Net transport due to noise-induced internal reciprocating motion
Yurii A. Makhnovskii, Viktor M. Rozenbaum, Dah-Yen Yang, and Sheng Hsien Lin

Citation: The Journal of Chemical Physics 130, 164101 (2009); doi: 10.1063/1.3116790
View online: http://dx.doi.org/10.1063/1.3116790
View Table of Contents: http://scitation.aip.org/content/aip/journal/jcp/130/16?ver=pdfcov
Published by the AIP Publishing

Articles you may be interested in
Controlling the conformations and transport of DNA by free energy landscaping

Distortion in the thermal noise spectrum and quality factor of nanomechanical devices due to finite frequency resolution with applications to the atomic force microscope
Rev. Sci. Instrum. 82, 095104 (2011); 10.1063/1.3632122

Highly efficient energy excitation transfer in light-harvesting complexes: The fundamental role of noise-assisted transport

Entropy driven unidirectional motion of Brownian particle inside a three-dimensional tube

Theory of electrical noise induced in a wire loop by the thermal motions of ions in solution
Net transport due to noise-induced internal reciprocating motion

Yuri A. Makhnovskii,1,2,a Viktor M. Rozenbaum,1,3 Dah-Yen Yang,1 and Sheng Hsien Lin1,4

1Institute of Atomic and Molecular Sciences, Academia Sinica, P.O. Box 23-166, Taipei 106, Taiwan
2Topchiev Institute of Petrochemical Synthesis, Russian Academy of Sciences, Leninsky Prospect 29, 119991 Moscow, Russia
3Chuiko Institute of Surface Chemistry, National Academy of Sciences of Ukraine, Generala Naumova str. 17, Kiev 03164, Ukraine
4Department of Applied Chemistry, National Chiao Tung University, Hsinchu 300, Taiwan

(Received 12 August 2008; accepted 21 March 2009; published online 22 April 2009)

We consider a system of two coupled Brownian particles fluctuating between two states. The fluctuations are produced by both equilibrium thermal and external nonthermal noise, the transition rates depending on the interparticle distance. An externally induced modulation of the transition rates acts on the internal degree of freedom (the interparticle distance) and generates reciprocating motion along this coordinate. The system moves unidirectionally due to rectification of the internal motion by asymmetric friction fluctuations and thus operates as a dimeric motor that converts input energy into net movement. The properties of the motor are primarily determined by the properties of the reciprocating engine, represented by the interparticle distance dynamics. Two main mechanisms are recognized by which the engine operates: energetic and informational. In the physically important cases where only one of the motion-inducing mechanisms is operative, exact solutions can be found for the model with linearly coupled particles. We focus on the informational mechanism, in which thermal noise is involved as a vital component and the reciprocating velocity exhibits a rich behavior as a function of the model parameters. An efficient rectification method for the reciprocating motion is also discussed. © 2009 American Institute of Physics.

[DOI: 10.1063/1.3116790]

I. INTRODUCTION

The emergence of directed motion in small-scale systems from unbiased nonequilibrium fluctuations (brought about by an energy releasing process) has attracted considerable recent attention. The problem has been discussed in manifold contexts by approaches of varying rigor and sophistication.1,2 These studies are primarily motivated by a desire to understand how molecular motor proteins3 and ion pumps4 operate, carrying out various particular physiological functions. Another motivation comes from artificial molecular5 and nanoscale machinery design,6 this rapidly developing field faces the challenge of building synthetic structures which, if supplied with energy and information, can controllably move and interface molecular-level systems with the macroscopic world.

Interaction between two dynamic levels, internal and external, has been recognized as an important factor in energy conversion by structured objects.7–9 In the present work, we address the case of motor systems consisting of two coupled particles, where the internal degree of freedom is essential for directional motion to occur. Several models of this type have been proposed.10–16 Most of them rely on the existence of a locally periodic and asymmetric (ratchet) potential in which the motors move.11,12 There are, however, alternative concepts: a transport effect can be achieved in a symmetric potential17 and, moreover, without any effective potential.8,14,15 It is usually postulated that the particles are linearly coupled and their order cannot change (resembling the inchworm walking in motor proteins)5 with notable exceptions10,16 in which a nonlinear particle interaction is considered and the particles are allowed to alternate in the lead (the head-over-head walking).16 Much of the previous work on the driving mechanisms of dimeric motors has been concerned with a role of intrinsic structures and symmetry properties of the systems operating in almost deterministic fashion at energies much higher than the thermal noise. Stochastically dominant mechanisms responsible for the appearance of dimer directed motion on the nanoscale have been comparatively less investigated, although a subtle interplay of thermal noise, nonlinearity, and different dynamic levels is definitely interesting and a promising topic.

In this paper, we consider a two-state model for a dimeric motor, placing particular emphasis on stochastic aspects of the system behavior. The considered system consists of two coupled Brownian particles fluctuating between two conformational states, generally with different interparticle interaction potentials, position-dependent rate constants of interstate transitions, and particle friction coefficients. An external action drives the interstate transition rates away from spontaneous values so that reciprocating motion “out of noisy states”17 occurs along the internal coordinate (the interparticle distance). Since the system dynamics is coupled to the internal dynamics and the internal motion is rectified by asymmetric friction fluctuations, the system moves unidirectionally and thus functions as a two-headed motor. By analogy with a macroscopic combustion motor, the motor con-
sists of a reciprocating engine capable to convert nonequilibrium fluctuations into reciprocating mechanical motion and a symmetry-breaking mechanism. We primarily focus on the reciprocating engine. In addition to a key role played in our approach, the concept of the reciprocating motion on the nanoscale is intriguing by itself. It also appears relevant in the treatment of optomechanical conversions in single-molecule devices, biochemical “futile cycles,” particle separation, a strategy for molecular motor design, and in other contexts.

For any nanoscale model of energy conversion to be physically reasonable and biologically relevant, it should include the spatial dependence of the system’s chemical activity. In a simplified version of the considered model, the dynamics for switching between competing states is assumed independent of particle spatial position and thermal noise. So the results and the conclusions of Ref. 15 are only applicable to systems switchable by extremely large on the nanoscale forces. As shown in Ref. 22, the incorporation of the position dependence of the interstate transition rate constants (i) gives proper weight to the effect of thermal noise not only for spatial motion but also for the interstate transitions and (ii) reveals two basic mechanisms (energetic and informational) causing the reciprocating motion with quite distinct physical origins and manifestations. Generally, a fully analytical treatment of the model under consideration is hardly possible. However, in the important limiting cases, where only one of the motion-inducing mechanisms is operative, exact solutions can be obtained for the model with linearly coupled particles. One of them (representing the energetic mechanism) has been found first in Ref. 15. The other, which nicely illustrates the stochastically dominant informational mechanism, is one of the main results of this work.

