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B. Lindner, Lutz Schimansky-Geier, Peter Reimann, Peter Hänggi

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Mass separation by ratchets

B. Lindner*, L. Schimansky-Geier*, P. Reimann†, and P. Hänggi†

*Humboldt-University at Berlin, Invalidenstr.110. D-10115 Berlin. Germany
†University of Augsburg, Memminger Str. 6, D-86135 Augsburg, Germany

Abstract. The fluctuation-induced transport of massive Brownian particles is investigated. Analytic approximations for their current in periodic 'ratchet'-potential driven additively by the Ornstein-Uhlenbeck noise are in qualitative agreement with the result of numeric simulations. The ability to separate particles with different masses in situations with a constant bias is discussed.

BROWNIAN PARTICLES IN RECTIFIERS

We consider the one-dimensional motion of a Brownian particle with coordinate $x = x(t)$, mass m, and viscous friction η,

$$m\ddot{x} = -\eta\dot{x} - V'(x) + F + y(t) + \sqrt{2D}\,\xi(t) \;, \qquad (1)$$

in an asymmetric periodic potential (ratchet) $V(x)$ of period L. F stands for an additional 'load force'. Both last expressions in (1) are noisy source terms. Thermal fluctuations are modelled by the Gaussian white noise $\xi(t)$. Its intensity D is given due to an Einstein relation by $D = \eta\, k_B T \equiv \eta/\beta$ and, hence, the particle performs Brownian motion in a thermal bath with temperature T. Furthermore, we introduce the action of external fluctuating forces $y(t)$ on the particle which exposes the system out of equilibrium.

We assume $y(t)$ to be an Ornstein-Uhlenbeck-process with zero average and correlation time τ. The intensity $\int\langle y(t)y(0)\rangle dt$ is labelled by Q and is independent of the correlation time τ. It is convenient to express Q in units of the thermal noise strength D introducing R by $Q = R\,D$.

Overdamped situations $\eta \to \infty$ of eq.(1) with different types of $y(t)$ was the topic of a lot of studies [1,2], recently, pointing in their application to biological systems. A rich material for several physical situations of driving, either by periodic or by stochastic forces y, was investigated in detail (for review see [2]). Also the fluctuation induced transport was verified experimentally [3].

Less well elaborated is the case where inertial effects of the particles come into play. Only in [4] a complex behaviour of the current for a periodic external force without thermal noise was reported. The inclusion of inertial effects.

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however, would generalize the effect of stochastic ratchets and achieves importance in technical applications, especially if particles should be separated by ratchets.

The quantity of foremost interest is the steady state particle current $\langle \dot{x} \rangle$ [1]- [4]. For zero load $F = 0$ in two limits, in the white noise limit $\tau \to 0$ as well as in the zero amplitude limit $\tau \to \infty$, an equilibrium-like situation is approached. The stationary distribution achieves a canonical like shape $P^{st} = P(H)$ with H being the Hamilton-function of the particle. The mean current vanishes in both limits. In the intermediate regime $0 < \tau < \infty$ the external force $y(t)$ violates the detailed balance in the systems and the non equilibrium situation will exhibit a non-vanishing current $\langle \dot{x} \rangle$ [2].

In the following sections two different approximation schemes are presented and compared with results of numerical simulations. Specifically, we will address the dependence of the current $\langle \dot{x} \rangle$ upon the correlation time τ and the particle mass m, assuming thereby all other parameters are kept fixed. In numerical evaluations we use the special potential: $V(x) = -[\sin(2\pi x) + 0.25\sin(4\pi x)]/(2\pi)$.

UNIFIED COLORED NOISE APPROXIMATION

The unified colored noise approximation (UCNA) has originally been developed for overdamped stochastic dynamics driven by OUP. Later refinements and generalisations have been elaborated [5]. It has proved to yield good approximations over wide parameter regimes in different situations [6] and was applied already to fluctuation induced transport [7].

The objective in the UCNA is to find an approximate Markovian description of the generally intractable non-Markovian dynamics (1) [6]. First a non-linear coordinate transformation to (approximately) decoupling stochastic variables is performed. In a second step, a separation of time scales for those new variables is established, thus admitting the adiabatic elimination of the 'fast' ones.

Adapting this general line to (1) we find expressions for small correlation times τ and, simultaneously, for a strongly overdamped dynamics $m/\eta \to 0$. Within these restrictions, the following approximate Langevin equation (in Stratonovich interpretation) as Markovian approximation of (1) is derived:

$$\eta\, g(x)\, \dot{x} = -V'(x) + F + \sqrt{2D(1+R)}\,\xi(t) \tag{2}$$

where the state- and mass-dependent dressing $g(x)$ of the friction reads

$$g(x) = 1 + \frac{d}{dx}\frac{\tau\, R\,[V'(x) - F]}{(1+R)(\eta + \frac{m}{\tau}) + \tau V''(x)}\,. \tag{3}$$

