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Autonomous energy transducer: proposition, example, basic characteristics

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Abstract

We propose a concept of autonomous energy transducer at a molecular scale, where output is produced with small input energy, not very much larger than the thermal energy, without restriction of magnitude or timing of input, and without any control after the input. As an example that satisfies these requisites, a dynamical systems model with several degrees of freedom is proposed, which transduces input energy to output motion on the average. It is shown that this transduction is robust and the coupling between input and output is generally loose. How this transducer works is analyzed in terms of dynamical systems theory, where chaotic dynamics of the internal degrees of freedom, as well as duration of excited conformation of an active part which is self-organized with the energy flow, is essential. We also discuss possible relationships to enzyme dynamics or protein motors.
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1. Introduction

How energy is converted from one form to another form has been extensively studied in these days. In biochemical reaction, some molecules are known to work for

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"energy transducer". Such energy transduction is important in enzyme function, molecular motor, and so forth, while recent progress in nanotechnology makes us possible even to design a microscopic machine that works as such energy transducer.

The question whether such molecular machine functions in the same way as a macroscopic machine was first addressed up by Oosawa [1,2] as a dichotomy between tight and loose coupling between input and output. In the tight coupling, chemical energy is converted into mechanical work via definitely scheduled successive conformational changes of molecules, and at each stage the conformational change has one-to-one correspondence to a mechanical work. This mechanism is similar to most of our macroscopic machine. Consider a typical machine with gears. It converts some form of energy to work via several rigid gears, following external operations. Each gear transforms one kind of motion to another directly and instantaneously, where fluctuations in the transformation process are negligible.

In contrast, in the loose coupling mechanism, the manner or the route to establish energy conversion does fluctuate by each event, and the energy is not necessarily converted all in once at each stage. Here, the amount of output work is not precisely specified, but varies by each event. By repeating trials, the output work extracted from the same amount of input energy (e.g., by a single reaction from ATP to ADP) is distributed with some fluctuations. Oosawa proposed that this loose coupling is a general property of a system that *robustly works* under large thermal fluctuations of the conformation of molecules even though the input energy is not very much larger than the energy of thermal fluctuations.

This problem was first posed in the study of molecular motors, where conversion from chemical energy to directional mechanical work within a fluctuating environment has been studied. Indeed, there are some experimental results suggesting loose coupling mechanisms. For instance, the energy is stored in a molecule over an anomalously long time between the chemical reaction event and emergence of directional motion [3], and multiple steps of conversion to work are repeated during molecular processes within one cycle of the chemical reaction [4]. There the resulting output steps are distributed as is expected in loose coupling mechanism. The required energy per one step could be as small as the order of the energy of thermal fluctuations. For instance, as ATP hydrolysis brings $20k_BT$ of available energy to biomolecules at room temperature, the estimated consumption of energy per one step will be $10k_BT$ if the output is two steps, and $5k_BT$ if it is four steps.

Whether the energy conversion of a biomotor is loose or tight may depend on detailed molecular structure. Still, the question how the energy conversion is possible in loose coupling mechanism is quite general, and can be discussed in any interacting molecules.

One possible mechanism for the loose coupling was proposed as thermal (or Brownian) ratchet [5–9] for a molecular motor. There, a unit exhibits a directional motion in an asymmetric potential, with the help of thermal fluctuations, and this ratchet model provides an example of a system converting energy from chemical to mechanical. This conversion is achieved in some non-equilibrium conditions, such as maintained difference of temperature, periodic forcing or switching of potentials.

In a molecular system, however, it is difficult to assume some external mechanism to maintain such non-equilibrium condition. Biomolecules often show large conformational fluctuations. Then controlled external operation to maintain some temperature difference or proper external forcing to specific switching in potential, is hardly available. Considering this difficulty, the question arisen in loose coupling can be restated as follows: *How is energy conversion achieved without external control*? To answer this question, we propose a concept of autonomous energy transducer in Section 2.

The scheme of *energy transduction of autonomous regulation* is proposed in Section 2, which works in a highly fluctuating flexible situation. In the section, we have proposed some conditions for a system to work as autonomous energy transducer. To construct an example of autonomous energy transducer, we introduce a system consisting of interacting molecules with internal dynamics, with referring some aspects of thermal ratchets, in Section 3. The specific choice of a model we adopt for this energy conversion is inspired by some experiments suggesting oscillatory molecular dynamics at a time scale of molecular work [10,11], whereas we do not pursue to make a direct correspondence with the experiment. Rather, we adopt the model to establish the concept of *autonomous energy transducer*.

By setting up an example of a dynamical systems model that satisfies the conditions given in Section 2, we will show in Section 4 that the system works as an autonomous energy transducer, and the energy transduction is possible within fluctuating environment. By analyzing the dynamical process of this energy transduction, we find some characteristic features of the dynamics that makes the coupling in this scheme generally loose. In Sections 5 and 6, robust transduction of energy within fluctuating conformation is discussed from the viewpoint of dynamical systems. The proposed mechanism may also shed new light on the function of enzyme in chemical reaction, design of a nano-machine that works at a molecular scale, and biomotors, as will be discussed in Sections 7 and 8.

2. Definition of autonomous energy transducer at molecular scale

We begin by defining a machine what we call "autonomous energy transducer" that works at a molecular scale in the absence of external controls. We postulate three requisites, by abstracting essential features of a system that converts energy within large fluctuations of conformation in molecules.

Consider a system composed of several degrees of freedom. 'Input' is injected into the system through some restricted degrees of freedom of it, which are pre-defined. Then, as a reaction to the input, there arises dynamical change in the system, which leads to 'output' as a typical motion of another set of restricted degrees of freedom. Here, the degrees of freedom for the input and for the output are distinct (for a schematic figure, see Fig. 1).

The dynamics of the system is given by the interaction among the degrees of the freedom, as well as noise from the heat bath. As a result, the system shows noisy fluctuating behavior, while, if it works as an autonomous energy transducer, input energy is transformed to stochastic output (directional motion or mechanical work)
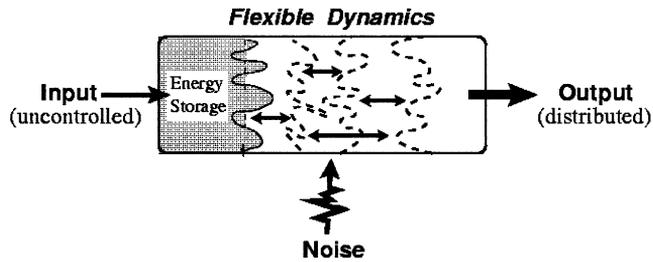
Fig. 1. Schematic figure for autonomous energy transducer.

through the dynamics. Such energy transducer can work with large fluctuations of conformation of the system, without any external control, once the energy is injected as input.

According to such consideration, at first, we postulate following requisite for the autonomous energy transducer:

 (i) Details in input event are not controlled. Neither the timing of the injection with regard to the molecule fluctuations nor the direction of the input motion is specified precisely. Even the magnitude of the input is not restricted.
 (ii) Once the input is injected, no external control is allowed, and the process is governed by a given rule for temporal evolution, while fluctuations at a molecular scale are inevitable.
(iii) In spite of this uncontrolled condition, mechanical work or directional flow can be extracted from the output motion, on the average. The system adapts itself to produce output, against the change of the input timing, direction, or magnitude.

Then, we address the question how such system is possible. In the present paper, we provide a specific example of a system satisfying this requisite, and discuss its characteristic features which realize the above three conditions.

In constructing a dynamical system satisfying these requisites, we note the following two postulates as a result of the requisites:

(A) *Flexible dynamics*: if the dynamics within the system were rigidly determined, the output should be determined by the input. Then the input–output relation should be tight, and depend on the details of the input such as its timing. To show robust average output motion without external control, some flexibility in the dynamics of the system will be required.

