii}(t;1) = \rho_{ii}(t)$, $\frac{\partial}{\partial z}F_{ii}(t;z)|_{z=1} = \sum_n n\rho_{ii}^{(n)}(t)$. The equations of motion for $F_{ii}(t;z)$ are

$$\frac{\partial}{\partial t}F_{00}(t;z) = \frac{1}{i\hbar}[H_{\text{osc}}, F_{00}(t;z)] - \frac{\Gamma_L}{2}\{e^{-2x/\lambda}, F_{00}(t;z)\}$$
$$+ \mathcal{L}_{\text{damp}}F_{00}(t;z) + z\Gamma_R e^{x/\lambda}F_{11}(t;z)e^{x/\lambda}$$
$$= \mathcal{L}_{00}F_{00}(t;z) + z\mathcal{L}_{01}F_{11}(t;z),$$

$$\frac{\partial}{\partial t}F_{11}(t;z) = \frac{1}{i\hbar}[H_{\text{osc}} - eEx, F_{11}(t;z)] + \mathcal{L}_{\text{damp}}F_{11}(t;z)$$
$$- \frac{\Gamma_R}{2}\{e^{2x/\lambda}, F_{11}(t;z)\}$$
$$+ \Gamma_L e^{-x/\lambda}F_{00}(t;z)e^{-x/\lambda}$$
$$= \mathcal{L}_{10}F_{00}(t;z) + \mathcal{L}_{11}F_{11}(t;z), \quad (5)$$

where we have introduced the block structure of the Liouvillean (super)operator $\mathcal{L} = \begin{pmatrix}\mathcal{L}_{00} & \mathcal{L}_{01}\\ \mathcal{L}_{10} & \mathcal{L}_{11}\end{pmatrix}$. Using the F's the shot noise formula can be rewritten as

$$\frac{S(0)}{2e^2\Gamma_R} = \left\{\text{Tr}_{\text{osc}}\left[e^{2x/\lambda}\left(2\frac{\partial}{\partial z}F_{11}(t;z)\bigg|_{z=1} + F_{11}(t;1)\right)\right] - 2\text{Tr}_{\text{osc}}[e^{2x/\lambda}F_{11}(t;1)]\text{Tr}_{\text{osc}}\left[\frac{\partial}{\partial z}\sum_{i=0}^1 F_{ii}(t;z)\bigg|_{z=1}\right]\right\}\bigg|_{t\to\infty}. \quad (6)$$

A Laplace transform of (5) yields

$$\begin{pmatrix}\tilde{F}_{00}(s;z)\\ \tilde{F}_{11}(s;z)\end{pmatrix} = \begin{pmatrix}s - \mathcal{L}_{00} & -z\mathcal{L}_{01}\\ -\mathcal{L}_{10} & s - \mathcal{L}_{11}\end{pmatrix}^{-1}\begin{pmatrix}f_{00}^{\text{init}}(z)\\ f_{11}^{\text{init}}(z)\end{pmatrix}, \quad (7)$$

where $f_{ii}^{\text{init}}(z) = \sum_n \rho_{ii}^{(n)}(0)z^n$ depends on the initial conditions. Defining the resolvent $\mathcal{G}(s) = (s - \mathcal{L})^{-1}$ of the full Liouvillean we arrive at

$$\begin{pmatrix}\tilde{F}_{00}(s;1)\\ \tilde{F}_{11}(s;1)\end{pmatrix} = \mathcal{G}(s)\begin{pmatrix}\rho_{00}^{\text{init}}\\ \rho_{11}^{\text{init}}\end{pmatrix}, \quad (8)$$

$$\frac{\partial}{\partial z}\begin{pmatrix}\tilde{F}_{00}(s;z)\\ \tilde{F}_{11}(s;z)\end{pmatrix}\bigg|_{z=1} = \mathcal{G}(s)\begin{pmatrix}0 & \mathcal{L}_{01}\\ 0 & 0\end{pmatrix}\mathcal{G}(s)\begin{pmatrix}\rho_{00}^{\text{init}}\\ \rho_{11}^{\text{init}}\end{pmatrix}$$
$$+ \mathcal{G}(s)\begin{pmatrix}f_{00}'^{\text{init}}(1)\\ f_{11}'^{\text{init}}(1)\end{pmatrix}. \quad (9)$$

