Disordered Markovian Brownian ratchets

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A model of a Brownian ratchet coupled to a heat bath and driven by a nonequilibrium Poisson white noise is discussed. The formula describing a generated current in terms of the statistical properties of a possible irregular or random potential is derived within the small nonequilibrium noise approximation and illustrated by a few concrete examples. The perturbation technique for Hilbert space operators is used as a mathematical tool. [S1063-651X(99)00609-1]

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Recently, different models of the so-called Brownian ratchets attracted attention and various mechanisms responsible for their operation as ''motors'' converting nonequilibrium noise into directed motion have been considered [1–9]. We restrict our discussion to a class of models formally described by the following one-dimensional Langevin equation in the overdamped regime:

$$\gamma \dot{x} = f(x) + \Gamma(t) + F(t), \tag{1}$$

where γ is a friction constant, $f(x)$ is a potential force [i.e., $f=-(\partial/\partial x)V$], $\Gamma(t)$ is a Gaussian white noise representing thermal fluctuations at the temperature T, and $F(t)$ is an external force modeling an interaction with the environment being out of the thermal equilibrium. Different proposals concerning the form of $F(t)$ including periodic in time deterministic forces [1,2], various types of colored noises of Gaussian and Poisson type [3–6], and white Poisson noises [7,8] have been analyzed numerically or analytically. In most papers the potential $V(x)$ is periodic and the noise is symmetric with respect to the reflection $x \mapsto -x$ and homogeneous. All authors agree that in this case the necessary condition for the generation of a macroscopic current is a loss of symmetry of the potential $V(x)$. However, some authors claimed that the additional necessary condition was the presence of correlations for $F(t)$, which means that the nonequilibrium random force could not be a white (generally non-Gaussian) noise [1,4,7]. In other words, the non-Markovian character of the stochastic process $x(t)$ should be essential for the mechanism of current generation. On the contrary, in Refs. [7,8] several special cases of models with piecewise linear periodic potentials and random forces $F(t)$ being Poisson white noise with a few selected simple forms of the jump distribution proved to generate a net current.

The purpose of this paper is to provide analytical expressions describing the generated current which are valid for a generic family of Brownian ratchets of the type (1) under the assumption of weak nonequilibrium perturbation. We relax the condition of periodicity for the potential $V(x)$ allowing its irregular character described by its statistical averaged properties. We assume that the random force $F(t)$ is a Poisson white noise symmetric with respect to the reflection and homogeneous. Under the assumptions above the Langevin equation (1) is completely equivalent to the following Chapman-Kolmogorov-Smoluchowski equation for the probability distribution $P(x,t)$ [10]:

$$\frac{\partial}{\partial t}P(x,t) = D\frac{\partial}{\partial x}\left[\frac{\partial}{\partial x} - \frac{f(x)}{kT}\right]P(x,t) + \lambda\int_{-\infty}^{\infty}\rho(z)[P(x-z,t)-P(x,t)]dz, \tag{2}$$

with the probability distribution of jumps

$$\rho(z)=\rho(-z), \quad \rho(z)\geqslant 0, \quad \int_{-\infty}^{\infty}\rho(z)dz=1, \tag{3}$$

the average frequency of jumps λ, the diffusion constant $D=\gamma kT$, and the appropriate initial and boundary conditions for $P(x,t)$. Equation (2) can always be written as a continuity equation

$$\frac{\partial}{\partial t}P(x,t) + \frac{\partial}{\partial x}J(x,t)=0. \tag{4}$$

The current $J(x,t)$ is a nonlocal functional of $P(x,t)$,

$$J(x,t) = -D\left[\frac{\partial}{\partial x} - \frac{f(x)}{kT}\right]P(x,t) + \lambda\int_{-\infty}^{\infty}G(x-y)P(y,t)dy, \tag{5}$$

with

$$G(z)=\int_{z}^{\infty}\rho(r)dr \quad \text{for } z>0, \quad G(-z)=-G(z). \tag{6}$$

The current $J(x,t)$ is uniquely determined by the condition

$$\lim_{x\to\pm\infty} J(x,t)=0 \quad \text{if} \quad \lim_{x\to\pm\infty} P(x,t)=0. \tag{7}$$