(B) *Energy storage*: If the system is in equilibrium with a heat bath, the directional output is not possible. Here, by an input, the system is set at a non-equilibrium condition. If the relaxation of the system to equilibrium were fast, the internal degrees of freedom would not be relevant to produce output. Then, the output would be directly determined by the input, and again the requisite would not be satisfied. To avoid such direct transduction, the input energy should be stored at some part of the system for a while. During this storage time, the system is not in equilibrium with the

heat bath, and the input energy is not directly transduced to the output as following reasons.

During the time while the energy is stored (B), detailed information of the input (such as the direction or the timing), except the energy value, is lost due to flexible dynamics (A) that are noisy and chaotic. This makes the output distributed. In other words, the input–output relationship is loose, in the sense that the output (i.e., displacement or extracted work) is distributed around its mean. There is a rather general relationship between the variance and the mean of the outputs, as will be shown.

For the energy storage, the interaction within the degrees of freedom have to be somehow restricted. For an output directional motion to appear, on the other hand, interaction with some other degrees of freedom becomes larger, after the stored energy starts to flow out. To make such a qualitative change in the system, flexible dynamics in (A) is required.

3. Model

To argue a possible loose coupling mechanism to extract work without external control, we have proposed autonomous energy transducer in Section 2, and we postulated two features, i.e., flexibility in dynamics and energy storage, to construct a dynamical systems model satisfying the requisites (i)–(iii).

In constructing a specific model, we refer to biomotors as a possible example of autonomous energy transducer. For example, in an acto-myosin system, a motor protein (e.g., myosin) moves along the chain of rail proteins, actin. Keeping the structure of acto-myosin system in mind, we adopt a model with a head particle (motor) that can move along a chain. Indeed, thermal ratchet models have this structure in common. In the thermal ratchet model, the head particle interacts with a fixed chain through a given potential with spatial asymmetry. Thermal noise is applied, while some non-equilibrium situation is sustained externally. It may be relevant to contrast our model satisfying the postulates (A) and (B) with the thermal ratchet models.

(A) *Flexible dynamics*: In thermal ratchet models, intrinsic conformational fluctuations are not explicitly discussed. Instead, external switch of potential is often introduced. In autonomous energy transducer, systems are expected to *behave autonomously* according to their dynamics, to avoid external control, and flexibility in dynamics is postulated. For this purpose we introduce a *flexible chain* as a basic structure for the model. Indeed, large conformational fluctuations are directly observed in single molecules of myosin or actin [12,13], which could be connected to the realization of loose coupling mechanism. By adopting spatially asymmetric interaction potential between the head and the elements of the chain, the effective potential is dynamically changing. From the standpoint of a ratchet model, our model might be regarded as a *deformable ratchet*.

(B) *Energy storage*: In contrast to thermal ratchet model, the system here is not sustained at non-equilibrium condition. After an input is introduced to a mode, without any specific control (with regard to the timing), the system evolves autonomously, during which energy is not dissipated immediately. The non-equilibrium situation
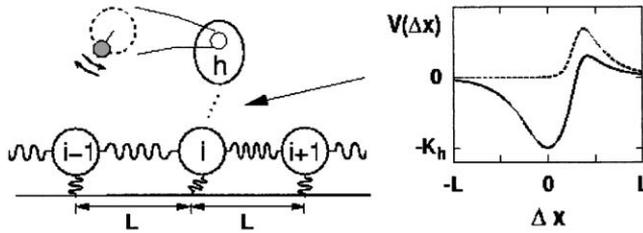
Fig. 2. Profile of the model. The form of potential V depends on the value of θ. The solid curve represents the form for $\theta = 0$ (the equilibrium state for θ), and the dotted curve for $\theta = \pi$. The latter case appears by excitation, due to the increase to E_0, the kinetic energy of the pendulum. In the simulation of this paper, the chain consists of 40 lattice sites with periodic boundary condition.

introduced by the input is sustained for a while, by using *a storage unit of energy*. Now the system includes a part that keeps energy for some time, following the energy input to it. Long-term relaxation dynamics is suggested in an experiment of a biomotor [3].

Now we reach a model consisting of a head interacting with a storage unit of energy and a flexible chain. To be specific, we adopt the following model. The motor part consists of a 'head', of position x_h, and an internal 'pendulum' represented by θ. The motor interacts with rail, represented by a one-dimensional chain of lattice sites positioned at x_i with index i. The internal pendulum is excited when energy is applied to the system. Every degree of freedom, except for θ, is in contact with a heat bath, generating random fluctuations described by a Langevin equation with damping. 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. 2). The periodic lattice is adopted as the chain, to study directional motion in an asymmetric periodic potential, as is often studied in the study of thermal ratchets.

The equations of motion for this system are chosen as

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

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

$$m_\theta \ddot{\theta} = -\sum_i \frac{\partial V(x_h - x_i, \theta)}{\partial \theta} \,, \tag{1}$$

where T is the temperature, γ is a friction coefficient and $\xi_\alpha(t)$ 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. To

observe directional motion of the head, the chain is also connected to a fixed ground via a spring with a constant K_c. Here, m_c, m_h and m_θ are mass of the respective degrees of freedom, $m_c = m_h = 1$ and $m_\theta = O(0.01)$. The inertia is not ignored, as small friction coefficient γ is adopted. Although this could be reasonable for the application to enzymatic reaction or to a design of nano-machine, one might think that biomotors should be treated as overdamped systems, considering that for small object that moves with a slow time scale, water is highly viscous fluid. Here, we introduce inertia term, because several experimental results by Yanagida's group may not necessarily match with this standard view [3,4,11–16]. Also, each variable in our model does not necessarily correspond to the atomic conformation of a protein. Rather it is a mesoscopic variable, for which effective inertia may be relevant to long-term storage of energy in dynamics of proteins, and allow for oscillatory dynamics among interacting degrees of freedom. We will come back to this 'inertia problem' in Section 8 again.

The potential form is asymmetric in space as shown in Fig. 2, where the characteristic decay length of the interaction is set at a smaller value than L, so that the interaction is confined mostly to the nearest lattice sites. Here we adopt the following potential form, $V(\Delta x, \theta) = V_x + V_\theta$ with $V_x = K_h \tanh(p(\Delta x - r))/\cosh(d \Delta x)$, and $V_\theta = K_h(1 - \cos \theta)/2 \cosh(d \Delta x)$. Here the parameters p and r determine the degree of asymmetry, while K_h and d^{-1} give the coupling strength and decay length of the interaction, respectively. Specific choice of this form is not important. We have simulated our model choosing several other potential forms with asymmetry, for instance $V(\Delta x, \theta) = K_h(1 - \cos \theta)/(\exp(p \Delta x) + \exp(-d \Delta x))$, and obtained qualitatively the same results with regard to the directional motion. In this paper, the parameters for the potential are fixed at $p = 10$, $r = 0.3$, $K_h = 0.2$, and $d^{-1} = 0.25$.

The pendulum mode without direct coupling to the heat bath is adopted here just as one representation of long-term storage of energy [17] experimentally suggested in molecular motors [3]. As long as there exists such slow relaxation mode, our results follow, and this specific choice is *just one example* for it. Any mode realizing slow relaxation can be adopted instead.

At last, we note that our model deals with each of single events of reaction process. The temporal evolution of each single event can be pursued, while the description of thermal ratchet models is at a *statistical* level. In recent single molecule experiments, each event of the conversion from chemical energy of ATP to mechanical work is pursued, and therefore the scheme of energy transduction in one single event should be investigated theoretically.

4. Output directional motion

In this section, we describe the basic properties of output directional motion for the model of autonomous energy transducer introduced in Section 3.