In order to extract the large-t behavior we study the asymptotics of the above expressions as $s \to 0+$. This is entirely determined by the resolvent $\mathcal{G}(s)$ in the small-s limit. Since $\mathcal{L}$ is singular (recall $\mathcal{L}\rho^{\text{stat}} = 0$) the resolvent is singular at $s = 0$. To extract the singular behavior we introduce the projector $\mathcal{P}$ on the null space of the Liouvillean: $\mathcal{P}\bullet = \begin{pmatrix}\rho_{00}^{\text{stat}}\\ \rho_{11}^{\text{stat}}\end{pmatrix}\text{Tr}_{\text{sys}}(\bullet)$. We also need the complement $\mathcal{Q} = 1 - \mathcal{P}$. Using the relations $\mathcal{P}\mathcal{L} = \mathcal{L}\mathcal{P} = 0$ and $\mathcal{L} = \mathcal{Q}\mathcal{L}\mathcal{Q}$, the resolvent can be expressed as $\mathcal{G}(s) = (s\mathcal{P} + s\mathcal{Q} - \mathcal{Q}\mathcal{L}\mathcal{Q})^{-1} = \frac{1}{s}\mathcal{P} + \mathcal{Q}\frac{1}{s-\mathcal{L}}\mathcal{Q} \approx \frac{1}{s}\mathcal{P} - \mathcal{Q}\mathcal{L}^{-1}\mathcal{Q}$, in leading order for small s. The object

$\mathcal{Q}\mathcal{L}^{-1}\mathcal{Q}$ (the pseudoinverse of $\mathcal{L}$) is regular as the "inverse" is performed on the Liouville subspace spanned by $\mathcal{Q}$ where $\mathcal{L}$ is regular (no null vectors).

Substituting the asymptotic behavior of the resolvent into Eqs. (8) and (9), keeping only the terms divergent at $s = 0$ in both equations and performing the inverse Laplace transform [23], we find the following large-t asymptotics:

$$\begin{pmatrix}F_{00}(t;1)\\ F_{11}(t;1)\end{pmatrix}\bigg|_{t\to\infty} \to \mathcal{P}\begin{pmatrix}\rho_{00}^{\text{init}}\\ \rho_{11}^{\text{init}}\end{pmatrix} = \begin{pmatrix}\rho_{00}^{\text{stat}}\\ \rho_{11}^{\text{stat}}\end{pmatrix},$$
$$\frac{\partial}{\partial z}\begin{pmatrix}F_{00}(t;z)\\ F_{11}(t;z)\end{pmatrix}\bigg|_{z=1,t\to\infty} \to \begin{pmatrix}\rho_{00}^{\text{stat}}\\ \rho_{11}^{\text{stat}}\end{pmatrix}(tI + C^{\text{init}}) - \begin{pmatrix}\Sigma_{00}\\ \Sigma_{11}\end{pmatrix},$$
$$(10)$$

where we have defined an auxiliary quantity $\Sigma = \mathcal{Q}\mathcal{L}^{-1}\mathcal{Q}\begin{pmatrix}\Gamma_R e^{x/\lambda}\rho_{11}^{\text{stat}}e^{x/\lambda}\\ 0\end{pmatrix}$ and C^{init} depends on initial conditions. Using these in (6) we arrive at the final expression for the Fano factor $F = S(0)/2eI$:

$$F = 1 - \frac{2e\Gamma_R}{I}\text{Tr}_{\text{osc}}(e^{2x/\lambda}\Sigma_{11}). \quad (11)$$

It is of crucial importance that this expression is independent on the initial conditions [in the algebra leading to (11) the linearly divergent terms in t and the initial condition terms cancel identically]. Σ satisfies

$$\mathcal{L}\,\Sigma = \begin{pmatrix} \Gamma_R e^{x/\lambda}\rho_{11}^{\text{stat}}e^{x/\lambda} - \frac{I}{e}\rho_{00}^{\text{stat}} \\ -\frac{I}{e}\rho_{11}^{\text{stat}} \end{pmatrix}, \quad \text{with } \mathrm{Tr}_{\text{sys}}\Sigma = 0.$$

(12)

Equations (11) and (12) together with the stationary version of the GME

$$\mathcal{L}\begin{pmatrix} \rho_{00}^{\text{stat}} \\ \rho_{11}^{\text{stat}} \end{pmatrix}= 0, \quad \text{with } \mathrm{Tr}_{\text{sys}}\rho^{\text{stat}} = 1$$

(13)

form the main theoretical result of this Letter and are the starting point for the calculation of the noise properties of the quantum shuttle.

