Energetics of thermal ratchet models

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Abstract

Several stochastic models called thermal ratchet models have been recently proposed to analyze the motor proteins such as myosin and kinesin, etc. We propose a method to study the energetics of those models, and show how the rate of energy consumption and the energy dissipation are evaluated. As a demonstration we consider "Feynman’s ratchet", a typical fluctuating heat engine.

The motor proteins, such as myosin or kinesin, act as the energy transducer in our lives, i.e., they produce mechanical work as they consume chemical energy. Motivated by such systems various phenomenological models have recently been proposed. [1, 2, 3, 4, 5] These models, which are called thermal ratchet models, share the common feature that the net work is obtained by rectifying the random thermal fluctuation of the system and that the energy of chemical reaction is implicitly supposed to be consumed for operating the rectifier, but not for driving the system directly.
By now there are no systematic study of the energetics of those models. In most of the literatures the model stochastic equation (see eq. (1) below) or the equivalent Fokker-Planck equation have been solved, and the average power output has been calculated, while no assessment has been done to the total consumption of the energy and/or the energy wasted into heat bath. To the author’s knowledge the only literatures on thermal ratchet model which refers the energetics are the following: Feynman invented what is called Feynman’s ratchet today and and analyzed in his textbook the energetics in a qualitative argument. Magnasco considered so-called Szilard’s heat engine and claimed an expression of the net power consumed by the machine in steady state (see eq.(7) below). Also there is a proposal of the formula of the total energy consumption (with no derivation) which is variant from our result.

It is of much interest to study the energetics of biological systems since, in actuality, some of the motor proteins is reported to have very high efficiency of energy conversion. Form theoretical point of view, the formalization of energetics is motivated in relation to the question: “what should the comprehensive phenomenological model of motor protein be?” If a model of motor protein incorporates explicitly the chemical reaction processes, that is, binding of adenosine triphosphate (ATP), hydrolysis of the ATP and releasing of the hydrolysis products, then the energetics such as the efficiency of energy conversion should be tested within the model, and the framework given below will play a decisive role for such analysis. The existing models of thermal ratchets, however, do not yet fully incorporate the reaction dynamics, but merely assume that the reaction dynamics is somehow correlated to the
dynamics of the model. The analysis of the energetics of such model and its comparison with real experimental results should, therefore, serve to judge how substantial part of the energetics is grasped within the model.

In regard to the present status mentioned above, we would like to present an approach to the energetics of stochastic models of thermal ratchet or, more specifically, to show how one can define the rate of total energy consumption or the rate of energy dissipation into heat. The main purpose of this Letter is to describe a basic framework and we will not exhaust the application to all the existing models. After establishing the framework the latter task can be done in principle with the knowledge of the pertinent probability distribution functions which are already given in the literatures. Below we firstly describe the general idea, and then we specify it for three typical categories of the existing models. After that we take up a version of so-called Feynman’s ratchet model, as a demonstration, and show several concrete results of energetics.

General argument: In the thermal ratchet models, the whole system consists of the following four parts:
(i) the energy transducer, whose state variable is denoted by $x$, which may be generalized to be more than one degree of freedom,
(ii) the external system, whose state variable is denoted by $y$,
(iii) the heat bath, and
(iv) the load $L$ to which the transducer does work.

The interaction of the transducer with the external system and the one with the load are assumed to be potential-like with the potential $U(x, y) \equiv U_0(x, y) + Lx$, where $U_0$ is a periodic function of $x$ with a period $\ell$, i.e.,
$U_0(x+\ell, y) = U_0(x, y)$. The interaction with the heat bath is treated stochastically so that the heat bath exerts an instantaneous force $-\gamma dx/dt + \xi(t)$, where $\gamma$ is the friction constant and $\xi(t)$ is, as usual, the white Gaussian process characterized by the ensemble averages, $\langle \xi(t) \rangle = 0$ and $\langle \xi(t)\xi(t') \rangle = (2\gamma/\beta)\delta(t - t')$ with $\beta = (k_B T)^{-1}$ being the inverse of the temperature of the bath times Boltzmann constant. The external system is assumed to be statistically independent of $\xi(t)$.

The dynamics of the system is described by the following Langevin equation;

$$-\frac{\partial U(x, y)}{\partial x} + \left[-\gamma \frac{dx}{dt} + \xi(t)\right] = 0, \quad x(t_i) = x_i. \quad (1)$$

The property of the external system is not specified at this point except that the variation of $y$ leads to a bounded variation for $U$, that is, whether $y(t)$ itself varies in a bounded region $[2, 5, 7, 10]$ or $U$ is assumed to be periodic with respect to $y$.