Once a sufficient energy is injected to the pendulum to drive the system out of equilibrium, we have observed that the head moves a few steps in one direction, on its way in the relaxation to thermal equilibrium [18]. An example of the time course of
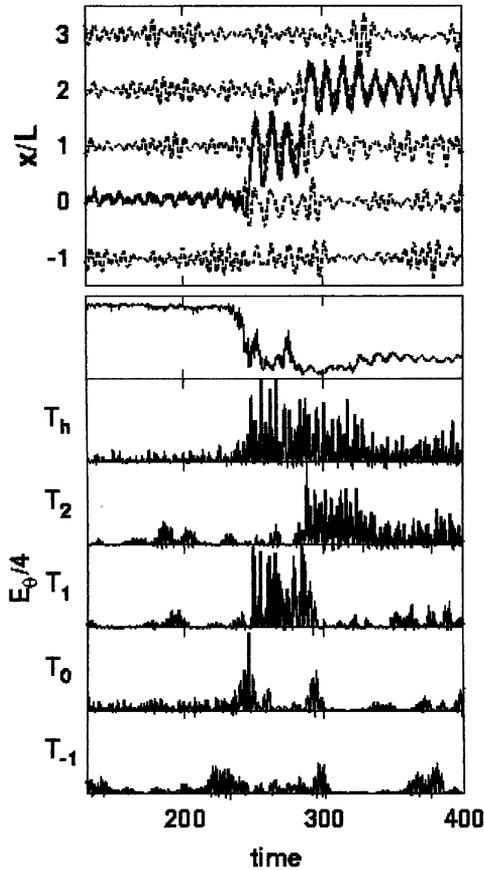
Fig. 3. A typical relaxation process following the excitation of the pendulum. $K_c = 0.5$, $M_\theta = 0.01$. In the simulation, the system was prepared in thermal equilibrium with $T = 0.01$ and $\gamma = 0.01$, and the pendulum was excited at *time* = 0 with $E_0 = 0.4$. At the thermal equilibrium with the temperature here, the head remains at one lattice site over a very long time. (Upper) Time series of the positions of the head x_h (solid line) and a few neighboring lattice sites x_i ($-1 \leqslant i \leqslant 3$, dotted lines). (Lower) Time series of the energy of the internal pendulum $E_\theta = T_\theta + V_\theta$ ($0 \leqslant E_\theta \leqslant E_0$), kinetic energy of each lattice site T_i and the head T_h ($0 \leqslant T_i \leqslant 0.16$) are plotted, where the vertical scale of T_θ is larger than those for the others.

the head motion is given in Fig. 3. How many steps the head moves after the energy injection depends on each run with different seed for the random force, even though the values of parameters including E_0 are kept constant.

In Fig. 4(a), the average step size is plotted as a function of temperature ($1/T$). The mean step size only weakly depends on the temperature for small T. It shows only slight decrease by decreasing the temperature. This is in strong contrast with the thermally activated process, in which the rate of crossing the potential barrier (for the head to shift) is given by $\exp(-U_0/T)$ with an activation energy U_0, according to Arrhenius law. At thermal equilibrium, indeed, the head shows such thermally activated motion. The resulting diffusion rate of the head Brownian motion obeys this exponential
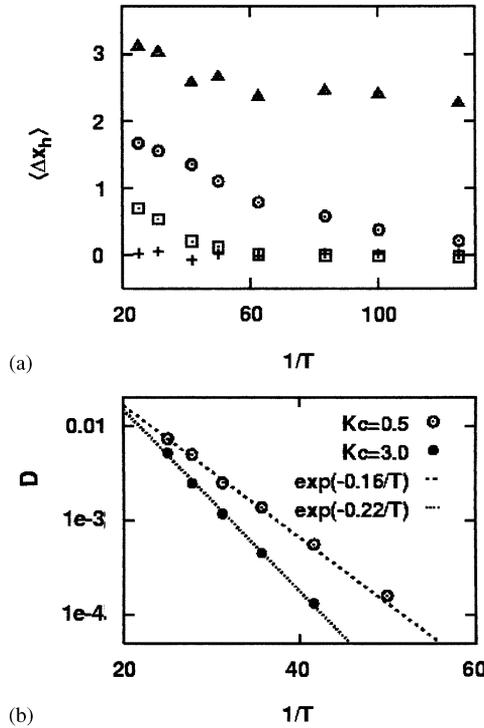
Fig. 4. (a) Mean displacement $\langle \Delta x_h \rangle$ of the head for four values of injected energy E_0, 0 (equilibrium), 0.1, 0.3 and 0.5. $K_c = 0.5$. $\gamma = 0.01$. (b) Diffusion coefficient of the head along the chain in thermal equilibrium with $\gamma = 0.01$. Here $D \equiv \langle (\Delta x_h - \langle \Delta x_h \rangle)^2 \rangle / \Delta t$. $\Delta t = 1000$.

form as shown in Fig. 4(b), whereas the values of U_0 agree with the activation energy derived analytically [19].

The dependence in Fig. 4(a) is distinct from such dependence, and the motion of the head is not thermally activated. This is natural, since the energy for the directional motion is extracted from the injected energy E_0. As a result, the head motion possesses different properties from the thermally activated motion as follows. For a fixed temperature, the average step of the head increases monotonically (almost linearly) with E_0, when the injected energy E_0 is larger than a threshold (see Fig. 5). This threshold is not equal to U_0 for the Brownian motion, but shows the following dependence upon temperature: For higher temperatures, this threshold energy goes to zero, and any small injected energy can lead to the directional motion on the average, whereas, with decreasing temperature, the threshold energy tends to converge to a certain value around 0.3. This result suggests that there is a certain minimum energy required for the head to shift to the next lattice site.

The temperature dependence suggests that the head motion is not thermally activated. Rather, it seems that the motion takes place when a suitable temporal correlation exists between the head motion and thermal fluctuations of the chain. It should also be noted
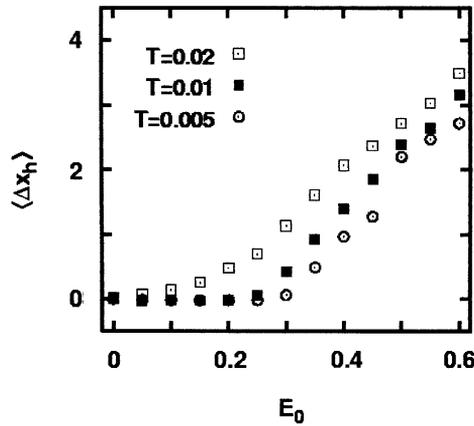
Fig. 5. Average displacement $\langle \Delta x_h \rangle$ as a function of E_0 for three values of temperature, computed as the ensemble average over 1000 samples. $K_c = 0.5$. For larger values of E_0, $\langle \Delta x_h \rangle$ increases as a function of E_0 similarly for all T.

that the directional motion is clearly observed even by the injection of the energy of $O(10)$ times of $k_B T$. For example, the average motion is about two steps, for the injection of the energy of $20 k_B T$, for $T = 0.02$. This input–output relation agrees with the experimental results in Ref. [4]. Even the broad distribution of step size per one event is rather similar (refer to Fig. 8(a)).

The linear increase of the step size with E_0 implies that the injected energy is not wasted even if it is larger than the required threshold value for the directional motion of the head. This implies that the injected energy is converted to the directional motion not at once but step by step with the successive step motion of the head. This feature is revisited in Section 6.

To make this successive energy conversion possible, it is important that the chain be sufficiently flexible. Indeed, as is shown in Fig. 6, if the spring constant K_c is too large, directional motion of the head is not observed. The directional motion is not possible, if the chain is too tight, or too flexible. The average step size has a peak around $K_c \sim 0.5$. This suggests that a flexible motion that appears under a proper stiffness, plays an important role to produce the directional motion as an output of the energy transduction. Indeed, around this parameter value, there is a transition in the dynamics of the head and neighboring few lattice points, to show correlated motion, and accordingly a rather long-range correlation appears there [19].