In general, these equations have to be solved numerically. However, there is an analytic solution to them in the limit of small bare injection rates compared to damping, i.e., $\Gamma_{L,R} \ll \gamma \ll \omega$. In this limit the oscillator gets equilibrated between rare tunneling events and, consequently, the state of the oscillator in a given charge state is close to its corresponding canonical state, i.e. $\rho_{00}^{\text{stat}} = p_{00}\rho_{\text{osc}}(0)$, $\rho_{11}^{\text{stat}} = p_{11}\rho_{\text{osc}}(eE)$, $\rho_{\text{osc}}(l) = e^{-\beta(H_{\text{osc}}-lx)}/\mathrm{Tr}_{\text{osc}}e^{-\beta(H_{\text{osc}}-lx)}$, where only the probabilities p_{00}, p_{11} of the respective occupations are to be determined from (13). By tracing Eq. (13) with respect to the oscillator we find $-\tilde{\Gamma}_L p_{00} + \tilde{\Gamma}_R p_{11} = 0$ (with $p_{00} + p_{11} = 1$) where $\tilde{\Gamma}_L = \Gamma_L \mathrm{Tr}_{\text{osc}}[e^{-2x/\lambda}\rho_{\text{osc}}(0)]$ and $\tilde{\Gamma}_R = \Gamma_R \mathrm{Tr}_{\text{osc}}[e^{2x/\lambda}\rho_{\text{osc}}(eE)]$ are the renormalized tunneling rates. Proceeding similarly in the evaluation of Σ (this intuitive approach can be easily justified with singular perturbation theory, see, e.g., Ref. [20]), we set $\Sigma_{00}^{\text{stat}} = s_{00}\rho_{\text{osc}}(0)$, $\Sigma_{11}^{\text{stat}} = s_{11}\rho_{\text{osc}}(eE)$ and tracing Eq. (12) with respect to the oscillator we arrive at $-\tilde{\Gamma}_L s_{00} + \tilde{\Gamma}_R s_{11} = \frac{I}{e}p_{11}$ (with $s_{00} + s_{11} = 0$). Solving the equations for p_{ii}, s_{ii} we find $I = e\frac{\tilde{\Gamma}_L\tilde{\Gamma}_R}{\tilde{\Gamma}_L+\tilde{\Gamma}_R}$, $F = \frac{\tilde{\Gamma}_L^2+\tilde{\Gamma}_R^2}{(\tilde{\Gamma}_L+\tilde{\Gamma}_R)^2}$, which is the standard result for the two-state sequential tunneling process [11,24]. The Fano factor depends only on the ratio between the rates: $\frac{\tilde{\Gamma}_R}{\tilde{\Gamma}_L} = \frac{\Gamma_R}{\Gamma_L}\exp\frac{2eE}{\lambda m\omega^2}$. This result provides us with the analytic asymptotical expressions for the current and the Fano factor for small hopping rates $\Gamma_{L,R}$ which we used to check our numerical routine.

In the general case Eqs. (13) and (12) must be solved by truncation of the oscillator Hilbert space by retaining the N lowest states of the oscillator and solving numerically the resulting $2N^2 \times 2N^2$ linear systems. Since the required N for a satisfactory convergence could reach $N = 100$ resulting in big (nonsparse) linear systems we employed the Arnoldi iteration and generalized minimum residual method for the solution of Eqs. (13) and (12), respectively [25]. When properly implemented these methods provided a fast solution with a modest memory requirement [21].

In Fig. 1 we present the plots of the mean current and the Fano factor as functions of the damping coefficient for different parameters λ, and $\Gamma = \Gamma_L = \Gamma_R$. The I vs γ curve shows the tunneling to shuttling crossover as damping is decreased, as explained in our previous work [4]. The crossover spans a narrower range of γ's in the case of

$\lambda = 2x_0$ ($x_0 = \sqrt{\hbar/m\omega}$) compared to the $\lambda = x_0$ case. Thus, already for $\lambda = 2x_0$ the shuttle behaves almost semiclassically, where a relatively sharp transition between the two regimes is expected. Around the transition the tunneling and shuttling regimes may coexist, as shown analytically in [6]. We see this phenomenon explicitly in Fig. 2 where we plot the Wigner distribution functions defined by

$$W_{ii}(X, P) = \int_{-\infty}^{\infty}\frac{dy}{2\pi\hbar}\left\langle X - \frac{y}{2}\,\Big|\,\rho_{ii}^{\text{stat}}\,\Big|\,X + \frac{y}{2}\right\rangle\exp\left(i\frac{Py}{\hbar}\right)$$

