Eur. Phys. J. B **52**, 501–505 (2006)
DOI: 10.1140/epjb/e2006-00321-8

THE EUROPEAN PHYSICAL JOURNAL B

Reciprocating nanoengine

Yu.A. Makhnovskii[1,2,a], V.M. Rozenbaum[1,3], D.-Y. Yang[1], S.H. Lin[1], and T.Y. Tsong[4]

[1] Institute of Atomic and Molecular Sciences, Academia Sinica, P.O. Box 23-166, Taipei 106, Taiwan
[2] Topchiev Institute of Petrochemical Synthesis, Russian Academy of Sciences, Leninsky Prospect 29, 119991 Moscow, Russia
[3] Institute of Surface Chemistry, National Academy of Sciences of Ukraine, Generala Naumova str. 17, Kiev-164, 03164, Ukraine
[4] Institute of Physics, Academy of Sciences, Taipei, National Chiao-Tung University and National Nanodevice Laboratory (NDL), Hsinchu, Taiwan

Received 5 April 2006 / Received in final form 1st July 2006
Published online 7 August 2006 –

Abstract. Brownian motion in a confining potential fluctuating between two spatially separated potential profiles is considered as a model of an engine converting nonequilibrium fluctuations into reciprocating motion on the nanoscale. We present two exact solutions obtained for the parabolic and step potential, which reveal the temperature and frequency-modulation behavior of the engine. The confining potential determines the interplay of the independent internal (thermal) and external (discrete) noises: the noises are cooperated for any potential, except the parabolic one. The engine can operate as a molecular motor, being supplemented by a rectifying mechanism.

PACS. 05.60.-k Transport processes – 05.40.-a Fluctuation phenomena, random processes, noise, and Brownian motion

1 Introduction

In everyday life, combustion motors provide a common solution to the ubiquitous problem of how to convert energy from forms supplied by nature to directed mechanical motion. The heart of a motor is an engine that processes the chemical fuel and generates the reciprocating motion of a piston. A gear ("crank mechanism") is used to transform piston oscillations into a continuous directed motion. Operating principles and conditions of macroscopic combustion motors can be understood and described in terms of thermodynamics and classical mechanics. Much less understood are the mechanisms of energy conversion on the nanoscale, where the underlying physics is completely different: the systems involved are isothermal, friction dominates inertia, and the motion effected by diffusion becomes stochastic. These mechanisms are now under intensive study [1,2] stimulated by applications to nanoscale machinery [3] and molecular biology, especially for modeling molecular motors [4] and ion pumps [5]. A general framework for building molecular combustion motor was formulated in the 1990s [6,7] offering a systematic view on the problem.

We consider a nanoversion of combustion motor by analogy to its macroscopic counterpart: (I) the energy produced by a chemical reaction (or any other external process) induces nonequilibrium fluctuations; (II) a nanoscale engine processes these fluctuations and generates reciprocating mechanical motion on time and length scales long compared to those of the microscopic (thermal) fluctuations; (III) the reciprocating motion is rectified by a symmetry-breaking mechanism (some kind of ratchet) into unidirectional motion. In this Letter we focus on the stage (II). As a model for the nanoscale reciprocating engine, we propose a Brownian particle moving in a confining potential fluctuating between two spatially separated potential profiles. This model is motivated in part by experimental observation of reciprocating motion during the process of optomechanical energy conversion in a single-molecule device [8]. Exact solutions for the reciprocating velocity obtained for the parabolic and step potentials allow us to reveal the physical properties of the engine and to clear up the role of the thermal noise in the mechanism of energy conversion. If and only if the potential profiles are parabolic, the thermal noise plays a neutral role and can be neglected. For any other potential shape, external and internal noises are coupled with the result that the velocity depends on temperature. The fact that the two noises acting together (even though their sources are independent) can generate motion, impossible in the presence of either of them alone, is strikingly illustrated by the case of the step potential, where the temperature dependence of the velocity exhibits a stochastic resonance-like behavior. Finally we show how the engine being supplemented by a phenomenological rectification mechanism based on asymmetrical friction fluctuations can operate as a molecular motor. For this purpose, we discuss a

