Interaction of Coupled Particles Based on Lennard-Jones and Spring Forces in Brownian Ratchet Devices

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ABSTRACT

The influence of the type of interacting force on the transport of two particles in one-dimensional flashing ratchet is considered. Lennard-Jones type interaction is compared to the classical case of elastically coupled particles. Parameter values where the Lennard-Jones force is not well approximated by a linearization of the force about the equilibrium distance are identified.

Keywords: Brownian motor; Coupled ratchet; Elastic coupling; Lennard-Jones potential; DNA separation

1 INTRODUCTION

The motion of Brownian particles in ratchet-like potentials [1] has attracted great interest due to its wide applications in connection with transport processes in many fields including nanotechnologies [2]. Experiments have demonstrated the possibility of particle transport in a ratchet-like potential generated by applying a voltage difference to interdigitated electrodes [3], [4]. The traps periodically 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 directional motion with shorter clusters moving faster then longer ones. This allows the separation of polymers with different lengths.

Directed motion of particles in ratchet devices has been studied recently by many workers. For a single particle, thermal noise and an asymmetric potential produce motion of particle in a direction that depends on the asymmetry of the potential [5]. It is desirable, however to study more complex systems then single particles. Several authors have studied the motion of two coupled particles in "flashing ratchets" [6]–[8], where the switching of the potential is governed by various stochastic or time-periodic processes. A net current in the presence of thermal noise occurs due to the fact that the slopes of the sawtooth potential of the ratchet are different in the forward and backward directions. The potential is switched on and off in time; in the case of alternating periodic dichotomous process for each particle [6], directional motion can be induced even in the absence of thermal fluctuations due to the compressibility of the spring and the independent switching of the potentials. In this regime the current decreases monotonically with increasing intensity of noise. For the case of strong coupling and switching governed by multiplicative nonwhite fluctuations [7], the current shows dependence on the correlation time of fluctuations and on the equilibrium distance between particles. The interaction between the particles clearly influences the directed motion — an effective potential for the center-of-mass of particles has been proposed [8] in order to understand this behaviour.

However, the models of interacting particles considered so far are based on spring-type coupling. In this work, we concentrate on the connection between the directed transport and the type of interaction force between the pair of particles. As an alternative to the spring model, we introduce a Lennard-Jones interaction between particles. The initial motivation to study this model emerges from the possibility of applying ratchet mechanisms in the sorting of DNA fragments by size using electric fields. The Lennard-Jones potential works reasonably well for electrically neutral, polarizable, spherical molecules. Although complex molecules such as polymer chains require complicated potentials to describe the interaction between monomers, we believe that the present study is the first step towards a more realistic model.

2 MODELS

Elastically coupled particles have been discussed extensively in the literature, but most models consider particles subject to additional forcing as well as to the ratchet potential [9]. We are interested here in the case where the driving mechanism is due to a flashing potential and particle interactions, with the presence of thermal noise.

The equations of motion of two interacting, overdamped particles are:

$$\gamma \dot{x_1} = -z(t)\frac{\partial W(x_1)}{\partial x_1} - \frac{\partial U}{\partial x_1} + \sqrt{2D}\xi_1, \qquad (1)$$

$$\gamma \dot{x_2} = -z(t)\frac{\partial W(x_2)}{\partial x_2} - \frac{\partial U}{\partial x_2} + \sqrt{2D}\xi_2, \qquad (2)$$

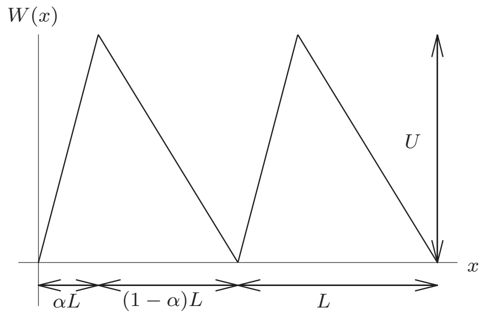

Figure 1: Sawtooth shaped periodic potential $W(x)$, with period L, height of potential U and parameter of asymmetry α.

