Stochastic Analysis of Particle -Pair Transport in Brownian Ratchet Device

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ABSTRACT

The motion of particle pairs in a Brownian ratchet device is studied using Langevin simulations. A Lennard-Jones interaction between the particles is added to a standard spring-bead model. The effects of such interaction upon a recent model for Brownian motors [3] is investigated, with emphasis on the steady-state current.

Keywords: electrophoresis, Brownian ratchet, Langevin equation, DNA

1 INTRODUCTION

Eletrophoresis is a technique used to separate polyelectrolyte strands with different lengths [1]. One of its fields of application in nanotechnology is use in separation of DNA [2]. Clusters of particles can undergo net transport on a potential energy that is externally driven to fluctuate between several states in Brownian ratchet device.

In [3], a model for coupled Brownian motors, inspired by the motion of individual two-headed molecular motors on cytoskeletal filaments was proposed. The motors were modelled as two elastically coupled Brownian particles, each moving in a flashing ratchet potential. With a view to modelling ratchet-separation devices for DNA, we examine in this paper the effect of a Lennard-Jones interaction [4] between the particle pair, in addition to the existing spring force.

Using Langevin simulations we obtain currents as a function of noise strength, the equilibrium separation of the particles and the rate of switching between potentials.

The outline is as follows. In Sec. 2 we introduce the Brownian ratchet mechanism. The model together with type of potential is discussed in Sec. 3. The numerical results are presented in Sec. 4.

2 BROWNIAN RATCHET

Noise induced transport has been recently become a widely studied area [5]–[7]. Much effort has been made to understand the dynamics of Brownian ratchets in the presence of stochastic forcing. The fluctuations and a broken symmetry are sufficient prerequisites for molecular transport to occur.

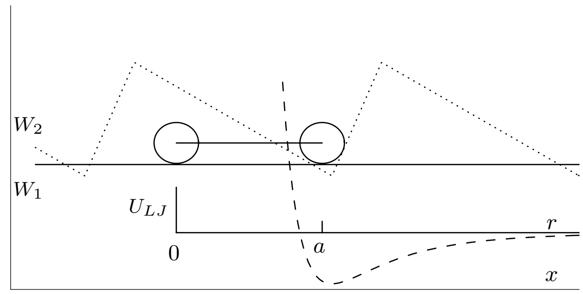

Figure 1: A simple Brownian ratchet device. Particles, with center at coordinate x, are subject to one of the two-state flashing ratchet potential, constant potential, W_1 and an asymmetric saw-tooth potential, W_2, which switches periodically with period τ. The interaction between particles, that are at the distance r apart, is modelled by the Lennard-Jones potential U_{LJ} , which has a minimum at equilibrium distance a.

Hammond et al [8] described the development and use of an integrated electrode array (IDEA) device for transportation of DNA based on a Brownian ratchet mechanism. The ratchet like potential is generated by applying a voltage difference to a series of pattern electrodes. The traps vanish and the particles undergo Brownian motion after the electrodes are discharged. When applying an ac electric field, because of the difference in the electrophoretic mobilities it is possible to observe a directional motion with shorter clusters moving faster then longer ones. This allows a separation of polymers with different lengths.

Material models of DNA frequently use elastic coupling between neighboring particles [9]. In order to investigate the effects of more realistic interaction between particles, we begin by adding a Lennard-Jones interaction to the ratchet model for Brownian motors described in [3].

3 MODEL

We consider two overdamped Brownian particles coupled through a spring of spring constant k and equilibrium length a. Graphical representation of the model is given in Figure 1. The excluded volume interaction between two particles, that are at the distance r apart,

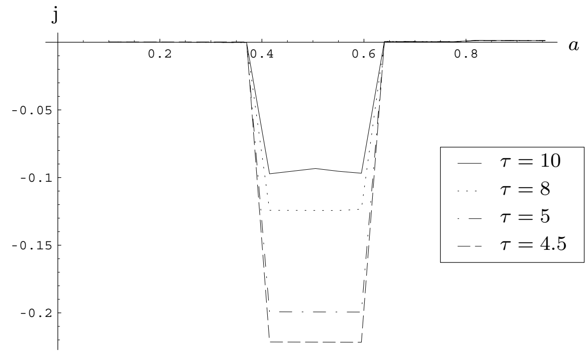

Figure 2: Deterministic case: the current j vs an equilibrium distance a for $\epsilon = 0.1$ and $k = 0.8$.

is modelled by the Lennard-Jones potential:

$$U_{LJ}(r) = 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right), \tag{1}$$

The potential of Eq. (1) is stiff for small distance r, and for strength of interaction $\epsilon = 0$ model would correspond to the standard spring-bead model [3]. We choose the value of parameter σ such that the minimum of Lennard-Jones potential is at the equilibrium distance, e.g. $\sigma = a \cdot 2^{-1/6}$.