The steady state probability current J in (2) follows by means of a standard calculation [8]. With $\langle \dot{x} \rangle = J\, L$ we arrive at

$$\langle \dot{x} \rangle = \frac{L\,(1+R)\,\left[1 - e^{\beta\Phi(L)}\right]}{\beta\eta \int\limits_0^L dx\, g(x)\, e^{-\beta\Phi(x)} \int\limits_x^{x+L} dy\, g(y)\, e^{\beta\Phi(y)}} \,. \tag{4}$$

Here we introduced an effective potential

$$\Phi(x) = \int_0^x \frac{g(y)}{1+R} \left[V'(y) - F\right] dy \,. \tag{5}$$

In the white noise limit $\tau \to 0$, the current $\langle \dot{x} \rangle_{\tau=0}$ predicted by (4) is independent of m and coincides with the exactly solvable case $F \neq 0$, $\tau = 0$, $m = 0$ [8]. If $F = 0$, the current is generically non-zero if $0 < \tau < \infty$ for non-symmetric potentials $V(x)$. The asymptotic behaviour of (4) for small τ and zero load $F = 0$ is obtained as

$$\langle \dot{x} \rangle = -\frac{\tilde{\tau}^2\, L\, R}{\eta^3 A (1+R)^2} \int_0^L V'(y) V''(y)^2\, dy \quad , \quad \tilde{\tau} = \frac{\tau}{1 + m/\eta\tau} \tag{6}$$

$$A = \int\limits_0^L dx \int\limits_x^{x+L} dy\, e^{\beta[V(y) - V(x) + (x-y)F]/(1+R)} \,. \tag{7}$$

Thus a τ^2 decay for moderately small τ is predicted, crossing over to a τ^4 decay for extremely small τ. The m-dependence of the UCNA result (4) can be completely absorbed into the renormalised correlation time $\tilde{\tau}$, for this reason the maximum of $\langle \dot{x} \rangle$ is independent of m.

To verify the approximative results we performed numerical simulations of the Langevin equation (1) using the algorithm of Fox [9]. For each set of parameter values we integrated the stochastic dynamics over 10^7 time steps $\Delta t = 10^{-2}$. This was repeated 20 times to obtain the average current and its estimated accuracy. Since the relative numerical error increases both with decreasing η and decreasing τ we could not reach the deep asymptotic regime, assumed in our derivation of the UCNA result (4). The comparison for moderately large η and moderate-to-small τ of the UCNA with the simulations is depicted in Fig. 1 (left) for different m-values. The maximum of the UCNA shifts in τ with increasing mass while the simultaneous decreasing of the maximum is not predicted.

PATH INTEGRAL APPROACH

In this section we aim the calculation of the steady state current by help of path-integrals. As in quantum mechanics the re-formulation of stochastic dynamics yields a compact representation [10,11]. In practise, however, a further analytical evaluation of the resulting expressions is possible for weak noise only, i.e. for situations where the (effective) potential barriers between adjacent local minima are large compared to the strength of the fluctuations.

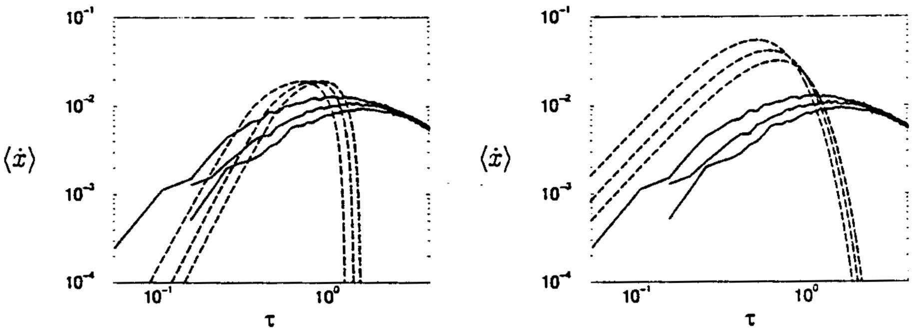

FIGURE 1. Particle current vs. correlation time. Left figure: UCNA (dashed) and numerical simulations (solid). From left to right: $m = 0.5, 1, 1.5$. ($\eta = 2$, $D = \eta/\beta = 0.1$, $Q = RD = 0.5$, $F = 0$). Right figure: Path-integrals (dashed) and simulations (solid).

Within this restriction the current can be approximated by

$$\langle \dot{x} \rangle = L\,[k_+ - k_-] \;, \tag{8}$$

where $k_+(k_-)$ are the hopping rates to the right (left) between neighbouring local minima.

For small temperatures (large β) these rates approach an Arrhenius-like dependence $k_\pm = \zeta_\pm \exp -\beta\Delta\Phi_\pm$ where $\Delta\Phi_\pm$ are temperature-independent 'effective' potential barriers. The $\zeta_\pm$ are prefactors with a much weaker temperature dependence.