(14)

for a specific set of parameters corresponding to the "most classical" curve around the transition in Fig. 1 denoted by the asterisk. The Wigner plots show the quasiprobability distributions in the phase space of the oscillator resolved with respect to its charge state and prove the coexistence of the tunneling regime (characterized by the spots around the phase-space origin) and the shuttling regime with the half-moon or ringlike shapes in W_{00}, W_{11}, or W_{tot}, respectively [4]. This semiclassical transition is accompanied by the nearly singular behavior of the Fano factor reaching the value ≈ 600 at the peak. This is in agreement with the recent classical study [17] where the singularity of the Fano factor at the transition was also predicted.
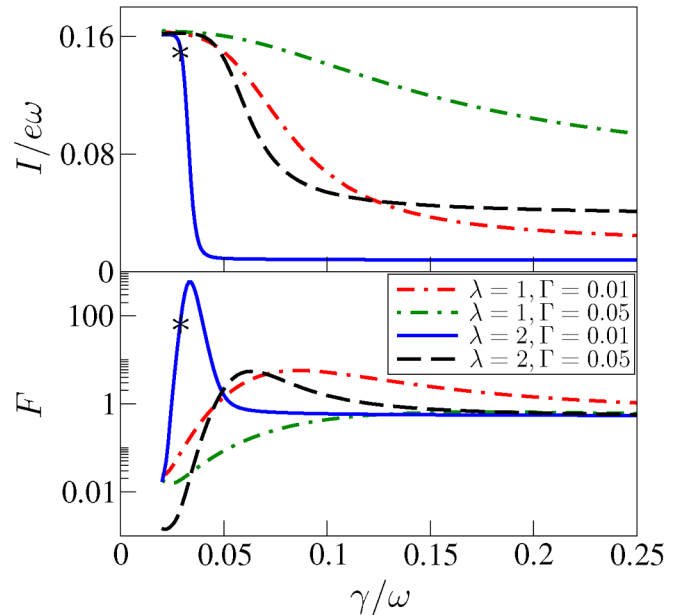

FIG. 1 (color online). Current I (upper panel) and Fano factor F (lower panel; log scale) vs damping γ for different transfer rates Γ and tunneling lengths λ. The parameters are $\lambda = x_0, \Gamma = 0.01\omega$ (dot-dash-dashed line); $\lambda = x_0, \Gamma = 0.05\omega$ (dot-dashed line); $\lambda = 2x_0, \Gamma = 0.01\omega$ (full line); $\lambda = 2x_0, \Gamma = 0.05\omega$ (dashes) with $x_0 = \sqrt{\hbar/m\omega}$. Other parameters are $eE/m\omega^2 = 0.5x_0$, $T = 0$. The asterisk defines the parameters of Wigner distributions in Fig. 2.
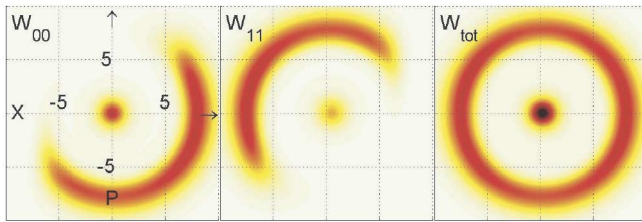
FIG. 2 (color online). Phase space picture of the shuttle around the transition where the shuttling and tunneling regimes coexist. From left to right we show the Wigner distribution functions for the discharged (W_{00}), charged (W_{11}), and both ($W_{\text{tot}} = W_{00} + W_{11}$) states of the oscillator in the phase space (horizontal axis: coordinate in units of $x_0 = \sqrt{\hbar/m\omega}$; vertical axis: momentum in $\hbar/x_0$). The values of the parameters are (corresponding to the asterisk in Fig. 1): $\lambda = 2x_0$, $eE/m\omega^2 = 0.5x_0$, $\gamma = 0.029\omega$, $\Gamma = 0.01\omega$, $T = 0$.

More important, however, is the behavior in the shuttling regime. We can see in Fig. 1 that the Fano factor is very small in the shuttling regime. This is true even in the strongly quantum case $\lambda = x_0$ where the transition peak characteristic of the classical case is almost totally missing. As found previously [4] the classical transition is strongly smeared by the quantum noise into a broad crossover which is reflected by the absence of the peak in the Fano factor. Nevertheless, the shuttling regime still persists and is again characterized by a low noise.

To conclude, we have presented a generic method of the calculation of the shot noise for quantum nanoelectromechanical systems and applied it to a quantum shuttle system. We show that even in the quantum case the shuttling regime is characterized by a highly ordered charge transfer mechanism accompanied by the low current noise compared to the tunneling regime. When approaching the semiclassical limit, the Fano factor shows a giant enhancement at the shuttling threshold, consistent with other classical studies and with the phase-space analysis of the stationary density matrix.

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