Transport properties and efficiency of elastically coupled Brownian motors

Akito Igarashi,[1] Shinji Tsukamoto,[2] and Hiromichi Goko[1]
[1]*Department of Applied Mathematics and Physics, Kyoto University, Kyoto 606-8501, Japan*
[2]*Sumitomo Electric Industries, Osaka 541-0041, Japan*

(Received 17 January 2001; revised manuscript received 17 July 2001; published 24 October 2001)

As models for biological molecular motors, Brownian motors have been studied recently by many workers, and their physical properties such as velocity, efficiency, and so on, have been investigated. They have also attracted much interest in an application to nanoscale technology. It is significant to study more complex systems, that is, coupled Brownian motors, in detail, since Brownian motors with a single particle have been mainly studied until now. In this paper, we consider Brownian motors coupled mutually with elastic springs, and investigate the dynamics of the model and the efficiency of energy conversion. In particular, we find that the center of the mass of the elastically coupled particles moves faster than the corresponding single-particle model, and also that the efficiency of the coupled-particle model is larger than that of the single-particle model.

DOI: 10.1103/PhysRevE.64.051908 PACS number(s): 87.10.+e, 05.40.−a, 02.50.−r

I. INTRODUCTION

Brownian motors have attracted much attention as models of molecular motors [1] and their physical properties such as velocity, efficiency, and so on have been studied in detail [2]. Recently, some workers have also paid attention to them in an application to nanoscale technology [3]. For example, Porto *et al.* [3] studied microscopic engines on the atomic scale that transform the fed energy into directed motion through a dynamical competition between the intrinsic length of the moving object and supporting carrier.

The molecular motors are involved in cell locomotion, some cellular transport and muscle contraction, and so forth. Many models have been proposed to comprehend theoretically the mechanism of the molecular motors. Doering *et al.* [4] investigated ''single-particle'' Brownian motor models, a ''rocking'' ratchet model where a periodic or random external force is applied to the system. A famous one among the single-particle models is a so-called ''flashing'' ratchet model [5]. It is shown that in the model, only thermal noise and a proper asymmetric potential are enough to produce macroscopic motion of the particle toward a particular direction that depends on the asymmetry of the potential. Next, ''coupled-particle'' models, where particles interact mutually, have been investigated. Csahók *et al.* [6] studied the dynamics of elastically coupled particles in a ''rocking'' ratchet model. On the other hand, Jülicher *et al.* [2] introduced and analyzed theoretically particles rigidly attached to a rigid backbone with equal spacing in a ''flashing'' ratchet. Recently, Elston and Peskin [7] investigated the characteristic of the elasticity between the motor and its cargo and showed that the elasticity allowed the motor to run faster than if they were linked rigidly. Klumpp *et al.* [8] studied the two harmonically coupled particles in the ratchet model and observed a driving mechanism different from the one in the case of a single particle, which does not need diffusion. As for the response to an external force, Reimann *et al.* [9] introduced another model of interacting Brownian particles and found some collective phenomena.

Studying the physical properties of coupled Brownian motors is interesting in itself. Moreover, it is quite significant to investigate the coupled systems, since in an application to nanoscale technology, coupled effects should be taken into account [3]. In an application to molecular motors, it is also interesting to study coupling effects, because, for example, molecular motors in muscle have a linear structure [1] that consists of many parts.

In this paper, we consider elastically coupled particles in a flashing ratchet model, in which each particle makes transition repeatedly between two states where interactions are expressed by their respective kinds of potential, and conduct numerical simulation. Unidirectional motion of the particles is confirmed in this model and the velocity for various values of the coupling constant, the temperature, and so on, is measured. Although an isolated single particle in flashing ratchet models cannot move in nonthermal conditions, that is, without thermal noise, elastically coupled particles in the flashing ratchet model may move due to the action of the interparticle springs restored to their natural length that is incommensurable with the period of the periodic potential, even if thermal diffusion is not allowed. It is also found that the velocity of the elastically coupled model under such conditions is larger than that of the corresponding single-particle model, and that the velocity has a maximum as a function of the coupling constant of the springs. Moreover, if we restrict the region where transition may be allowed, we find that the velocity of the model is enhanced by the restriction. We also apply various loads externally to our system to investigate the efficiency of energy conversion, and find that the efficiency has a peak as a function of the load. We also find that the peak values are larger when we restrict the region of transitions and are improved by the coupling effect in comparison with the single-particle model.