The outline of the paper is as follows. In Sec. II, we formulate a model for a dimeric motor, reduce this model to one dimension, and show how the directional motion of the system arises from the noise-induced internal reciprocating motion. The reduced model (called the reciprocating engine) is considered in Sec. III. Our main results are presented in Sec. IV, where an exact solution for the informational reciprocating engine is obtained and analyzed. Section V contains a short discussion of a possible rectifying mechanism.

II. TWO-STATE MODEL FOR DIMERIC MOTOR

Consider a system consisting of two coupled Brownian particles moving on a track. The system is assumed to have two conformational states, \( \sigma = + \) and \( \sigma = - \). The discrete variable \( \sigma(t) \) determines the potential profile of interaction between the particles \( U_+(x) = x_2 - x_1 \) with \( x_1 \) and \( x_2 \) denoting the locations of the particles along the track, the particle friction coefficients \( \zeta_1(\sigma) \) and \( \zeta_2(\sigma) \), and the standard chemical potentials \( \mu_{1r}(\sigma) \) and \( \mu_{2r}(\sigma) \) (the position-independent parts of the chemical potentials which reflect the contribution of internal degrees of freedom). The potentials \( U_+(x) \) and \( U_-(x) \) may have various shapes (e.g., be multiwell) and are assumed to tend to infinity for \( |x| \to \infty \). Depending on the behavior of \( U_{\pm}(x) \) at small \( |x| \), two scenarios are possible. If the potentials become high enough as the particles approach each other, the particles cannot overtake and one of them always leads (inchworm mode). Otherwise the particles can alternate their order randomly (hand-over-hand mode).

The interstate switching dynamics is governed by the rate equation

\[
\gamma_+(x) = \frac{\partial U(x_2 - x_1; \sigma)}{\partial x} + \sqrt{2\xi(\sigma)T\xi(t)}, \quad i = 1, 2, \tag{1}
\]

with the position-dependent transition rate constants \( \gamma_+(x) \) and \( \gamma_-(x) \). We assume that

\[
\gamma_+(x) = \gamma_{\pm,0}(x) + \omega(x), \tag{2}
\]

where \( \gamma_{\pm,0}(x) \) are the rate constants for the transitions caused by equilibrium (thermal) fluctuations and \( \omega(x) \) represent the excitation introduced by an external (nonthermal) noise.

By introducing the center of mass \( X = (x_1 + x_2)/2 \) as a system variable and the relative coordinate \( x \) as an internal variable, Eqs. (1) and (3) can be written in terms of the equivalent master equation for 2D joint probability densities \( P_\sigma(X, x, t) \), \( \sigma = +, - \), for finding the system in state \( \sigma \) near point \( (X, x) \) at time \( t \). The master equation reads

\[
\frac{\partial P_\sigma(X, x, t)}{\partial t} = \left[ \frac{1}{2} \frac{\partial I_\sigma(X, x, t)}{\partial X} + \frac{\partial i_\sigma(X, x, t)}{\partial x} \right]
- \alpha \left[ \gamma_+(x) P_\sigma(X, x, t) - \gamma_-(x) P_\sigma(X, x, t) \right], \tag{4}
\]

where

\[
I_\sigma(X, x, t) = -\frac{1}{\beta\sigma} \left[ \frac{1}{2} \frac{\partial P_\sigma(X, x, t)}{\partial X} + e^{\beta U_{\sigma}(x)} \frac{\partial \left[ e^{\beta U_{\sigma}(x)} P_\sigma(X, x, t) \right]}{\partial x} \right], \tag{5}
\]

\[
i_\sigma(X, x, t) = -\frac{1}{\beta\sigma} \left[ e^{\beta U_{+}(x)} \frac{\partial \left[ e^{\beta U_{+}(x)} P_\sigma(X, x, t) \right]}{\partial x} - e^{\beta U_{-}(x)} \frac{\partial \left[ e^{\beta U_{-}(x)} P_\sigma(X, x, t) \right]}{\partial x} \right]
\]

are the probability currents, \( \beta = T^{-1} \), and \( \xi_\sigma \) are the effective friction coefficients

\[
\xi_\sigma = \xi_1(\sigma) + \xi_2(\sigma), \tag{6}
\]

The dimensionless coefficients \( \epsilon_{\sigma} = [\xi_1(\sigma) - \xi_2(\sigma)]/\xi_1(\sigma) + \xi_2(\sigma) \) represent the coupling between the internal motion and the translation of the system as a whole. Both the system variable \( X \) and the internal variable \( x \) vary from \( -\infty \) to \( \infty \).
(even if the order of particles is fixed, the range of definition of x may be safely extended to include negative values, which are not populated). The boundary conditions to Eqs. (4) and (5) imply that the probability densities and currents vanish when |x| or |x| goes to infinity.

As it follows from Eqs. (4) and (5) and the boundary conditions at infinity, the marginal probability density associated with the internal motion

\[ \rho_\sigma(x,t) = \int_{-\infty}^{\infty} P_\sigma(X,x,t) dX, \quad \sigma = +,- \]  

satisfies the following equation:

\[ \frac{\partial \rho_\sigma(x,t)}{\partial t} = - \frac{\partial J_\sigma(x,t)}{\partial x} - \sigma [\gamma_+(x) \rho_+(x,t) - \gamma_-(x) \rho_-(x,t)], \]

where \( J_\sigma(x,t) \) is the probability current along the x-coordinate in state \( \sigma \),

\[ J_\sigma(x,t) = \int_{-\infty}^{\infty} i_\sigma(X,x,t) dX \]

\[ = - \frac{1}{2\beta \epsilon_\sigma} e^{-\beta U_\sigma(x)} \frac{\partial}{\partial x} \left[ e^{\beta U_\sigma(x)} \rho_\sigma(x,t) \right]. \]  

The average velocity of the motion in state \( \sigma \) is defined as

\[ v_\sigma(t) = \int_{-\infty}^{\infty} J_\sigma(x,t) dx. \]

Note that the dynamics along the internal coordinate evolves independently of the system motion, since both the potential and the transition rate profiles are determined solely by \( x \).

