Precise Numerics versus Theory for Correlation Ratchets

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Fluctuation-induced transport in a correlation ratchet driven by both additive Gaussian white and additive Ornstein-Uhlenbeck (colored) noise is studied numerically and interpreted against theoretical predictions. The current, as well as the current-load curve, exhibits a different behavior depending on the scaling of the colored noise strength. This archetypal correlation ratchet is capable of changing the direction of current (passing through zero at a particular value of noise color) if only the *shape* of the ratchet potential is chosen appropriately.

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The ability of a Brownian particle to extract useful work from nonequilibrium fluctuations when rattling in a periodic structure with broken spatial symmetry ("ratchet") has recently attracted much attention [1]. Apart from the general effort of understanding this novel nonequilibrium phenomenon, it entails interesting technological applications such as novel mass separation and trapping schemes [2] and, likely, is also of relevance for intracellular transport processes [1–3]. In the simplest case, such a "*Brownian rectifier*" is modeled by an overdamped particle moving in a periodic ratchet potential $V(x) = V(x + L)$ of period L under the simultaneous action of Gaussian white, δ-correlated thermal noise $\xi(t)$, $\langle \xi(t)\xi(s)\rangle = \delta(t - s)$, of strength $2D$ and an additional *state-independent* fluctuating force $\epsilon(t)$ of vanishing mean $\langle \epsilon(t)\rangle$, i.e.,

$$\dot{x} = -\frac{\partial V}{\partial x} + \epsilon(t) + \sqrt{2D}\,\xi(t). \qquad (1)$$

Equation (1) describes a *correlation ratchet* [4–6]. If the additive fluctuation $\epsilon(t)$ is a second Gaussian stationary white noise, the dynamics in (1) obeys detailed balance; hence the stationary current $J = \langle \dot{x}\rangle$ is zero in accordance with the second law of thermodynamics. Our focus here is on the simplest, nontrivial colored noise driven correlation ratchet: With Gaussian noise being abundant in physical applications [7], we choose for $\epsilon(t)$ an Ornstein-Uhlenbeck (OU) process, which is the archetype model for free Brownian motion [7]. This Markovian Gaussian process $\epsilon(t)$ satisfies the Langevin equation

$$\dot{\epsilon} = -\frac{1}{\tau}\epsilon + \frac{\sqrt{2Q(\tau)}}{\tau}\eta(t), \qquad (2)$$

with $\eta(t)$ Gaussian white noise, $\langle \eta(t)\eta(s)\rangle = \delta(t - s)$, which is independent of $\xi(t)$. Its stationary correlation reads

$$\langle \epsilon(t)\epsilon(s)\rangle = \frac{Q(\tau)}{\tau} e^{-|t-s|/\tau}. \qquad (3)$$

With $Q(\tau) = Q$ a constant, $\epsilon(t)$ describes for small noise correlation time τ a deviation from the white noise limit, yielding a constant integrated intensity $2Q$. In contrast, the case with a constant variance $\langle \epsilon^2\rangle = \tilde{Q}$ implies the different scaling $Q(\tau) = \tilde{Q}\tau$. In this latter case, the noise intensity vanishes as $\tau \longrightarrow 0$. Both scalings are of practical relevance, but entail different physical consequences. With $Q(\tau) = Q$ the colored fluctuations approach zero amplitude in the adiabatic limit $\tau \longrightarrow \infty$, whereas in the second case the Gaussian stationary fluctuations $\epsilon(t)$ explore a continuous spectrum of amplitudes, which extends over the whole real axis and is independent of τ.

Equation (1) together with (2) provide our setup for directed transport generated by colored nonequilibrium fluctuations $\epsilon(t)$. The problem at hand is challenging from several points of view: First, the dynamics of the particle motion $x(t)$ is non-Markovian in nature. This means that the application of familiar tools from the theory of stochastic processes is met with distinct difficulties [7]. These queries become even more pronounced in the presence of two noise sources, with one being nonwhite. Second, a finite stationary current J occurs only when internal forward and backward transitions do not cancel "on average." Hence, good approximations for the individual internal transition rates do not necessarily guarantee good results for the overall current J, which at weak noise is sensitive to the *difference* of the two exponentially small rates (see below).