where γ is the friction coefficient, $x_1(t)$ and $x_2(t)$ are the positions of the particles, $W(x)$ is the ratchet potential, D is the diffusion coefficient, and $\xi_i(t)$ denotes white noise with zero mean and correlation given by $\langle \xi_i(t)\xi_j(s)\rangle = \delta(t-s)\delta_{ij}$. The time dependence of the ratchet, $z(t)$, is a periodic dichotomous process taking the values 0 and 1:

$$z(t) = \begin{cases} 0, & 0 \le t < \tau/2, \\ 1, & \tau/2 \le t < \tau. \end{cases} \tag{3}$$

We consider a piecewise linear but asymmetric ratchet potential $W(x)$ with period L, shown in Figure 1:

$$W(x) = \begin{cases} \frac{U}{\alpha}x, & 0 \le x < \alpha L, \\ \frac{U}{(L-\alpha)}(L-x), & \alpha L < x \le L, \end{cases} \tag{4}$$

where U is the height of the potential and α is an asymmetry parameter. If $\alpha < \frac{1}{2}$ the transport is in the positive direction, and in the negative direction otherwise. We nondimensionalize appropriately and use the following parameter values throughout the paper: $\gamma = 1$, $\alpha = 0.1$, $L = 1$ and $U = 1$.

The potential function for elastic spring interaction takes the form:

$$U_{SP}(x_1, x_2) = \frac{k(x_2 - x_1 - a)^2}{2}. \tag{5}$$

where k and a are the spring constant and equilibrium distance, respectively. The Langevin equations (1)-(5), are solved by employing the second order Runge-Kutta method [10] for stochastic differential equations (SDE) with a time step of $\Delta t = 10^{-3}$. All quantities of interest are averaged over 200 different realizations, each single trajectory consisting of 10^6 integration steps. The main quantity of interest here is the current j, which is the average velocity of the mid-point of the two particles, defined by

$$j = \lim_{T\to\infty} \frac{\langle x_{MP}(T) - x_{MP}(0)\rangle}{T},$$

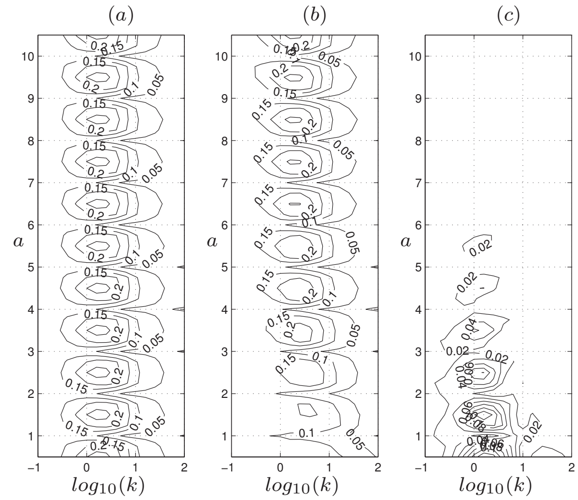

Figure 2: Contours of the average current as a function of the equilibrium distance and spring constant for $D = 0.01$: (a) Spring model, (b) Lennard-Jones model, and (c) absolute difference of the average current between two models.

where x_{MP} is the coordinate of the mid-point of the pair of particles.

An important feature of the spring-coupled model is that, for certain parameter values, transport of particles can occur even when no random fluctuations are present. The condition on the parameters [11]

$$nL + 2\alpha L < a < nL + L - 2\alpha L, \tag{6}$$

(where n is an integer) means that this noiseless current can appear for a wide variety of values of equilibrium length a. This mode of motion arises when the spring is stretched and compressed during 'on' and 'off' phases of the ratchet. If the equilibrium length of the spring is larger then the short section of the sawtooth potential, one particle can be pushed or pulled to a neighboring minimum of the potential, see [11] for details.