We introduce the three quantities concerning the energetics of the system: (a) the work $W$ done by the transducer to the load during the period, say, $t_i < t < t_f$, which is formally given as

$$W = U(x(t_f), y(t_f)) - U(x(t_i), y(t_i)), \quad (2)$$

(b) the dissipation of energy $D$ to the heat bath, and (c) the total consumption of energy $R$ coming from the external system in the meantime. The law of energy conservation requires the relation $W + D = R$. As noted before, there are many calculation of the first quantity in the form of average power, $\langle dW/dt \rangle = L \langle dx/dt \rangle$, where $\langle dx/dt \rangle$ can be directly obtained
from the simulation of the Langevin equation (1) or by solving the equivalent Fokker-Planck equation and integrating the probability current over a section perpendicular to the $x-$axis.

Our reasoning for obtaining the remaining two quantities is based on the following observation: The equation (1) embodies the balance of forces acting on the transducer and, therefore, the transducer exerts the reaction force $[-\gamma dx/dt + \xi(t)]$ to the heat bath. Then, the dissipation, which is the work done by the transducer onto the heat bath, is given as the following Stieltjes integral

$$D = -\int_{t_i}^{t_f} \left[-\gamma \frac{dx}{dt} + \xi(t)\right] dx(t)$$

$$= \int_{t_i}^{t_f} \left[-\frac{\partial U((x(t), y(t)))}{\partial x} \right] dx(t).$$

(3)

To move on to the second line on the right hand side we have used (1). We should note here that the probability theory tells that the above integrals should be interpreted as the stochastic one in the Storatovitch sense, (3) and that we can perform the usual integration rules such as integration by parts or the change of integration variable. By the conservation law $W + D = R$ the total consumption of the energy becomes

$$R = \int_{t_i}^{t_f} \left[dU(x(t), y(t)) - \frac{\partial U(x(t), y(t))}{\partial x} dx(t) \right]$$

(4)

Below we apply the above formula of $R$ to the three categories of models with different assumptions on the variable $y(t)$, and show how this formula can be transformed into a physically appealing expression.

Category 1: $y(t)$ is a given periodic function, $y(t + T) = y(t)$. [2, 4] In this case we may write $U(x, y(t))$ as $U(x, t)$ and using the identity $dU =$
\begin{align*}
(\partial U/\partial x)dx + (\partial U/\partial t)dt, \quad & (3) \text{ becomes,} \\
R = \int_{t_i}^{t_f} \frac{\partial U(x(t), t)}{\partial t} dt, \quad & (\text{Category 1}).
\end{align*}

This expression tells that the input of energy from the external system is done by lifting the potential \( U \) while the state of the transducer, \( x \), is virtually fixed. Suppose that the probability distribution function \( P(x, t) \) is available as the solution of the Fokker-Planck equation which corresponds to (3), \( \partial P/\partial t = -\partial J/\partial x \), where \( J \equiv -\gamma^{-1} (\beta^{-1} \partial P/\partial x + P \partial U/\partial x) \) is the probability current, and the initial condition \( P(x, 0) = \delta(x - x_i) \) is satisfied. The average \( \langle R \rangle \) is then given as
\begin{align*}
\langle R \rangle = \int_{t_i}^{t_f} dt \int_{\Omega} \frac{\partial U(x, t)}{\partial t} P(x, t) dx,
\end{align*}
where \( \Omega \) is the domain of the variable \( x \). Although we treat \( x \) as a single degree of freedom for the simplicity of explanation, the generalization to more than two degrees of freedom [12] is straightforward. We can show after integration by parts that (3) is equivalent to the following expression for \( \langle D \rangle \),
\begin{align*}
\langle D \rangle = \int_{t_i}^{t_f} dt \int_{\Omega} dx \left[ -\frac{\partial U}{\partial x} \right] J,
\end{align*}
Magnasco [8] has discussed a similar expression in the case of steady state probability distribution, for a time independent potential.

\textit{Category 2:} \( y(t) \) obeys discrete Markov process. [4, 6, 12] The value of \( x(t) \) is assumed to be continuous upon the jump of \( y(t) \) from one discrete value to the other. Let us denote by \( \{ t_j \} \) the times at which such jumps occur upon a particular realization of \( y(t) \). Then \( R \) in (4) becomes
\begin{align*}
R = \sum_j [U(x(t_j), y(t_j + 0)) - U(x(t_j), y(t_j - 0))],
\end{align*}
\( (\text{Category 2}), \quad (8) \)
where the sum is taken for all the jumps occurred during $t_i$ and $t_f$. This result shows that, as in (3), the external system puts energy into the transducer by lifting the potential with $x$ taking its instantaneous value.