Given these theoretical challenges, it is an important task to *test* analytical predictions vs precise numerical results. In fact, it is only very recently that the theoretical qualifications for this class of two-noise driven colored flows have been developed [8–12].

Before we engage in our objective of calculating both the stationary current as well as the current-load characteristics, we comment on the general features of the archetypal correlation ratchet in (1) and (2): When the noise color τ approaches zero, the current J vanishes since for both scalings of the noise strength the stochastic dynamics is driven by *additive Gaussian white* noise only. This result holds true also for the constant intensity scaling $Q(\tau) = Q$ in the adiabatic limit $\tau \longrightarrow \infty$. The latter feature is valid *independently* of the Gaussian statistics of $\epsilon(t)$. In contrast, for constant variance scaling $\tilde{Q}$ we encounter in the adiabatic limit a Gaussian distribution of arbitrary large barrier heights. In this limit a rate description fails

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[9]. Nevertheless, there exists a limiting adiabatic average transition time and current as well [9,12]. Moreover, it should not be overlooked that with our form in (1) we implicitly use a scaling of physical time t, which is inversely proportional to the physical friction strength [7]. Hence, instead of varying τ in (1) and (2), one could keep τ "fixed," and vary instead the friction in the original (unscaled) system. This feature calls for interesting consequences when the current changes sign as a function of the noise color τ (see below).

Starting from the Fokker-Planck equation (FPE) for the probability density $W_t(x, \epsilon)$,

$$\frac{\partial W_t(x,\epsilon)}{\partial t} = \left[\frac{\partial}{\partial x}\left(\frac{\partial V}{\partial x}\right) - \epsilon \frac{\partial}{\partial x} + \frac{1}{\tau}\frac{\partial}{\partial \epsilon}\epsilon + D\frac{\partial^2}{\partial x^2} + \frac{Q(\tau)}{\tau^2}\frac{\partial^2}{\partial \epsilon^2}\right] W_t(x,\epsilon), \qquad (4)$$

we evaluate by use of the matrix-continued fraction (MCF) method (see [7,10,13]) the x-periodic stationary probability $W_{\mathrm{st}}(x,\epsilon) = W_{\mathrm{st}}(x + L, \epsilon)$, normalized to unity within a spatial period, i.e., $\int_0^L dx \int_{-\infty}^{\infty} d\epsilon W_{\mathrm{st}} \times (x,\epsilon) = 1$. With the probability current in the x direction given by $J_x(x,\epsilon) = (-\partial V/\partial x + \epsilon - D\partial/\partial x) W_{\mathrm{st}}(x,\epsilon)$, the total fluctuation-induced nonequilibrium current J is obtained as

$$J = \int_0^L dx \int_{-\infty}^{\infty} d\epsilon J_x(x,\epsilon). \qquad (5)$$

In applying the MCF, we expand the potential $V(x)$ as well as the solution $W_{\mathrm{st}}(x,\epsilon)$ into Fourier series in x, and the ϵ dependence into a series of Hermite functions. For the ratchet potential we use two different shapes,

$$V(x) = V_2(x) = -[\sin(2\pi x) + 0.25\sin(4\pi x)]/2\pi, \qquad (6)$$

and a model with three Fourier modes,

$$V(x) = V_3(x) = -\sin\{(2\pi x) + 0.2\sin[4\pi(x - 0.45)] + 0.1\sin[6\pi(x - 0.45)]\}/2\pi. \qquad (7)$$

Both these ratchet potentials exhibit a smaller *average* force in *forward* direction, see Fig. 1. Hence, the current in a correlation ratchet is intuitively expected to flow always towards the *positive* direction. Nevertheless, the characteristic quantity [see (9) below]

$$-\int_0^L dx\, V'(x)[V''(x)]^2 \equiv c^- - c^+ \qquad (8)$$

is positive for $V_2(x)$, but *negative* for $V_3(x)$. This difference will be of crucial importance for the phenomenon of current reversal in *OU process driven ratchets*.