Following [3], particles are subject to one of the two-state flashing ratchet potential which switches periodically with period τ. $W_j(x)(j = 1, 2)$ defines the potential in state j at point x. W_1 is a flat potential and we choose the following asymmetric potential W_2:

$$W_2 = U\left(\frac{1}{2}\sin\left(\frac{2\pi x}{L}\right) + \frac{1}{8}\sin\left(\frac{4\pi x}{L}\right)\right), \tag{2}$$

where U and L represent depth and period of potential, respectively. We set $L = 1$ and $U = 1$. The span of this potential is about 1.1 and its ratio of downhill region to the uphill region is around 1/4.

The equations of motion of the particles are

$$\begin{aligned} \gamma\dot{x_1} &= -z_1(t)\frac{\partial W_2(x_1)}{\partial x_1} + k((x_2 - x_1) - a) \\ &+ \frac{\partial U_{LJ}(x_2 - x_1)}{\partial x_1} + \sqrt{D}\xi_1, \end{aligned} \tag{3}$$

$$\begin{aligned} \gamma\dot{x_2} &= -z_2(t)\frac{\partial W_2(x_2)}{\partial x_2} - k((x_2 - x_1) - a) \\ &- \frac{\partial U_{LJ}(x_2 - x_1)}{\partial x_2} + \sqrt{D}\xi_2, \end{aligned} \tag{4}$$

where x_i denote position of particle i^{th}. $\xi_i(t)$ denotes white noise with zero mean and correlation given by $\langle\xi_i(t)\xi_j(s)\rangle = \delta(t - s)\delta_{ij}$. D represents the intensity of fluctuations. We set the physical scales of the problem by putting the friction constant γ to unity.

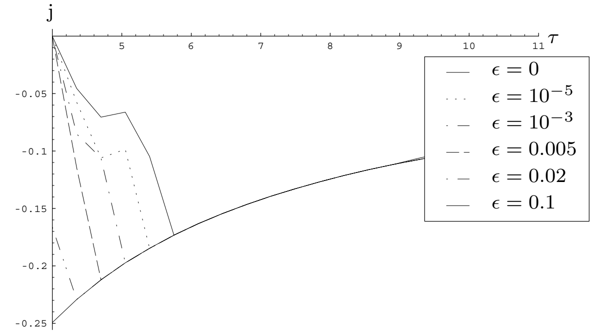

Figure 3: Deterministic case: the current j vs the potential switching period τ for $a = 0.5$ and $k = 0.8$.

The z_i are periodic functions with period τ, given by $z_1(t) = 1$, $z_2(t) = 0$ for $0 \le \tau < \tau/2$ and $z_1(t) = 0$, $z_2(t) = 1$ for $\tau/2 \le t < \tau$.

The quantity of our interest is the current, which we define by:

$$j = \frac{\langle x(T) - x(t_0)\rangle}{T - t_0}, \tag{5}$$

where $\langle\rangle$ denotes the ensemble average.

We obtain currents as a function of noise strength D, the equilibrium separation of the particles a, strength of Lennard-Jones potential ϵ and the period of switching between potentials τ.

4 RESULTS AND DISCUSSION

4.1 Deterministic case

Particles in an asymmetric potential can drift on average in one direction even when operated at zero noise level, e.g. when $D = 0$. The phase space of the system can be either periodic or diffusive, depending on the value of the control parameter.