In order to calculate the average $\langle R \rangle$, we introduce the transition probability of $y$: If we distinguish by $\{\sigma\}$ the possible discrete values of $y$, the probability distribution function, of $x$ and $y$, $P_\sigma(x, t)$, obeys the Fokker-Planck equation like the following form, [4, 5, 13]

$$\frac{\partial P_\sigma}{\partial t} = -\frac{\partial J_\sigma}{\partial x} + \sum_{\sigma'} P_\sigma W_{\sigma'\sigma} - \sum_{\sigma'} P_\sigma' W_{\sigma'\sigma}, \quad (9)$$

where $J_\sigma \equiv -\gamma^{-1} (\beta^{-1} \partial P_\sigma / \partial x + \gamma P_\sigma \partial U_\sigma / \partial x)$ and $U_\sigma(x)$ denote, respectively, the probability current in the domain of $x$-variable, $\Omega$, and the potential with $y$ taking its $\sigma$-th value, and $W_{\sigma\sigma'}$ is the transition rate of $y$ from $\sigma$-th to $\sigma'$-th value. ($W_{\sigma\sigma'}$ can be a function of $x$ and $t$.) Using $W_{\sigma\sigma'}$ and the probability $P_\sigma(x, t)$ the average consumption $\langle R \rangle$ is given as,

$$\langle R \rangle = \frac{1}{2} \int_{t_i}^{t_f} \int_\Omega dx \sum_{\sigma} \sum_{\sigma'} (P_{\sigma} W_{\sigma'\sigma} - P_{\sigma'} W_{\sigma'\sigma}) \times [U_{\sigma'} - U_\sigma], \quad (10)$$

where the argument $x$ has been suppressed. From this expression it is clear that the net consumption of the energy comes out from the lifting of potential due to the breaking of the detailed balance with respect to $y$-values.

Category 3: $y(t)$ is a stochastic process influenced by the second heat bath. [1, 7] $y(t)$ is assumed to obey the following Langevin equation,

$$-\frac{\partial U(x, y)}{\partial y} + \left[-\gamma \frac{dy}{dt} + \dot{\xi}(t)\right] = 0, \quad y(t_i) = y, \quad (11)$$
where the second heat bath is characterized by $\hat{\gamma}$ and $\hat{\beta}(\neq \beta)$ through the conditions, \(\langle \hat{\xi}(t) \rangle = 0\) and \(\langle \hat{\xi}(t)\hat{\xi}(t') \rangle = (2\hat{\gamma}/\hat{\beta})\delta(t - t')\). The above equation tells the balance of forces on the degree of freedom, \(y\), just as \(x\) does on \(x\). By the same reasoning as we derived eq. (3), the consumption of energy from the second heat bath, \(R\), is given as

\[
R = -\int_{t=t_i}^{t=t_f} \left[ -\frac{\partial U(x(t), y(t))}{\partial y} \right] dy(t),
\]

\[
\equiv -\hat{D} \quad \text{(Category 3).} \tag{12}
\]

Using the identity \(dU = (\partial U/\partial x)dx + (\partial U/\partial y)dy\) we can verify that \(D + \hat{D} + W = 0\) holds.

In the present case the above stochastic integral \(R\) should be evaluated directly, not via the form like (3) above. The evaluation of \(\langle R \rangle (= -\langle \hat{D} \rangle \) or \(\langle D \rangle\)), therefore, requires some care about the Storatonovich calculus. \(\text{[6]}\)

Noting that the probability distribution of \(dx(t)\) and \(dy(t)\) obeys the Fokker-Planck equation with the initial condition specified at the time \(t\), and that \(\partial U/\partial x\) or \(\partial U/\partial y\) should be evaluated at the midpoint, \(t + dt/2\), as a rule of Storatonovich calculus, we arrive at the expressions;

\[
\langle D \rangle = \int_{t_i}^{t_f} dt \int_{\Omega} dx \int_{\hat{\Omega}} dy \left[ -\frac{\partial U(x, y)}{\partial x} \right] J, \tag{13}
\]

\[
\langle \hat{D} \rangle = \int_{t_i}^{t_f} dt \int_{\Omega} dx \int_{\hat{\Omega}} dy \left[ -\frac{\partial U(x, y)}{\partial y} \right] \hat{J}, \tag{14}
\]

where \(\hat{\Omega}\) is the range of the variable, \(y\), and \(\hat{J} \equiv -\hat{\gamma}^{-1} (\hat{\beta}^{-1}\partial P/\partial y + P\partial U/\partial y)\) is the probability current of \(y\). In the absence of the load, \(L = 0\), the transducer described by (3) and (11) acts as a passive heat conductor. Especially, for harmonic coupling \(U(x, y) = (k/2)(x - y)^2\) with \(k > 0\), we
can directly calculate the energy conduction rate; 

\[-\langle d\dot{D}/dt \rangle = \langle dD/dt \rangle = k(\hat{\beta}^{-1} - \beta^{-1})/\gamma + \dot{\gamma}].\]

