A Dynamic Mechanism of Energy Conversion to a Mechanical Work

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We propose a dynamic 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, irrespectively 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. The mechanism is shown to be robust and efficient. Some suggestions are given for molecular machines.

Recently, how energy is converted from one form to another form has been extensively studied. In biochemical reaction, some molecules are known to work for “energy converter”. On the other hand, recent progress in nanotechnology enables us to design a microscopic machine that works as energy converter. Since such molecular machine has to function under thermal fluctuations comparable to the input energy, it is questionable if it works in the same way as a macroscopic machine. This question was first addressed up by Oosawa as a dichotomy between tight and loose couplings. In the tight coupling, energy is converted one-to-one, as in our macroscopic machine. In contrast, in the loose coupling, conversion from chemical energy to mechanical work does not occur all in once, but step by step. Here, the output work is not precisely specified, but is distributed with some fluctuations.

It is important to propose possible mechanisms for the energy conversion with loose couplings, since they are relevant to consider a molecular machine working under thermal fluctuations that cannot be negligible at that scale. One of the well-known and successful models for such loose coupling mechanism is thermal ratchet. The model gave one plausible mechanism for the energy conversion to a mechanical work, and statistical analysis was carried out successfully. Here we propose another possible mechanism, that fully takes advantage of nonlinear dynamics of the system in concern. By taking a Hamiltonian dynamical model, we can trace each process of energy conversion, without using probability distribution, and study the mechanism in terms of dynamical systems. Since our model is self contained, we do not have to assume external switch of potential or specific non-white noise.

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 a mechanical work is extracted. Temporal evolution of the system is given by a set of equations with Hamiltonian dynamics with damping and noise coming from a heat bath. Since the system has several degrees of freedom, the motion generally generates fluctuations from their chaotic dynamics in addition to those by heat bath. Relevance of Hamiltonian dynamics to a rectifier is also presented by Terraneo et al.

Here we demonstrate that mechanical work is extracted as a directional motion, among all the degrees of the system, even though input is not specifically controlled with regards to its timing or direction, and without any ‘supervisor’ (i.e., external control). The model is capable of functioning with the injection of energy that is slightly larger than the energy associated with the thermal fluctuations in the system.

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 $\theta$. 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 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 damping. The equations of motion for this system are chosen as

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

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

where \( T \) is the temperature, \( \gamma \) is a friction coefficient and \( \xi_n(t) \) represents Gaussian white noise. Here, we use the units Boltzmann constant \( k_B = 1 \). \( K_c \) and \( L \) are the spring constant and the natural interval between two neighboring lattice sites in the chain. \( m_c, m_h \) and \( m_\theta \) are mass 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 Letter, we adopt the following potential form,

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

where the parameters \( p \) and \( r \) determine the degree of asymmetry and \( K_h \) and \( d \) gives a strength and decay length of interaction, 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.

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 for 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 obtained from 1000 random sequences \( \xi_n(t) \), where, at the energy injection, configuration of the system and the direction of the rotation of the internal pendulum are not taken into account. The direction of the head motion is independent of the direction of the rotation of the pendulum and other situation of the system. Therefore, the system functions robustly.

The presently studied energy conversion mechanism 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 efficiency of the energy conversion 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 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 conversion is carried out, by closely examining the dynamics of the model. As depicted in Fig.2, 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 (stage 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, in possible relationship with the Boltzmann-Jeans conjecture.

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 (stage 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 neighboring site immediately to the left of the original (stage 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 neighboring site immediately to the right of the original after a few period of synchronization (stage 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 mechanical work 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 conversion is efficient. 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.

This is in strong contrast with thermal ratchet models, popular in the theoretical study of molecular motors 10,11. In such models, to attain reasonable efficiency, it is necessary to assume a rather fine-tuned timing for the switching from one potential form of the interaction to another, or to tune the time scale of the colored noise present. When there is such fine-tuning, the motion of the ratchet and this switching are synchronized, and the energy conversion is no longer loose. Furthermore, either the switching or the specific form of the noise is externally given. In the present model, such external condition required for the thermal ratchet is generated through the dynamics. In addition, in the present model we can trace each event of the conversion of the energy to mechanical work, as in recent single-molecule experiments.

An advantage of using Hamiltonian 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 to function 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 interval allows for efficient conversion, which results in directional motion.

We have demonstrated how a coupled dynamical system with an internal degree of freedom can carry out robust conversion of energy to mechanical work generating directional motion. Note that the efficiency of our mechanism is lost when the spring of the chain is stiff as shown in Fig.4(b). This is in strong contrast with a consequence from the tight machine, where the efficiency should be higher as the chain is stiffer.

Although we have demonstrated the behavior of our mechanism only in a weakly dissipative system, this type of mechanism is common in dynamical systems, and proper extension of the present study to over-damped systems should be possible. Such an extension would be useful in constructing a more realistic model of a biomotor based on the present mechanism. It is interesting to note that the broad distribution form of steps in the present model is similar to that observed in some experiments of molecular motors 10,11, where very large time-lag between the injection of the energy and the directional motion is also observed 11.

Because the mechanism studied here operates in a Hamiltonian system, it 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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FIG. 1. Profile of the model. The form of $V$ depends on the value of $\theta$, where, the solid curve represents the form for $\theta = 0$ (the equilibrium state for $\theta$), 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 Letter, 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. $\gamma$ 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 $d = L/4$. 
FIG. 2. A typical relaxation process following excitation of the pendulum. $K_c = 0.5$. 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 ($T_\theta$), the lattice sites ($T_i$) and the head ($T_h$), where the vertical scale of $T_\theta$ is larger than that of the others. In the lower schematic figures, a - d correspond to each stage shown in the upper figure.

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

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.
Nakagawa and Kaneko  Figure 1
Nakagawa and Kaneko  Figure 4