The quantity of foremost interest is the average velocity of the center of mass

\[ V(t) = \frac{d}{dt} \int_{-\infty}^{\infty} dX dX' \left[ P_+(X,x,t) + P_-(X,x,t) \right]. \]

Using Eqs. (4) and (5) and the boundary conditions at infinity, Eq. (11) can be rewritten as

\[ V(t) = \int \int_{-\infty}^{\infty} dX dX' \left[ \frac{\partial P_+(X,x,t)}{\partial t} + \frac{\partial P_-(X,x,t)}{\partial t} \right] \]

\[ = \frac{1}{2} \int \int_{-\infty}^{\infty} dX dX' \left[ I_+(X,x,t) + I_-(X,x,t) \right] \]

\[ = \frac{1}{2} \left[ \epsilon_+ J_+(x,t) + \epsilon_- J_-(x,t) \right] dx. \]  

At long times, the motion along the internal coordinate approaches a steady state, so that \( v_\sigma(t) \to \pm \nu \) and \( V(t) \to V \). In this regime, the total current \( J_+(x) + J_-(x) = 0 \) for all \( x \) as it must be for bounded motion. Using this fact and Eq. (10), we can rewrite Eq. (12) to obtain the relation between the steady-state values of the system velocity \( V \) and the internal velocity \( \nu \) (Ref. 25),

\[ V = \epsilon_\nu, \quad \epsilon = \frac{1}{2} (\epsilon_+ - \epsilon_-) = \frac{\xi_+(\epsilon_+) - \xi_-(-\epsilon_-)}{[\xi_+(\epsilon_+) + \xi_-(-\epsilon_-)][\xi_+(\epsilon_+) + \xi_-(-\epsilon_-)]}. \]

Thus, the original two-dimensional problem is reduced to the one-dimensional problem of finding the reciprocating velocity \( \nu \) of Brownian motion in a confining fluctuating potential. The reduced model contains essentially the dominant dynamics of the system.

A simple physical picture emerges from our analysis. An external excitation does not directly interact with the state variable \( x \) but rather acts on the internal degree of freedom and induces reciprocating (bidirectional) motion along this coordinate with time and length scales long compared to those of the microscopic (thermal) fluctuations. The internal dynamics drives the motion of the whole system via the coupling represented by the coefficients \( \epsilon_+ \) and \( \epsilon_- \). The rectification mechanism exploits the left-right asymmetry of friction fluctuations which determines the rectification coefficient \( \epsilon \). As a result, the system motion appears as the rectified reciprocating motion of the internal degree of freedom, i.e., the system operates like a two-headed motor. The motor consists of an engine converting nonequilibrium fluctuations into reciprocating motion and a symmetry-breaking rectifier. In Secs. III and IV we study mechanisms by which the reciprocating engine operates within the one-dimensional reduced model. An example of a symmetry breaking mechanism is briefly discussed in Sec. V.

III. RECIPROCATING ENGINE

A. Model

The reduced model considers the confined motion of a Brownian particle fluctuating between two conformational states \( \sigma=+ \) and \( \sigma=- \). The conformational variable \( \sigma \) specifies the potential profile \( U_\sigma(x) \), the particle friction coefficient \( \zeta_\sigma \) [Eq. (6)], and the standard chemical potential \( \mu^0_\sigma = \mu^0_+(\sigma) + \mu^0_-(\sigma) \). The switching dynamics is described by rate Eqs. (4) with the position-dependent transition rate constants \( \gamma_+(x) \) and \( \gamma_-(x) \) [see also Eq. (2)]. In fact, the reduced model is the model of a nanoscale reciprocating engine recently proposed by the present authors. In the next two paragraphs, we briefly review the major points of the model formulation, which are needed for understanding the engine operation and in further calculations (for a more detailed description see Sec. II in Ref. 22).

The dynamics of the model is governed by the master Eq. (8) for the time evolution of probability densities \( \rho_\sigma(x,t), \sigma=+,- \) for finding the particle in state \( \sigma \) near point \( x \) at time \( t \). The total probability of both states is normalized to unity [see Eq. (7) in Ref. 22]. In the steady-state regime, all the quantities become time independent and Eq. (8) takes the form
where \( J_\sigma(x) \) is the probability current in state \( \sigma \) at point \( x \) defined by Eq. (9) [see also Eqs. (5) and (6) in Ref. 22]. The currents \( J_\sigma(x) \) vanish at \( x \to \pm \infty \). From Eq. (14) and the reflecting boundary conditions at \( x=\pm \infty \), it follows the integral balance condition

\[
\int_{-\infty}^{\infty} [\gamma_+(x)\rho_+(x) - \gamma_-(x)\rho_-(x)]dx = 0, \tag{15}
\]

which is the condition of existence and stability of the steady state. The quantity of concern, viz., the reciprocating velocity \( v=v_+=-v_- \) is defined by Eq. (10).

Without external forcing, \( \omega(x)=0 \) for all \( x \), the system is at equilibrium: the probability densities \( \rho_{\sigma,0} \), \( \sigma=+,- \), obey the Boltzmann distribution

\[
\rho_{\sigma,0}(x) = Z^{-1} e^{-\beta \mu_{\sigma}^0 + U_{\sigma}(x)}, \quad Z = \sum_{\sigma=+,-} e^{-\beta \mu_{\sigma}^0} \int_{-\infty}^{\infty} e^{-\beta U(x)}dx \tag{16}
\]

and the detailed balance holds

\[
[\Gamma(x)Q(x)/\gamma(x)]' + \beta Q(x)[(1-\Delta)\alpha(x)U'_+(x) + (1+\Delta)[1-\alpha(x)]U'_-(x)] = 2\Delta W'(x) - \beta W(x) [(1-\Delta)U'_+(x) - (1+\Delta)U'_-(x)]',
\]

\[
\{Q'(x) + \beta Q(x)[\alpha(x)U'_+(x) + (1-\alpha(x))U'_-(x)] + \beta W(x) [U'_+(x) - U'_-(x)] \}' = 2\beta \xi \Delta \gamma(x) W(x), \tag{19}
\]