II. THE MODEL

We consider elastically coupled particles (Fig. 1). In this paper, our model is described by dimensionless quantity. It is assumed that the particles are put in a heat bath represented by white noise. Particles are subjected to one of the two substrate potential stochastically. $W_j(x)$ $(j=1,2)$ defines the potential in state j at point x. W_1 is a flat potential and we

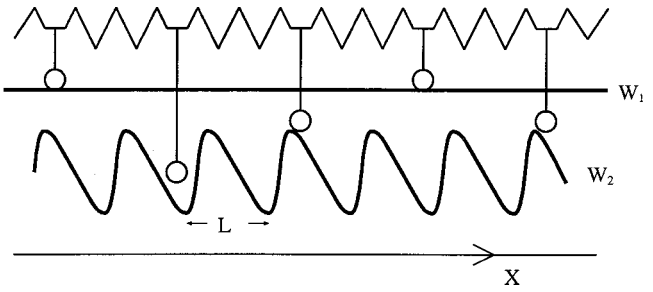

FIG. 1. In our simulation, the period of the potential is not equal to the natural length of the springs. This ''incommensuration'' leads to the easy movement of the particles to a particular direction (to the right direction in this figure). Some particles are subjected to W_1 and the others to W_2.

choose the following asymmetric interaction potential W_2:

$$W_2=\left[\frac{1}{2}\sin\left(\frac{2\pi x}{L}\right)+\frac{1}{8}\sin\left(\frac{4\pi x}{L}\right)\right]\times U, \tag{2.1}$$

where U and L represent the depth and period of the potential, respectively. In state one, no force from the substrate is exerted on the particles because the substrate potential W_1 is flat. Therefore, state one is called the detached state. Since, in state two, the particles feel periodic substrate potential, state two is called the attached state.

The equations of motion of the particles read

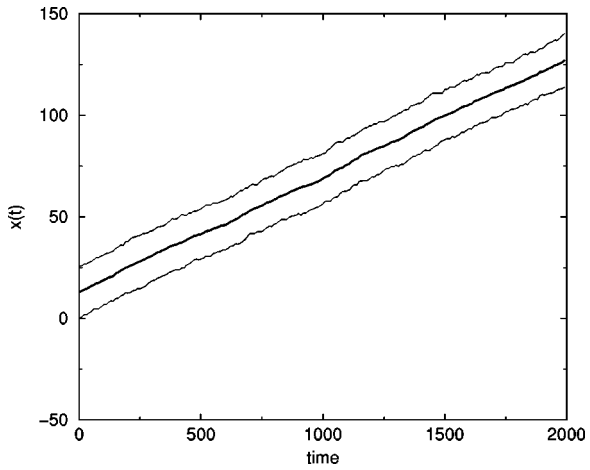

FIG. 2. x_1, x_N, and the center of mass as a function of time. We find that finite temperature is not necessarily needed for the finite velocity of the elastically coupled particles in an asymmetric potential. This figure shows finite velocity for zero temperature ($k=4.0, N=20$).

$$\gamma\dot{x_i}=k(x_{i+1}-2x_i+x_{i-1})-h_i(t)\frac{\partial W_j(x_i)}{\partial x_i}+\sqrt{2D}\xi_i(t),$$
$$2\leqslant i\leqslant N-1, \tag{2.2}$$

where x_i denotes the position of the ith particle and we consider the overdumped case. $\xi_i(t)$ denotes white noise of zero