For $\epsilon > 0$, direct current is possible if the equilibrium separation of the particles is larger that the smaller arm of the potential $W_2(x)$, L_{min}, and smaller then the longer arm of the potential $W_2(x)$, L_{max}. Lengths L_{min} and L_{max} given by:

$$L_{max} = \frac{2L}{\pi}\arcsin\left[\frac{1}{2}\sqrt{1 + \sqrt{3}}\right], \tag{6}$$

$$L_{min} = L - L_{max}. \tag{7}$$

For period of potential equal to one particles move away from the initial coordinates if the equilibrium separation satisfies: $0.38 < a < 0.62$. This is investigated in Figure 2, which shows the dependance of current on the equilibrium distance and period switching. Zero value of current corresponds to closed orbits in the phase space of the system.

In Figure 3 we plot current j as function of τ for $a = 0.5$

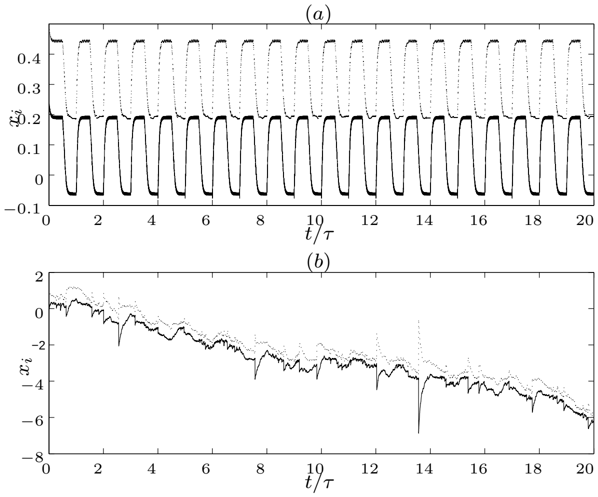

Figure 4: Position of particles for (a) deterministic case $D = 0$ and (b) stochastic case $D = 0.01$, for $a = 0.25$, $\epsilon = 0.1$, $\tau = 5$, $k = 0.8$. The current arises as a result of the presence of noise in the system.

and $k = 0.8$, for different values of ϵ. As the switching period increases, current for different values of ϵ does not differ significantly. For the case where $\epsilon = 0$, the values of the equilibrium distance for which a direct current occurs depends on switching period τ [10]. The length of the window for nonzero current is smaller for smaller values of τ, although the dependance is not monotonic, see, for example the $\epsilon = 10^{-5}$ curve in Figure 3.

4.2 Stochastic case

We have already discussed in Section 4.1 that for zero-noise case, the transport of particles occurs only when the equilibrium distance a satisfies the condition $L_{min} < a < L_{max}$. The addition of thermal fluctuations to the system permits net motion (non-zero current) even for values of a outside the deterministic limits. Figure 4 shows the position of particles for (a) deterministic case $D = 0$ and (b) stochastic case $D = 0.01$, for $a = 0.25$, $\epsilon = 0.1$, $\tau = 5$, $k = 0.8$. The phase space of the particle pair is a closed orbit for the deterministic case, whilst for the stochastic case the particles are moving in the negative direction.

Since the model under consideration has seven parameters, we have analyzed the dependance of current only on two parameters. In our calculations we fixed $\tau = 5$ and $a = 0.5$. For convenience, we have plotted absolute values of current.

Figure 5 shows the absolute value of current j as a function of spring constant k and intensity of interaction ϵ, for $D = 0.01$. Note $\epsilon = 0$ corresponds to the case studied in [3]. For any fixed value of ϵ, introducing stronger coupling between the particles causes current to increase

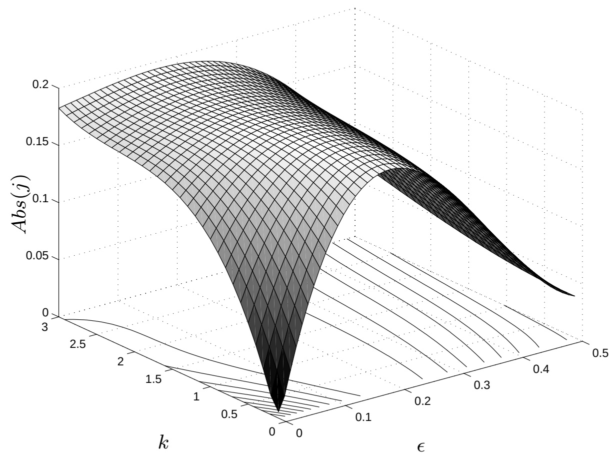

Figure 5: Stochastic case: the absolute value of current j vs spring constant k and intensity of interaction ϵ, for $D = 0.01$, $\tau = 5$ and $a = 0.5$.

initially, and for $k \simeq 2.5$ the currents saturates. On other hand, for any fixed value of k, the current has a maximum in the range of ϵ from 0.1 to 0.3. The location of the peak in $k - \epsilon$ space is governed by the strength of the Lennard-Jones potential.