[a] e-mail: yuam@ips.ac.ru

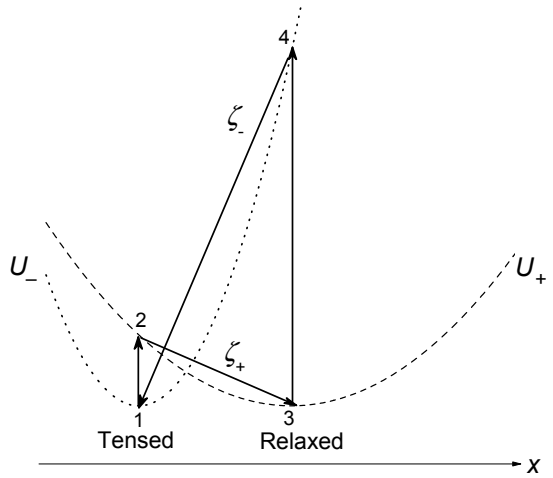

Fig. 1. Set-up for the problem. Brownian particle is moving in the potential which fluctuates between the two profiles U_+ (dashed line) and U_- (dotted line). The profiles correspond to the relaxed and tensed conformational states which also determine the particle friction coefficients, ζ_+ and ζ_-. The arrows schematically represent the working cycle of the reciprocating engine.

two-particle model in which the dynamics of an internal degree of freedom, playing the role of the engine, leads to the directional motion of the system. Energetic aspects of the problem will be considered elsewhere.

2 The model

As a model for the engine, we consider a Brownian particle moving in a one-dimensional potential in a thermal bath at temperature T. The state of the particle is characterized by its spatial coordinate x and conformational variable z. The particle can exist in two conformations, relaxed ($z = +$) and tensed ($z = -$) (see Fig. 1). Chemical reactions (or another source of nonequilibrium fluctuations) trigger transitions between these two states. The switching dynamics $z(t)$ depends neither on x nor on the thermal noise and is considered as a stationary Markov process described by the rate equation

$$\text{Relaxed}\,(+) \underset{\gamma_-}{\overset{\gamma_+}{\rightleftharpoons}} \text{Tensed}\,(-). \tag{1}$$

According to this scheme, the average time spent by the particle in the relaxed/tensed state is $\gamma_\pm^{-1}$. The conformational state determines both the particle friction coefficient $\zeta(z)$ and the potential profile $U(x;z)$, i.e., the potential and the friction fluctuations are parametrized by a single Markovian noise process $z(t)$. The potential profiles $U_\pm(x) \equiv U(x; z = \pm)$ are spatially separated and may have various shapes (e.g., be multiwelled but without any infinitely high wells). They are assumed to tend to infinity for $|x| \to \infty$ or to be defined in a finite domain with reflecting boundary conditions.

The overdamped dynamics of the model is governed by the extended Langevin equation [9]

$$\zeta(z)\dot{x} = -U'(x;z) + \sqrt{2\zeta(z)k_BT}\,\xi(t) \tag{2}$$

conjointly with the rate equation (1). A dot and a prime in equation (2) denote derivatives with respect to time and position, and $\xi(t)$ is a Gaussian white noise, i.e. $\overline{\xi(t)} = 0$, $\overline{\xi(t)\xi(s)} = \delta(t-s)$, where the overbar represents the average over the thermal noise. The corresponding master equation for the time evolution of probability densities for finding the particle in the relaxed/tensed state at position x at time t, $\rho_\pm(x,t) \equiv \rho(x,t,z=\pm)$, reads

$$\frac{\partial \rho_\pm}{\partial t} = -\frac{\partial J_\pm}{\partial x} - \gamma_\pm \rho_\pm + \gamma_\mp \rho_\mp, \tag{3}$$