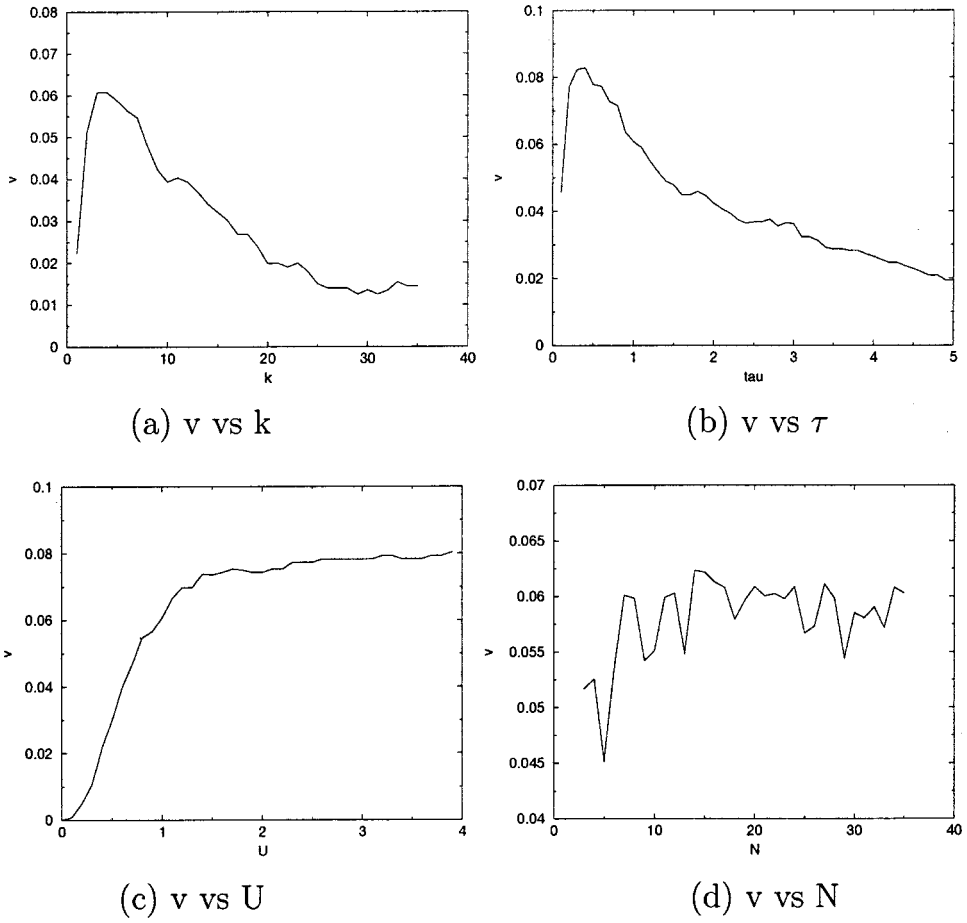

FIG. 3. Velocity as functions of various parameters. The velocity shows various dependence on the parameters. From these figures, we can understand the characteristics of the model more profoundly.

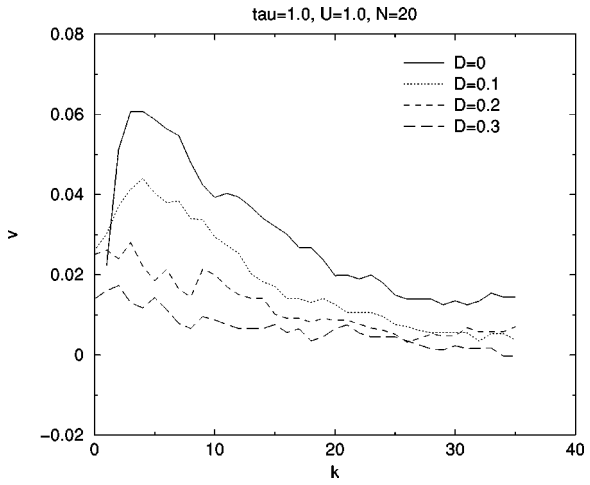

FIG. 4. V vs k. The lower the temperature is, the faster the particles move in general. For high temperature, the peak almost disappears since the particles tend to move more randomly.

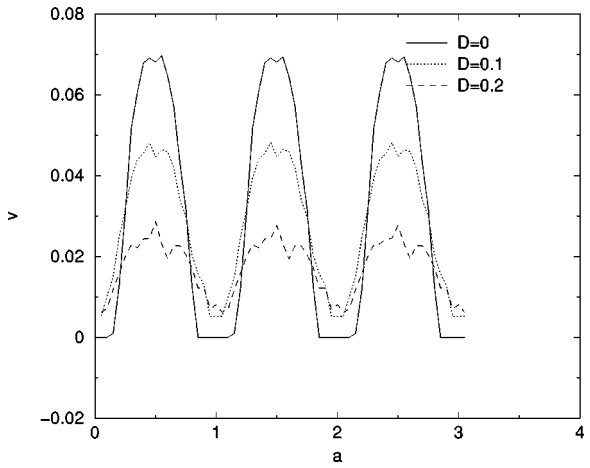

FIG. 5. V vs a. When the natural length of the spring is almost equal to an integer times the period of the potential, the model moves so slowly because each particle is caught to a minimum of the potential and cannot escape from it easily.

mean and correlation $\langle \xi_i(t)\xi_j(s)\rangle = \delta(t-s)\delta_{ij}$. k is the spring constant and N the number of particles. Since the boundary condition of the particles is free, the forces due to springs of Eq. (2.2), the first term of the right-hand side, is

$$k(x_2 - x_1 - a) \tag{2.3}$$

for the first particle and

$$k(x_{N-1} - x_N + a) \tag{2.4}$$

for the Nth particle, where a stands for the natural length of the springs. A friction constant γ is set to be 1.0 and D stands for the temperature. In our simulation, U, L, and a are set to be 1.0, 1.0, and 1.35, respectively, if not mentioned.

