

Dynamical mechanism for the conversion of energy at a molecular scale

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We propose a dynamical mechanism of a molecular machine for energy conversion, by considering a simple model describing the dynamics of two components, the head and the chain. After injection of energy to the head region, the energy is stored at one part for some time, and is used step by step, allowing the head to move directionally along the chain, irrespective of the direction of the input, under a fluctuating environment. Our system can adjust the timing with which the head crosses the energy barrier by taking advantage of internal dynamics and the flexibility of components. Some suggestions are given for molecular machines.

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Recently, how energy is converted from one form to another form has been extensively studied, in biochemical reaction, biomotor, and other biological processes. Often, biological processes are flexible, and work in fluctuating environment. Indeed, a mechanism of a flexible machine that works under large fluctuations was proposed by Oosawa as “loose coupling” [1,2]. In contrast to our macroscopic machine like a gear, where energy is converted one-to-one, conversion from chemical energy to mechanical work in the loose coupling does not occur all in once, but step by step. Here, the output work is distributed with some fluctuations. Indeed, such a step-by-step conversion and broad distribution of the output work are observed in some biological molecular motors [3]. This loose coupling mechanism is expected to work under fluctuations of a comparable order to the input energy.

One of the well-known and successful models for such loose coupling mechanism is thermal ratchet [4–7], which gives one plausible mechanism for the conversion of energy to mechanical work under thermal fluctuations. It is a statistical model and steady directional motion is computed from the steady current in probability distribution, under continuous supply of chemical energy. On the other hand, the energy conversion seems to proceed even by a single event of excitation of a motor protein by a chemical reaction with ATP [8]. Then, it is natural to study a model in which energy is converted only by autonomous dynamics without any external mechanism, once the system is excited by a single chemical reaction. Without going into details of specific processes of molecular motors, we introduce such dynamical model here, to propose a different general mechanism of energy conversion with loose coupling that fully takes advantage of dynamics of internal degrees of the system, neglected in a ratchet model. Although long-term dynamics adopted in the model might not be realistic for protein dynamics, it is interesting to note that, in molecular motors, existence of dynamical process with long time scale is suggested in some experiments on biological molecular motor; gradual conversion of energy which is stored in a motor for an anomalously long time [8], slow wave propagation along long filament of proteins [9], and oscillatory force generation in some molecular motors [10].

In general, we are interested in a system composing of several degrees of freedom. The system has an “input part” to which energy is injected, and an “output part” from which mechanical work can be extracted. Temporal evolution of the system is given by a set of equations with nonlinear dynamics with damping and noise coming from a heat bath [11]. From numerical simulations, it is shown that a directional motion is extracted, among all the degrees of the system, even though input is not specifically controlled with regards to its timing or direction. The model is capable of functioning with the injection of energy that is slightly larger than the energy associated with the thermal fluctuations.

The model system consists of a motor that interacts with a chain composed of N -lattice sites, positioned at x_i with index i . The motor consists of a “head” of position x_h and one internal degree of freedom in the form of a “pendulum” represented by θ . The injection of energy into the system is represented by the transfer of energy to this pendulum. The interaction potential $V(x_h - x_i, \theta)$ between the chain and the head is spatially asymmetric and its form depends on the angle of the pendulum (see Fig. 1). The periodic lattice is assumed in the chain, to consider directional motion in an

