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

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ABSTRACT

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

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

1 INTRODUCTION

Brownian particles motion in ratchet like potential [1] gained great interest due to its wide applications in connection with transport processes in many fields including nanotechnologies [2]. Physical experiments 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 to separate polymers with different length.

Directed motion of particles in ratchet devices has been studied recently by many worker. For single particle, only thermal noise and an asymmetric potential are enough to produce motion of particle toward a particular direction that depends on the asymmetry of the potential [5]. It is significant to study more complex systems then single particle. Several authors studied the motion of two coupled particles in "flashing ratchet" [6]–[8], where switching of potential governed by different stochastic processes. The net current occurs due to the fact that the slopes of sawtooth potential are different along the forward and backward direction as well as presence of thermal noise. The potential is switched on and off in time. In the case of periodic dichotomous process independently taking two values 0 and 1 [6], directional motion can be induced even in the absence of thermal fluctuations due to the compressibility of the spring and independent switching of potential. In this regime, the current decreases monotonically with increasing intensity of noise. For the case of strong coupling and switching govern by multiplicative nonwhite fluctuations [7], current showed dependance on correlation time of fluctuations and on equilibrium distance between particles. In the case of two particles subject to periodic ratchet, it has been found [8] that interaction between the particles influence the directed motion. The effective potential for the center-of-mass of particles has been proposed in order to understand this behaviour.

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

2 MODELS

The elastically coupled particle have been discussed in the literature, but most models considered particles subject to ratchet as well as additional forcing [9]. We are interested in the case where driving mechanism is initiated when particles interacted with each other and flashing potential in the presence of thermal noise.

The equations of motion of interacting two particles reads:

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

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

where γ is a constant friction coefficient, $x_1(t)$ and $x_2(t)$ are positions of first and second particles, $W(x)$ the potential energy it experience, D is diffusion coefficient, and $\xi_i(t)$ denotes white noise with zero mean and correlation given by $\langle \xi_i(t)\xi_j(s)\rangle = \delta(t-s)\delta_{ij}$. z(t) is a

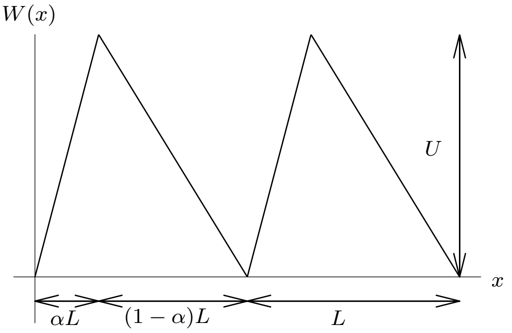

Figure 1: Sawtooth shaped periodic potential $W(x)$, with period L, height of potential U and parameter of asymmetry α.

periodic dichotomious process taking two values 0 and 1:

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

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

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

where U is the height of potential and α is parameter of asymmetry. If $\alpha < \frac{1}{2}$ the transport is in positive direction, and in the negative direction otherwise. We will use the following values of parameters if not stated otherwise: $\gamma = 1$, $\alpha = 0.1$, $L = 1$ and $U = 1$.

Elastic interaction takes form:

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

where k and a are spring constant and equilibrium distance, respectively.

The Langevin equations (1)-(5), as well as any other equation within this paper is solved by employing second order Runge-Kutta method [10] for Stochastic Differential Equations (SDE) with a small time step of $\Delta t = 10^{-3}$. All quantities of interest were averaged over 200 different realisations. Each single trajectory consist of 10^6 integration steps.

The quantity of interest here is the net current of mid point between particles, defined by

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

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

Important feature of coupled via spring model is the ability to have transport of particles when no random fluctuations are present for certain values of parameters, satisfying the following condition [11]:

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

where n is an integer.

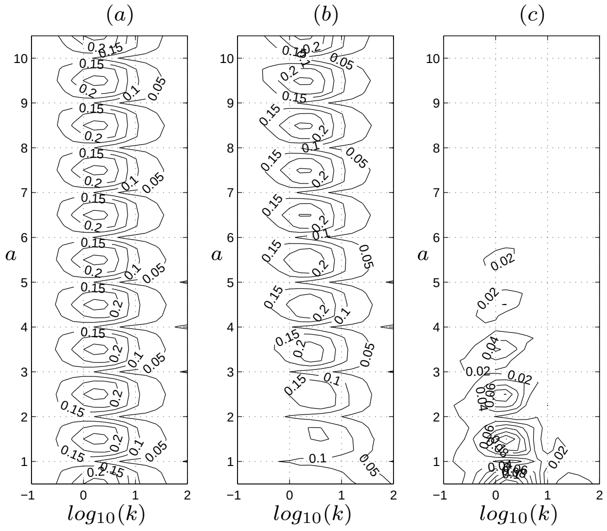

Figure 2: Contours of the average current as a function of the equilibrium distance and spring constant for $D = 0.01$: (a) Spring model, (b) Lennard-Jones model, and (c) absolute difference of the average current between two models.

A way to get directed motion is that particles are stretched and compressed during 'on' and 'off' phases of ratchet. If the equilibrium distance of the particles is large then short section of the sawtooth potential, one particle can be pushed or pulled to neighbour minimum of potential.

In order to investigate the effects of more realistic interaction between particles, instead of classical spring model we use a Lennard-Jones (LJ) interaction. The Lennard-Jones potential is mildly attractive as two particles approach one another from a distance, but strongly repulsive when they approach too close. At equilibrium, the pair of particles tend to go toward a separation corresponding to the minimum of the Lennard–Jones potential.