$h_i(t)$ is a dichotomous random modulation that rules the time-dependent change expected 0 or 1. We determine $h_i(t)$ process as follows. An Ornstein-Uhlenbeck process Z_i ($i = 1,2,\ldots,N$), where

$$\langle Z_i(t)Z_j(s)\rangle = \delta_{ij}(D'/\tau)e^{-|t-s|/\tau},$$

$$\langle Z_i(t)\rangle = 0, \quad D' = 0.4 \tag{2.5}$$

is considered and if $Z_i(t)$ is less than 0, then $h_i(t)$ is set to be 0, if $Z_i(t)$ is more than 0, then $h_i(t)$ is set to be 1. Consequently, $h_i(t)$ changes with a correlation time τ stochastically. In our simulation, τ is set to be 1.0 if not mentioned. Thereby we can change only three parameters, that is, k, D, and N. If not mentioned, k, D, and N are set to be 4.0, 0.2, and 20, respectively. At the beginning of our simulations, the ith particle is always located at $x = ia$.

III. NUMERICAL SIMULATION

A. Zero-temperature case

1. Dynamics of elastically coupled particles

First of all, we investigate a zero-temperature case ($D = 0$). Figure 2 shows the motion of two boundary (first and Nth) particles (thin lines), and the center of mass of the coupled particles (thick line). A particle trapped to the potential W_2 is likely to be near a minimum of it and going to move by the elasticity when trapped to W_1. When it is attached to the substrate again under the influence of W_2, it goes down to a minimum of the potential W_2 to the $+x$ direction more frequently than to the $-x$ direction because of the asymmetry of the potential W_2. Consequently, the particles move unidirectionally in an average sense.

2. Parameter dependence of the velocity

Figure 3 shows the velocity of the center of mass of the N particles as functions of various parameters. As a function of k, the velocity has a maximum at $k \simeq 4.0$ [Fig. 3(a)]. When we change τ, the velocity has also a maximum [Fig. 3(b)], and the graph is bell shaped. The correlation time τ has to be appropriate if it is nearly equal to the time for particles

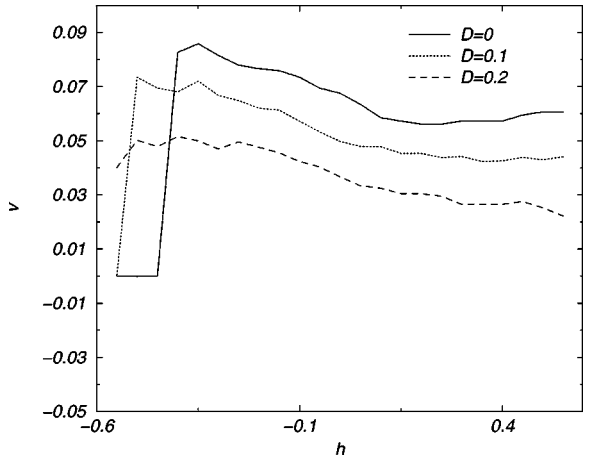

FIG. 6. V vs h. The model moves faster when the transition is restricted. Each line indicates the velocity of the center of mass at different temperature. We can see that the value of the peak and the position of the peak depend on D (k=4.0,N=20).

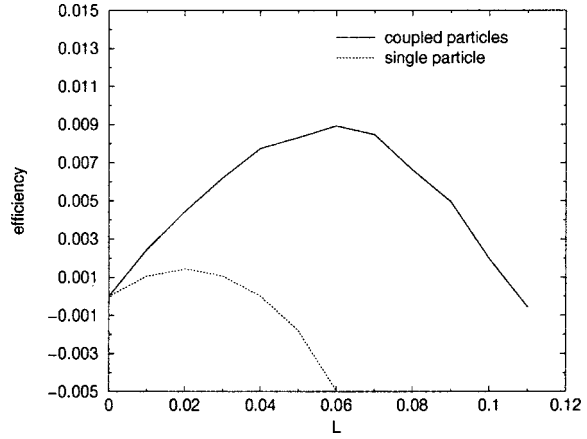

FIG. 7. Load vs efficiency at $D=0.1$ and $k=4.0$. The efficiency has a maximum at $F_{ext}\simeq 0.06$ for the coupled system, and it is less than 0 for $F_{ext}\geqslant 0.11$, which means that the model moves in $-x$ direction. Efficiency for a single particle is lower than for the coupled model.