where

$$J_\pm = -\left(\beta\zeta_\pm\right)^{-1} \frac{\partial \rho_\pm}{\partial x} - \zeta_\pm^{-1} \frac{\partial U_\pm}{\partial x}\rho_\pm$$

is the probability current, $\beta = (k_BT)^{-1}$, $\zeta_\pm \equiv \zeta(z = \pm)$, and k_B is the Boltzmann constant. The quantity of interest is the particle velocity in each state defined as

$$v_\pm(t) = \int_{-\infty}^{\infty} dx\, J_\pm(x,t). \tag{4}$$

After transient effects, the system approaches a steady state $\rho_\pm^{\rm ss}(x)$. So the long-time velocity $v_\pm \equiv \lim_{t\to\infty} v_\pm(t)$ can be written in the following form:

$$\begin{aligned} v_\pm &= \gamma^* \int_{-\infty}^{\infty} dx \int_{-\infty}^{x} dy\, \left[p_\mp(y) - p_\pm(y)\right] \\ &= \pm\gamma^* \int_{-\infty}^{\infty} dx\, x\left[p_+(x) - p_-(x)\right] = \pm\gamma^* \left(\langle x\rangle_+ - \langle x\rangle_-\right) \end{aligned} \tag{5}$$

(from here on $\pm$ signs refer to the upper and lower subscript, respectively). We have introduced the effective frequency of modulation $(\gamma^*)^{-1} \equiv \gamma_+^{-1} + \gamma_-^{-1}$, the probability density for the particle position distribution in the relaxed/tensed state $p_\pm(x) = (\gamma_\pm/\gamma^*)\,\rho_\pm^{\rm ss}(x)$ (normalized to unity), and the averages $\langle x\rangle_\pm = \int_{-\infty}^{\infty} dx\, x p_\pm(x)$. Note that the functions $p_\pm(x)$ satisfy the system of coupled ordinary differential equations

$$\frac{d}{dx}\left[e^{-\beta U_\pm}\frac{d}{dx}\left(e^{\beta U_\pm}p_\pm\right)\right] = \beta\gamma_\pm\zeta_\pm\left(p_\pm - p_\mp\right). \tag{6}$$

Thus the model under consideration generates bidirectional (reciprocating) motion transforming the energy coming from the source of nonequilibrium. The particle moves back and forth with the same absolute value of the velocity $v \equiv |v_\pm|$ (the complete average, $(v_+ + v_-)$, is zero, as it must be for bounded motion). This value is determined by the difference $\langle x\rangle_+ - \langle x\rangle_-$ which can be found from the solution to equation (6) or its following reduced form

$$\left\langle U_\pm'\right\rangle_\pm = \mp\gamma_\pm\zeta_\pm\left(\langle x\rangle_+ - \langle x\rangle_-\right), \tag{7}$$

valid for any confining potentials defined in the infinite interval $-\infty < x < \infty$.

3 Illustrative examples

A particularly simple (exact) result is obtained when both conformational states are characterized by the parabolic potentials: $U_{\pm}(x) = \frac{1}{2}k_{\pm}\,(x - a_{\pm})^2$, where $k_{\pm}$ and $a_{\pm}$ are the curvatures and the locations of potential well minima separated by the distance $L = a_+ - a_-$. In this case, it immediately follows from equations (5) and (7) that

$$v = \frac{\gamma^* L}{1 + \gamma_+\zeta_+/k_+ + \gamma_-\zeta_-/k_-}. \qquad (8)$$

Interestingly, the difference $\langle x\rangle_+ - \langle x\rangle_-$ is temperature-independent implying no contribution to the reciprocating velocity from the thermal noise. This is a signature of the parabolic potential involved: equilibrium and nonequilibrium fluctuations are not coupled. Moreover, the thermal noise can be ignored if and only if the potentials U_+ and U_- are parabolic.