5. Characteristics of dynamics in energy transduction with loose coupling

Now we discuss how the above directional motion is achieved in terms of dynamical systems. We note that the present mechanism works only as a loose coupling mechanism in this section.
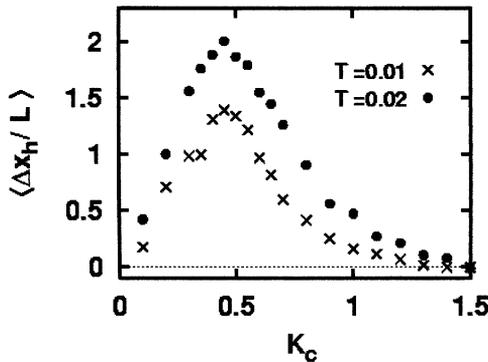
Fig. 6. Dependence of average displacement $\langle \Delta x_h \rangle$, on K_c for two temperature $T = 0.01$, 0.02 with $E_0 = 0.4$. Directional motion is most prominent in a particular range of stiffness of the chain ($K_c \approx 0.5$), where the fluctuations of the lattice are slightly larger than those of the head. The directional motion is suppressed both for larger values of K_c and smaller values of K_c. The former decrease is due to the decrease of the magnitude of lattice fluctuations, while the latter decrease is due to the interaction of the head not only with the adjacent lattice site, but also with neighboring sites, resulting in an effectively stronger potential experienced by the head.

First, let us discuss how the system 'forgets' initial conditions and how broad distribution of output step motion appears. Before the directional motion of the head, the motion of the triplet {head, pendulum, rail} shows a weakly chaotic motion, with which the input information (e.g., the conformation of the system when the input is applied) is lost. The chaotic motion here only works as weak perturbation to the two-body problems consisting of the interactions between the head and the pendulum and that between the head and the adjacent lattice site. On the other hand, when the head exhibits a step motion, there is strong interaction between the head and the lattice sites, which lead to a stronger chaotic instability arising from three- or five-body (including the neighboring lattice points) motions [19].

The change of the degree of instability is demonstrated in Fig. 7, where the evolution of difference between two close orbits is plotted. As shown, there are two rates of exponential divergence, one that continues during the energy storage, and the other with the flow of energy from the pendulum part. The former is given by perturbations to the two-body motions, and the latter is induced by strong interaction with the three- or five-body motion. The orbital instability here is examined by taking two identical initial conformations, and applying identical input energy and identical random noise (i.e., sequence of random number). A slight disturbance is added to the reference system at the timing of energy injection. The evolution of these two systems with tiny difference in conformations results in quite different number of output steps (see Fig. 7(a)). Then, it is impossible to predict or control the number and the direction of steps by the conformation of the system at the excitation. On the other hand, the directional motion appears rather independently of the conformation and, therefore, the energy conversion of the system is robust against thermal noise, and disturbances in the input event.
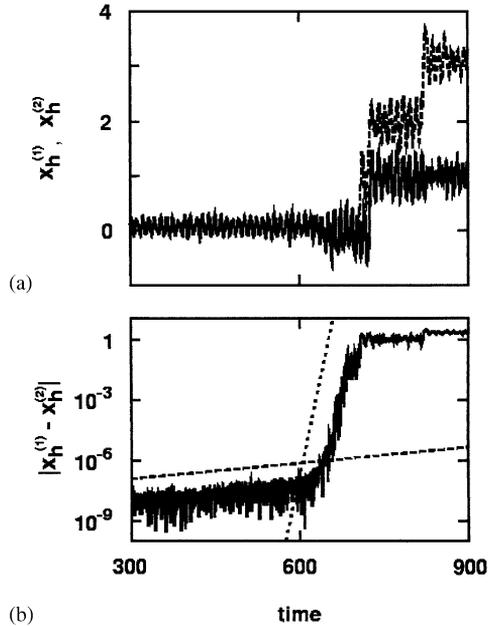
Fig. 7. (a,b) Sensitivity of the dynamics to small disturbances. The small difference at the event of excitation induces very large difference between $x_h^{(1)}$ and $x_h^{(2)}$. In the simulation, the system was prepared in thermal equilibrium before excitation with $T = 0.01$ and $\gamma = 0.01$, and the pendulum was excited at *time* $= 0$ with $E_0 = 0.35$. At the same time, small disturbance of the order 10^{-10} is added to the value of x_h. Initial conditions and applied random sequence are common to the two time sequence.

One consequence of these chaotic dynamics together with the influence of the heat bath is a *loose* relationship between the input and the output. In fact, the output number of steps shows a rather broad distribution, as shown in Fig. 8(a), where one step means the displacement of the head for one lattice site along the chain. The distribution was obtained by taking 1000 samples with arbitrarily chosen conformations at the moment of energy injection, while satisfying thermal equilibrium, and also by taking different random sequences $\xi_\alpha(t)$. The resulting distribution is rather broad, although the input energy E_0 is identical for all the samples. The difference in the output step comes mainly from intrinsic chaotic dynamics of the system mentioned above.

In the distribution of the number of steps, we note that at low temperatures the mean displacement is almost equal to its variance (sea Fig. 8(b)). If the step motion is a result of rare stochastic events, one could expect Poisson distribution. Indeed, if one disregards the small tail of the distribution at negative steps, the obtained distribution is not far from Poissonian, for low temperatures. Even for high temperatures, the linear relationship between the mean and the variance is still valid with an offset depending on the temperature. This Poisson-type distribution suggests that random process underlies the output head motion, as expected from the above chaotic dynamics.
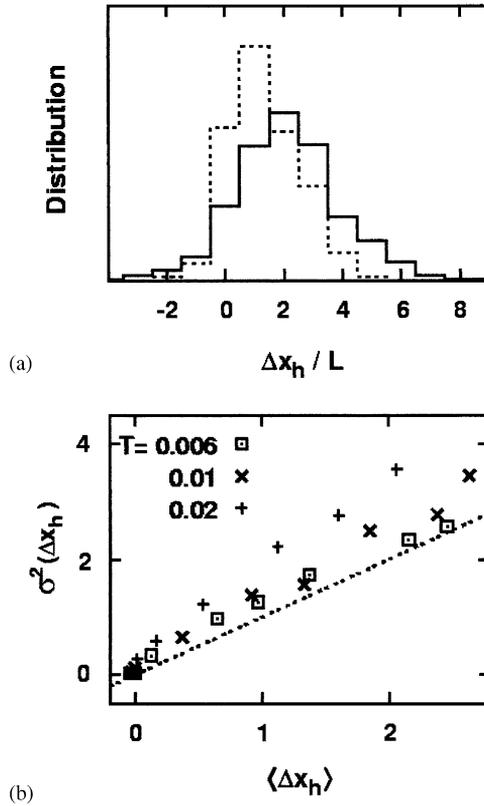
Fig. 8. (a) Frequency distribution of the displacement (number of steps) of the head position x_h per excitation for $K_c = 0.5$ and $\gamma = 0.01$. (Solid line) $T = 0.02$ with $E_0 = 0.4\,(20k_BT)$. (Dotted line) $T = 0.01$ with $E_0 = 0.4\,(40k_BT)$. (b) Relation between the mean and the variance for the step distribution in (a). $K_c = 0.5$, $\gamma = 0.01$ for three kinds of temperatures. The graph displays data for various values of E_0.

The relationship in Fig. 8(b) indicates that to obtain a sufficient output amount in directional motion, large fluctuations are inevitable. Indeed, it is not possible, at least in the present model, to make the step distribution sharp while keeping sufficient directional motion of the head, even if the parameter values are changed. For example, one could make our model rigid, by increasing stiffness K_c in the rail and suppressing the fluctuations of the conformation. Then, the directional motion is highly suppressed, as already shown in Fig. 6. The average displacement as a function of the stiffness has a maximum around $K_c \sim 0.5$, where the fluctuations of the displacement of rail elements are rather large. On the other hand, for $K_c = 1.3$, i.e., for a rigid spring of the rail, the average displacement is only 2% of the maximum. There, most of the input energy then is wasted. Accordingly, to achieve larger directional steps without wasting input energy, the step distribution has to be broad. This demonstrates the relevance of loose coupling mechanism to energy transduction.