Figure 6 shows the absolute value of current j vs spring constant k and intensity of noise D, for $\epsilon = 0.1$. The maximum of the current is at $D = 0$. On increasing the noise strength and keeping spring constant k small, random hopping in both directions dominates the ratchet mechanism and the absolute value of the current tends to zero. However, for any fixed value of noise intensity D, the current increases monotonically with increasing k.

Our preliminary results from exploring a subset of parameter space indicate that the addition of Lennard-Jones interaction to a standard spring-bead model can have important effect upon current. A fuller understanding of particle-particle interaction as well as particle-ratchet interaction is required for modelling of DNA transport and separation devices.

5 ACKNOWLEDGMENT

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REFERENCES

[1] G.W. Slater, S. Guillouzic, M.G. Gauthier, "Theory of DNA electrophoresis (1999-2002 1/2)," Electrophoresis, 23, 3791-3816, 2002.

[2] J. S. Bader, R. W. Hammond, S. A. Henck, "DNA Transport by a Micromachined Brownian Ratchet Device," PNAS, 96, 13165-13169, 1999.

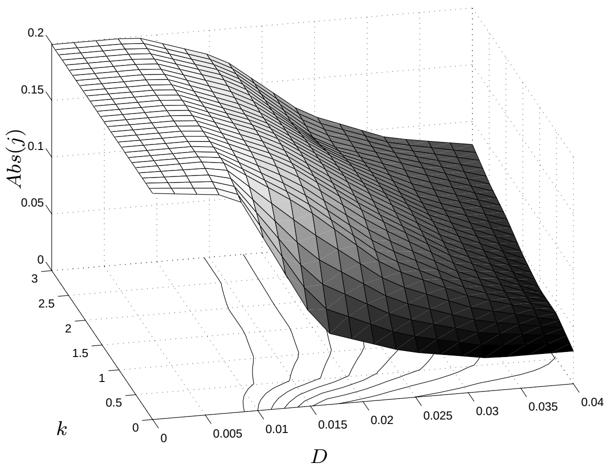

Figure 6: Stochastic case: the absolute value of current j vs spring constant k and intensity of noise D, for $\epsilon = 0.1$, $\tau = 5$ and $a = 0.5$.

[3] D. Dan, A.M. Jayannavar and G.I. Menon, "A biologically inspired ratchet model of two coupled Brownian motors," Physica A, 318, 40-47, 2003.

[4] D. Ceperlay and M.H. Kalos, "Computer simulations of dynamics of a single polymer chain," Phys Rev Lett, 45, 313-316,1978.

[5] B. Yan, R.M. Miura, Y. Chen, "Direction Reversal of Fluctuation-induced Biased Brownian Moion on Distorted Ratchets," J. theor. Biol., 210, 141-150, 2001.

[6] H. Linke, T.E. Humphrey, P.E. Lindelof, "Quantum Ratchets and Quantum Heat Pumps," Appl.Phys. A, 75, 237-246, 2002.

[7] P. Reimann, P. Hänggi, "Introduction to the Physics of Brownian Motors," Appl. Phys. A, 1-10, 2002.

[8] R.W. Hammond, J.S. Bader, S.A. Henck, M.W. Deem, G.A. McDermott, J.M. Bustillo, J. M. Rothberg, "Differential transport of DNA by a rectified Brownian motion device," Electrophoresis, 21, 74-80, 2000.

[9] Z. Csahok, F. Family, T. Viscek, "Transport of Elastically Coupled Particles in an Asynnetric Period Potential," Physical Review E, 55, 5179-5183, 1997.

[10] A. Igarashi, S Tsukumoto, H. Goko, "Transport properties of elastically coupled Brownian motors," Physical Review E, 64, 0519081-0519085, 2001.