Even small nonparabolicity of the confining potential leads to the coupling of the noises (even though their sources are statistically independent) and to the temperature-dependent velocity [10]. The temperature effect on the velocity may be manifested differently depending on the potentials. In particular, the thermal noise can have a constructive effect enhancing the velocity for a judiciously chosen potential pair. An especially illustrative example is a model of a potential box with a step barrier of height u as shown in Figure 2a, which has the advantage of being fully analytically tractable. For this model, $U_{\pm}(x) = u\theta\,(\pm L \mp x)$, where $\theta(x)$ is the Heaviside step function, and $p_{\pm}(x)$ can be found from two coupled second-order differential equations (6) supplemented with the condition of the probability current continuity and the jump conditions at $x = L$ [11]. The result for the velocity is

$$v = \gamma^* L\,\tanh\frac{\beta u}{2}\,\mathrm{sech}\,\omega\left[\frac{\sinh(\omega/2)}{\omega/2}\right]^2, \qquad (9)$$

where the dimensionless parameter $\omega^2 = \beta(\gamma_+\zeta_+ + \gamma_-\zeta_-)L^2$ represents the coupling between the external and internal noises.

Upon variation of the temperature, the velocity v given by equation (9) exhibits a bell-shaped behavior shown in Figure 2b, which is totally different from that we have seen for the parabolic potential. Such a stochastic resonance-like effect admits a simple explanation. At high temperatures, the + and − states become almost identical and the velocity decays as $u/(k_BT)$. At zero temperature, the transduction mechanism stops because the motion in the flat potential invoked is frozen. For small T, the velocity increases linearly with the temperature.

The reciprocating velocity as a function of the flipping rate $\gamma_{\pm}$ appears much the same for both considered models with the parabolic or step potential. With one of the rates, say γ_+, varied and the other fixed, the velocity exhibits a nonmonotonic dependence on γ_+. It becomes zero in the limiting cases of $\gamma_+ = 0$ and $\gamma_+ = \infty$ since either of them implies the reduction of the two-state model to the one-state model. A more interesting situation arises when $\gamma_+ = \gamma_- \equiv \gamma$. Then, v monotonously increases with γ approaching a nonzero limit at $\gamma = \infty$ (see Eqs. (8) and (9)). To account for this fact, let us consider how the difference $\langle x\rangle_+ - \langle x\rangle_-$ varies with γ. In the low frequency limit, the probability distribution $p_{\pm}(x)$ has enough time to adjust to the new potential after each state flip. Thus, the quasiequilibrium densities p_+ and p_- are well separated and the difference $\langle x\rangle_+ - \langle x\rangle_-$ is close to its equilibrium value L (see Fig. 2c). With an increase in γ, the adjustment becomes more and more difficult, so that p_+ and p_- approach each other, and the value of $\langle x\rangle_+ - \langle x\rangle_-$ diminishes. As $\gamma \to \infty$, the system