where \( \xi=(\xi_+ + \xi_-)/2 \) is the average friction coefficient, \( \Delta = (\xi_+ - \xi_-)/ (\xi_+ + \xi_-) \) represents the friction asymmetry of the states, \( \Gamma^{-1}(x) \) is the characteristic relaxation time

\[
\Gamma(x) = (1+\Delta)\gamma_+(x) + (1-\Delta)\gamma_-(x), \tag{20}
\]

and the prime denotes a derivative with respect to \( x \). In derivation of the first of Eq. (19), we essentially used the fact that the total probability current takes the zero value at any point \( x \), \( J_+(x)+J_-(x)=0 \). The second equation of system (19) is obtained simply by summing up the equations derived from Eq. (14) with \( \sigma=+ \) and \( \sigma=- \), after multiplying them by \( \xi_+ \) and \( \xi_- \), respectively. Both \( Q(x), W(x) \) and \( Q'(x), W'(x) \) vanish when \( x \to \pm \infty \). Additionally, the normalization condition for the \( \rho_{\sigma,0} \) and the integral balance condition (15) imply that \( Q(x) \) and \( W(x) \) must satisfy

\[
\langle 1 \rangle_Q = 1, \quad \langle \gamma(x) \rangle_W = 0, \tag{21}
\]

where notations \( \langle \cdots \rangle_Q = \int_{-\infty}^{\infty} \cdots Q(x)dx \) and \( \langle \cdots \rangle_W = \int_{-\infty}^{\infty} \cdots W(x)dx \) have been introduced for future convenience. In these notations, the desired reciprocating velocity (10) reads

\[
v = \langle x\gamma(x) \rangle_W. \tag{22}
\]

\[\gamma_{+,0}(x)\rho_{+,0}(x) - \gamma_{-,0}(x)\rho_{-,0}(x) = 0 \text{ for all } x. \tag{17}\]

The condition of detailed balance implies zero current and zero average velocity in each state. With a source of nonequilibrium noise, additional transitions between the states occur, the detailed balance is broken, and nonzero values of the velocity in each of the states are allowed. The particle moves back and forth with the same absolute value of the velocity \( v \). So the model operates as a reciprocating engine: a part of the free energy coming from the source of nonequilibrium is converted into mechanical energy of reciprocating motion.

For our goals it is useful to introduce the marginal probability density of the position variable \( Q(x) \) and the function \( W(x) \), which serves as a direct measure of detailed balance breaking

\[
Q(x) = \rho_+(x) + \rho_-(x),
\]

\[
W(x) = [\gamma_+(x)\rho_+(x) - \gamma_-(x)\rho_-(x)]/\gamma(x) = [1 - \alpha(x)]\rho_+(x) - \alpha(x)\rho_-(x), \tag{18}
\]

where \( \alpha(x)=\gamma_+(x)/\gamma(x) \) is the conditional probability to find the particle in state +, given the particle is at point \( x \), and \( \gamma(x)=\gamma_+(x) + \gamma_-(x) \). From Eqs. (9) and (14) it follows that the functions \( Q(x) \) and \( W(x) \) satisfy the following system of differential equations

\[
\{Q'(x) + \rho_+(x)U'_+(x) + (1-\alpha(x))U'_-(x)] + \beta W(x) [U'_+(x) - U'_-(x)] \}' = 2\beta \xi \Delta \gamma(x) W(x), \tag{19}
\]

While at equilibrium \( Q_0(x) \) is determined by Eq. (16) and \( W_0(x)=W_0'(x)=0 \), in a state of nonequilibrium, generally, Eq. (19) does not admit analytic solutions. In what follows, we show that there exist particular physically meaningful cases where exact solutions for \( v \) are available and focus on their analysis.

B. Two basic operational mechanisms

The energy required for the engine to operate is provided by a source of noise that modulates the equilibrium values of transition rates. It is instructive to characterize this source of unbalance by the chemical potential \( \mu_{\text{eff}}(x) \), which specifies the free energy released on “burning of the effective fuel” at point \( x \). For the reciprocating engine, \( \mu_{\text{eff}}(x) \) has been expressed in terms of the model parameters in Ref. 22,

\[
\mu_{\text{eff}}(x) = \mu_0 - \mu_0 + U_+(x) - U_-(x) + T \ln \frac{\gamma_+(x)}{\gamma_-(x)} = T \ln \frac{1 + \omega_+(x)/\gamma_+(x)}{1 + \omega_-(x)/\gamma_-(x)}. \tag{23}
\]

A more accurate derivation of this formula is given in the Appendix to make the paper self-contained.
coefficient (or temperature)\textsuperscript{28} and position-dependent mobility\textsuperscript{29} (or friction\textsuperscript{30}). Within a microscopic description of the environment in terms of a harmonic oscillator bath, the nonequilibrium noise associated with these inhomogeneities represents the nonthermal part of the energy in the nonequilibrium bath coupled to the system and acts as a source or sink of negentropy.\textsuperscript{31} So the informational mechanism stands for “possibilities rather than forces.”\textsuperscript{29} Both the energy\textsuperscript{32} and information ratchets\textsuperscript{33} have been implemented chemically in the form of catenanes (interlocking rings) and rotaxanes (a dumbbell threaded through a ring).

Of primary interest are two limiting cases, where only one of the motion-inducing mechanisms is operative. If the position-dependent part of the chemical potential of the effective fuel $\mu_{\text{eff}}(x)$ is simply $U_{a}(x) = U_{b}(x)$, the reciprocating engine is driven solely by the energetic mechanism [see Fig. 1(a)]. This occurs when the barrier between the conformational states is very high compared to $T$, so that the thermally activated jumps vanish and the interstate transitions are caused only by a homogenous (position-independent) strong (on the nanoscale) excitation, i.e., $\gamma_{\pm}(x) = \omega_{\pm}$. At these conditions, the model is reduced to that considered in Ref. 15, where an exact solution for the velocity $v$ has been found, with the parabolic potential profiles of the conformational states given by (apart from additive constants) $U_{\pm}(x) = \frac{1}{2} k_{\pm} (x \mp a_{\pm})^2$, where $k_{\pm}$ and $a_{\pm}$ are the curvatures and the locations of the potential well minima separated by the distance $L = a_{+} - a_{-}$. The solution reads\textsuperscript{15}

$$\nu = \frac{\omega_{+} \omega_{-}}{\omega_{+} + \omega_{-} + k_{+} / k_{-} + \zeta_{+} \omega_{+} / k_{-} + \zeta_{-} \omega_{-} / k_{+}}.$$  \hfill (24)

This formula also follows from Eqs. (19), (21), and (22) under the conditions formulated above.