This relevance of loose coupling is expected to be general under our postulates for the molecular transducer. Note that rigid process in tight coupling mechanism can transfer energy very well when conformations of every two parts between which the energy is transferred is precisely determined, but the efficiency will go down drastically if this precise condition for the conformations is not satisfied. In the molecular energy transducer we are concerned, such a precise control of conformations of molecules is impossible. Furthermore, as detailed information on the input is lost, control of the motion gets more difficult. Hence, the tight coupling mechanism is difficult to maintain high efficiency for a molecular transducer.

On the other hand, in the present loose coupling mechanism for the energy trans-duction, there exists chaotic motion. Then, the efficiency could be much lower than the maximum efficiency achieved by tuning initial condition in the tight coupling. However, the probability to achieve 'good' conformations starting from any initial conditions or from a variety of boundary conditions remains to be large. Hence, energy transduction in present loose coupling mechanism works over a wide range of initial conditions, and therefore is robust.

6. Characteristics of energy flow leading to directional motion

In spite of chaotic motion mentioned above, the output should be directional, in order to extract some work from the system. Here, recall that there is some time lag between the injection of energy and the emergence of the step motion, during which chaotic motion is maintained. Even after the stronger chaos appears with the flow of energy from the pendulum, there is a certain time lag before the emergence of the step motion (see Fig. 7). During such time lag, the energy may be sustained or may be used degree by degree to bring about the step motion. In this section, we examine the energy flow in detail during this 'active state' preceding to the directional motion. We will show that the duration of active state is relevant to realize the directional motion under large fluctuations of the conformations of molecules.

In Fig. 3, we have plotted the time course of energy flow to the chain from the head–pendulum part. Here, the time series for the kinetic energy of each lattice site is plotted together with that of the head. As shown, the energy flow from the head to farther lattice site is suppressed, before the step motion occurs. This restriction in the energy flow is generally observed whenever the directional motion is observed. In other words, the energy injected from the pendulum is stored for a while to the head and the adjacent three lattice sites, which we term *active part*. In contrast, there is a continuous gradual flow when the step motion is not possible.

To examine if the energy is stored at the active part with some restriction in the energy dissipation, and check its relevance to the directional motion, we have computed the following two quantities:

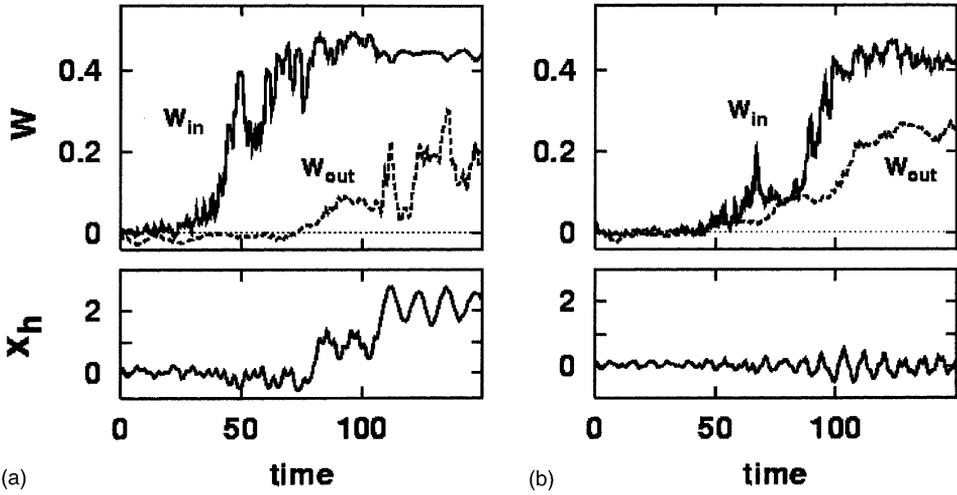$$W_{in}(t) \equiv - \sum_{j=i_0-1}^{i_0+1} \int_0^t \dot{x}_j \, \frac{\partial V_\theta}{\partial x_j} \, dt \,, \qquad (2)$$

Fig. 9. Time sequence of W_{in} and W_{out} for (a) $K_c = 0.5$, $T = 0.01$, $E_0 = 0.5$ and $m_\theta = 0.02$, and (b) $K_c = 1.0$, $T = 0.01$, $E_0 = 0.5$ and $m_\theta = 0.02$. Lower figures are corresponding time series of the position x_h for the head. For detailed explanation, see the text.

$$W_{out}(t) \equiv - \int_0^t \dot{x}_{i_0-2} \left\{ \frac{\partial V}{\partial x_{i_0-2}} - \frac{K_c}{2} (x_{i_0-1} - x_{i_0-2} - L) \right\} dt$$

$$- \int_0^t \dot{x}_{i_0+2} \left\{ \frac{\partial V}{\partial x_{i_0+2}} - \frac{K_c}{2} (x_{i_0+1} - x_{i_0+2} - L) \right\} dt . \qquad (3)$$

$W_{in}(t)$ is the energy that has flowed from the pendulum to the active part, up to time t since the energy injection, and $W_{out}(t)$ is the energy dissipated from the active part (in particular three lattice sites adjacent to the head) to farther lattice sites, again up to the time t.[1] In the present set of simulations for the measurement of W_{in} and W_{out} (and only in this set of simulations), the contact with the heat bath to the active part is eliminated, to distinguish clearly the stored energy from the wasted energy to other lattice sites. Hence, $W_{in} - W_{out}$ gives the energy storage to the active part.

A time course of W_{in} and W_{out} is shown in Fig. 9. In a certain range of parameters where the step motion frequently occurs, dissipation from the active part is delayed for some time after the energy flow from the pendulum into the system (Fig. 9(a)). During the interval for this delay, the energy is sustained in the active part (i.e., at the head and the adjacent lattice sites) for a while to keep it in excited conformation. As is shown in Fig. 9(a), the sustained energy is dissipated to the residual chain, together with the event of the step motion.[2] In contrast, for the parameters with much smaller

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[1] We note the measured values here is not "useful mechanical work" but energy transfer, because we are interested in the origin of robustness of unidirectional motion from the viewpoint of energy localization and dissipation.

[2] Note that steep changes in W_{in} and W_{out} after the step motion is an artifact since the computation here is based on the active part consisting of the head that is adjacent with the i_0, and loses its meaning after the head steps from the i_0th site.
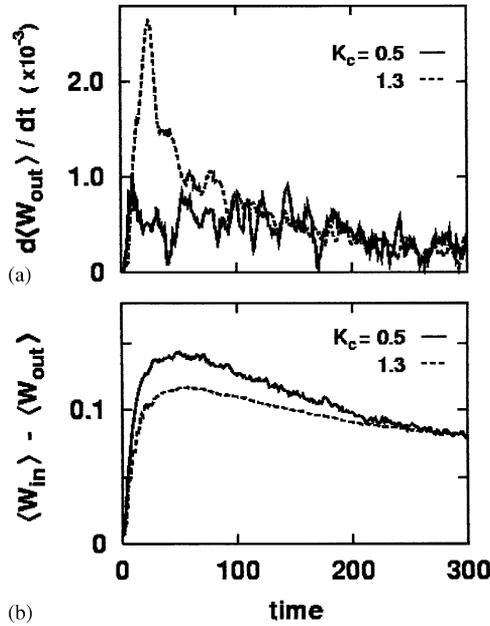
Fig. 10. Time sequence for (a) the mean energy flow $d\langle W_{out}\rangle/dt$ and (b) the mean energy $\langle W_{in} - W_{out}\rangle$ in the active part, for $K_c = 0.5$ (solid line) and $K_c = 1.3$ (dotted line). $E_0 = 0.35$ and $m_\theta = 0.02$. In this simulation, lattice sites satisfying $i \leqslant i_0 - 3$ and $i \geqslant i_0 + 3$ are contacted with the heat bath with $\gamma = 0.05$ and $T = 0.01$, in order to make the relation in energy flow clear around the active part.

directional motion, the increase of W_{in} and W_{out} begins simultaneously with the energy flow from the pendulum to the system (Fig. 9(b)). Then the system cannot keep excited conformation of the active part.