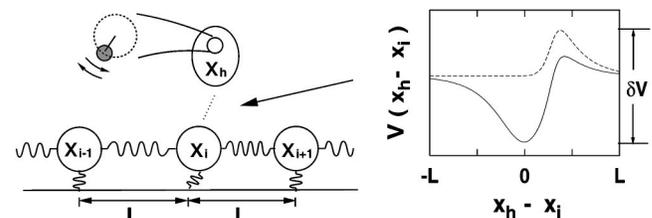


FIG. 1. Profile of the model. The form of V depends on the value of θ , where the solid curve represents the form for $\theta=0$ (the equilibrium state for θ), and the dotted curve for $\theta=\pi$. The latter value appears upon excitation, consisting of the instantaneous increase to E_0 of the kinetic energy for the pendulum. In this paper, the following parameters are fixed as $m_c = m_h = 1$, $m_\theta = 0.02$, and $L = 1$. The chain consists of 40 lattice sites with periodic boundary condition. K_c is used as a control parameter. γ is 0.01. The parameters for the potential $V(\Delta x, \theta)$ (see the text) are $p = 10$, $r = 3$, $K_h = 0.2$, and $d = L/4$.

asymmetric periodic potential as is often studied in the study of thermal ratchet. Every degree of freedom, except for the internal pendulum, is in contact with a heat bath, generating random fluctuations described by a Langevin equation with weak damping. The equations of motion for this system are chosen as

$$m_c \ddot{x}_i = -m_c \gamma \dot{x}_i + \sqrt{2m_c \gamma T} \xi_i(t) - K_c \left\{ (x_i - iL) + \left(x_i - \frac{x_{i-1} + x_{i+1}}{2} \right) \right\} - \frac{\partial V}{\partial x_i},$$

$$m_h \ddot{x}_h = -m_h \gamma \dot{x}_h + \sqrt{2m_h \gamma T} \xi_h(t) - \sum_i \frac{\partial V}{\partial x_h},$$

$$m_\theta \ddot{\theta} = - \sum_i \frac{\partial V}{\partial \theta},$$

where T is the temperature, γ is a friction coefficient, and $\xi_\alpha(t)$ represents the Gaussian white noise. Here, we use the units Boltzmann constant $k_B=1$. K_c and L are the spring constants and the natural interval between two neighboring lattice sites in the chain. m_c , m_h , and m_θ are masses of the respective degrees of freedom.

The potential form is asymmetric in space as shown in Fig. 1, where the characteristic decay length of the interaction is set at a smaller value than L , to assure that the interaction is confined mostly to the nearest lattice sites. In this paper, we adopt the following potential form:

$$V(\Delta x, \theta) = K_h \frac{\tanh(p\Delta x - r) + (1 - \cos \theta)/2}{\cosh(\Delta x/d)},$$

where the parameters p and r determine the degree of asymmetry and K_h and d give a strength and a decay length of interactions, respectively. Specific choice of this form is not important. We have simulated our model choosing several other potential forms with asymmetry and obtained qualitatively the same results for the directional motion. The pendulum mode without direct coupling to the heat bath is adopted here just as one representation of long-term storage of energy experimentally suggested in molecular motors [8]. As long as there exists such slow relaxation mode, our results follow, and this specific choice is *just an example* for it. Any mode realizing slow relaxation (even in the form of conformational change) is adopted instead.

In thermal equilibrium, no directional motion is possible on the average. However, when energy is imported to the pendulum, directional motion is observed, after a time lag. One realization of time series of the positions of the head, pendulum, and neighboring lattice sites is plotted in Fig. 2. Although this time series represents a typical example of the head motion, the particular motion differs from each event, since it includes a chaotic component and is subject to thermal noise. We computed the distribution of the number of steps as displayed in Fig. 3. In this distribution, there appears a peak at two steps, which is shifted to larger values as the amount of injected energy is increased. The distribution was

