Stochastic pump of interacting particles

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received 3 January 2011; accepted in final form 24 March 2011
published online 27 April 2011

PACS 05.70.Ln - Nonequilibrium and irreversible thermodynamics
PACS 05.40.-a - Fluctuation phenomena, random processes, noise, and Brownian motion
PACS 05.60.-k - Transport processes

Abstract – We consider the overdamped motion of Brownian particles, interacting via particle exclusion, in an external potential that varies with time and space. We show that periodic potentials that maintain specific position-dependent phase relations generate time-averaged directed current of particles. We obtain analytic results for a lattice version of the model using a recently developed perturbative approach. Many interesting features like particle-hole symmetry, current reversal with changing density, and system size dependence of current are obtained. We propose possible experiments to test our predictions.

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Introduction. – Stochastic pumps refer to systems where overall directed motion of particles are obtained under the influence of external driving forces that are unbiased in the sense that they vanish either on spatial or temporal averaging. However, in order to generate directed motion, it is necessary that the external forces have some form of time-reversal symmetry breaking inbuilt into them. A large number of models of pumps have been studied and there have also been many experimental realizations [1–4]. Natural examples of stochastic pump include ion pumps associated with the cell membrane (e.g., Na\textsuperscript{+}, K\textsuperscript{+}-ATPase pump [5]), molecular motors (kinesin/dynein, myosin) moving on polymeric tracks (microtubule, F-actin) [3], etc.

Most studies of particle pumps focussed on systems of non-interacting particles, though, there have been some numerical [6] and analytical work [7] on interacting Brownian motors. Recently the effect of interactions in ratchet models has been studied analytically using mean-field theory and dynamical density functional theory and also numerically in [8]. Some other studies involving ratchet models have focussed on interaction effects that leads to transport of one species of particles due to driving of another species [9]. Recently a model of a classical pump, similar to those used in the study of quantum pumps [10], has been proposed in ref. [11]. They studied directed current (DC) in the presence of inter-particle interactions. The model studied was the symmetric exclusion process on a ring which closely mimics a system of diffusing particles with short-ranged repulsive interaction in one dimension. It was shown that for time oscillatory hopping rates between two neighbouring points a DC current was established in the system. The hopping rates were taken to be symmetric around every point, and this made it difficult to make a direct connection of this model to a system of particles in an oscillatory external potential. In this letter we consider a stochastic exclusion dynamics which directly mimics hard-core particles moving in a time-dependent external potential. We show that the perturbative approach of ref. [11] can be used for this case as well, and thence obtain a number of interesting predictions for this system.

Model. – The dynamics of small thermally diffusing interacting particles confined within a narrow tube is well described by overdamped Langevin equations in one dimension. Consider \(N\) particles interacting with each other through a short-ranged repulsive pairwise interaction potential and in an external potential \(V\). We denote the total interaction potential energy by \(U\). Let \(x_r\) denote the position of the \(r\)-th particle. The equations of motion are then given by

\[
\frac{dx_r}{dt} = -\frac{\partial U}{\partial x_r} - \frac{\partial V}{\partial x_r} + \xi_r, \quad r = 1, 2, \ldots, N,
\]

where \(\xi_r(t)\) is white Gaussian noise with \(\langle \xi_r \rangle = 0\), \(\langle \xi_r(t)\xi_s(t') \rangle = 2\gamma k_B T \delta_{rs} \delta(t - t')\), \(k_B\) is the Boltzmann
constant and $T$ the ambient temperature. We assume the interaction potential to be of the form of hard-core repulsion between particles of radii $a$. It is expected that many of our results should be qualitatively similar for other short-range potentials. The choice of hard-core repulsive potential allows a mapping to the exclusion process which we now discuss. In the absence of an external potential, hard-core colloidal particles of diameter $a$, confined within a narrow channel of width $\leq 2a$, are well described by the symmetric exclusion process (SEP) [12]. Discretizing space by the particle size are well described by the symmetric exclusion process (SEP) [12]. Discretizing space by the particle size.