The mean profile of the energy flow from the active part is given by the time course of $d\langle W_{out}\rangle/dt$, where the ensemble average $\langle \cdot \rangle$ is computed by setting the origin of *time* as the time of the energy injection, since, for the parameters adopted here, the energy flows rapidly (in less than 10 time units) from the pendulum to the other degrees of freedom. The flow $d\langle W_{in}\rangle/dt$ takes a large value only in the initial stage (*time* < 10) of the relaxation process.[3]

As is seen in Fig. 10(a), the out-flow $d\langle W_{out}\rangle/dt$ of the energy is kept small at the early stage (up to *time* ≃ 100) of the relaxation, for $K_c = 0.5$. This is in strong contrast with the temporal profile for larger values of K_c (e.g., =1.3). Comparing the cases with large and small K_c, the active part in the flexible system does not respond instantaneously to the sudden flow of energy, and therefore the energy is sustained for a while in the active part without dissipation into the residual chain. This ensemble average of the sustained energy up to t is given by $\langle W_{in}(t) - W_{out}(t)\rangle$, as plotted in

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[3] The ensemble average at time t is computed only over the samples in which the head stays at the site i_0 up to time t. Accordingly, the number of samples decreases with the increase of the time.
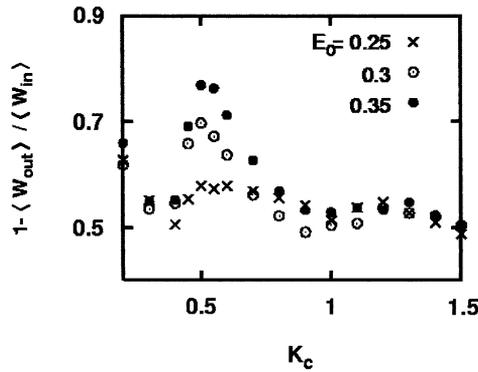
Fig. 11. The rate $\langle W_{in} - W_{out} \rangle / \langle W_{in} \rangle$, at the mean waiting time t_w. The contact with the heat bath is given in the same manner as in Fig. 10, where $\gamma = 0.05$ and $T = 0.01$. The rate is almost constant over a wide range of K_c for small injected energy $E_0 = 0.25$, which is smaller than the threshold energy for the directional motion even for $K_c \approx 0.5$ (see Fig. 5). For larger values of E_0, the rate depends strongly on K_c. Approximately half of the energy flowing into the active part is sustained even though the chain is very stiff. This is because t_w is as short time as 100. Indeed, if we choose larger t_w, this rate becomes smaller.

Fig. 10(b). The energy is sustained up to the time $t \approx 100$ when $K_c = 0.5$ and dissipated more quickly when $K_c = 1.3$.

If the injected energy were dissipated completely into a large number of degrees of freedom, the conversion of energy into mechanical work would suffer a rather large loss. Contrastingly, the motion generated by our mechanism remains confined within just a few degrees of freedom where some correlation among degrees of freedom is maintained. Supplied energy to the pendulum is not diffused as heat immediately. As a result, the conversion is efficient. The restriction of energy transfer to the farther lattice sites comes from the correlated motion among the pendulum, head, and the lattice sites [18,19].

The effective rate for the sustained energy in the active part is estimated by $\langle W_{in}(t_w) - W_{out}(t_w) \rangle / \langle W_{in}(t_w) \rangle$ by suitably choosing t_w. (As t_w is increased to infinity, these quantities go to zero, of course). By choosing the time t_w as an average waiting time for the step motion, one can estimate the sustained energy within the time scale for the step motion. The K_c dependence of this rate is shown in Fig. 11, which shows that approximately 80% of the energy flow is sustained in the active part for $K_c \approx 0.5$, where the average steps in directional motion becomes maximum. The mean waiting time t_w is almost 100 for parameter values given in Fig. 11, which is much shorter than the time for the complete dissipation of the energy.

Now, it is shown that the combination of chaotic motion (for the loss of details of input) and the restriction of dissipation (that leads to directional motion) gives a basis of our mechanism how the energy is transduced in a microscopic system under large fluctuations of their conformations. Due to the chaotic motion, if the head shifts to the next site by crossing the energy barrier or not is probabilistic. Here, the active part can keep excited conformation with sustaining the excess energy. Therefore, the head
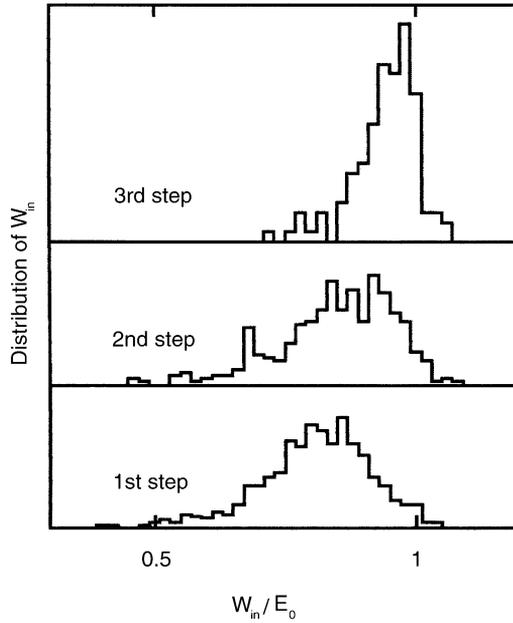
Fig. 12. Frequency distribution for the extracted energy $W_{in}(t_n)$ from the pendulum up to nth step. $W_{in}(t_n)$ is measured at the time when the head crosses nth energy barrier. $T = 0.01$, $\gamma = 0.01$, $E_0 = 0.4$, $m_\theta = 0.02$ and $K_c = 0.6$.

comes close to the barrier several times even if it fails in the first trial. Hence, the motion to cross the barrier can be robust and adaptive.

Revisiting Fig. 3, it is noted that the amount of the stored energy E_θ in the pendulum decreases step by step, corresponding to the step motion of the head. The energy once extracted from the pendulum is partly restored after the completion of the step motion. The fact that the energy is restored to the pendulum allows the delayed use for the multiple step motion. Thus, in our mechanism the energy is used step by step.

To confirm the delayed use in multiple steps, we have measured W_{in}, by restricting only to such case that multiple steps are observed (Fig. 12). Here we have computed W_{in} up to the time of the first, second, and third steps respectively. These measurements show that the extracted energy W_{in} from the pendulum up to the n-step motion increases with n. These results imply that the multiple step motion is supported by the delayed step-by-step use of the stored energy. This is why output motion with more and more steps is possible as the injected energy is increased.

In Fig. 12, one may note that the amount of the available energy in the pendulum for the next steps is smaller than that for the previous step. Indeed, the extracted energy in Fig. 12 is estimated to take a rather large value due to the timing to measure it, i.e., W_{in} is measured at the timing when the head crosses the energy barrier to move to the next site. Then, the energy stored in the pendulum is expected to be larger than expected. This is because some part of the energy is restored to the pendulum when

the head approaches the bottom of the potential for the next site, as is seen in several rises of E_θ after the first step motion shown in Fig. 3.

7. Discussion

In the paper, we have proposed a concept of autonomous energy transducer at a molecular scale. In this transducer, we have set constraints (i)–(iii) in Section 2: Output is produced, even though input energy is not very much larger than the thermal energy, and even though the magnitude or the timing of input is not specified, nor any control after the input is introduced. This requisite is postulated so that the function of the autonomous energy transducers is robust at a molecular scale.

