Controlling the collective motion of interacting particles: Analytical study via the nonlinear Fokker-Planck equation

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Abstract

We propose a nonlinear Fokker-Planck equation for the description of stochastic transport in systems of short-range interacting particles. We develop a perturbation scheme, valid for high-frequencies, for particles driven by a time-dependent temperature ratchet. For a particular type of asymmetric potential, the net DC current shows two current inversions when increasing either the particle density or the interaction strength.

Key words: Collective transport of short-range interacting particles; particles driven by a time-dependent temperature;

Stochastic transport on spatially–asymmetric periodic ("ratchet") potentials has been intensively studied in systems far from equilibrium, and mostly in the context of molecular motors (see, e.g., the reviews [1]). In such Brownian motors, a net motion of particles may occur even in the absence of any DC driving force, due to the rectification of non-equilibrium thermal fluctuations.

Analytical studies of ratchets are usually performed using the *linear* Fokker-Planck equation, which is valid for an assembly of *non*-interacting particles. It is important to study the physically relevant case of how particle-particle interactions influence the stochastic transport in Brownian motors. In this paper, we derive and analyze the nonlinear equation describing stochastically-moving particles with short range interaction. Here we consider the so-called temperature ratchet [2], where the time-oscillations of the temperature drive the motion of particles.

Our starting point is the overdamped equation of motion for pairwise-interacting particles in an asymmetric periodical potential $\mathcal{U}$,

$$\dot{x}_i = -\frac{\partial \mathcal{U}(x_i)}{\partial x_i} - \sum_{j\neq i} \frac{\partial}{\partial x_i}\mathcal{W}(x_i - x_j) + \sqrt{2k_B T}\,\xi^{(i)}(t), \tag{1}$$

with temperature T, Boltzmann constant k_B, and pair potential $\mathcal{W}$. The Gaussian white noise $\xi^{(i)}$ satisfies the relation $< \xi_\alpha^{(i)}(t)\xi_\beta^{(j)}(t+\tau) >= \delta(\tau)\delta_{\alpha\beta}\delta_{i,j}$. Applying the Bogolyubov method, an infinite set of many-particle distribution functions can be constructed. Such a hierarchy can be truncated in the "mean field" approximation by replacing the binary distribution function with the product of two one-particle distribution functions $F_1(t,x)$; hence we obtain the nonlinear integro-differential equation:

$$\frac{\partial F_1(t,x)}{\partial t} = \frac{\partial}{\partial x}\left[F_1(t,x)\frac{\partial \mathcal{U}^{\rm eff}}{\partial x} + k_B T\frac{\partial F_1(t,x)}{\partial x}\right] \tag{2}$$

with the "mean-field" potential

$$\mathcal{U}^{\rm eff} = \mathcal{U}(x) + \int dx' \mathcal{W}(x-x')F_1(t,x') \tag{3}$$

which is periodic and has the same spatial period l as the substrate potential $\mathcal{U}$. The distribution function

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$F_1(t,x)$ can be normalized, for instance, by the total number of particles in the system. In this case the spatial average of the function $F_1(t,x)$ coincides with the density of particles $\bar{n}$. If the interaction range of the particles is the smallest distance in the problem, the interaction potential can be taken in the local limit $\mathcal{W}(x) = g\delta(x)$. This simplifies considerably the nonlinear Fokker-Planck equation under study:

$$\frac{\partial F_1}{\partial t} = \frac{\partial}{\partial x}\left[F_1 \frac{\partial \mathcal{U}}{\partial x} + k_B T(t)\frac{\partial F_1}{\partial x} + gF_1\frac{\partial F_1}{\partial x}\right]. \qquad (4)$$

Now the temperature T is chosen to be a periodic time-dependent function [2], say $T(t) = T(1 + a\cos(\omega t))$, $a < 1$. In the high frequency limit, $[\max_x(\mathcal{U}) - \min_x(\mathcal{U})]/(\omega l^2) \ll 1$, $k_BT/(\omega l^2) \ll 1$, and $g\bar{n}/(\omega l) \ll 1$, the solution of Eq. (4) can be expanded with respect to the reciprocal of the frequency $1/\omega$:

$$F_1(\tau,x) = \sum_{i=0}^{\infty} \frac{1}{\omega^i}\,\phi_i(\tau,x) \qquad (5)$$