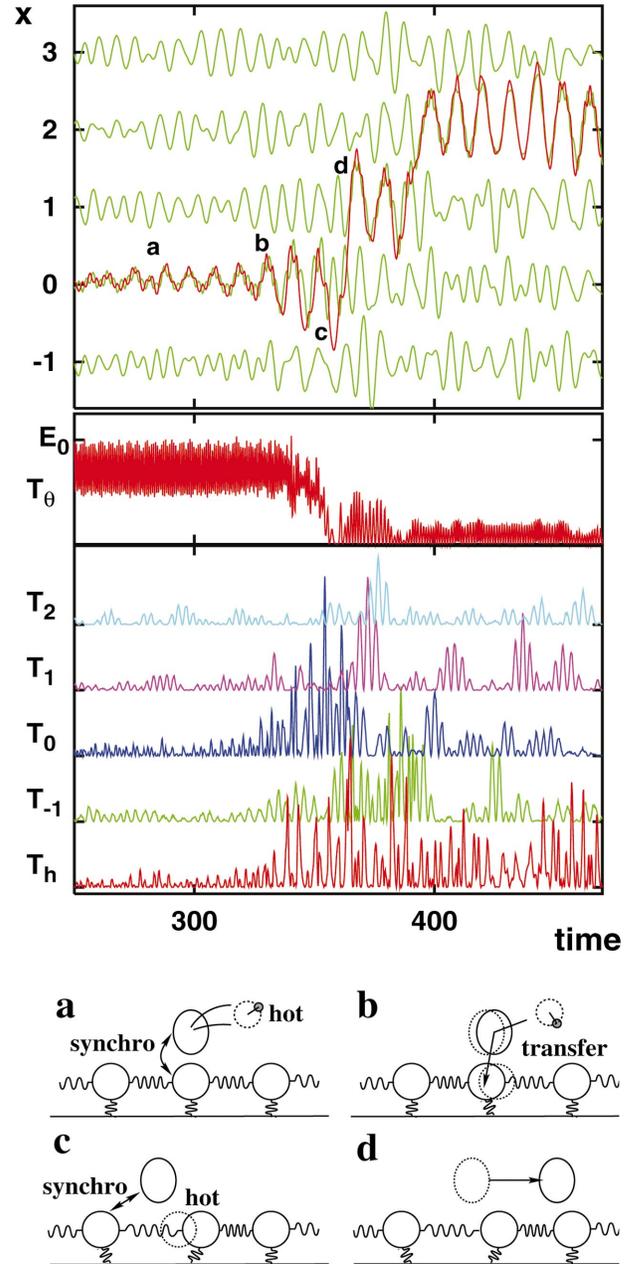


FIG. 2. (Color) A typical relaxation process following the excitation of the pendulum for $K_c=0.5$. In the simulation, the system was prepared in thermal equilibrium with $T=0.02$, and the pendulum was excited at $time=0$ with $E_0=0.4$. With the temperature used here, the head remains at one lattice site for a very long time in thermal equilibrium. Upper, time series of the positions of the head x_h (red) and a few neighboring lattice sites x_i ($-1 \leq i \leq 3$, green). Middle, time series of the kinetic energy of the internal pendulum (T_θ), the lattice sites (T_i), and the head (T_h), where the vertical scale of T_θ is larger than that of the others. In the lower schematic figures (a)–(d) correspond to each stage shown in the upper figure.

obtained from 1000 random sequences $\xi_\alpha(t)$, where, at the energy injection, configuration of internal degrees of the system is not specified. The direction of the head motion is independent of the direction of the rotation of the pendulum

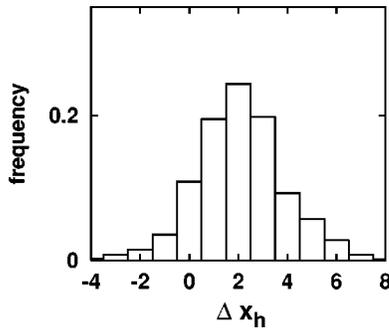


FIG. 3. Frequency distribution of the displacement (number of steps) of the head position (x_h) per an excitation. $K_c=0.5$, $T=0.02$, and $E_0=0.4$ ($=20k_B T$).

and other situation of the system. Therefore, the system functions robustly.