In the case of small τ [12] we obtain

$$\Delta\Phi_\pm(\tau) = \frac{V(x^\#) - V(x_\pm) + (x_\pm - x^\#)F}{1+R} + \tau^2 \frac{\eta R}{(1+R)^2} \int_{-\infty}^{\infty} \ddot{q}_\pm^2(t)\, dt \;, \tag{9}$$

where $x^\#$ is one of the local maxima of $V(x) - xF$ and x_+ and $x_- = x_+ - L$ its neighbouring local minima to the right and left, respectively. The functions $q_\pm(t)$ are the trajectories found from $m\ddot{q}_\pm(t) = -\eta\dot{q}_\pm(t) - V'(q_\pm(t)) + F$ with boundary conditions $q_\pm(t=-\infty) = x^\#$ and $q_\pm(t=\infty) = x_\pm$.

Concerning $\zeta_\pm$ we restrict ourselves to the 0-th order approximation $\zeta(\tau) \simeq \zeta(\tau = 0)$ with the effective temperature $T(1+R)$. Closer inspection involving detailed-balance arguments as well as explicit perturbation calculations [13] have shown that the identity $\zeta_+(\tau=0) = \zeta_-(\tau=0)$ should hold true in the spatial diffusion regime whenever the concept of an escape rate makes sense. We thus infer that (with $\Delta\Phi_\pm^{(1)}$ being the second term in (9))

$$\langle \dot{x} \rangle = B\big[e^{-\beta\tau^2\Delta\Phi_+^{(1)}} - e^{-\beta\{\tau^2\Delta\Phi_-^{(1)} + LF/(1+R)\}}\big] \tag{10}$$

and where $B = L\,k_+(\tau = 0)$. We will utilise here our observation from the previous section that the current $\langle \dot{x} \rangle_{\tau=0}$ is apparently almost m-independent.

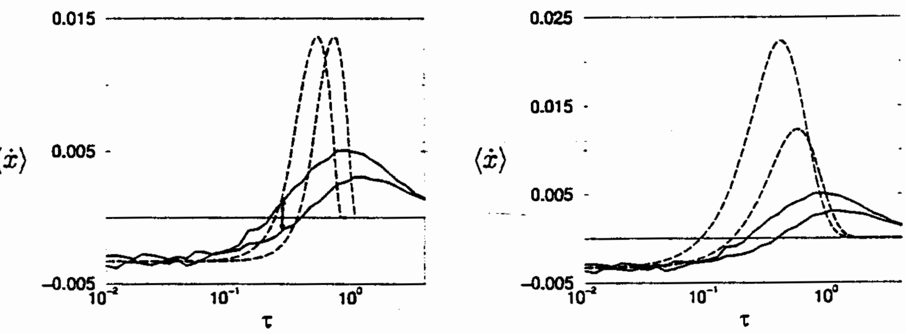

FIGURE 2. Same as in Fig.1 but for $F = -0.01$, $Q = 0.25$, $m = 0.5$ (curve, that reaches first the maximum), $m = 1.5$. The arrow indicates a τ-value allowing for mass separation.

So, the same m-independence is inherited by B and by setting $m = 0$ we obtain the approximative prefactor

$$B = L\,(1 + R)/\beta\eta\,A \tag{11}$$

and A is due to (7). For zero load $F = 0$ this yields the leading order small-τ behaviour

$$\langle\dot{x}\rangle = -\frac{\tau^2 L\,R}{A(1+R)} \int_{-\infty}^{\infty} [\ddot{q}_+(t)^2 - \ddot{q}_-(t)^2]\,dt. \tag{12}$$

The comparison of the path integral prediction (10), (11) with numerical simulations is shown in Fig. 1. The agreement is rather satisfactory up to about $\tau = 0.5$. The shift and the decreasing of the maximum are well described. In particular, the asymptotics (12) seems to agree better with the numerics than that from the UCNA approach (7).

MASS SEPARATION

Above we obtained a displacement of the maximal current for increasing values of the mass m. This shift can be used with the purpose to separate mesoscopic particles with different masses. Beside a size-depending separation due to different friction constants of the particles, the separation by mass is a new and independent possibility, as easy to survey in the case of particles of different masses but of the same size.

With zero load $F = 0$ flux reversals do not occur in the considered case. Otherwise, adding a constant force against the preferred direction of the ratchet a flux reversal will be exhibited in a finite region of τ. Beginning from a value τ_1 until a second value τ_2 the noise-induced current overcompensates the action of the (small) load force. Both values, τ_1 and τ_2 depends on the mass of the particle. Hence for two different values of the mass non-overlapping regions of the flux reversals are possible which yields the separation of the two species of particles.

Results of simulations and of the estimations from the UCNA and the path-integral approach are depicted in Fig. 2. For a specific range of τ the particles have different signs of velocity, and hence flow in the average in different directions. An increase of the differences of the masses would strengthen the speed of separation and enlarge the region of possible correlation times.

In conclusion we have investigated inertial effects of Brownian particles in sawtooth-like potential. In the region of moderate to strong damping and for small correlation times of the considered external forces we found numerically a shift of the maximal flux with increasing mass towards larger τ. The observation was confirmed by two approximation schemes. This dependence of the flux on the mass can be exploited for separation of particles with different inertial properties.

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