We have shown a possible scheme that satisfies this requisite, by providing a simple example, with a dynamical system of several degrees of freedom. In the model, the energy transducer is robust by the following two properties: The first one is chaotic dynamics. The chaotic dynamics amplifies difference of initial conditions by each input and thus detailed condition on the input event is lost. Chaotic dynamics also brings mixing of orbits, and each orbit from different initial condition has a chance to visit a certain part of phase space that is necessary to generate directional motion. Hence, an output motion can be obtained on the average, independently of details of the input.

The second property is energy "storage" at "active part" in the system. The active part consists of several degrees of freedom, and is self-organized as a conformation excited by absorbing energy from the input degrees of freedom. This excited conformation is sustained over rather long time interval, with very weakly dissipating the energy. During this long time span, each orbit has more chances to visit the part of phase space inducing directional motion. Then, the ratio of the events with the directional output motion is increased.

In addition, a "storage unit", like a pendulum, enhances the potentiality of autonomous regulation of the system. [4] The dynamic linking between the storage and the active parts makes restorage of the extracted energy possible, which makes the delayed use for multiple steps easier. Such regulation would not be possible if the energy were simply provided to the active part, as assumed for a single conformational change per one chemical process.

As a consequence of our scheme of energy transduction, the output has large fluctuations by each event. There exists variance of the same order with the mean of the output. Hence input–output relationship is not one-to-one, but the output from the same input is distributed. Now, a mechanism is provided for a molecular machine with loose coupling between the input and the output, as was originally proposed by Oosawa.

For the autonomous energy transducer, the output has to be extracted without specifying input conditions, even under the fluctuations of the same order of the in-

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[4] Use of internal mode is also adopted for energy transduction, where ratchet-like motion is obtained as an output, see Ref. [20].

put. Hence, in order for the transducer to work at a molecular scale, several degrees of freedom are necessary to exhibit flexible change. The input energy is first stored into some of these degrees of freedom, and then is used step by step. Accordingly, the output is not directly coupled to the input. In contrast with a tight-coupling machine consisting of "rigid gears", the machine with this loose coupling is flexible.

After the output is extracted from the transducer, a stationary final state is restored, that is identical with the initial state before the input, except the change for the output (i.e., translational motion). In the model we presented, such stationary state is represented by a combination of stable two-body motions, that are almost decoupled each other. During the transduction process, however, several degrees of freedom in the internal states are coupled. This mode coupling leads to flexible dynamics on the one hand, but also brings about the directional motion, on the other hand. Relevance of the change of effective degrees of freedom to energy transduction has also been discussed in relationship with chaotic itinerancy [19].

Although we presented our scheme by a specific model with a head and a rail, the mechanism proposed here is expected to appear rather generally. Recalling that the essence of our model consists of flexibility in (chain) dynamics, asymmetry of potential and energy storage to some mode, we have studied some variants of the model keeping these features, to examine the generality of proposed mechanism.

Already, we have explicitly pointed out the importance of flexibility of the chain, as shown in Fig. 6 or 11. As long as the stiffness of the chain is low, the directional motion is observed independent of the form of the dynamics of the chain. To be specific, we have confirmed the directional motion in the non-linear lattice (such as FPU) instead of the harmonic chain. If the chain becomes stiff, on the other hand, the system fails to sustain energy in an excited conformation of the active part and the robust directional motion is not obtained.

As for the shape or the asymmetric potential between the head and the chain, we have also studied some variants of the model. For instance, the properties obtained here are qualitatively reproduced in an asymmetric potential form $V(\Delta x, \theta) = K_h(1 - \cos\theta)/(\exp(p\Delta x) + \exp(-d\Delta x))$ with $p \neq d$. This asymmetry in the potential here is given only as a function of the distance Δx, and the degree of asymmetry is controlled by varying the values of p and d. Up to some degree of asymmetry the directional motion is not clearly discernible, while it is left for future studies to clarify the condition for the asymmetry quantitatively.

Without the storage unit, the output directional motion is not available, unless some external operation is introduced to keep non-equilibrium situation. For instance, we have imposed and maintained the temperature difference between the head and the chain by attaching heat baths of different temperatures to each. Statistically speaking, this model shows similar output motion to the original model with the storage unit. There appears average output motion, as computed in terms of 'signal-to-noise ratio' as in Fig. 7(b), although the ratio seems to be lower than the original model with a storage unit. The dynamic link between the storage unit and the 'active part' would allow the original system to use energy effectively (refer Fig. 12). Furthermore, the two-heat-bath model above can be treated only at a statistical level, as

in a ratchet model, and the dynamics of each single input event cannot be discussed.[5]

So far we have discussed the mechanism of autonomous energy transducer for a system with a head moving along a chain. Is it generalized to a much broader class of systems? To address this question, we note that we have postulated the flexible dynamics in a system and energy storage, in Section 2. Indeed, the model in the present paper is adopted as an example satisfying these two postulates. Recollecting the dynamical systems study throughout the paper, only these two postulates are essential. Hence, it is expected that the autonomous energy transducer is possible rather generally, if a system in concern possess asymmetry for output motion, and flexibility in the system dynamics, energy storage at some part after energy is injected to the system as an input. These features are expected to be rather general in a system with interacting units at a molecular scale, whose conformation exhibits flexible dynamics, following energy input to it.

We note here that each degree of freedom we used in the model does not necessarily have to correspond to an atomic motion. Rather, it may represent a collective variable consisting of a large number of atoms. It should be also noted that the present scheme for the energy transduction is not necessarily restricted to a Langevin system with weak damping, but it is hoped that a model with overdamped dynamics will be constructed that realizes energy transduction with loose coupling by the present scheme. In this sense, the concept of autonomous transducer at a molecular scale, which we have proposed here, would be general and applied widely.

The importance of loose coupling mechanism lies in its adaptability to different conditions. Although the motion is not precisely optimized with regard to the efficiency of the transduction, instead, the present transducer works even if external conditions are changed.

As an extreme case, consider such external condition that makes directional motion much harder. For example, by adding a load to the transducer, it is expected that the output motion is suppressed. Then the question is raised if the fluctuations in the output may also be decreased. If the answer is in the affirmative, the coupling between input and output will be more tight, as added load is increased. In other words, a transducer with loose coupling can show tight coupling depending on external condition. On the other hand, a system designed to have a tight-coupling cannot work as a machine with a loose-coupling, under the change of external condition. It just does not work when the condition is changed.

To check this plasticity of energy transducer with loose-coupling, we have carried out a numerical experiment of our model by adding a load. In order to study the effect of a load, we make a slight modification of the present model; We reverse a condition for fixing the total system, i.e., the head is fixed (e.g., by attached to a glass plate), and the rail (chain) is set free, and its center of mass can move. Due to the friction

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[5] One may notice that the above variant models are quite similar to Feynman's thermal ratchet model [5]. In this case, some output motion can be obtained even in sufficiently stiff chains, where the direction of output motion is opposite to the case with the flexible chains, and is same to the direction in thermal ratchet models.
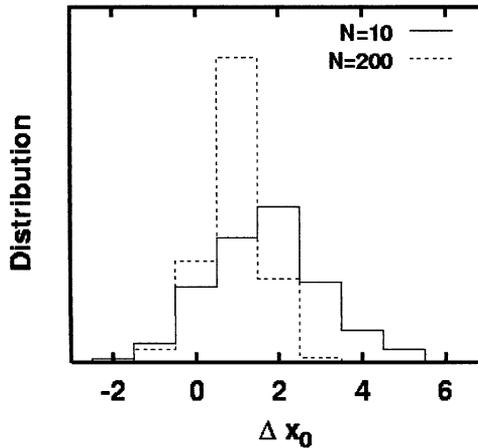
Fig. 13. Dependence of the distributions of the rail displacement upon imposed load. Frequency distributions of Δx_0 is plotted, by using the conformation of the system described in the text. $T = 0.01$, $\gamma = 0.01$, $E_0 = 0.6$, $K_c = 0.5$ and $m_\theta = 0.02$. The solid and dotted lines give distributions for a short ($N_c = 10$) and a longer rail ($N_c = 200$), respectively.

from the heat bath, the rail itself imposes a certain amount of load to the head. The amount of the load increases with the length of the rail given by N_c.