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\[ J = \frac{1}{L \tau} \sum_{l=1}^{L} \int_0^t dt J_{l-1,l}(t). \]

Using the form of the hopping rates we then get

\[ J = \frac{\lambda f_0}{2L \tau} \sum_{l=1}^{L} \int_0^t dt (u_l - u_{l-1})(\rho_{l-1} + \rho_l - 2C_{l-1,l}). \]

To evaluate $J$ we need to evaluate $\rho_l$’s and $C_{l-1,l}$’s and this we do using perturbation theory. For weak driving potential we make a perturbative expansion of $\rho_l$, $C_{l,m}$ in a series in the dimensionless parameter $\lambda$

\[ \rho_l = \bar{\rho} + \sum_{k=1,2,\ldots} \lambda^k \rho_l^{(k)}, \]

\[ C_{l,m} = C_{l,m}^{(0)} + \sum_{k=1,2,\ldots} \lambda^k C_{l,m}^{(k)}. \]

The $\lambda = 0$ terms in the above expansions correspond to the absence of any external potential and this is then just the symmetric exclusion process with uniform hopping rate $f_0$. For that case the steady state is the equilibrium state obeying detailed balance and is characterized by the position-independent densities and correlations. These are all known exactly, for example $\bar{\rho} = N/L = \rho$, $C_{l,m}^{(0)} = \rho(N-1)/(L-1)$, etc. [13].

As noted in ref. [11] the time evolution of the first-order terms $\rho_l^{(1)}(t)$ and $C_{l,m}^{(1)}(t)$ are given by the following equations:

\[ \frac{d\rho_l^{(1)}}{dt} = f_0(\Delta \rho_l^{(0)} + f_0 q_0 \Delta u_l), \]

\[ \frac{dC_{l,m}^{(1)}}{dt} = f_0(\Delta_1 + \Delta_m) C_{l,m}^{(0)} \]

\[ + f_0 q_0 (\Delta_1 u_l + \Delta_m u_m) \text{ for } l \neq m \pm 1, \]

\[ \frac{dC_{l,l+1}^{(1)}}{dt} = f_0(C_{l-1,l+1}^{(0)} + C_{l-1,l+2}^{(0)}) - 2C_{l,l+1}^{(0)} \]

\[ + f_0 q_0 (u_l - u_{l+1} - u_l - u_{l+1}), \]

where $\Delta g_{l,m} = g_{l+1,m} + g_{l-1,m} - 2g_{l,m}$ defines the discrete Laplacian, and $q_0 = \bar{\rho} - C_{l,m}^{(0)}$, $k_0 = C_{l,m}^{(0)} - C_{l,m}^{(0)}$ with equilibrium three-point correlation $C_{l,m,n}^{(0)} = C_{l,m}^{(0)}(N-2)/(L-2)$. These linear homogeneous equations can be solved exactly to obtain the long-time oscillatory solution [11]. We find

\[ \rho_l^{(1)}(t) = \text{Re}[A_l e^{i\Delta t}], \]

where the vector $A = \{A_1, A_2, \ldots, A_L\}$ is given by

\[ A = \frac{q_0 f_0}{\iota \Delta - f_0 \Delta} \hat{\Delta} \eta = -q_0 \eta + \frac{i \tilde{f} q_0}{\iota - f_0 \Delta} \eta \]

with $\eta = \{\eta_1, \eta_2, \ldots, \eta_L\}$ and $\hat{\Delta}$ the discrete Laplacian operator. The eigenfunctions of $\hat{\Delta}$ are given by $(1/\sqrt{L}) e^{-i \xi q}$ with corresponding eigenvalues $\epsilon_q = -2(1 - \cos q)$. Expanding $\hat{\Delta}$ using its