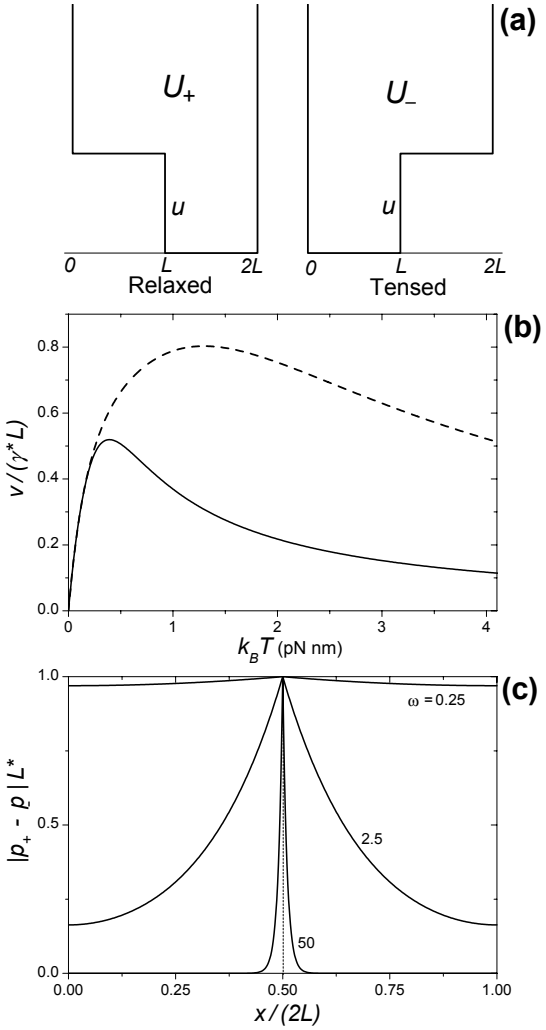

Fig. 2. The model of a potential box with a fluctuating step barrier. (a) A sketch of the potential profiles U_+ and U_-. (b) The reciprocating velocity vs temperature for the step barrier height $u = 1$ and 5 pN nm (solid and dashed line, respectively), as calculated from equation (9) with $L = 20$ nm, $\gamma_+ = \gamma_- = \gamma = 10^3$ s^{-1}, $\zeta_+ + \zeta_- = 1.5 \times 10^{-6}$ pN s/nm. (c) Reduction of the difference $|p_+(x) - p_-(x)|$ for increasing values of the parameter $\omega = \sqrt{\beta\gamma\,(\zeta_+ + \zeta_-)}L$ indicated by the numbers near the curves. Here the parameter ω represents the frequency modulation and $L^* = L\coth(\beta u/2)$.

is not capable of tracking the potential modulations and feels an effective potential. The probability distributions for the tensed and relaxed states become almost identical except for a very narrow domain with the width (and consequently $\langle x\rangle_+ - \langle x\rangle_-$) decaying as γ^{-1}. As a result, $v \to [\beta L(\zeta_+ + \zeta_-)]^{-1} \tanh(\beta u/2)$ when $\gamma \to \infty$. The same mechanism holds for parabolic and presumably for any other potential [12].

4 Rectification due to friction asymmetry

We have a mechanism to transduce, at the mesoscale level, chemical energy into mechanical energy of reciprocating motion. To obtain a molecular motor, which converts chemical energy into directed motion, it remains to equip the engine with any appropriate gear rectifying reciprocating motion ("crank gear"). With this in mind, consider a system consisting of two mutually interacting Brownian particles moving on the track [13]. Like in the above-discussed one-particle model, the system is assumed to have two conformational states, relaxed (+) and tensed (−). The discrete conformational state variable $z(t)$ determines both the interaction potential $U(x_2 - x_1; z)$ (with x_1 and x_2 denoting the locations of the left and the right particles along the track) and the friction coefficients $\zeta_1(z)$ and $\zeta_2(z)$ of the particles. The overdamped dynamics of the model in a thermal bath at temperature T is now described by the two coupled extended Langevin equations:

$$\zeta_i(z)\dot{x}_i = -\frac{\partial U(x_2 - x_1; z)}{\partial x_i} + \sqrt{2\zeta_i(z)k_BT}\xi_i(t), \quad i = 1, 2 \tag{10}$$

and the rate equation (1) for the conformational state variable $z(t)$. Here $\xi_1(t)$ and $\xi_2(t)$ are not correlated standardized Gaussian white noises: $\overline{\xi_i(t)} = 0$, $\overline{\xi_i(t)\xi_k(s)} = \delta_{ik}\delta(t-s)$.

By introducing the center of mass $X = \frac{1}{2}(x_1 + x_2)$ and the internal variable $x = x_2 - x_1$, one obtains two stochastic equations of motions in terms of the new variables. It can be ascertained that one of them, the equation for x, coincides with the Langevin equation (2) with $\zeta^{-1}(z)$ replaced by $\left[\zeta_1^{-1}(z) + \zeta_2^{-1}(z)\right]$, whereas the other relates $\dot{X}$ to $\dot{x}$. This implies that the dynamics along the internal coordinate (i) is governed by external modulation, as specified by equation (1), and evolves independently of the system motion; (ii) represents the reciprocating engine discussed above; (iii) underlies the system motion. In the long-time limit, the relation between $\dot{X}$ and $\dot{x}$ averaged over both external and thermal noises can be written as follows:

$$V = \mu v, \quad \mu = \frac{\zeta_1(+)\zeta_2(-) - \zeta_2(+)\zeta_1(-)}{[\zeta_1(+) + \zeta_2(+)]\,[\zeta_1(-) + \zeta_2(-)]}, \tag{11}$$

where $V = \lim_{t\to\infty}\langle \dot{X}(t)\rangle$ is the system velocity and $v \equiv |v_\pm|$ is reciprocating velocity, equation (5). The rectification coefficient μ represents the left-to-right/right-to-left asymmetry of the model. The rectification mechanism exploits the asymmetry of friction fluctuations. Thus in the absence of any macroscopic gradients, the system moves unidirectionally due to rectification of internal movement driven by the energy absorbed from the source of the nonequilibrium fluctuations (such as ATP successive hydrolysis cycles), i.e., the system operates as a two-head molecular motor.

A mechanism providing the asymmetric friction fluctuations can be exemplified within the framework of a simple phenomenological model. This model includes two channels of energy dissipation for the protein head sliding with the constant velocity on the microtubule track: the viscous dissipation due to hydrodynamic Stokes-type resistance of the solvent and the dissipation due to continuous making and breaking of weak chemical bonds between the protein and the microtubule, which is called *protein friction* [14]. If the time scale for protein motion is much longer than the times associated with the binding/unbinding kinetics, the friction forces are linear in the velocity, with the friction coefficients ζ_v and ζ_p for the viscous and protein friction, respectively. In this case, the protein friction dominates, $\zeta_p \gg \zeta_v$, and the viscous friction can be neglected. However, if the protein motion is so fast that the chemical bonds have no enough time to form, the viscosity friction is solely responsible for energy dissipation. Turning back to our two-particle model, imagine now that only one of the particles, say the first, is able to interact with the track. Moreover, assume that the potential associated with the relaxed (tensed) state implies a sufficiently slow (fast) dynamics to allow (suppress) protein friction. Then, the friction coefficient of the left particle fluctuates, $\zeta_1(+) = \zeta_p$ and $\zeta_1(-) = \zeta_v$, while the friction coefficient of the right particle is constant $\zeta_2(\pm) = \zeta_v$. Thus, the rectification coefficient is $\mu_p = \frac{1}{2}\left(\zeta_p - \zeta_v\right)/\left(\zeta_p + \zeta_v\right)$. This expression, along with equations (5) and (11), gives the velocity of the two-head motor which involves rectification of reciprocating motion by the protein friction mechanism for any potential of the inter-head interaction [15]. It is noteworthy that the biologically relevant model of molecular motor based on the protein friction concept was suggested by Mogilner et al. [16]. Our two-particle model generalizes the Mogilner et al. model to the case of arbitrary interaction between the motor heads [17]. In the particular case of the parabolic setup (an effective spring considered in Ref. [16]), our result for the velocity, given by equations (8) and (11) with $\mu = \mu_p$, coincides with that obtained by Fogedby et al. [18] within the Mogilner et al. model. Importantly, the parabolic potential used in references [16,18] leads to a chemically driven power stroke mechanism, while the thermal noise can play a key role in the energy transduction for a nonparabolic potential.

5 Summary

In summary, we have devised a nanoscale reciprocating engine by using Brownian motion in a fluctuating confining potential. We have found an interesting interplay of external and internal noises underlain by the action of the confining potential. Among other aspects, we have also

discussed the problem of how to construct a molecular motor based on the reciprocating engine.

The authors thank A.A. Villaeys for many inspiring discussions and P. Talkner and M.L. Dekhtyar for helpful comments on the manuscript. This work was supported by Academia Sinica. V.M.R. thanks NSC of Taiwan for support (Contract No. NSC 94-2811-M-001-064). Yu.A.M. and V.M.R. gratefully acknowledge the kind hospitality received from the Institute of Atomic and Molecular Sciences.