enough to go beyond maximums of W_2 in the detached state and for the springs to go back to the natural length in the attached state in order to pull the particles forward before they are detached again. The larger the depth of the potential W_2, U, becomes, the faster the particles go down toward the minimum of W_2. Since the correlation time τ is finite, the velocity of the particles increases as the depth increases until the velocity saturates for large U such that particles probably arrive at minimums of the potential W_2 within the correlation time [Fig. 3(c)]. Finally, we investigate the velocity as a function of N [Fig. 3(d)]. The velocity is almost independent of the number of particles except for small N. The dependence of velocity on the size in biological experiments of muscle system is similar to our results.

B. Finite-temperature case

Figure 4 shows the velocity versus k at $D=0,0.1,0.2,0.3$. The velocity decreases as the temperature increases. At $D=0.3$, the velocity is almost independent on the spring constant k. The influence of the springs is weak in comparison with that of thermal diffusion for high-temperature $D=0.3$.

TABLE I. Lv and γv^2 is shown for various loads. The energy used to the dissipation is much larger than that used to the total motion of the model.

Load	$L\times v$	$\gamma\times v^2$
0.000000	0.000000	1.386913
0.010000	0.002441	1.383389
0.020000	0.004427	1.392557
0.030000	0.006206	1.388566
0.040000	0.007744	1.393150
0.050000	0.008313	1.397241
0.060000	0.008928	1.397302
0.070000	0.008471	1.398886
0.080000	0.006630	1.404158
0.090000	0.004963	1.412609
0.100000	0.001967	1.420848
0.110000	−0.000569	1.417309

Until now, the natural length of the springs a has been set to be 1.35. Now we investigate the relation between the velocity and the natural length in Fig. 5. The velocity disappears when a/L is an integer for $D=0$. That is because particles are trapped at minimums of W_2 tightly and cannot escape without thermal noise. At $D=0.1$ and 0.2, however, the average velocity is finite even when a/L is an integer, where particles in the detached state diffuse thermally enough to go over the maximum of W_2 against the force of springs.

C. Restricted transition

Until now, transitions between detached and attached states has been allowed to occur everywhere in the potential. Now we restrict the region where transition toward the detached state can be allowed. This restriction is defined by parameter h. That is, when a particle is located at x and if $W_2(x)<h$, transition may be allowed and if $W_2(x)\geqslant h$ it cannot be allowed. In our simulation, transitions from the detached state to the attached state may occur without any restriction of the positions of the particles. Figure 6 shows the velocity as a function of h. For a certain region of h, the velocity is larger than that of the unrestricted transition case, which is the right end of Fig. 6. One reason for this, we think, is that the possibility of the particles going over the maximum W_2 is larger when transition is restricted near minimums of the potential.

IV. EFFICIENCY

A. Calculation of efficiency

Recently, Sekimoto [10] has defined the efficiency for thermal ratchet models with a load F_{ext}. Derényi *et al.* [11] has also defined the efficiency in another way.

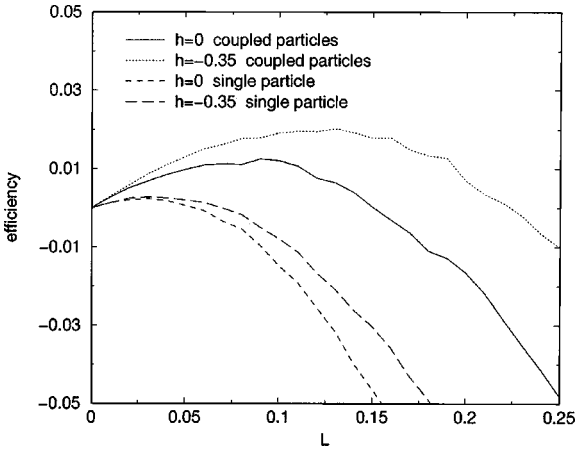

FIG. 8. Load vs efficiency at $D=0.1$, $k=4.0$, and $h=0,-0.35$ where h is the parameter to restrict the transition region. The maximum is located at larger F_{ext} than in the unrestricted case of Fig. 7, and the model moves $+x$ direction even for larger F_{ext} than the load where motions to $-x$ direction occurs in the unrestricted transitions. Efficiency for the single-particle model is lower than the coupled-particle model in this case as well as in the case of Fig. 7.