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eigenbasis we get $A_l = -q_0 \eta_l + \sum_m R_{l,m} \eta_m$, where $R_{l,m} = (\Omega q_0 / L) \sum q \left\{ q^{i(l-m)}/(\Omega - f_0 \epsilon_q) \right\}$ with $q = 2\pi j / L$, $j = 1, 2, \ldots, L$. The equation of two-point correlations can also be solved and it is easy to verify the following steady-state solutions (for all $l, m$):

$$C_l(t) = \frac{k_0}{q_0} [\rho_l(t) + \rho_{-l}(t)].$$

Then using eq. (3) one can find the general expression for the directed current,

$$J = -\frac{\lambda^2 f_0}{2L} \left( 1 - \frac{2k_0}{q_0} \right) \sum_{l=1}^L 2 \text{Re} \left( (\eta_l^* - \eta_{l-1}^*)(A_{l-1} + A_l) \right)$$

$$= -\frac{\lambda^2 f_0}{L} \left( 1 - \frac{2k_0}{q_0} \right) \text{Re} \left( \sum_{l,m} \eta_l^* (R_{l-1,m} - R_{l+1,m}) \eta_m \right)$$

$$= -\frac{2\lambda^2 f_0 \Omega}{L} (q_0 - 2k_0) \text{Re} \left( \sum_q \tilde{\eta}_q^2 \sin q / (\Omega - f_0 \epsilon_q) \right),$$

where $\tilde{\eta}_q = (1/\sqrt{L}) \sum_l \eta_l e^{-iql}$.

Note that the effect of interaction is entirely contained in the prefactor $(q_0 - 2k_0)$, which in the large-$L$ limit equals $\rho(1 - \rho)(1 - 2\rho)$. Several interesting features follow. The current vanishes at half-filling and its sign reverses with increasing particle density. The dynamics has particle-hole symmetry, and this is explicit in the density dependence. At low densities we obtain $J \propto \rho$ and this corresponds to the case where interactions can be neglected. This differs from the result in ref. [11] where the current vanished in the absence of interactions. We now investigate the solution in eq. (10) for different choices of the oscillating potential. We consider the following two cases.

**Case i): localized pump.** – Here we consider the specific case of a localized pump with time-varying potentials acting only on two consecutive sites such that $\alpha_l = \alpha_L = 1$ with all other $\alpha_l = 0$, and $\phi_l = \phi$, $\phi_L = 0$. For this case eq. (10) leads to the DC current

$$J_2 = -\lambda^2 (q_0 - 2k_0) \Omega \sin \phi \frac{\Omega \sin \phi}{2L} \text{Re} \left[ \frac{z_- - z_-^{L-1}}{1 - z_-} \right],$$

where $z_- = y/2 - \sqrt{(y/2)^2 - 1} = y/2 + i\Omega / f_0$. Note that $J_2$ has a sinusoidal dependence on the phase difference of external driving $\phi$, leading to maximal driven current at $\phi = \pm \pi / 2$. $J_2$ decays as $1/L$ with the system size $L$.

In fig. 1 we plot density dependence of $J_2$ obtained from Monte Carlo simulations. In this stochastic simulation, in each time step, all the lattice sites are visited randomly with uniform probability. In case a particle is found at a site $l$, a trial move is generated to place it in one of its nearest-neighbouring sites (right or left) with rate $w_{l,l+1}$. The trial move is accepted if the new site is empty, otherwise the move is rejected. We used periodic boundary conditions. In the steady state the instantaneous current across each bond is obtained by averaging over initial conditions and then this is averaged over many time periods. The parameter values used in the simulation are list in the caption of fig. 1. The data show good agreement with eq. (11). The small difference is expected since our analytic prediction is based on second-order perturbation theory. At $\rho = 1$ the current vanishes due to complete jamming of particles. Note the zero in the current at the point of half-filling $\rho = 1/2$, and the reversal in the direction of current as the density crosses this point (fig. 1). The maximal currents are obtained at $\rho = (1 \pm 1/\sqrt{3})/2$. We re-emphasize that the density dependence is general, and independent of whether the pumping is localized or spatially distributed.

Recently, both experimental works [14] and theoretical studies based on Brownian dynamics simulations [15] have discussed the diffusion mechanisms of interacting colloidal particles in quasi-one-dimensional geometries and under the influence of external periodic potentials. Note that the tagged particle diffusion in SEP is expected to show a crossover from a single-file diffusion behaviour $(\langle x(t) - x(0)^2 \rangle \sim t^{1/2})$ at short times to Fickian diffusion $(\langle x(t) - x(0)^2 \rangle \sim t)$ at long times [16]. We have verified from our simulation that, once the drift due to the pump effect is subtracted out, our model also shows this crossover.