In order to investigate the effects of more realistic interaction between particles, we compare the classical spring model to a Lennard-Jones (LJ) interaction. The Lennard–Jones force between two molecules is given by the potential function [14]:

$$U_{LJ}(r) = 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right), \tag{7}$$

where ϵ is the strength of interaction and the distance between particles is $r = |x_2 - x_1|$. We choose the value of parameter σ such that the minimum of Lennard-Jones potential is at the spring equilibrium distance, e.g. $\sigma = a \cdot 2^{-1/6}$. The Lennard-Jones potential is mildly attractive as the two particles approach one another from a distance, but strongly repulsive when they

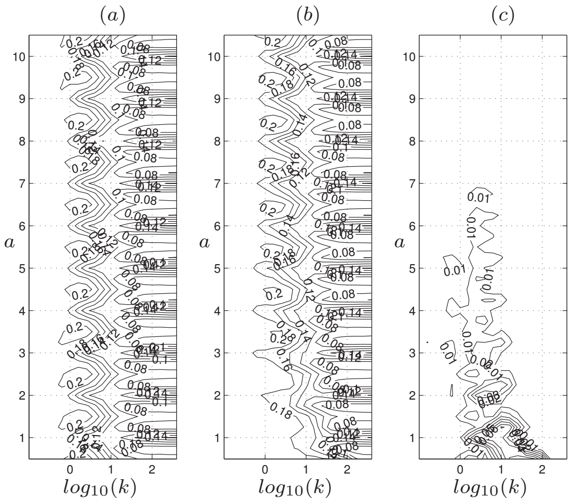

Figure 3: Contours of the average current as a function of the equilibrium distance and spring constant for $D = 0.05$: (a) Spring model, (b) Lennard-Jones model, and (c) absolute difference of the average current between two models.

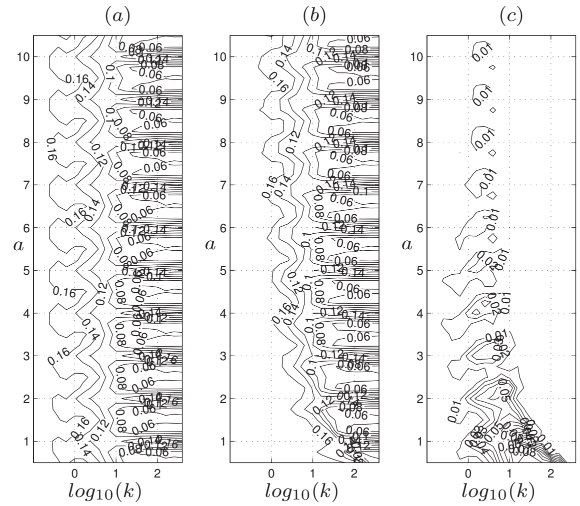

Figure 4: Contours of the average current as a function of the equilibrium distance and spring constant for $D = 0.1$: (a) Spring model, (b) Lennard-Jones model, and (c) absolute difference of the average current between two models.

approach too close. At equilibrium, the pair of particles reach a separation corresponding to the minimum of the Lennard–Jones potential.

A somewhat similar situation was studied in [12], [13], where the particles were assumed to be hard rods and the interaction between two particles was approximated with a hard core repulsion. The average velocity dependence on the particle size was shown to be a discontinuous function in the limit where the average distance between the two particles goes to zero. In this paper we focus on investigating whether the usual elastic coupling assumption can accurately model more complicated potentials such as LJ.

