# Two-dimensional model of elastically coupled molecular motors*

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A flashing ratchet model of a two-headed molecular motor in a two-dimensional potential is proposed to simulate the hand-over-hand motion of kinesins. Extensive Langevin simulations of the model are performed. We discuss the dependences of motion and efficiency on the model parameters, including the external force and the temperature. A good qualitative agreement with the expected behavior is observed.

**Keywords:** Brownian motors, ratchet, current, efficiency

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## 1. Introduction

The dynamics of molecular motors is an important topic in the features of life appearing on levels ranging from flocks of animals to single cell motility and intracellular transport. The majority of biological molecular motors, also known as motor proteins, include a considerable number of different molecules: myosins, kinesins, RNA polymerases, topoisomerases, etc. Most studies of molecular motors have focused on the case of directed transport or rotary motion, which constitutes the key ingredients of any complex structure. Most of the theoretical studies suggest that molecular motors move along spatially asymmetric potentials under the influence of thermal and/or other external forces.[1−7]

In this paper, we focus on the problem of directed motion over a two-dimensional bar, which is used to simulate the microtubule. The kinesin is a two-head protein linked by a neck and a tail, which is attached to a cargo or a vesicle to be carried. Its processive walks consist of about 100 steps within a few seconds. Each motor step consists of an 8-nm displacement along the microtubule via the hand-over-hand movement of its two identical motor heads.[8−10] During each step, the motor hydrolyzes one adenosine triphosphate (ATP) molecule into one adenosine diphosphate (ADP) molecule and inorganic phosphate, transforming chemical fuel ATP into mechanical work.[11]

The rest of the present paper is organized as follows. First we propose a two-dimensional model, which can mimic the motion of the motor. Within reasonable values of parameters, we explore different regimes of motion. In the conclusion section, we discuss the validity of the results to model a molecular motor.

## 2. Model

In this work, we consider a kinesin as a molecular motor moving along a two-dimensional track via hand-over-hand motion. The model also takes into account the properties of the microtubule substrate. An external force $\boldsymbol{F}$ against the motion is exerted on the leading motor.

For simplicity, we consider the simplest case of single-motor dynamics within a two-state isothermal ratchet. We define the Langevin equations for the motor positions as

$$\gamma \frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}x} = -\nabla V(\boldsymbol{r}) + \boldsymbol{F}(\boldsymbol{r}, t) + \boldsymbol{\xi}(t),$$

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where $\boldsymbol{F}(\boldsymbol{r},t)$ denotes the external force, and $\boldsymbol{\xi}$ is the thermal noise,

$$\left\langle \xi_{j(t)}\xi_{k(t')}\right\rangle = 2\gamma k_{\mathrm{B}}T\delta(t-t')\delta_{jk},$$

with $\xi_j$ and $\xi_k$ being the Cartesian components of vector $\boldsymbol{\xi}$, $\gamma = 4\times10^{-11}$ the damping coefficient, $k_{\mathrm{B}}$ the Boltzmann constant, and $\delta$ the delta function.

We consider the kinesin as two interacting particles moving in a flashing ratchet substrate potential. The potential energy of the system is given by

$$V(\boldsymbol{r}_1,\boldsymbol{r}_2) = V_1(\boldsymbol{r}_1,t) + V_2(\boldsymbol{r}_2,t) + V_{12}(\boldsymbol{r}_1-\boldsymbol{r}_2),$$

where $V_{12}$ is the elastic interacting potential between the motors,

$$V_{12} = \frac{1}{2}k(|\boldsymbol{r}_1-\boldsymbol{r}_2|-a)^2,$$

with $k$ and $a$ being constants and assumed to be 1.5 and 0.5, respectively. The two components of $V_1(\boldsymbol{r})$ take the following forms in the Cartesian coordinates (see Fig. 1):

$$V_{1x}(x) = -\frac{1}{\pi}\left[\sin(\pi x) + 0.25\sin(2\pi x)\right],$$
$$V_{1y}(y) = \frac{1}{2}y^2.$$

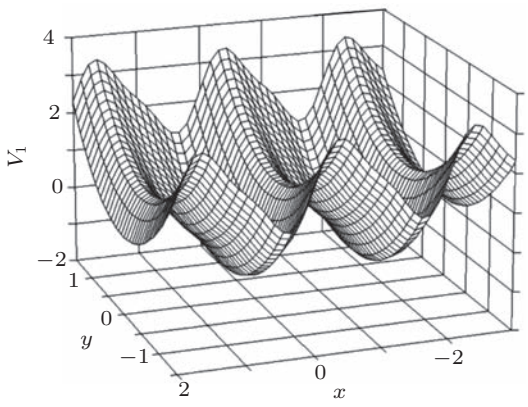



**Fig. 1.** Asymmetric potential the two heads subjected to in our model.

According to the hand-over-hand model, we assume four states: at $t=0$, head one and head two are both subject to the ratchet potential; at $t=t_1$, head one is not subject to the ratchet potential; at $t=t_2$, head one and head two are both subject to the ratchet potential; at $t=t_3$, head two is not subject to the ratchet potential. At $t=t_4$, the states repeat from $t=0$. For simplicity, we denote $t_{\mathrm{f}} = t_2-t_1 = t_4-t_3$ and $t_{\mathrm{d}} = t_1 = t_3-t_2$.