What is particularly noteworthy about this result is the temperature-independent reciprocating velocity, which implies no contribution to the effect from thermal noise. As shown earlier,\textsuperscript{15} this is a signature of the parabolic potential involved: equilibrium and nonequilibrium fluctuations are not coupled. Even a small nonparabolicity of the potential leads to noise coupling and the temperature-dependent velocity. Generally, an interesting interplay of the noises underlain by the action of the confining potential takes place. Thus the energetic mechanism is not purely deterministic: thermal noise comes into play with nonlinear potential effects.

\section*{IV. INFORMATIONAL MECHANISM}

Consider the opposite limiting case: the engine is driven solely by the informational mechanism. Let the potential profiles of the conformational states be identical, $U_{a}(x) = U_{b}(x)$; hence the interstate transitions do not change the particle energy. Then the position-dependent part of the chemical potential $\mu_{\text{eff}}$ is determined only by the entropic term $T \ln \gamma_{\pm}(x) / \gamma_{\pm}(x)$ [cf. Eq. (23)]. So the engine operates at the expense of increased entropy. The active sites represented by the peaks of the nonequilibrium noise distributions $\omega_{\pm}(x)$ work as sources and sinks of the information about the particle position. The particle converts this information into reciprocating motion [see Fig. 1(b)].

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig1}
\caption{Schematic illustrations of the energetic (panel a) and informational (panel b) mechanisms. (a) A Brownian particle is moving in the potential that fluctuates between the two profiles $U_{i}$ (dashed line) and $U_{f}$ (dotted line) corresponding to $+$ and $-$ conformational states. The arrows designate the working cycle of the engine. This mechanism essentially exploits the difference between the state potential profiles. (b) The state potential profiles are identical, $U_{i}(x) = U_{f}(x)$ ($U_{i}(x)$ is vertically shifted for clarity). Interstate transitions occur only at “active sites” located at $x_{1}$ and $x_{2}$ with zero energy cost. The rate constants are $\gamma_{\pm} = \hat{\gamma}_{\pm,1} \delta(x-x_{1}) + \hat{\gamma}_{\pm,2} \delta(x-x_{2})$. If the relation $\hat{\gamma}_{\pm,1} / \hat{\gamma}_{\pm,2} = \hat{\gamma}_{\pm,2} / \hat{\gamma}_{\pm,1}$ holds, then $\mu_{\text{eff}}(x) = 0$, i.e., the system is at equilibrium implying probability current in neither state. If this relation is violated, the system is out of equilibrium: one of the active sites, say at $x_{1}(x_{2})$, can be treated as a source (sink) of particles in, say, state $+$($-$), while the other site in this state serves as a sink (source). As a result, Brownian motion in $+$($-$) state is biased in the positive (negative) direction. The reciprocating motion occurs due to the presence of a sink or source of information about the particle position.

As Eq. (23) shows, a generalized force that drives the reciprocating motion may be treated as the sum of two forces: one arising from the difference between the state potential profiles and the other stemming from the difference between the position-dependent rate constants of interstate transitions. This suggests two ways to modify the system stability properties and, correspondingly, two mechanisms responsible for the engine operation with quite distinct physical origins and manifestations: (i) the energetic mechanism [see Fig. 1(a)] implies that the energy fed into the system in each transition from one state to the other is converted into the particle potential energy and then used to push the particle forward or back upon relaxation and (ii) the informational mechanism [see Fig. 1(b)] makes nonequilibrium noise act as a source or sink of physical information about the particle position. The former is mainly based on mechanical nonequilibrium and the latter on chemical nonequilibrium.

It is worth mentioning that the concept of the two mechanisms underlying the fluctuation-induced transport\textsuperscript{26} has been often invoked in modeling molecular motors and pumps.\textsuperscript{5} The deterministicly dominant energetic mechanism is usually discussed in the framework of the so-called power-stroke model.\textsuperscript{27} The stochastically dominant informational mechanism is involved to account for transport in inhomogeneous systems with the position-dependent diffusion
With identical potentials, Eq. (19) is greatly simplified. In particular, the first of them can be integrated to obtain

\[
Q(x) = \frac{\gamma(x)}{\Gamma(x)} 2\Delta W(x) + C Q_0(x) 
\]

(25)

with \( \gamma(x) = \gamma_+(x) + \gamma_-(x) \), the characteristic relaxation time \( \Gamma^{-1}(x) \) defined by Eq. (20) and the equilibrium probability density \( Q_0(x) = e^{-U(x)}/\int e^{-U(x)} dx \). The integration constant \( C \) (independent of \( x \) but generally dependent on the model parameters) is determined to satisfy condition (21).

\[
\left[ \frac{\gamma(x)}{\Gamma(x)} W(x) \right]' - \frac{C}{2} \left[ \frac{\gamma_+(x) - \gamma_-(x)}{\Gamma(x)} \right] Q_0(x) + \frac{\gamma(x)}{\Gamma(x)} BU'(x) W(x) \]  

\[
\rightarrow = \beta \zeta \gamma(x) W(x). 
\]

(27)

In fact, we do not need \( W(x) \) itself but the integral (22) with this function. This suggests use of a reduced form of the differential equation, which is obtained by integration of Eq. (27) over \( x \) after multiplying it by \( x \). Then, in view of Eqs. (22) and (26) and the boundary conditions at infinity, we are led to the following relation:

\[
T \left( \frac{\Gamma(x)}{Q_0} \right) \frac{\gamma(x)}{\Gamma(x)} \left[ \frac{\gamma_+(x) - \gamma_-(x)}{\Gamma(x)} \right] \Bigg[ \frac{\gamma(x)}{\Gamma(x)} U'(x) \Bigg] = \zeta w. 
\]

(28)

As demonstrated below, in the parabolic setup the desired reciprocating velocity \( v \) [Eq. (22)] is found exactly from this relation by assuming that the characteristic relaxation time \( \Gamma^{-1}(x) \) is position independent,

\[
\Gamma(x) = (1 + \Delta) \gamma_+(x) + (1 - \Delta) \gamma_-(x) = \Gamma. 
\]

(29)

Note that in the symmetric case the condition (29) implies the position-independent \( \gamma(x) = \Gamma \) (remind that the transition rates \( \gamma(x) \) are anyway position dependent).