Two remarks: Firstly the derivation of the expressions (7), (13) and (14) from the stochastic integrals (3) or (12) can be done more shortly but symbolically by regarding \(v \equiv -\gamma^{-1}(\beta^{-1}\partial/\partial x + \partial U/\partial x)\) or \(\dot{v} \equiv -\dot{\gamma}^{-1}(\hat{\beta}^{-1}\partial/\partial y + \partial U/\partial y)\) as the velocity operators along \(x\) and \(y\) directions, respectively, and rewriting, for example, \(\int_{t_i}^{t_f} dt \langle [-\partial U/\partial x]v(t) \rangle\) as \(\int_{t_i}^{t_f} dt \langle [-\partial U/\partial x]v \rangle\), etc.

Secondly in the above description the probabilities and the currents have been assumed to be the solutions of the initial value problem with a definite initial value of \(x\) (and of \(y\)) at the initial time \(t = t_i\). We can show, however, that in the long-time limit the integrals in (6), (7), (10), (13) and (14) may be alternatively evaluated by using the solutions of Fokker-Planck equation which are periodic along \(x\)-direction with the period \(\ell\) (and, for Category 1, along \(t\)-direction with the period \(T\)) under the normalization condition imposed within the spatial period. If we use such solutions, the integral \(\int_0^\ell dx\) in the equations mentioned above should be replaced by that over the period \(\ell\), say, \(\int_0^\ell dx\).

Example: Feynman’s ratchet. [7] Feynman invented a thoughtful heat engine consisting of a ratchet wheel joined tightly to a rotatable vane immersed in a first heat bath, and a pawl that is loosely attached by an elastic spring to the ratchet’s tooth and is immersed in a second heat bath. The profile of the tooth of the ratchet is asymmetric and the temperatures of the two heat baths are made different. It has been shown [7] that in this non-equilibrium system the ratchet wheel can generate a torque even under a load. Depending on the temperatures of the heat baths, one of the baths acts as a source
of energy, while the other bath acts as a breaking media, or a cooling media, which absorbs the kinetic energy of the part immersed therein. If the effect of inertia is neglected, his model is a typical example of the transducer of the Category 3 described above. Since Feynman has left only qualitative discussion on his model, the concrete description given below would be of some interest to demonstrate the feasibility of our framework.

The valuable $x$ in our notation corresponds to the angle of rotation of a ratchet wheel and $y$ represents the displacement of the pawl. The potential $U(x, y)$ can be given in the following form,

$$U(x, y) = U_1(y - \phi(x)) + U_2(y) + Lx,$$

(15)

where $\phi(x)$ is the periodic function with a period $\ell$ that represents the asymmetric saw-tooth profile of the ratchet and $U_1(z)$ stands for the short-range repulsion between the pawl and the ratchet. In the original model it is hard-core like; $U_1(z) = \infty$ for $z < 0$ and $= 0$ for $z \geq 0$. The second term $U_2(y)$ is the potential devised so that the pawl is elastically pressed down onto the ratchet tooth. We show in Fig. 1 the contour plot of the potential energy $U(x, y)$ as well as the profile of $\phi(x)$, which we used in our calculation. The values of the other parameters are also given in the figure caption.

As noted in the above remarks, in order to evaluate $\langle D \rangle$ or $\langle \dot{D} \rangle$ we need only the stationary and periodic solution of the Fokker-Planck equation

$$\frac{\partial P}{\partial t} = -\frac{\partial J}{\partial x} - \frac{\partial \dot{J}}{\partial y},$$

normalized within the range, $0 \leq x \leq \ell$. Using such solution, $\langle dD/dt \rangle$ is given as

$$\left\langle \frac{dD}{dt} \right\rangle = \int_0^\ell dx \int_\Omega dy \left[ -\frac{\partial U}{\partial x} \right] J,$$

(16)
and $\langle d\hat{D}/dt \rangle$ is obtained similarly. The average velocity $\langle dx/dt \rangle$ can be calculated as $\ell \int_\Omega dy J$. The stationarity condition $\partial J/\partial x + \partial \hat{J}/\partial y = 0$ assures that the last integral is independent of the variable $x$.