For the potential $V_2(x)$ the behavior of the current J in the (OU) ratchet is depicted in Figs. 2(a)–2(c) as a function of the noise parameters $\{D, Q, \tau\}$. Figure 2(a) is for the constant intensity scaling $Q(\tau) = Q$, where the current $J(\tau)$ for fixed Q starts out from zero at $\tau = 0$, reaches a maximum, and approaches zero again as

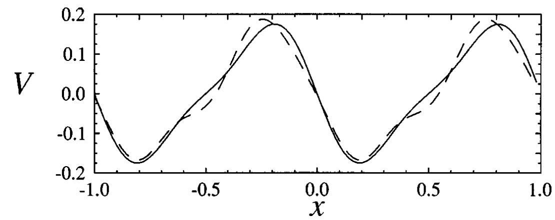

FIG. 1. Shape of the two ratchet potentials $V_2(x)$ (solid) and $V_3(x)$ (dashed) used in this work.

$\tau \to \infty$. We note that this increase and decrease occurs monotonically as τ is varied. For fixed variance scaling $Q(\tau) = \tilde{Q}\tau$, the current is depicted as a function of $\tilde{Q}$ and noise color τ in Fig. 2(b). We note that for fixed $\tilde{Q}$, the current $J(\tau)$ is maximal in the adiabatic fluctuation limit $\tau \to \infty$, and always *monotonically* decreases to zero as $\tau \to 0$. The global adiabatic maximum occurs near $\tilde{Q} \simeq 3$. With τ held fixed, the current $J(\tilde{Q})$ exhibits

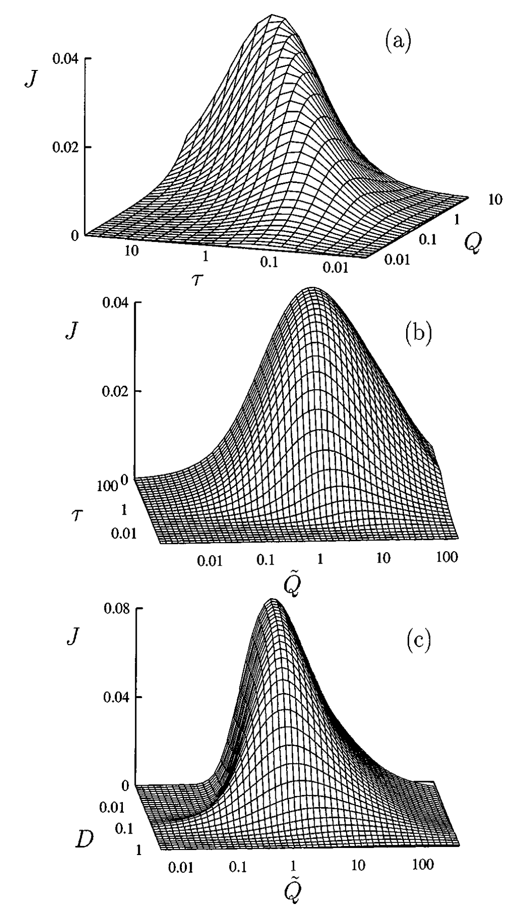

FIG. 2. Numerical (MCF) results for the current J in $V_2(x)$ are depicted in (a) and (b) for the two different noise scalings $Q(\tau) = Q$ and $Q(\tau) = \tilde{Q}\tau$ at fixed thermal noise strength $D = 0.1$. The dependence on both noise sources is exhibited in panel (c) at $\tau = 1$. The prediction for $J(\tau \to \infty)$ of the familiar adiabatic approximation [1] agrees within line thickness with the MCF results in (b).

a bell-shaped maximum as $\tilde{Q}$ is varied within $[0, \infty]$. Moreover, we note that this maximum does *not occur* at a fixed value $\tilde{Q}$, but moves towards larger $\tilde{Q}$ values as $\tau \to 0$. For $\tau = 1$ (i.e., $\tilde{Q} = Q$) the influence of the thermal noise strength D is depicted in Fig. 2(c). Over most parts of the parameter regime $(\tilde{Q}, D)$ the effect of increasing the thermal noise intensity D yields a *smaller* current. An exception occurs for small $\tilde{Q}$ values $\lesssim 0.5$, where small thermal noise can increase the current.