The following remark is to be made before we proceed. With identical potentials, the ratio \( \gamma_+(x)/\gamma_-(x) \) is constant, as followed from Eqs. (16) and (17). Then, in view of condition (29), the rate constants for the transitions caused by thermal fluctuations are \( x \)-independent, \( \gamma_{+,0}(x) = \gamma_{+,0} \) and \( \gamma_{-,0}(x) = \gamma_{-,0} \). So the \( x \)-dependence of the transition rate constants arises due to the position-dependent excitations \( \omega_+(x) \). This enables condition (29) to be rewritten,

\[
\Gamma = (1 + \Delta) \gamma_{+,0} + (1 - \Delta) \gamma_{-,0}. 
\]

(30)

For convenience of notation, let

\[
\omega_+(x) = (1 - \Delta) \omega f(x), \quad \omega_-(x) = -(1 + \Delta) \omega f(x), 
\]

(31)

where \( \omega \) and \( f(x) \) characterize the amplitude and distribution of external noise with \( 2|\omega| < \min(\gamma_{+,0}, \gamma_{-,0}) \) and \( |f(x)| \leq 1 \) for all \( x \).

Note that if \( \zeta = \zeta = \zeta \), the picture becomes especially simple because in this case \( \Gamma(x) = \gamma(x) \), \( C = 1 \), and \( Q(x) = Q_0(x) \) for any values of \( \gamma(x) \). Thus in the symmetric case, the equilibrium distribution of the position variable persists even in the absence of global equilibrium.

The second from Eq. (19) when combined with Eq. (25) gives an equation for the function \( W(x) \), which can be written as

\[
C = \frac{\langle \gamma(x) \rangle Q}{\langle \gamma(x) \rangle Q_0}. 
\]

(26)

Then for the parabolic potential \( U(x) = kx^2/2 \) and, accordingly, \( Q_0(x) = \sqrt{\beta k / (2\pi)} \exp(-\beta k x^2/2) \), it follows from Eqs. (28)–(31) that

\[
v = \omega \frac{\sqrt{\beta k}}{k} \frac{s}{2} \left( \frac{\Gamma}{Q_0} \right) \frac{\gamma(x)}{\Gamma(x)} \frac{U'(x)}{w}. 
\]

(32)

The parameter \( \chi = \zeta / k \) compares two relevant time scales: the typical sliding time in the potential \( \zeta / k \) and the characteristic relaxation time \( \Gamma^{-1} \) related to the position-independent thermally driven interstate transitions. The parameter

\[
s = \frac{\Gamma}{\gamma_0 - 2\Delta \omega f(x) Q_0} 
\]

(33)

with \( \gamma_0 = \gamma_{+,0} + \gamma_{-,0} \) accounts for the effect state asymmetry (in the symmetric case \( s = 1 \)).

Formula (32) is one of the main results of this work. This formula is the exact solution for the informational engine with the transition rates related by condition (30). It explicitly emphasizes two important points: (i) the reciprocating motion occurs due to the difference between the position-dependent rate constants of interstate transitions and (ii) a symmetric excitation must be shifted relatively to a symmetric potential for the effect to occur.

This formula also clearly shows that the role of thermal noise in the informational mechanism is substantially different from that in the energetic mechanism [cf. Eq. (24)]. At low temperatures \( T \to 0 \), the velocity exhibits a universal behavior (in the sense that it is insensitive to the specific form of external excitation): \( v \propto T \). Thus the informational engine can operate only in the presence of both thermal and nonthermal noises. Taking into account that \( f(x) \) is a bounded function of \( x \), one can verify that at high temperatures \( T \to \infty \), the velocity goes to zero with a law depending on the specific form of external excitation. So strong thermal noise essentially destroys the confining effect of the potential. Accordingly, the velocity exhibits a nonmonotonic behavior upon temperature variation, thus reflecting the constructive
and destructive roles of thermal fluctuations. For any set of the model parameters, there exists an optimal value of $T$ which maximizes the velocity $v$. Another evidence of the dual role played by thermal fluctuations in the informational mechanism is provided by the effect of thermal transitions rates on the reciprocating velocity. In the limit of slow thermal transitions, where $\gamma_0 \to 0$ and hence $\omega \to 0$, the velocity $v$ vanishes. In the opposite limit of fast spontaneous transitions, $\Gamma \to \infty$ and $v$ vanishes again.

A closer examination of the solution [Eq. (32)] reveals that the interplay of thermal and external noises leads to a rich behavior of the reciprocating velocity as a function of the relevant model parameters. To illustrate the physics of the informational mechanism, we present two simple prototypical examples in which the function $f(x)$ is explicitly used.

### A. Local excitation

Let us consider an excitation normally distributed around point $c$ with a width $q$ [see Fig. 2(a)],

$$f(x) = e^{-(x-c)^2/2q^2}.$$  

(34)

With this local excitation, the solution given by Eq. (32) takes the form

$$v = c\omega s \frac{T/(kq^2)}{1 + \chi(1 + T/(kq^2))^{3/2}} \exp\left[-\frac{1}{2} \frac{(c/q)^2}{1 + T/(kq^2)}\right],$$  

(35)

where $s$ is given by Eq. (33) with $(f(x))_0 = [1 + T/(kq^2)]^{-1/2} \exp\left[-\frac{1}{2c} (c/q)^2 / [1 + T/(kq^2)]\right]$. Note that external noise leads to a shift in the equilibrium temperature. Then as Eq. (35) suggests, the nonequilibrium steady state is characterized by the effective temperature $T_{\text{eff}} = T + kq^2$. The notion of “effective temperature” was first used in this context in Ref. 34.

Figure 2 [panels (b)–(d)] illustrates the behavior of the reciprocating velocity [Eq. (35)] as a function of the model parameters. Upon temperature variation, the velocity exhibits a stochastic resonancelike behavior shown in Fig. 2(b). At low temperatures, $T \ll T_{\text{eff}}$, the velocity goes to zero, thus demonstrating that thermal noise is a necessary ingredient for the informational engine operation. The velocity also vanishes at very high temperatures, $T \gg T_{\text{eff}}$, since the effect of the potential is drowned out by the noise in this case.