In the following we shall apply quantum-mechanical-like perturbation techniques to the evolution equation (2) written now in an operator form on the Hilbert space $L^2(\mathbf{R})$,

$$\frac{\partial}{\partial t}\psi = -i\hat{\mathcal{K}}\psi. \tag{8}$$

Here $\hat{\mathcal{K}}$ is a nonself-adjoint operator on $L^2(\mathbf{R})$ which can be represented as a function of self-adjoint ''momentum'' and ''position'' operators

$$\hat{P}\psi(x)=-i\frac{\partial}{\partial x}\psi(x),\quad \hat{Q}\psi(x)=x\psi(x) \tag{9}$$

as

$$\hat{\mathcal{K}}=-iD\hat{P}[\hat{P}+iU'(\hat{Q})]+i\lambda[\tilde{\rho}(\hat{P})-1]. \tag{10}$$

In the formula (10)

$$U'(\hat{Q})=-\frac{1}{kT}f(\hat{Q}) \tag{11}$$

and $\tilde{\rho}$ denotes the Fourier transform of ρ. The operator $\hat{\mathcal{K}}$ can be expressed in terms of the current operator $\hat{\mathcal{J}}$

$$\hat{\mathcal{J}}=iD\hat{P}-DU'(\hat{Q})+\lambda\tilde{G}(\hat{P})=-iDe^{-\hat{U}}\hat{P}e^{\hat{U}}+\lambda\tilde{G}(\hat{P}),$$
$$\hat{\mathcal{K}}=i\hat{P}\hat{\mathcal{J}}. \tag{12}$$

In order to compute the stationary current in our system we shall use the approximative spectral resolution of the current operator $\hat{\mathcal{J}}$. To simplify the problem we consider the diffusion process on the finite interval $[0,L]$ with the periodic boundary conditions. Here L is not a period of the potential as in many papers on Brownian ratchets but the total length of the system which finally will tend to infinity. Hence the Hilbert space $L^2(\mathbf{R})$ is replaced by $L^2([0,L])$ and we must assume that $V(L)=V(0)$. Then the operators $\hat{\mathcal{J}}$ and $\hat{\mathcal{K}}$ given by Eqs. (12) are well defined on $L^2([0,L])$ and possess discrete spectra. The ''momentum operator'' $\hat{P}$ has the following spectral representation:

$$\hat{P}=\sum_{k\in\mathbf{Z}}\left(\frac{2\pi k}{L}\right)|\phi_k\rangle\langle\phi_k|,\quad \phi_k(x)=\frac{1}{\sqrt{L}}\exp\left(i\frac{2\pi kx}{L}\right). \tag{13}$$

Using general Frobenius-Perron type arguments [11] one can show that the stationary equation

$$\hat{\mathcal{K}}\psi=0 \tag{14}$$

possesses a unique solution ψ_0 which can be chosen positive and satisfying the normalization condition

$$\int_0^L\psi_0(x)dx=L=\sqrt{L}\langle\phi_0,\psi_0\rangle. \tag{15}$$

With the above normalization we obtain from Eqs. (4), (5), and (12) the formula for the normalized stationary current

$$j=\hat{\mathcal{J}}\psi_0=j\sqrt{L}\phi_0,\quad \psi_0=j\sqrt{L}\hat{\mathcal{J}}^{-1}\phi_0 \tag{16}$$

and finally using Eq. (15)

$$j=(\langle\phi_0,\hat{\mathcal{J}}^{-1}\phi_0\rangle)^{-1}. \tag{17}$$

We apply now the standard quantum-mechanical perturbation technique with respect to the small parameter λ/D. Using Eq. (12) we can write

$$\hat{\mathcal{J}}^{-1}=D^{-1}e^{-\hat{U}}\hat{\mathcal{R}}^{-1}e^{\hat{U}}, \tag{18}$$

with

$$\hat{\mathcal{R}}=-i\hat{P}+\frac{\lambda}{D}e^{\hat{U}}\tilde{G}(\hat{P})e^{-\hat{U}}. \tag{19}$$

In the lowest order approximation with respect to λ/D the eigenvectors of $\hat{\mathcal{R}}$ coincide with the eigenvectors of $\hat{P}$ and the eigenvalues acquire the first order correction producing the following approximative expression

$$\hat{\mathcal{R}}\simeq\sum_{k\in\mathbf{Z}}\left(-\frac{i2\pi k}{L}+\frac{\lambda}{D}\Gamma_k\right)|\phi_k\rangle\langle\phi_k|, \tag{20}$$

with

$$\Gamma_k=\langle\phi_k,e^{\hat{U}}\tilde{G}(\hat{P})e^{-\hat{U}}\phi_k\rangle. \tag{21}$$