In order to compute the efficiency of the motion, we use a definition from Ref. [12], i.e.,

$$\eta = \langle v\rangle\, A_0/\langle P\rangle_{\mathrm{in}},$$

where $\langle v\rangle A_0$ is the average mechanical work done per unit of time against a working load $A_0$, and $\langle P\rangle_{\mathrm{in}}$ is the average net power pumped into the system by the external drives, no matter how they are applied.

# 3. Results and discussion

## 3.1. Motion without external load

In this section, we discuss in detail the directed transport in the asymmetric periodic potential. A particle initially placed at the bottom of the potential well is mostly confined to that well or performs random motions around the minimum potential energy position. However, during the quarter cycle, when one of the substrate potentials is switched off, the corresponding particle is still subjected to the noise and diffuses freely with Einstein's constant. By switching the potential on again, the substrate cuts the probability density into smaller peaks of different sizes, one for each well surrounding initial one. Due to the asymmetry of the potential, the minimum more frequently corresponds to the one on the right-hand side of the original one, the asymmetric potential applied to the motors is expected to induce a net positive current, as shown in Fig. 2. A closer look at the $x$ positions of the two particles enables us to believe that this movement is hand-over-hand. While one head is attached to the microtubule, the other head switches between free and loosely bounded states until it lands in a strongly bounded state.

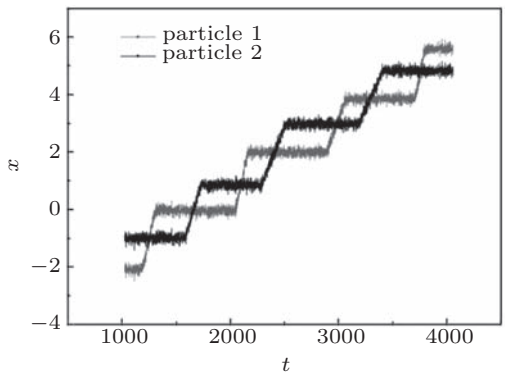



**Fig. 2.** The $x$ positions for the two particles versus time $t$, showing flashing dynamics of the substrate potentials.

As said above, when the ratchet potential is switched on and off periodically, the particle initially

set at $x = 0$ diffuses symmetrically, which is driven only by the noise and finally retrapped in the neighboring well at the beginning of the next cycle. From Fig. 3, we can see that as the left peak of $p_0$ decreases with time, the right peak at $x = 2$ increases, which also indicates that the net current is positive.

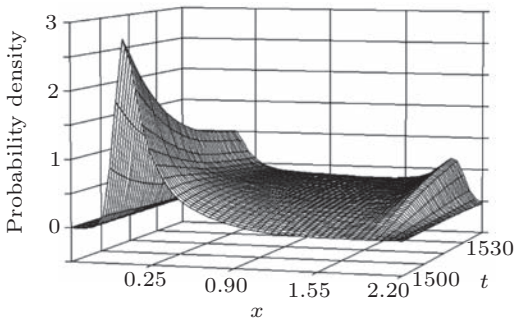



**Fig. 3.** Time evolution of probability distribution projected on the $x$ axis.

In Fig. 4, we show the probability density of the particles in the $x$–$y$ phase space. The peak has widths both in the $x$ and the $y$ directions. It is clearly observed that as $y$ increases, the probability of finding such a particle decreases. This overall feature indicates that the Brownian motor moves along the $x$ direction but may not move along a straight line.

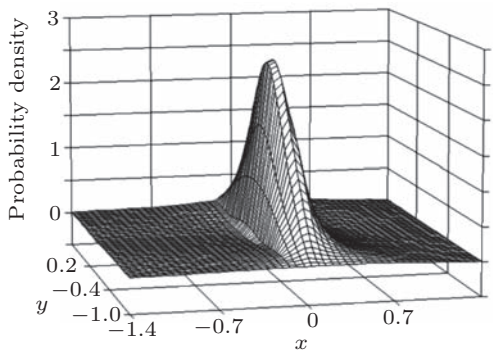



**Fig. 4.** Probability density in the $x$–$y$ plane.

In Fig. 5, we present the velocity of the system varying with temperature and time. When $t_\mathrm{d} = t_\mathrm{f} = 0$, which means that the system is subject to a constant substrate potential, the velocity is zero, and this is the conventional Brownian motion with zero mean velocity. As $t_\mathrm{d}$ increases, the velocity generally tends to increase for given $T$ values, as shown in Fig. 5, which indicates that the velocity depends sensitively on $t_\mathrm{d}$ representing the potential change. For a given $t_\mathrm{d}$, the velocity remains almost unchanged for temperatures higher than 180 K. Another important feature found in Fig. 5 is that the velocity is positive within the parameter range.