Equation (35) indicates that the excitation inducing the reciprocating motion must be shifted relative to the potential. The shift is needed to split the degenerate conformational states with identical potentials and hence to modify stability properties of the states. When the shift $c$ is small, $c \ll \sqrt{T_{\text{eff}}/k}$, the velocity $v$ grows linearly with $c$. However, when the excitation is far enough from the potential well bottom (located at the origin), i.e., in a sparsely populated region, the velocity decays exponentially as one might expect. Thus the dependence of $v$ on $c$ has a bell-shaped profile, as shown in Fig. 2(c).

Figure 2(d) presents $v$ plotted versus $q$. Note that with our setup [see Eq. (34)], the parameter $q$ characterizes not only the width but also the strength of the excitation. Since the smallness of $q$ implies not only the narrowness of the distribution $f(x)$ but also the excitation weakness, the velocity tends to zero linearly when $q \to 0$. As the distribution broadens, $q \to \infty$, the function $f(x)$ becomes increasingly flat. In this limit, $v \approx 1/q^2$. While the small-$q$ behavior of the velocity is attributed to the particular form of the local excitation considered here, the large-$q$ decay is universal. In contrast to the energetic engine, here the velocity changes non-
monotonically with the stiffness coefficient $k$. In the limit of $k$ going to zero, the points of stability disappear, the motion becomes delocalized in either state, and the energy-transduction mechanism stops, $v \propto k^{3/2}$. In the opposite limit of $k \to \infty$, the motion is confined to a very narrow region around the origin, the average $\langle f'(x) \rangle_{Q_0}$ becomes independent of $k$, and the velocity therefore decays as $k^{-1}$.

**B. Periodic excitation**

Consider a periodic excitation [see Fig. 3(a)]

$$f(x) = \cos \left( \frac{2\pi}{\lambda} x - \phi \right),$$  
(36)

where $\lambda$ is the excitation wavelength and $\phi$ is the phase shift between the excitation and the confining potential. With periodic driving, the solution given by Eq. (32) takes the form

$$v = \frac{2\pi T}{k} \sin \phi \exp \left( -\frac{2\pi^2 T}{k \lambda^2} \right) = \frac{\omega \lambda \sin \phi}{2\pi} e^{-e^{-e^{-2}}},$$

(37)

where $e=4\pi^2 T/(k \lambda^2)$, $\chi=\xi^2/k$, and $\xi$ is found from Eq. (33) at $\langle f'(x) \rangle_{Q_0} = e^{-\xi^2} \cos \phi$. We see again that a finite phase shift between the excitation and the potential is required for reciprocating motion to occur.

The dimensionless parameter $e$ reflects the combined effect of thermal noise, the periodic excitation, and the confining potential. Figure 3 [panel (b)] illustrates how the interplay of these three factors affects the reciprocating velocity. As would be expected, in both limiting cases, $e \ll 1$ and $e \gg 1$, the velocity vanishes. The maximum velocity is reached at $e$ of the order unity. As Eq. (37) shows, the velocity behavior with varying temperature (or potential strength) is qualitatively the same as that for the local excitation case. The difference is that the velocity in the present example decays exponentially rather than algebraically at large $T$ and small $k$. Equation (37) also shows that the velocity as a function of the excitation wavelength $\lambda$ exhibits a bell-shaped behavior. At short wavelengths, $\lambda \ll \sqrt{T/k}$, the effect is small since the potential change over the distance $\lambda$ is small as compared to $T$. So the velocity rapidly falls to zero with $\lambda$, $v \propto e^{-\xi^2}$. In the opposite limit of long wavelengths, $\lambda \gg \sqrt{T/k}$, the spatial dependence of the transition rates becomes very weak and the velocity vanishes, $v \propto \lambda^{-1}$.

**V. DISCUSSION**

Let us return to the dimeric motor model introduced in Sec. II. In this model, the noise-driven dynamics along the internal coordinate represents the reciprocating engine discussed in Secs. III and IV. The role of a gear that rectifies the reciprocating motion is played by asymmetric friction fluctuations. To specify the motor operation, a mechanism to produce these fluctuations should be incorporated into the model. The simplest way by which to accomplish this goal involves variation in the size or shape of the dimer heads upon the conformational changes. However, only very low rectification efficiency can be obtained in this way.

A more efficient rectification can be achieved when, along with the omnipresent viscous drag, there is an additional channel of energy dissipation provided by specific particle-track interaction, which is different for two motor heads. Several realizations of this approach are possible. A known example is the dissipation due to continuous making and breaking of weak chemical bonds between the particle and the track, which is called protein friction. The corresponding additive friction forces are linear in the velocity with the friction coefficients $\xi_v$ and $\xi_p$ for the viscous and protein friction, respectively. In contrast to the hydrodynamic drag, the protein friction takes place only if (i) the particle and the track are able to interact and (ii) the binding/unbinding kinetics is much faster than the particle motion (characterized by the sliding time and the mean residence time). In case the conditions (i) and (ii) are fulfilled, the friction coefficient is $\xi = \xi_p + \xi_0$. If the particle-track interaction is absent or the motion is so fast that the chemical bonds do not have enough time to form, the viscosity is solely responsible for the dissipation, i.e., $\xi = \xi_v$. Suppose that only one of two particles in each state is able to interact with the track, say the first particle in state + and the second in state −. Moreover, assume that the sliding along the potential profiles and interstate transitions are sufficiently slow to allow protein friction. Then the switching between the states causes the friction coefficients to fluctuate, $\xi_1(+) = \xi_p + \xi_v$ and $\xi_1(-) = \xi_v$, while $\xi_2(+) = \xi_v$ and $\xi_2(-) = \xi_p + \xi_v$. Thus, noise gives rise to left-to-right/right-to-left asymmetry that provides a rectifying action. With two “operating heads,” the rectification coefficient defined by Eq. (13) takes the value.
\[ \epsilon_p = \frac{\zeta_p}{\zeta_p + 2\zeta_v}. \]  

Substituting Eqs. (22) and (38) into Eq. (13), we obtain the velocity of the dimeric motor with an arbitrary interhead interaction in which the noise-induced internal motion is rectified by the protein friction. Since protein friction dominates, \( \zeta_p \gg \zeta_v \) the coefficient \( \epsilon_p \) is very close to unity, i.e., high rectification efficiency is achieved, \( |V| \approx |v| \). If only one of the motor heads is operative, the rectification efficiency is twice smaller, \( \frac{1}{2} \epsilon_p \).