Similar situation was studied in [12], [13], where the particles were assumed to be hard rods and the interaction between two particles has been approximated with a hard core repulsion. The average velocity dependence on size of the particles has been showed to be discountinious function in the limit where the average distance between two particles goes to zero.

The Lennard–Jones force between two molecules is given the equation [14]:

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

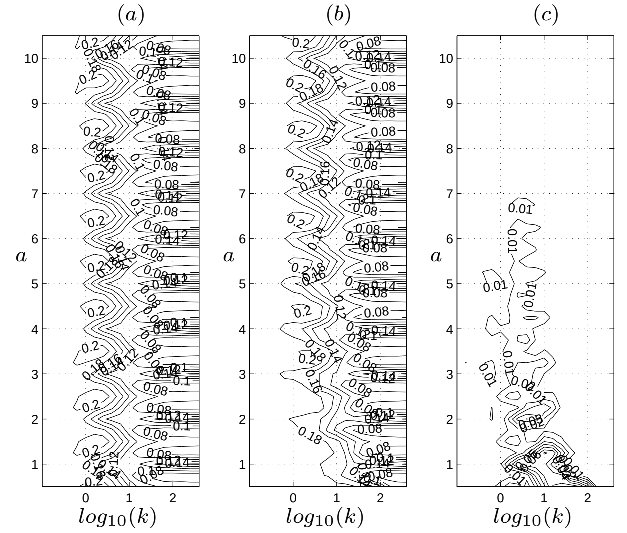

Figure 3: Contours of the average current as a function of the equilibrium distance and spring constant for $D = 0.05$: (a) Spring model, (b) Lennard-Jones model, and (c) absolute difference of the average current between two models.

where ϵ is strength of interaction and distance between particles is $r = |x_2 - x_1|$. The potential of Eq. (7) is stiff for small distance r. We choose the value of parameter σ such that the minimum of Lennard-Jones potential is at the equilibrium distance, e.g. $\sigma = a \cdot 2^{-1/6}$. Parameter σ describes basically where the potential equals zero. Parameter ϵ describes the strength of the interaction or the depth of the potential well. It can be shown that the depth of the well is just $-\frac{\epsilon}{4}$.

3 RESULTS AND DISCUSSION

We are interested in comparison of our proposed model of Lennard -Jones force with classical spring model. If we assume that particles oscillate around the equilibrium distance, a, with a very small amplitude, we can expand the potential around a and find the effective value of spring constant in terms of 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 spring constant, k, with strength of noise taking values $D = 0.01$ (Figure 2), $D = 0.05$ (Figure 3) and $D = 0.1$ (Figure 4). It can be seen that the difference between two models is observed for small a values and k values in the range from 10^{-1} to 10^{1}: for a fixed value of k, spring model show periodic response as a function of a, but Lennard-Jones model is lacking 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 that explains 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 $D = 0.1$.

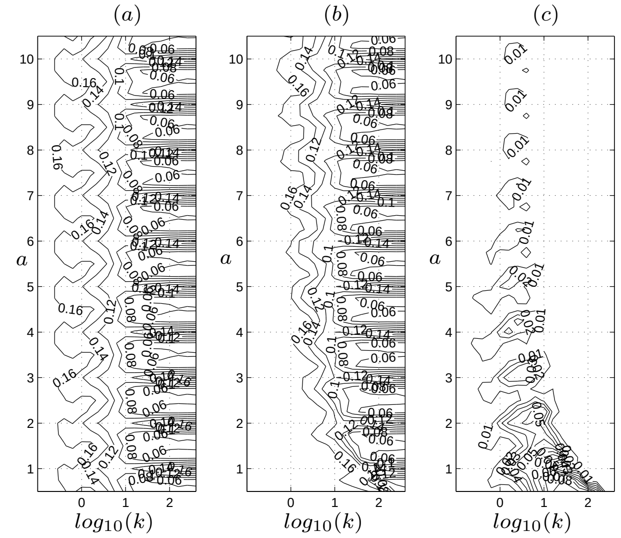

Figure 4: Contours of the average current as a function of the equilibrium distance and spring constant for $D = 0.1$: (a) Spring model, (b) Lennard-Jones model, and (c) absolute difference of the average current between two models.

In the case of strong coupling, i.e. $k \to \infty$, we have that particles are rigidly coupled to each other. Our numerical simulations indicate that 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.

Details of the results for moderate coupling are rather complex and show strong dependency on value of D. This difference can be explained by the fact that harmonically coupled particles are able to move directionally in the absence of thermal noise, while transport in LJ models requires nonzero noise intensity.

Our simulations showed 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 $k = 1$. In the second regime, maximum current $j = 0.14$ is at $k = 0.1$ and minimum current $j = 0.04$ is at $k = 10$.

For larger noise intensities, introducing stronger coupling between the particles causes current to decrease until the currents saturates.

4 CONCLUSIONS

In the present work, we have explored the influence of type of interacting force on the transport of two particles moving in one-dimensional ratchet. Our main objective has been to identify if LJ interaction can produce any qualitatively different results compared to elastic coupling.

We have discussed how current depends on strength of thermal noise, D, equilibrium distance, a, and strength of interaction, k, in LJ model compared to harmonically coupled particles. We have identified few regimes where both models showed similar behaviour: (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 value of D.

Our results from exploring a subset of parameter space indicate that the Lennard-Jones interaction can have important effect upon current compared to a standard spring-bead model. Further refinement of the model would be necessary to describe polymer chains more realistically. For example to have more that two interacting particles.

5 ACKNOWLEDGMENT

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