The result of our numerical calculation is given in Fig. 2. In the top figure we show the mean velocity $\langle \frac{dx}{dt} \rangle$ and the mean energy consumption rate for four values of the load. The efficiency $\eta$ can be calculated from these data as $\eta \equiv L \langle \frac{dx}{dt} \rangle / \langle \frac{dR}{dt} \rangle$ and is shown in the bottom figure of Fig. 2. Since both $\langle \frac{dx}{dt} \rangle$ and $\langle \frac{d\hat{J}}{dt} \rangle$ depend almost linearly on the load, we can safely extrapolate to find that the velocity and the efficiency vanishes when the load is about 0.0057. In the steady states $J$ and $\hat{J}$ generally compose a finite circulation $\partial J/\partial y - \partial \hat{J}/\partial x$ and, as Magnasco has pointed out, these states are qualitatively different from equilibrium states even if $\langle \frac{dx}{dt} \rangle$ vanishes; the coupling between $x$ and $y$ allows the transfer of energy even without doing work. The efficiency of the model turned out to be very small. It is because we have chosen a rather moderate potential variation (the difference of $\beta U(x, y)$ between the minima and the saddle points is about one) in order to assure the numerical accuracy. The feasibility of our formalism, however, should be understood by the present example.

In this Letter we have developed the framework to analyze the energetics of thermal ratchets that work as energy transducers while keeping contact with heat bath(s). We have developed here the point of view that Langevin equations imply the balance of forces and that the energetics of the system can be analyzed based on this balance relation with the aid of a standard probability theory. We have not exhausted the possible application of our scheme; for example, the external system may be a chaotic dynamical sys-
tem. It is a future task to construct the comprehensive phenomenological model of motor proteins in which we should specify a biochemically correct expression of the external system.

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References

[1] R. D. Vale and F. Oosawa: Adv. Biophys. 26 (1990) 97.

[2] A. Ajdari and J. Prost: C. R. Acad. Sci. Paris II 315 (1993) 1635.

[3] N. J. Cordova, B. Ermentrout and G. F. Oster: Proc. Nat. Acad. Sci. USA 89 (1992) 339.

[4] M. O. Magnasco: Phys. Rev. Lett. 71 (1993) 1477.

[5] R. D. Astumian and M. Bier: Phys. Rev. Lett. 72 (1994) 1766.

[6] C. W. Gardiner: “Handbook of Stochastic Methods” 2nd ed. (Springer-Verlag, Berlin, 1990) Chap. 4.

[7] R. P. Feynman: in “Lectures in Physics” ed. by R. P. Feynman, R. B. Leighton and M. Sands, (Addison-Wesley Publ. Co., Reading, Massachusetts, 1963), vol. I.
[8] M. O. Magnasco: *Europhys. Lett.* **33** (1996) 583.

[9] R. C. Woledge, N. A. Curtin and E. Homsher, “Energetic Aspects of Muscle Contraction” (Academic Press, New York, 1985).

[10] F. Jülicher and J. Prost: *Phys. Rev. Lett.* **75** (1995) 2618.

[11] M. O. Magnasco: *Phys. Rev. Lett.* **72** (1994) 2656.

[12] I. Derényi and T. Vicsek: *Proc. Nat. Acad. Sci.* **93** (1996) 6775.

[13] J. Prost, J. Chauwin, L. Peliti and A. Ajdari: *Phys. Rev. Lett.* **72** (1994) 2652.

[14] T. Hondou and S. Sawada: *Phys. Rev. Lett.* **75** (1995) 3269.
Figure 1: In the top figure the contour plot of the potential $U(x,y)$ is shown. The parameters we have chosen for (15) in the text are such that $U_1(z) = e^{-z}$ and $U_2(y) = \frac{1}{2}y^2$, and the profile of $\phi(x)$ is given in the bottom figure. The brighter region indicates the higher potential, and the spacing between the contours corresponds to the height of 0.5. We have discretized the region of $0 < x < \ell \equiv 1$ and $-0.25 < y < 1.65$ into $50 \times 35$ points and imposed the periodic boundary condition at $x = 0$ and $x = \ell$. As for the boundaries $y = -0.25$ and $y = 1.65$ we required $\tilde{J}$ to vanish so that the probability is conserved within the region of calculation. The inverse temperatures and the friction constants are chosen to be $\beta = 2$, $\hat{\beta} = 4$, $\gamma = 1$ and $\hat{\gamma} = 1$. 