3 RESULTS AND DISCUSSION

We are interested in comparing the effect of Lennard-Jones interaction with the classical spring model. If we assume that the distance between the particles $|x_2 - x_1|$ is close to the equilibrium length of the spring or LJ force, we can Taylor-expand the potential (7) around a and find the effective value of the spring constant, $k = k_{eff}$, in terms of the LJ parameters:

$$k_{eff} = \frac{72\epsilon}{a^2}. \tag{8}$$

Figures 2, 3 and 4 show the contours of the average current as a function of the equilibrium distance a, and (effective) spring constant k, with noise intensity $D = 0.01$ (Figure 2), $D = 0.05$ (Figure 3) and $D = 0.1$ (Figure 4). It can be seen that the difference between the two models is observable for small a values and k values in the range from 10^{-1} to 10^1. Note that for a fixed value of k, the spring model shows a periodic response as a function of a, but the Lennard-Jones model lacks periodicity for small values of a.

In the limit of weak coupling $k \to 0$, both models approach the case of two single particles and so give similar results. Further, numerical simulations for coupled particles agreed well with results on current for a single particle [15]. We calculated the following values of net current for coupling $k = 0.01$: $j = 0.12$ for $D = 0.01$, $j = 0.21$ for $D = 0.05$ and $j = 0.18$ for $D = 0.1$.

In the case of strong coupling, i.e. $k \to \infty$, the particles are rigidly coupled to each other. Our numerical simulations indicate that the actual threshold for k to observe this type of behaviour depends on the value of noise strength D: asymptotic behaviour requires larger values of k as the intensity of noise increases. For larger noise intensities, introducing stronger coupling between the particles causes the current to decrease until the spring and LJ the currents both reach the $k \to \infty$ limit.

Details of the results for moderate coupling are rather complex and show strong dependency on the value of D as well as periodicity in a [15]. This can be explained by the fact that harmonically coupled particles are able to move directionally in the absence of thermal noise (see equation (6) above), while transport in the LJ model requires nonzero noise intensity for small values of a.

Our simulations show that for small noise $D = 0.01$, the current has a maximum in the range of k from 10^{-1} to 10^1. For any fixed value of a, two regimes of current can be identified. If parameters satisfy formula (6), the maximum current $j = 0.24$ is observed near $k = 1$.

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In the second regime, maximum current $j = 0.14$ is at $k = 0.1$ and minimum current $j = 0.04$ is at $k = 10$.

Some understanding of the differences between the two coupling models may be obtained using the approach of Wang and Bao [8], who examined elastically coupled pairs of particles. They show that when the noise intensity D is sufficiently low and the coupling k is sufficiently strong, the distance between the particles $y = x_1 - x_2$ has a Gaussian distribution of mean a and standard deviation $\sqrt{D/k}$. This prediction is verified by our numerical simulations (not shown), though we note it applies only to the case where noiseless transport is absent, i.e. when (6) is not satisfied. Since the linearization of the LJ potential about $y = a$ gives the effective spring coupling (8), we expect that if $y(t)$ remains confined near a then LJ and spring effects will coincide. Thus we have a simple condition: if $\sqrt{D/k} \ll a$, then the LJ coupling current is indistinguishable from the equivalent spring coupling case. We note that the case of noiseless transport obeying (6) requires further refinement of this rule-of-thumb.

4 CONCLUSIONS

In the present work, we have explored the influence of the type of interacting force on the transport of two coupled particles moving in a one-dimensional ratchet. Our main objective has been to identify the parameter regimes where LJ interaction produces qualitatively different results compared to elastic coupling.

We have discussed how current depends on the strength of thermal noise D, equilibrium distance a, and strength of interaction k. Regimes where both LJ and spring models show similar behaviour have been identified: (a) for weak coupling $k \to 0$, (b) strong coupling $k \to \infty$ and (c) large equilibrium distance a. Details of the results for moderate coupling are rather complex and show strong dependency on the value of D.

Our results from exploring a subset of parameter space indicate that the Lennard-Jones interaction can have important effects upon the current which are not captured by linearizing the force to a spring model. Further refinement of the model, for example increasing the number of interacting particles, is necessary to describe polymer chains more realistically.

5 ACKNOWLEDGMENT

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