**Case ii): traveling wave.** – A spatially distributed external potential of the form $V(x,t) = V_0 \sin(\Omega t + \phi x)$ where $\phi$ is constant generates a directed traveling wave of external force. The motion of a single Brownian particle in such a traveling-wave potential in the under-damped regime was studied in [17]. We use $\alpha_l = 1$ and $\phi_l = \phi l$ with a constant $\phi$, i.e., $\eta_l = \exp(i\phi l)/2i$ for all $l$. Hence we have $\tilde{\eta}_q = (1/2i) \sqrt{L} \delta_{q,\phi}$, and using this expression in eq. (10)
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Definite phase difference between the oscillatory forcing at neighbouring sites breaks the time-reversal symmetry to yield directed current. The mechanism works even in the limit of very low densities where particles rarely interact. However, with increasing density we found a non-monotonic variation of the DC current, entirely due to the exclusion interaction between particles. Most interestingly, the system showed a current reversal around half-filling: at density $> 1/2$, the driven DC current flows in a direction opposite to that in the non-interacting limit. This behaviour is associated with the particle-hole symmetry —the dynamics of holes at high densities is equivalent to the dynamics of particles at low densities.

Our predictions may be tested experimentally by using oscillatory force on colloids moving in confined geometries. There have been several experimental observations in colloidal systems of single-file diffusion which is one of the signatures of diffusing interacting particles moving in one dimension [12, 20–22]. Recently, ref. [23] experimentally verified theoretical predictions of particle velocity and diffusivity in a tilted periodic potential [24]. It is possible to apply localized AC drive on confined colloids by, e.g., exploiting AC electro-kinetic effects, or localized oscillatory pressure. Alternatively in the setup of ref. [22] one could impose oscillatory trapping potential by using laser traps of tunable power. Yet another experimental realization could be possible using the setup in ref. [14] where macroscopic dissipative particles moving in confined channels are subjected to random mechanical shaking.

A setup similar to that used in ref. [19] to generate directed Brownian motion appears to be best suited to test our predictions. In ref. [19], charged silica beads were trapped by means of scanning optical tweezer to form a channel between two lines of particles. A test particle placed inside the channel underwent oscillatory driving generated by periodic movement of the position of particles belonging to the channel walls. Reference [19] used an increasing frequency of driving from one end of the channel to the other. In order to test our predictions, the driving frequency needs to be kept constant and the phase at which the driving is applied has to be increased linearly from one end of the channel to the other.

Consider the motion of colloidal particles of diameter $a \approx 2 \mu m$ moving in water inside a narrow tube of diameter $\lesssim 2a$. At room temperature $k_B T = 4.2 \times 10^{-21}$ Nm using water viscosity $\nu \approx 10^{-3}$ Ns/m² one finds the Stokes-Einstein self-diffusion constant $D_0 = k_B T/3\pi \nu a \approx 0.2 \mu m^2/s$. This gives hopping rate $f_0 = D_0/a^2 \approx 0.05 s^{-1}$. Then for the case of extended driving corresponding to the result in eq. (12), the maximum current is obtained at a density of $\rho = (1 - 1/\sqrt{3})/2 \approx 0.2$ and a driving frequency of $\Omega = 2f_0 \approx 0.1 Hz$. Since the value of the maximal current $J_L \approx \lambda^2 f_0/40$, this means that we can get particle flow velocities $\sim J_{L,a} \sim 0.0025 \mu m/s$. This compares with the drift velocity that would be attained by a colloidal particle of the same radius and carrying a charge of 10 electrons, when placed in an electric field $\sim 30 V/m$.  

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The work of DC is part of the research program of the “Stichting voor Fundamenteel Onderzoek der Materie (FOM)”, which is financially supported by the “Nederlandse organisatie voor Wetenschappelijk Onderzoek (NWO)”. DC thanks the Raman Research Institute for hospitality during a short visit which initiated this work, and N. Becker for a critical reading of the manuscript.

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