Here we briefly discuss the characteristics of the step distribution. In lower temperature, $\langle \Delta x_h \rangle$ is nearly equal to the variance of Δx_h . In fact, the step distribution is nearly Poissonian, i.e., the probability occurring at n steps jump is given by $P(n) = e^{-\lambda} \lambda^n / n!$ with $\lambda = \langle \Delta x_h \rangle$. With increasing the temperature, the distribution becomes broad, as is displayed in Fig. 3. It is interesting to note that this broad distribution form of steps is similar to that observed in some experiments of molecular motors [3].

The energy conversion mechanism presented here functions over a rather broad range of temperatures, as shown in Fig. 4(a). The average number of steps is a linearly increasing function of the injected energy above a certain threshold value. This implies that as the amount of injected energy increases, the ratio of converted energy to directional motion does not decay to zero, but, rather, approaches some finite constant. For low temperatures, there exists a critical value of E_0 around $\delta V = 0.34$ (see Fig. 1), below which the directional motion is suppressed. For higher temperatures, the head exhibits directional motion even for small values of E_0 . It is thus seen that the system's directional motion is robust with respect to changes of the environmental temperature and can adjust itself in response to the amount of input energy. To make this energy conversion possible, it is important that the chain should be sufficiently flexible. Indeed, if the spring constant K_c is too large, no directional motion of the head is generated [see Fig. 4(b)].

Now, we discuss how energy is converted, by closely examining the dynamics of the model. When the pendulum motion is fast, and is essentially decoupled from the head motion, the head and the nearest lattice site exhibit highly correlated vibration as depicted in Fig. 2(a). Since their motion is governed mainly by a two-body interaction, this coherent vibration is not surprising. Here the energy is stored at the pendulum for some time, as was already studied [12].

As an initially excited pendulum relaxes, their motion is eventually no longer decoupled from the rest of the system, and the pendulum, head, and the corresponding lattice site come to exhibit three-body motion. Since this motion possesses instability, the coherent motion of the head and the lattice site is lost. As a result, the vibration amplitude of the head becomes larger with energy transfer from the pendulum

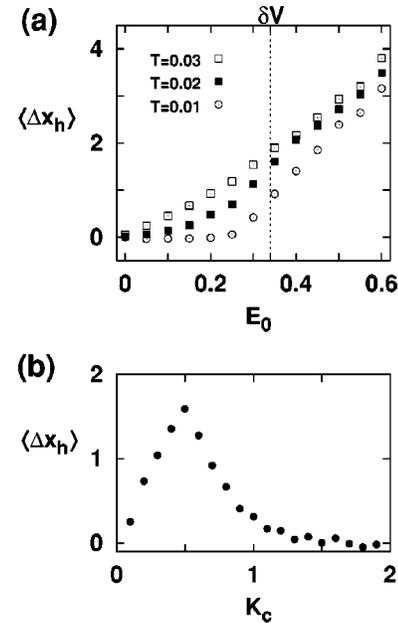


FIG. 4. (a) Average displacement $\langle \Delta x_h \rangle$ as a function of E_0 for three values of temperature computed as the ensemble average over 1000 samples. $K_c=0.5$. For larger values of E_0 , $\langle \Delta x_h \rangle$ increases as a function of E_0 in similar manners for all T . (b) Dependence of $\langle \Delta x_h \rangle$ on K_c for $T=0.02$ and $E_0=0.35$. Directional motion is most prominent in a particular range of stiffness of the chain ($K_c \approx 0.5$), where the fluctuations of the lattice are slightly larger than those of the head. The directional motion is suppressed both for larger values of K_c , because lattice fluctuations decrease in magnitude, and for smaller values of K_c , because the head interacts not only with the lattice site at which it is positioned, but also with neighboring sites, resulting in an effectively stronger potential experienced by the head.

