

# The Finitely Numerable Effect in the Coupled Molecular Motor Model

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## 1 Introduction

Molecular motors perform many kinds of activities in living organisms such as cellular transport processes, muscular contraction, and so on. The components of motors are protein molecules that can exchange chemical energy of adenosine triphosphate (ATP) for mechanical work. We now know that there are some different kinds of motors in the cell. One of them slides along filaments which guide the movement of motors as a track. Myosins move along actin filaments, and dyneins and kinesins move along microtubules. Recently, many kinds of researches have been given in the molecular level experiments. For example, one-molecule experiments showed that a single myosin motor moves along an actin filament stochastically, and the regular steps of it are filament-periods. But in many case, motor molecules cooperate in groups and form a multimotor. In those backgrounds, another experiments showed that a Ncd mutant NK11, which lacked directionality as an individual motor, could generate bi-directional motion of filaments in motility assay experiments [2].

At the same time, many people have studied the molecular motor models. Magnasco proposed the basic thermal ratchet model [5]. This model assumes that a particle moves on the piecewise linear potential called ‘ratchet’, and a particle of the model moves stochastically like a real motor. But it has the problem that the energetic efficiency is low. Then F. Jülicher and J. Prost proposed the coupled molecular motor model [3]. This model assumes that particles are rigidly coupled each other, and the number of motors in it are infinite. In this condition the energetic efficiency of the model is high (around 50%). And it predicts that the motion of motors can be bi-directional. Now, we want to understand the reason why the efficiency of the coupled motor model becomes high. In order to achieve this purpose, we use the finitely numerable molecular motor model proposed by M. Baoual, et al [1], which can analyze the system that has several motors. They showed the force-velocity relationships for the finitely numerable molecular motor model, and it represents bi-directional motion. In this paper, we want to discuss the energetic efficiency of such models.

## 2 Methods

Motor proteins are coupled with each other, and form a filament. This filament moves directionally to either the plus or minus end of microtubules or actin filaments. The analysis of this filament’s movement has been given in motility assay experiments[2]. Molecular motor models of the filament also has been studied [1], and basically we used this model. We consider a simple one dimensional situation similar to motility assay. We assume  $N$  motors are attached to a rigid rod. Length of this is  $L_{\text{rod}} = (N - 1)q$ , and  $q$  is fixed space of the motor period. The relative displacement between rod and substrate is denoted by  $x$ . Each of the motors is represented by a two-state model [3, 4]. We assume that the motor can exist in two different conformations or chemical states  $\sigma = 1$  and 2. The interaction

between motors and filament depends on  $\sigma$  and is described by potentials  $W_\sigma(X)$  at position  $X$ . The potentials are periodic,  $W_\sigma(X) = W_\sigma(X + L)$ , because cytoskeletal filaments are periodic. When we think about the relationships between motor and potential, the displacement of the  $n$ -th motor is  $x_n = x + q(n-1)$ . The distance  $q$  between adjacent motors is taken incommensurate relative to the period  $L$ , i.e.,  $q/L$  is an irrational number. We can write the total force exerted by all motors on the filament as

$$F_W(x, \sigma_1, \sigma_2, \dots, \sigma_N) = - \sum_{n=1}^N \partial_x W_{\sigma_n}(x + q(n-1)). \quad (1)$$

We represent the filament velocity,  $v(t) = dx(t)/dt$ , as

$$\frac{dx}{dt}(t) = \frac{1}{\lambda}(f_W + f_{\text{ext}} + \xi(t)), \quad (2)$$

where  $\lambda$  is a friction coefficient,  $f_W = F_W/N$  and  $f_{\text{ext}} = F_{\text{ext}}/N$  are normalized forces exerted by the motors and the externally applied force.  $\xi(t)$  represents the effect of thermal noise applied per motor. It implements zero average  $\langle \xi(t) \rangle = 0$  and  $\langle \xi(t)\xi(t') \rangle = 2kT\lambda/N\delta(t-t')$ .

We now consider a chemical reaction mechanism for the two state model. The scheme of chemical reactions about kinesin and myosin molecules has been previously discussed [4]. We modeled the following chemical scheme: (i)  $\text{ATP} + \text{M}_1 \rightleftharpoons \text{M}_2 + \text{ADP} + \text{P}$ , (ii)  $\text{M}_1 \rightleftharpoons \text{M}_2$ , where  $\text{M}_i$  denote the motor state. When a chemical reaction occurs, the transitions between state 1 and 2 take place. Then we define chemical reaction rates, (i)  $\alpha_1(\rightarrow)$  and  $\alpha_2(\leftarrow)$ , (ii)  $\beta_1(\rightarrow)$  and  $\beta_2(\leftarrow)$ . With these chemical reaction mechanism, we can get ATP consumption rate for the Langevin equations. We define the number of transitions  $n_1$  and  $n_2$ .  $n_i$  means the number of them caused by  $\alpha_i$ . With these expression, the ATP consumption rate we can give is  $r(t) = (n_1 - n_2)/(tN)$ . Finally, we can get the energetic efficiency of the finite-number model,  $\eta(t) = -f_{\text{ext}}v(t)/(r(t)\Delta\mu)$ .

### 3 Results and Discussion

In 1995, F. Jülicher and J. Prost proposed the coupled molecular motor model that has high (around 50%) energetic efficiency [3]. This model assumes an infinite number of motors are rigidly coupled with each other. Does the system require an infinite number of motors to achieve such a high efficiency? To answer this question we analyze the models which have a finite number of motors, and obtain the results of force-velocity ( $f-v$ ) and force-efficiency ( $f-\eta$ ) relationships for them. The relationships of  $f-v$  are almost linear with  $N = 1$ , but they become nonlinear with  $N \geq 2$ . At last, they become discontinuous and contain bi-directional motions at certain values of  $f$  with  $N \geq 50$ . On the other hand, the efficiency is the lowest with  $N = 1$  and gradually increases as the number of motors become high until  $N \sim 20$  (the value of it is almost the same with the mean-field limit), but it decreases with  $N \geq 20$ . These results conflict with the mean-field limit for large  $N$ . Consequently, we can see the system does not require an infinite number of motors to attain the high energetic efficiency.

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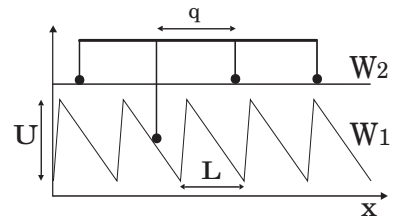


Figure 1: Schematic representation of  $N$  rigidly coupled motors.