For this class of two-noise driven colored flows a generalized unified colored noise approximation (GUCNA) has been developed in Ref. [10]. The upshot of this theory is that the non-Markovian dynamics is approximated by a white-noise driven effective Fokker-Planck equation with a color and state dependent diffusion. Given this, the current $J[\tau, Q(\tau), D]$ itself can be evaluated readily in terms of two quadratures; see, e.g., Refs. [6,13]. Notably, the GUCNA is *not restricted* to small noise intensities only. The path integral approach is another tool for obtaining approximative results; however, it is restricted to small noise intensities. Within this restriction, the current J can be approximated by $L[k^+(\tau) - k^-(\tau)]$, wherein $k^\pm$ are the forward and backward transition rates between adjacent minima of the ratchet potential $V(x)$. The Arrhenius factors for these rates can be evaluated by invoking the "small-γ" path integral theory put forward in [12]. With a constant intensity scaling $Q(\tau) = Q$, the regime of validity of this approximation is governed by the expansion parameter $\gamma = (Q/D\tau)^{1/2} < 1$, see Ref. [12]. At small noise color τ, yet a different path-integral analysis [8,10,12] for weak noise D and $Q(\tau)$ similarly predicts for the current

$$J \approx L \frac{|V''(x_0)V''(x^\#)|^{1/2}}{2\pi} \exp\left[-\frac{\Delta V}{D + Q(\tau)}\right] \times \exp\left\{-\frac{\tau^2 Q(\tau) c^+}{[D + Q(\tau)]^2}\right\} \times \left(1 - \exp\left\{-\frac{\tau^2 Q(\tau)}{[D + Q(\tau)]^2}(c^- - c^+)\right\}\right). \quad (9)$$

Here, x_0 is the minimum of the ratchet potential, with the left- (right-) sided transition states x^- (x^+), obeying $V''(x^-) = V''(x^+) \equiv V'(x^\#)$. The quantity $c^\pm$ is dependent solely on the potential shape, $c^\pm = \int_{x_0}^{x^\pm} dx [V''(x)]^2 V'(x) > 0$, and $\Delta V = V(x^\#) - V(x_0)$ denotes the Arrhenius energy of the periodic ratchet. At large noise color $\tau \to \infty$, with $D \neq 0$ but small, an adiabatic approximation yields for the current a limiting behavior of the form

$$J(\tau \to \infty) = C\left\{1 - \exp\left[\frac{Q(\tau)}{2D^2\tau}(L_-^2 - L_+^2)\right]\right\}, \quad (10)$$

where C is positive valued and $L_\pm = |x^\pm - x_0|$.

The predictions of the various theories are compared in Fig. 3 for constant noise intensity $Q(\tau) = Q$ for the ratchet potential $V_2(x)$. The small-γ theory (dashed line) yields qualitatively the correct behavior over the whole τ regime, predicting correctly the location of the maximum, although being off for J by a factor $\lesssim 10$. In contrast, the GUCNA (dash-dotted line) is limited in the regime of validity to small τ values. There, it predicts rather correctly the current, and is in agreement superior to the small-τ path integral result in (9) (dotted line).

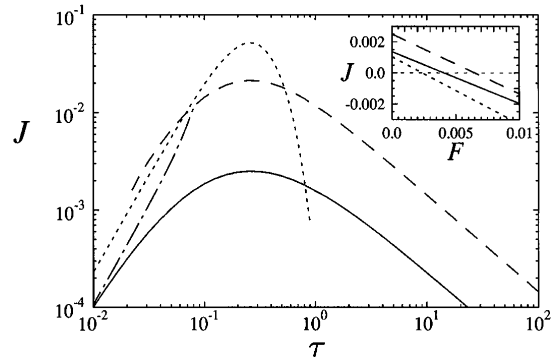

FIG. 3. The numerical result (solid line) is compared to theories of Eq. (9) (dotted line), GUCNA of [10] (dash-dotted line), and small-γ theory in [12] (dashed line) for the noise parameters $D = 0.1$ and $Q = 0.025$. The inset shows the current in the tilted potential $V_2(x) + xF$, which flows "uphill" for small F. D and Q are as above, $\tau = 1.25$ (solid line), $\tau = 0.25$ (dashed line), and $\tau = 0.05$ (dotted line). As $\tau \to 0$, the numerics of the small-γ theory become increasingly intractable.