[Fig. 2(b)]. The energy is localized at the corresponding lattice site and the head for a certain interval (see T_0 and T_h). Then, due to the large amplitude, the head begins to interact with the neighboring lattice sites. As it does so, head begins to experience the asymmetry of the potential, and its motion becomes synchronized with that of the next site to the left of the original [Fig. 2(c)]. Because the interaction between the head and the left lattice site is repulsive [see $V(x_h - x_i)$ in $x_h - x_i > L/2$], the head bounces back eventually to the next site to the right of the original after a few period of synchronization [Fig. 2(d)]. In this process, the head absorbs energy from the chain, so that it can cross over the energy barrier to the next site to the right. The timing of this crossing is spontaneously determined by the interaction of the head, pendulum, and lattice sites.

If the injected energy were dissipated completely into a large number of degrees of freedom (as heat), the conversion of energy into directional motion would suffer a rather large loss. Contrastingly, the motion generated by our mechanism remains confined to just a few degrees of freedom and highly correlated in space and time. In other words, supplied energy to the pendulum is not diffused randomly as heat, and, as a result, the injected energy can effectively be transduced to produce directional motion. For the robustness of this conversion mechanism, it is important that the motion is not

periodic but chaotic. Since chaotic motion allows continuous spectrum of frequency, in contrast to resonant periodic motion, flexible adaptation of the energy conversion mechanism to changes of the governing parameters is possible. Hence, neither fine-tuning of parameters nor external control for a driving force is needed.

If the internal modes and the rail motion are regarded to give a kind of external potential to the head, the present model can be regarded as an extension of ratchet models. An important consequence of our model, however, is that a suitable change of such external potential is formed through mutual feedback between the head motion and the other modes. The robust behavior against several parameters is a consequence of this feedback. For instance, it is observed in Fig. 2 that the energy is kept from diffusion at the site x_0 (not at the pendulum) until the head moves directionally. Such self-organized dynamics of the system allows for the energy conversion to a directional motion, while the standard ratchet models do not behave in this manner.

An advantage of using dynamics is that in this case the energy transfer can be traced directly, as shown in Fig. 2. We have found that for the present mechanism, energy must be localized within the head and neighboring lattice sites. This condition is not satisfied, for example, when the spring is stiff (i.e., when K_c is large). In that case, energy rapidly diffuses from the head to all lattice sites, and the conversion mechanism does not work, as shown in Fig. 4(b). The localization of energy in the few lattice sites near the head over some time intervals allows for effective conversion, which results in directional motion. It is interesting to note that in real molecular motor, the directional motion is suppressed when the stiffness of actin filament is increased by attaching proteins to it [13].

Although we have demonstrated the behavior of our mechanism only in a weakly dissipative system, this type of mechanism is common in dynamical systems. An extension to overdamped systems might be useful in constructing a more realistic model of a biomotor based on the present

mechanism, although it is still an open problem if the overdamped model can explain experimental data of Yanagida's group [3,8,10,14,15], where very large time lag between the injection of the energy and the directional motion is observed as in our model [8]. In addition, the time scale for the stepping motion, once it started moving, is suggested to be faster than that generally believed, and could occur in the order of nanoseconds [14], while the waiting time before stepping is in milliseconds. The ratio of inertia to viscous terms is often estimated by the Reynolds number Re . Then, for the two terms to be of comparable order [i.e., $Re \sim O(1)$], the time scale for an object of 10 nm to move over the same scale under water should be about 0.1 ns. Although it may still be smaller than the experimental data, it is not sure if one can rely upon such estimate based on macroscopic property of water. The head in our model represents a mode relevant to the interaction between a molecular motor and a rail protein, and may not be subject directly to the macroscopic water as heat bath. Note also that in equilibrium, proteins show slow thermal fluctuations of the order of seconds [15], much slower than the stepping motion. Summing up, it is still open if the stepping of the protein motor should be definitely treated as an overdamped motion.

The mechanism studied here represents a possible type of energy conversion mechanism at a molecular scale. It would be interesting to study enzyme function using this mechanism. Furthermore, it seems that designing a nanomachine for energy conversion employing our mechanism would not be too difficult, because this mechanism functions in the presence of thermal fluctuations corresponding to energies that are of the same order as the injected energy.

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