In Fig. 13, the step distributions are displayed for two different lengths of chain, ($N_c = 10$ and 200). When the length of the chain is short, the mean step size is multiple that is distributed rather broadly by samples, similarly to the original system (refer Fig. 8(a)). On the other hand, for a sufficiently long chain, the mean is still kept positive but becomes smaller in amount. Moreover, the distribution gets much sharper. The fluctuations of the output are very small, i.e., the output is almost constant, as is expected in the tight coupling mechanism. Such trend is also observed in the experiments of molecular motors [15].

8. Possible application of autonomous energy transducer

A good candidate of the autonomous energy transducer is protein. In applying the present idea to proteins, it is interesting to recall that several reports show that protein is not rigid, but flexible. Actin, a rail protein, is known to be not so stiff, as assumed in the chain of our model. Some proteins are known to take several forms and spontaneously switch over these forms under thermal energy.

Recently, there are several reports on single-molecule protein dynamics, by adopting fluorescent techniques. Some enzymes show long-term relaxation of a time scale of ms to seconds [21,22]. In particular, oscillatory dynamics with order of seconds are observed in the conformational change of single enzyme molecules, which suggest cyclic dynamics over transient states [22]. Anomalously long-term energy storage is also observed by Ishijima et al. [3]. There the chemical energy from ATP hydrolysis is stored in the motor for 0.1–1 s and then the energy is used for the directional motion gradually. The energy is used step-by-step for multiple steps [4]. Oscillatory dynamics

are also suggested in Dynein motor [11]. Summing up, several experiments support long-term dynamics in the relaxation of protein after excitations, as assumed in the dynamics of our model.

If the output is simply provided by chemical reaction, for instance by hydrolysis of ATP, such dynamical behavior would not be possible. For the dynamics, the proteins in concern should possess a "storage unit" between the domain for chemical reaction and the active part. In the present model, the storage unit is a simple pendulum and is not directly contacted with the heat bath. This is just an idealization, and the storage unit need not be so simple. Also, the obtained results would be valid qualitatively even though a weak contact with the heat bath is added.

From our result, it is postulated that the storage unit should interact with the active part bi-directionally, and the dissipation of energy from the unit is rather weak. Then, multiple step-by-step motion with restorage of the energy is possible. We hope that the storage unit that satisfies the above requisite is discovered in motor proteins.

Although the purpose of our paper is to propose a new general mechanism for loose coupling for energy conversion, application of the idea to a molecular motor may look straightforward. In doing so, however, one might claim that one should construct a model with overdamped dynamics, rather than a model with inertia. Although it should be important to construct an overdamped-dynamics version of the present mechanism, still the present model may be relevant to some molecular motors, for the following reasons.

First, it is not completely sure if the model for biomotor should be definitely over-damped. Proteins there exhibit fluctuations of very slow time scales, while the dynamics to realize directional motion is considerably rapid. The time scale for the stepping motion is suggested to be faster than microsecond order [16] and could be of nanosecond order, while the waiting time before stepping is milliseconds. In equilibrium, proteins show slow thermal fluctuations of the scale of millisecond or so [12,13]. Thus, the time scale of the relaxation of protein might be slower than, or of the same order as the stepping motion, in contrast with the standard estimate. It is still open if the stepping of the protein motor should be definitely treated as a overdamped motion. It should also be noted that in the usual estimate for the damping, one uses the viscosity of macroscopic water, whereas if the water around a protein can be treated just as macroscopic water or not is an open question [23].

Second, as already mentioned, each variable in our model does not necessarily correspond to the atomic conformation of a protein. Rather it can correspond to some mode at a mesoscopic scale, and the inertia term in our model does not directly correspond to that of an atomic motion. When the head swings along the chain, microscopic conformations do not necessarily return to the original, but may change along the relaxation. As long as some collective mode swings, the present mechanism works. A protein includes a large number of atoms. To understand energy transduction with such large molecule, it is important to use a reduced model with a smaller number of degrees of freedom representing a collective mode consisting of a large number of atoms.

Third, numerical results of the model show rather good agreement with the experimental results in Ref. [4]. Indeed, the directional motion is obtained by setting the input energy of $20k_BT$, corresponding to the available energy via ATP hydrolysis in room

temperature. [6] Furthermore, the mean step size and the distribution of steps obtained from the present model agree rather well with those in the experiment (see Fig. 8(a)).

As a theory for loose coupling, thermal ratchet models of various forms are proposed, and they have captured some features of energy conversion. However, some problems remain. First, to attain a reasonable efficiency, one needs to assume a rather tuned timing for the change of switching of potential or the time scale of colored noise. When tuned, the energy conversion often becomes one-to-one. Second, such external switching or a specific form of noise is given externally, and is not given within the theory in a self-contained form. On the other hand, in a Feynmann-type ratchet, use of different temperatures is assumed, but the temperature localized at one part of a molecule is not necessarily well defined. Some exogenous process is required. Third, the ratchet model adopts statistical description, and a single event of dynamics is not pursued, while in the recent single molecule experiments, each event of the conversion from chemical energy of ATP to mechanical work is pursued.

Whether the concept of 'autonomous energy transducer' is valid for biomotor or not has to be judged in experiments. We discuss here possible predictions that can be tested experimentally in molecular motors.

- The mean step size per one ATP hydrolysis is modified by the change of stiffness for the rail filament (see Fig. 6 for the stiffness dependence of the mean step size.) With the increase of the stiffness, the step motion is expected to decrease. In actin filaments, even longitudinal and rotational stiffnesses of the rail are quite different. Moreover, the stiffness we considered here may correspond to local flexibility on the surface of proteins in the rail, which might be difficult to detect. In spite of these subtle problems for comparison, it should be important to measure *stiffness dependence* of the step motion, to compare our prediction.
- The mean step size is modified also by the change of the amount of energy from ATP hydrolysis. If the amount of input energy is modified, the step size is predicted to change, roughly in proportion to it. Although artificial modification of the available energy by ATP is not easy experimentally, such modification of E_0, might be already realized by the long-term storage of energy in molecules. If the molecule can store the energy over several times of ATP hydrolysis, the amount of available energy will simply increase. Then, the step size realized in a single sequence would be observed to be significantly large, compared with the usual step size of molecular motors. In such cases, one-to-one correspondence would be lost between ATP hydrolysis and one sequence of stepping.
- Molecular motors can step occasionally even without activation by ATP hydrolysis. A rail element which has experienced stepping of motors accompanied by ATP hydrolysis could possess long-term memory and store a part of energy transduced from the motors during these events. Then, a motor attached to this rail protein would later receive this stored energy and use it for the stepping motion. Similarly,

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[6] There is no absolute temperature scale in the present model, and the comparison to experiment is possible by magnitude of input energy (or the potential height). The directional output is obtained by a condition experimentally plausible.

stepping events without ATP may occur due to the energy propagated from the neighboring active motors with sufficient energy from ATP hydrolysis.

- More definite proof for the relevance of autonomous dynamics in the stepping motion could be provided by direct observation of proteins dynamics. Detection of oscillation in conformation over a few periods preceding to the stepping motion will confirm the validity of the autonomous dynamics to biomotors. Measurement of conformational fluctuations with using FRETs or with using optical traps might be effective to explore this point, although for complete test of the theory, rather fine time precision, say nano or microseconds, might be required.

To conclude, we note that design of a nano-scale machine will be interesting that works under the present mechanism. Since our scheme is general and the model is simple, there can be several ways to realize the required situation. With the recent advances in nano-technology, the design of autonomous energy transducer at a molecular scale may be realized in near future.

Acknowledgements

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