If we define v as an average velocity of the model, the conventional expression of the efficiency η is

$$\eta = \frac{F_{ext} v}{P_{in}}, \tag{4.1}$$

where P_{in} is the power input [10]. If we define P_{out} as the power output, it seems more appropriate to define it as

$$P_{out} = F_{ext} v + \gamma v^2, \tag{4.2}$$

rather than only $F_{ext} v$, the numerator of Eq. (4.2) [11]. The term γv^2 denotes, of course, the dissipation via friction. In our simulation, the load F_{ext} is dispersedly exerted to each particle, that is, $-F_{ext}/N$ is applied to each particle.

We show in Fig. 7 the efficiency defined by Eq. (4.2). It has a maximum as a function of F_{ext} and at a certain threshold it has a value less than 0, which means that the model moves in the $-x$ direction. The efficiency for a single particle is shown also in Fig. 7. The efficiency for the coupled model is higher than for the single-particle model.

In Table I, we compare $F_{ext} v$ with γv^2. We find that γv^2 is always much larger than $F_{ext} v$ for any load, which makes sure that most of the energy of the molecular motor is used for the Brownian motion and therefore for the dissipation. This is a reason why the efficiency of the molecular motor is not so high.

Since muscle is known to have much higher efficiency than in our simulation, we do not succeed in reproducing the real situation if we apply our model to muscle contraction. This is mainly because of the simplicity of our model.

B. Efficiency for the restricted transitions

Figure 8 shows the efficiency defined by Eq. (4.2) versus load F_{ext} when we introduce the restricted transitions that we have mentioned in Sec. IIIC. When transition is restricted, the peaks appear for larger loads than for unrestricted transitions, and the peak values of efficiencies are also larger. We think that in the restricted transitions, it is easy for the particles to go forward since when the particles makes transition from W_2 to W_1, they are comparatively near the neighbor maximum of W_2 in $+x$ direction, which they must go beyond in order to move forward.

V. CONCLUSION

We demonstrate that elastically coupled particles in a flashing ratchet model move co-operatively. An important result is the generation of directed motion in a no-thermal condition. Though an isolated particle in flashing models cannot move in a no-thermal condition, elastically coupled particles in flashing models may move by the effects of springs even if thermal diffusion is not allowed. It is also found that the velocity of the particles has a maximum at a specific coupling constant of springs. The maximum of the velocity as a function of h, the restriction parameter, appears when we restrict the region of transitions as well. Changing other various parameters, we confirm the complicated behaviors of the elastically coupled particles.

On the efficiency of energy conversion, the effects of the coupling between particles are also found to be very important. The elastically coupled particles may pull a heavier load than a single particle, and the efficiency for the coupled model is larger than the single-particle model. Most of the energy, however, is used for Brownian motion, that is, for the dissipation.

[1] L. Stryer, *Biochemistry*, 4th. ed, (Freeman, San Francisco, 1995).

[2] F. Jülicher, A. Ajdari, and J. Prost, Rev. Mod. Phys. **69**, 1269 (1997), and references cited therein.

[3] M. Porto, M. Urbakh, and J. Klafter, Phys. Rev. Lett. **84**, 6058 (2000).

[4] C.R. Doering, W. Horsthemke, and J. Riordan, Phys. Rev. Lett. **72**, 2984 (1994).

[5] J. Prost, J-F. Chauwin, L. Peliti, and A. Ajdari, Phys. Rev. Lett. **72**, 2652 (1994).

[6] Z. Csahók, F. Family, and T. Vicsek, Phys. Rev. E **55**, 5179 (1997).

[7] T.C. Elston and C.S. Peskin, SIAM (Soc. Ind. Appl. Math.) J. Appl. Math. **60**, 842 (2000).

[8] S. Klumpp, A. Mielke, and C. Wald, Phys. Rev. E **63**, 031914 (2001).

[9] P. Reimann, R. Kawai, C. Van Den Broeck, and P. Hänggi, Europhys. Lett. **45**, 545 (1999).

[10] K. Sekimoto, J. Phys. Soc. Jpn. **66**, 1234 (1997).

[11] I. Derényi, M. Bier, and R.D. Astumian, Phys. Rev. Lett. **83**, 903 (1999).