References

1. P. Reimann, Phys. Rep. **361**, 57 (2002)
2. J. Phys.: Condens. Matter **17**, S3661-S4024 (2005), special issue containing papers on molecular motors, edited by J. Klafter, M. Urbakh
3. See, e.g., K.E. Drexler, *Nanosystems: Molecular Machinery, Manufacturing and Computation* (Wiley, New York, 1992)
4. See, e.g., J. Howard, *Mechanics of Motor Proteins and the Cytoskeleton* (Sinauer Associates, Sunderland, 2001)
5. See, e.g., B. Hille, *Ionic Channels of Excitable Membranes* (Sinauer Associates, Sunderland, 1992); T.Y. Tsong, T.D. Xie, Appl. Phys. A **75**, 345 (2002)
6. M.O. Magnasco, Phys. Rev. Lett. **72**, 2656 (1994); M.O. Magnasco, Phys. Rev. Lett. **71**, 1477 (1993); R.D. Astumian, M. Bier, Phys. Rev. Lett. **72**, 1766 (1994); C.R. Doering, W. Horsthemke, J. Riordan, Phys. Rev. Lett. **72**, 2984 (1994); J. Prost, J.-F. Chauwin, L. Peliti, A. Ajdari, Phys. Rev. Lett. **72**, 2652 (1994)
7. R. Bartussek, P. Hänggi, J.G. Kissner, Europhys. Lett. **28**, 459 (1994); F. Jülicher, A. Ajdari, J. Prost, Rev. Mod. Phys. **69**, 1269 (1997); K. Sekimoto, J. Phys. Soc. Jpn **66**, 1234 (1997)
8. T. Hugel, N.B. Holland, A. Cattani, L. Moroder, M. Seitz, H.E. Gaub, Science **296**, 1103 (2002)
9. R. Rozenfeld, J. Łuczka, P. Talkner, Phys. Lett. A **249**, 409 (1998); J. Łuczka, P. Talkner, P. Hänggi, Physica A **278**, 18 (2000)
10. Discussion of the constructive role of thermal noise in fluctuation driven transport began a few years ago. See, e.g., R.D. Astumian, F. Moss, Chaos **8**, 533 (1998); A. Fuliński, P.F. Góra, Phys. Rev. E **64**, 011905 (2001)
11. H. Risken, *The Fokker-Planck Equation. Methods of Solution and Apllications* (Springer-Verlag, Berlin, 1989)
12. It is noteworthy that when $\gamma \to \infty$ the characteristic length and time scales of the reciprocating motion tend to zero, though their ratio remains finite
13. Several models consisting of two coupled particles were proposed to elucidate noise-induced transport of structured objects. See, e.g., A. Ajdari, J. Phys. I France **4**, 1577 (1994); I. Derényi, T. Vicsek, Proc. Natl. Acad. Sci. USA **93**, 6775 (1996); S. Klumpp, A. Mielke, C. Wald, Phys. Rev. E **63**, 031914 (2001); M. Porto, Eur. Phys. J. B **25**, 345 (2002) and reference [16]
14. K. Tawada, K. Sekimoto, J. Theor. Biol. **150**, 193 (1991); S. Leibler, D.A. Huse, J. Cell Biol. **121**, 1357 (1993)
15. The rectification mechanism based on the protein friction breaks down when the the flipping rates are comparable with the rates of binding/unbinding process
16. A. Mogilner, M. Mangel, R.J. Baskin, Phys. Lett. A **237**, 297 (1998)
17. The rectification mechanism discussed in reference [16] and here does not involve the interaction between the motor heads and the protein filament (the motor track) which plays the key role in the protein motor operation, as shown experimentally [4]. Thus this mechanism may serve as a robotic model for molecular motors rather than for existing, known protein motors
18. H.C. Fogedby, R. Metzler, A. Svane, Phys. Rev. E **70**, 021905 (2004)