The two theoretical predictions in (9) and (10) call for interesting effects: First, we observe that with $L_+ > L_-$ (i.e., a forward ratchet), the current is *always positive* as $\tau \to \infty$, independent of the noise scaling (cf. Fig. 2). For $Q(\tau) = Q$, it vanishes exponentially inversely proportional to τ. Turning to the behavior at small τ, the rub is that the quantity $(c^- - c^+)$ in (8) can assume for a *forward* ratchet both positive as well as *negative* values. Indeed, for $V_2(x)$, $c^- - c^+ \simeq 14.8$, and for $V_3(x)$, $c^- - c^+ \simeq -6.19$! Hence, with $(c^- - c^+) < 0$, the current in (9) starts out from $\tau = 0$ with negative values. Upon noting

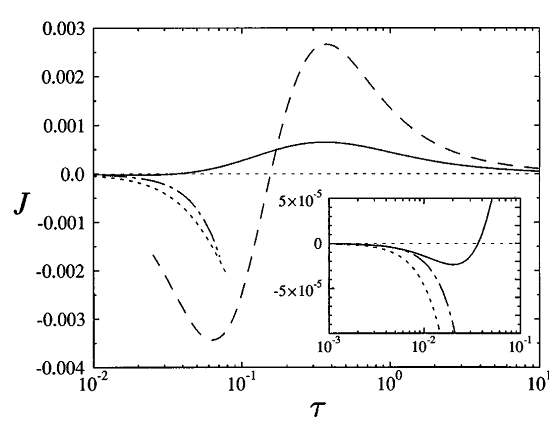

FIG. 4. The current reversal in $V_3(x)$ is depicted for $D = 0.05$ and $Q(\tau) = Q = 0.025$: Numerical results (solid line) are compared to GUCNA (dash-dotted line), small-τ (dotted line), and small-γ (dashed line) theory. The inset gives a magnification of the behavior at small τ.

(10), i.e., $J(\tau \to \infty) \geq 0$, this implies at least one current reversal of J vs τ for the OU noise driven $V_3(x)$ ratchet. Moreover, this reversal occurs independently of the chosen form of the noise scaling $Q(\tau)$. The vanishing (!) of $J(\tau)$ itself typically occurs at moderate noise color τ_R, which is outside the regime of validity of the small-τ path integral approach as given in (9). Figure 4 depicts this new current reversal [14], where precise numerics (solid) are compared with the GUCNA (dash-dotted line), the "small-τ" theory in (9) (dotted line), and the small-γ theory (dashed line). The reversal occurs near $\tau_R \simeq 0.037$, while the small-γ theory—being presently the only theory that captures the *change of sign*—yields $\tau_R \simeq 0.16$. At small τ, the GUCNA again exceeds in accuracy the prediction (9), see inset in Fig. 4. It is worth mentioning that the current reversal is *not* caused by the slight extra "shoulder" of the potential $V_3(x)$ in comparison with $V_2(x)$ (cf. Fig. 1) as can be demonstrated by examples; rather it is the proper interplay of the higher x derivatives of $V(x)$ in (8) which matters.

The inset in Fig. 3 displays the current for $V_2(x)$ in the presence of an additional constant bias F ("current-load curve") for different τ values. For small bias, the particle *can move uphill* until a critical value F_s (the stopping force) is reached, where $J(F_s) = 0$. This phenomenon of uphill motion against an external gradient has been observed recently for the directed motion of ions in a biological system [15]. The stopping force $F_s(\tau)$ on the almost *linear* load curve depicted in Fig. 3 exhibits a *bell-shaped behavior* as a function of noise color τ.

In summary, we have presented the first precise numerical (MCF) calculations over extended parameter regimes (cf. Fig. 2) for the simplest Gaussian colored noise driven correlation ratchet. We compared the results vs recent, nontrivial theoretical predictions. The discovered novel features of the stopping force $F_s(\tau)$ and—most surprisingly—the simple scheme of current reversal calls for intriguing applications in the natural sciences in both microtechnology and biophysics.

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[14] This novel and simple mechanism for reversing the current in a correlation ratchet distinctly differs from both the scheme where the reversal is due to a change in the "flatness" of the noise statistics [4], and the one that results if one modifies the noise spectrum $\phi(\omega)$ so that a *minimum* for $\phi(\omega)$ occurs at $\omega = 0$ (e.g., for Gaussian *harmonic* noise) [5]. In contrast, for our OU noise driven ratchet, the spectrum $\phi(\omega) = 2D + 2Q(\tau)/(1 + \omega^2\tau^2)$ is monotonically decreasing as $|\omega| \to \infty$.
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