The idea to exploit the concept of protein friction in rectifying noise-induced internal fluctuations was proposed by Mogilner et al.\textsuperscript{14} In their model, the motor is represented by two heads connected by an effective spring that fluctuates between two conformational states with different rest lengths and stiffness coefficients. Because the conformational changes caused by nucleotide binding/hydrolysis are linked to the protein friction fluctuations, the net result is directed motion. The effect was analyzed by means of a numerical simulation technique. With the biologically relevant values of the model parameters, the calculated velocity of the motor based on protein friction well reproduces the typical velocity of dimeric motor proteins. So the heuristic model exhibits qualitatively similar behavior to that observed for the protein motors. A noteworthy point is that the rectification mechanism relies on protein friction does not require any potential interaction between a motor and its track in contrast to ratchet-type models\textsuperscript{1,2} where a periodic asymmetric potential acts as a rectifier.

A shortcoming of the model developed in Ref. 14 is that the dynamics of switching between states was assumed independent of motor-head spatial positions and thermal noise, which oversimplifies the problem and leads to a motor with the only power-stroke (energetic) operational mechanism. Our model that includes the position dependence of transition rate constants overcomes the above shortcoming, so that we give proper weight to the effect of thermal noise and get an insight into the interplay of two main mechanisms: energetic and informational. Thus the model of Mogilner et al.\textsuperscript{14} is a particular case of the model considered here (with the rectification relied on protein friction), in which the interstate transition rates are position independent, the interhead interaction potential is parabolic, and the only energetic mechanism is operative. In this limiting case (with the only working head), our result for the motor velocity [see Eq. (13) with \( \epsilon = \frac{1}{2} \epsilon_p \) and \( v \) given by Eq. (24)] coincides, as it should be, with the exact solution obtained by Fogedby et al.\textsuperscript{10} for the model of Mogilner et al.\textsuperscript{14}

VI. CONCLUSIONS

Summing up, we have presented a model of a motor that operates due to rectification of the noise-induced internal movement. The model consists of a reciprocating engine that converts unbiased nonequilibrium fluctuations into reciprocating mechanical motion and a symmetry breaking mechanism. As a model for the engine, we have considered the confined motion of a Brownian particle fluctuating between two states with different potential profiles and different position-dependent rate constants of the interstate transitions. Two main mechanisms are recognized by which the engine operates in the steady-state regime: the energetic mechanism relies on the difference between the potential profiles of the competing states and the informational mechanism takes advantage of the difference between the position-dependent rate constants. While the problem is too complicated to be solved analytically in a general case with arbitrary profiles of the confining potentials, exact solutions for parabolic potential profiles have been found in the important limiting cases where only one of the motion-inducing mechanisms is operative. These solutions reveal the properties of the engine. The most notable observation is that the informational mechanism involves thermal noise as a vital component of the energy conversion process, whereas in the energetic mechanism thermal noise manifests itself only through nonlinear effects. Another notable observation is a nonmonotonic behavior of the reciprocating velocity as a function of the model parameters. This allows for the possibility of tuning the engine to optimum performance, which may be useful for applications. The rectification method is based on the asymmetry of noise-induced friction fluctuations resulting from specific particle-track interaction, which is different for two motor heads. This method not involving any effective periodic potential may serve as a possible alternative to the most common approach relied on the rectified action of the ratchet potential.

We hope that the model developed here provides a better understanding of mechanisms of energy conversion on the nanoscale and may be relevant to some aspects of the behavior of protein and artificial molecular motors. In the present paper, we have focused on physically meaningful limiting cases amenable to a fully analytical treatment. The model deserves a more detailed study including numerical simulations. In particular, it is of interest to look at a more general situation in which both the motion-inducing mechanisms are involved and an alternation of two particles is possible (a rigid ordering of particles has been tacitly assumed in the derivation of the main results of the paper). This will be the subject of the future work.

ACKNOWLEDGMENTS

The authors thank M. L. Dekhtyar for helpful comments on the manuscript. This work was supported by Academia Sinica, Y.A.M. and V.M.R. gratefully acknowledge the kind hospitality received from the Institute of Atomic and Molecular Sciences.

APPENDIX: CHEMICAL POTENTIAL OF EFFECTIVE FUEL

The derivation of Eq. (23) is based on the simple idea that the system can be driven out of equilibrium in several equivalent ways. With this in mind, consider the transitions between the conformational states caused by the chemical reaction [cf. Eq. (1)],

\[
\xi \rightarrow \xi' 
\]

\[
\xi \rightarrow \xi'. 
\]

(A1)
The processes represented by Eqs. (1) and (A1) are distinguished by the sources of unbalance. In the former case, the system is driven out of equilibrium by external noise modulating the transition rates [see Eq. (2)]. In the latter case, the process involves the unbalanced chemical species $\mathcal{F}$ or $\mathcal{F}$ so that $\nu_0(x)$ may be considered as pseudo-first-order rate coefficients: $\gamma_1(x)\nu_0(x)$ and $\gamma_1(x)\nu_0(x)$ obey the detailed balance condition

$\gamma_1(x)\nu_0(x)\rho_{\gamma_0}(x) = \gamma_1(x)\nu_0(x)\rho_{\gamma_0}(x)$.

(A4)

To establish a correspondence between the two cases, first note that $\gamma_1(x)$ and $\gamma_1(x)$ can be considered as pseudo-first-order rate coefficients: $\gamma_1(x)\nu_0(x)$ and $\gamma_1(x)\nu_0(x)$. Then Eqs. (16) and (A2)–(A4) are used to rewrite the ratio $\gamma_1(x)/\gamma_1(x)$,

$\gamma_1(x)\nu_0(x)\rho_{\gamma_0}(x) = \gamma_1(x)\nu_0(x)\rho_{\gamma_0}(x)$

(A5)

where $\mu_{\gamma_0}(x) = \mu_{\gamma_0}(x) - \mu_{\gamma_0}(x)$ is the chemical potential of the effective fuel. This expression, together with Eqs. (2), (16), and (17), leads to the result in Eq. (23).