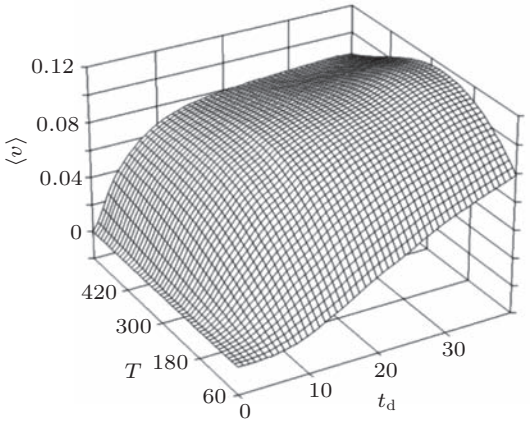



**Fig. 5.** Velocity as a function of temperature $T$ and $t_\mathrm{d}$ ($t_\mathrm{d} = t_\mathrm{f}$).

## 3.2. Under external load

In this section, we will further explore the velocity when the external load is present. As reported in Ref. [13], backward stepping was observed when high backward loads were used in their experiments. This current reversion is highly interesting, so it is worth studying how the system behaves under the effect of an external force.

Then we need to determine how the total load is divided into the two heads of the protein. Here we use a method used in Ref. [14]. If only one head is attached to the microtubule, it will bear the whole load; if both heads are attached to the microtubule, each bears half of the load.

Figure 6 shows the velocity as a function of temperature $T$ and the external load. A distinct feature is the observed current reversion shown in Fig. 6(b). We can see that the velocity decreases nonlinearly with the increase of the load, and the critical load varies with temperature, which is similar to the case in Ref. [11].

We also study the efficiency of the system. The results are shown in Fig. 7, where the efficiency versus the temperature and the external load is plotted. When the temperature and the load are either too high or too low, $\eta$ is low, so there exist optimal values for the temperature and the external load to achieve the highest efficiency.

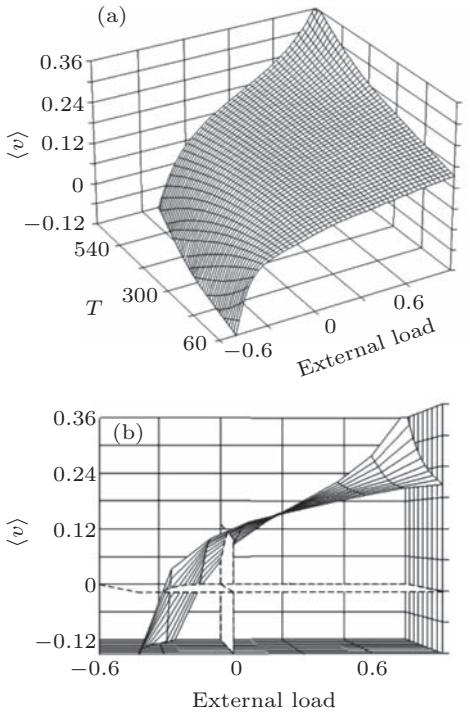



**Fig. 6.** Velocity as a function of temperature $T$ and external load. Panels (a) and (b) are drawn from different angles. Dashed lines are drawn to guide the eye.

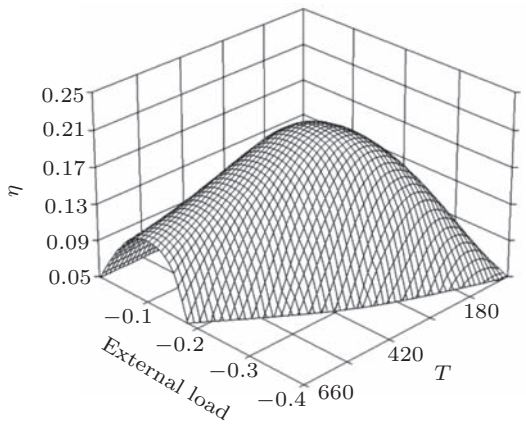



**Fig. 7.** Efficiency versus temperature and external load.

# 4. Conclusion

We present a simple mechanical model for the hand-over-hand motion in two dimensions. In our model, the directed motion is obtained along the $x$ direction, although the probability finding the particle along the $y$ direction is nonzero. When the external load is present, the current reversion is observed. The critical load varies with temperature, that is, a high temperature requires a low load, and vice versa. The efficiency varies with both the temperature and the load, and there is a maximum value for a certain temperature and a certain load, which accords with experimental observations.

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