where $\tau = \omega t$ is a dimensionless time. The following periodic and normalizing conditions can be taken: $\phi_i(\tau+2\pi,x) = \phi_i(\tau,x) = \phi_i(\tau,x+l)$, $\int_0^l dx\phi_{i\neq 0}(x) = 0$, and $\int_0^l dx\phi_0(x)/l = \bar{n}$. Omitting the detailed description of the iterative procedure, here we concentrate on the physical results. Instead of the usual Boltzmann distribution, the equilibrium distribution function $\phi_0(x)$ of the very short-range interacting particles is described by the transcendental equation:

$$\phi_0(x) = C(\bar{n})\exp\left(-\frac{\mathcal{U}(x) + g\,\phi_0(x)}{k_BT}\right) \qquad (6)$$

with a constant $C(\bar{n})$ defined by the normalization condition. By solving equation (4) up to the third approximation with respect to $1/\omega$, we obtain the equation for the DC net current related to the nonequilibrium state induced by the time oscillating temperature:

$$J(\,\bar{n}\,,\omega,T) = \frac{k_B^2T^2a^2}{2\omega^2\int_0^l\frac{dx}{\phi_0}}\int_0^l dx\left\{\frac{(\mathcal{U}'')^2\mathcal{U}'(4k_BT+5g\phi_0)}{(k_BT+g\phi_0)^3} - \frac{2k_BT(\mathcal{U}')^3\mathcal{U}''(4k_BT+5g\phi_0)}{(k_BT+g\phi_0)^5} - \frac{g\phi_0(\mathcal{U}')^5\left(6k_B^2T^2+10gk_BT\phi_0+3g^2\phi_0^2\right)}{(k_BT+g\phi_0)^7}\right\}, \qquad (7)$$

with $' \equiv \partial/\partial x$. This expression can be simplified in the limit of zero interaction, giving the known result [1]:

$$J = \frac{2a^2l\bar{n}\int_0^l dx\mathcal{U}'(\mathcal{U}'')^2}{\omega^2\int_0^l dx\exp\left(\frac{\mathcal{U}}{k_BT}\right)\int_0^l dx\exp\left(-\frac{\mathcal{U}}{k_BT}\right)} \qquad (8)$$

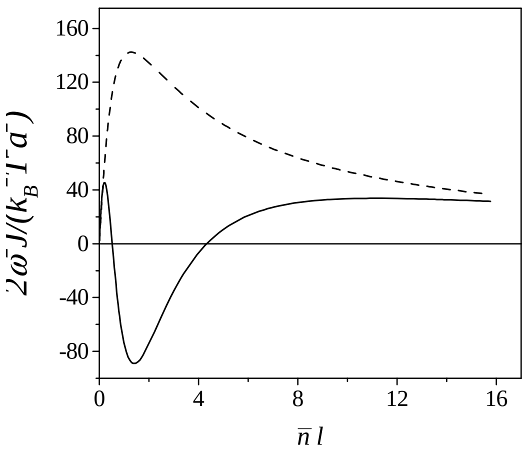

Fig. 1. The DC probability current versus particle density for for the potential $\mathcal{U}/k_BT = a_0\sin(2\pi x/l) + a_1\sin(4\pi x/l - \beta_1) + a_2\sin(6\pi x/l - \beta_2)$. Two sets of parameters are shown here: $a_0 = 1$, $a_1 = 0.2$, $a_2 = -0.06$, $\beta_1 = 0.45$, $\beta_2 = 0.45$ for the solid curve with *two current inversions*; and $a_0 = 1$, $a_1 = 0.01$, $a_2 = 0$, $\beta_1 = 0.45$ for the dashed curve with *no current inversions*. These two examples illustrate two types of allowed $J(n)$'s for interacting particles driven by a time-oscillating temperature $T(t)$ and moving on a spatially asymmetric periodic potential.

and can also provide the current in the strong interaction limit, $\max(k_BT; \max_x\mathcal{U} - \min_x\mathcal{U}) \ll g\bar{n}\,l \ll \omega l^2$,

$$J = \frac{5k_B^2T^2a^2}{2\omega^2g^2l^2\bar{n}}\int_0^l dx\mathcal{U}'(\mathcal{U}'')^2. \qquad (9)$$

It is clear from the last two equations, that the sign of the current is the same in the case of weak and strong interactions for *any* asymmetric potential. This means that *either there is no current inversion or that the current inverts an even number of times when increasing either the strength g of interaction or the particle density* $\bar{n}$. Numerical calculations of the integral in expression (7) show examples of these two scenarios.

In conclusion, we have derived the nonlinear Fokker-Planck equation for systems of locally interacting particles and obtained the expression for the net DC current for temperature ratchet in high frequency limit.

References

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