Putting the inverse of $\hat{\mathcal{R}}$ into Eq. (18) and then into Eq. (17) one can notice that the leading term is given by a single term with $k=0$ in the sum (20). Therefore we obtain the following approximative formula for the net current:

$$j\simeq\lambda\Gamma_0(Z_-Z_+)^{-1}. \tag{22}$$

The parameters which appear in Eq. (22) can be rewritten for large L in terms of certain averages over the system

$$\Gamma_0=\lim_{L\to\infty}\frac{1}{L}\int_0^L dx\int_0^L dy\,G(x-y)e^{[U(x)-U(y)]}$$
$$=2\int_0^\infty dz\,G(z)\left\{\lim_{L\to\infty}\frac{1}{L}\int_0^L\sinh[U(z+x)-U(x)]dx\right\} \tag{23}$$

$$Z_\pm=\langle\phi_0,e^{\pm\hat{U}}\phi_0\rangle=\lim_{L\to\infty}\frac{1}{L}\int_0^L dx\,e^{\pm U(x)}. \tag{24}$$

The averages over x in Eqs. (23) and (24) can be replaced by the averages with respect to a certain ensemble of potentials (random potential model) denoted by $\langle\ \rangle$,

$$\Gamma_0=-2\int_0^\infty dz\,G(z)\left\langle\sinh\left[\frac{1}{kT}\int_0^z f(x)dx\right]\right\rangle,$$
$$Z_\pm=\left\langle\exp\left\{\pm\frac{1}{kT}V\right\}\right\rangle. \tag{25}$$

It follows from formulas (22) and (25) that a nonzero current appears if the distribution of the force $f(x)$ is not symmetric with respect to the change of its sign (ratchetlike potential). Remembering that the average force should be zero ($\langle f\rangle=0$) the leading term in the high temperature limit is given by

$$j \simeq -\frac{\lambda}{3(kT)^3}\int_0^{\infty} dz G(z)\left\langle\left[\int_0^z f(x)dx\right]^3\right\rangle. \quad (26)$$

It means that the current flows in the direction of a steeper climb and its value decreases asymptotically when the temperature grows. More explicit expression for the current can be obtained under the assumption that the average jump length is smaller than the typical length scale of the force's variation. It follows that in formula (25) we can use the estimation

$$\int_0^z f(x)dx \simeq f(0)z. \quad (27)$$

Therefore the current (22) can be written in terms of the three probability distributions: $\rho(z)$ for the jumps, $\mu(f)$ for the force, and $\nu(V)$ for the potential

$$\Gamma_0 = -kT\int_{-\infty}^{+\infty} df \int_{-\infty}^{+\infty} dz \mu(f)\rho(z) f^{-1}\left[\cosh\left(\frac{fz}{kT}\right)-1\right], \quad (28)$$

$$Z_{\pm} = \int_{-\infty}^{+\infty} dV \nu(V)\exp\left\{\pm\frac{V}{kT}\right\}. \quad (29)$$

As the force f is related to the potential V then in principle the probability distributions $\mu(f)$ and $\nu(V)$ might not be independent. On the other hand, $\mu(f),\nu(V)$ do not contain any information about the correlations of $f(x)$ and $V(x)$ at different points and therefore the only consistency condition is $\langle f\rangle = 0$, which is implied by $V(0)=V(L)$. The obtained formulas can be illustrated by the following examples involving concrete probability distributions:

$$\rho^{(1)}(z) = \begin{cases} \frac{1}{2a} & \text{if } |z| \leqslant a \\ 0 & \text{otherwise}, \end{cases} \qquad \rho^{(2)}(z) = \frac{1}{a\sqrt{2\pi}} e^{-z^2/2a^2} \quad (30)$$

$$\nu^{(1)}(V) = \begin{cases} \frac{1}{2V_0} & \text{if } |V| \leqslant V_0 \\ 0 & \text{otherwise}, \end{cases} \qquad \nu^{(2)}(V) = \frac{1}{V_0\sqrt{2\pi}} e^{-V^2/2V_0^2}. \quad (31)$$

For the probability distribution of f we select a very simple one corresponding to a piecewise linear ''saw shape'' potential with possible different (random) sizes of the teeth

$$\mu(f) = \frac{1-\epsilon}{2}\delta(f+(1+\epsilon)f_0) + \frac{1+\epsilon}{2}\delta(f-(1-\epsilon)f_0), \quad (32)$$

where the parameter $\epsilon \in (-1,1)$ describes the asymmetry of the force distribution. In the small asymmetry regime ($|\epsilon| \ll 1$) we obtain from Eqs. (28), (29), and (32) the expression for the current

$$j \simeq \epsilon\lambda kT\left(\Psi'(f_0) - \frac{2}{f_0}\Psi(f_0)\right)R, \quad (33)$$

where $R = (Z_- Z_+)^{-1}$ and

$$\Psi(f) = \int_{-\infty}^{+\infty} dz \rho(z)\left[\cosh\left(\frac{fz}{kT}\right)-1\right]. \quad (34)$$

For the probability distributions (30) and (31) we have

$$\Psi^{(1)}(f) = \frac{kT}{af}\sinh\frac{af}{kT} - 1, \quad \Psi^{(2)}(f) = \exp\left\{\frac{1}{2}\left(\frac{af}{kT}\right)^2\right\} - 1, \quad (35)$$

$$R^{(1)} = \left(\frac{V_0}{kT}\right)^2 \sinh^{-2}\left(\frac{V_0}{kT}\right), \quad R^{(2)} = \exp\left\{-\left(\frac{V_0}{kT}\right)^2\right\}. \quad (36)$$

The high temperature regime (26) yields now the following result:

$$j \simeq \epsilon\lambda a\left(\frac{f_0 a}{kT}\right)^3 c, \quad (37)$$

where $c = \frac{1}{60}$ for $\rho^{(1)}$ and $c = \frac{1}{8}$ for $\rho^{(2)}$, respectively.

The low temperature regime together with the assumption (27) means that

$$kT \ll af_0 \ll V_0. \quad (38)$$

The asymptotic forms of the current at low temperature, small asymmetry, and weak nonequilibrium noise calculated with the probability distributions (30)–(32) read

$$j \simeq \begin{cases} \epsilon\lambda a\left(\frac{kT}{f_0 a}\right)\left(\frac{V_0}{kT}\right)^2 \exp\left\{-\frac{1}{kT}(2V_0 - f_0 a)\right\} & \text{for } \rho^{(1)},\nu^{(1)} \quad (39) \\ \epsilon\lambda a\left(\frac{kT}{f_0 a}\right)\exp\left\{-\left(\frac{V_0}{kT}\right)^2 + \frac{f_0 a}{kT}\right\} & \text{for } \rho^{(1)},\nu^{(2)} \quad (40) \\ \epsilon\lambda a\left(\frac{f_0 a}{kT}\right)\left(\frac{V_0}{kT}\right)^2 \exp\left\{\frac{1}{2}\left(\frac{f_0 a}{kT}\right)^2 - \frac{V_0}{kT}\right\} & \text{for } \rho^{(2)},\nu^{(1)} \quad (41) \\ \epsilon\lambda a\left(\frac{f_0 a}{kT}\right)\exp\left\{-\left(\frac{V_0}{kT}\right)^2 + \frac{1}{2}\left(\frac{f_0 a}{kT}\right)^2\right\} & \text{for } \rho^{(2)},\nu^{(2)} \quad (42) \end{cases}$$

The examples above show that in contrast to the high temperature behavior (26) and (37), which is rather universal, the moderate and low temperature ones depend on the details of the probability distributions ρ,μ,ν. Typically, one can expect the existence of the optimal temperature for which the generated current has at least a local maximum. Such phenomena can be important in biophysical applications of the theory.

Summarizing, we have confirmed in a more general setting the prediction of Refs. [8,9] that a white Poisson noise can generate current in systems modeled by Brownian ratchets. Moreover, we can deduce the following rough dependence of the current on the fundamental parameters: the temperature T, the asymmetry of the force ϵ, the typical potential variation V_0, the length scale l_0 of the potential variation (defined by $f_0 l_0 = V_0$), the average jump frequency λ, and the typical jump length a,

$$j \simeq \epsilon \lambda a H\left(\frac{a}{l_0}, \frac{V_0}{kT}\right). \tag{43}$$

Here the function $H(\alpha,\beta)$ depends on the details of the model but for $\alpha,\beta = O(1)$ we expect $H(\alpha,\beta) = O(1)$ while for $\beta \to 0$, $H(\alpha,\beta) \sim (\alpha\beta)^3$.

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