Generalized Efficiency and its Application to Microscopic Engines

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(Received 10 March 1999)

We generalize the definition of the energy output of an engine as the minimum energy input required to accomplish the same task as the engine. Applying this new concept to molecular motors makes it possible to measure their efficiency even without attaching any external load to them. This way we can compare and characterize the operation of molecular motors in various situations. We also investigate how the thermally driven motors differ from other motors.

PACS numbers: 05.40.Jc, 02.50.Ey, 05.70.Ce, 87.10.+e

Recently, micron-scale devices have been built [1] to drive the forward motion of microscopic particles not with a net macroscopic field but with small imposed fluctuations of an anisotropic periodic "ratchet" potential [2]. Motor proteins have been experimentally studied on the level of individual proteins [3,4] and appear to work by the same principles. It seems only a matter of time before the first man-made molecular motors will be assembled [5]. Such small engines are subject to a physics that is fundamentally different from the physics of our macroscopic world. First of all, when the length scales go down the Reynolds number goes down also, and we approach the overdamped limit in which inertia no longer plays a role and where the velocity of a particle is directly proportional to the force acting on that particle at that moment. Second, there is Brownian motion. Particles are being randomly kicked around by molecules of the surrounding medium and any deterministic motion comes on top of a thermal noise term. The motion of such an overdamped Brownian particle is described by the Langevin equation

$$\dot{x}(t) = -U'(x,t)/\gamma - F_{\text{ext}}/\gamma + \sqrt{2D(x,t)}\,\xi(t), \quad (1)$$

where x denotes the position of the particle, $U(x,t)$ is the periodic ratchet potential along which the particle moves, F_{ext} is an externally applied opposing force, and $\xi(t)$ is a Gaussian white noise with the autocorrelation function $\langle \xi(t)\xi(t')\rangle = \delta(t - t')$. In general, $U(x,t)$ can depend on time explicitly, or can fluctuate between different potentials with position dependent rate constants. The diffusion coefficient $D(x,t)$ and the viscous drag coefficient γ are connected by the fluctuation-dissipation theorem $D(x,t) = k_{\text{B}}T(x,t)/\gamma$, where k_{B} denotes the Boltzmann constant and $T(x,t)$ is the absolute temperature.

One of the most important characteristics of a molecular motor is its *efficiency*. It is widely accepted that to measure the efficiency (or more precisely, the energy output) a constant external force must be applied against which the motor advances and does "useful work," which, in turn, can be stored in a battery [6]. But not all molecular motors are designed to pull loads. Some of them are designed to achieve high velocity, e.g., motor proteins that transport chemicals inside the cells. These motors operate in the Brownian regime, where thermal fluctuations are of vital importance. In contrast with our macroscopic world, where frictional forces acting on an engine can always be replaced by externally applied forces, such a replacement would drastically change the operation of microscopic engines, because the viscous friction is inseparably connected to the thermal fluctuations by the fluctuation-dissipation theorem. In order to overcome this problem and be able to measure the efficiency of such motors without the necessity of attaching any external load to them, we must generalize the concept of efficiency.

We define the energy output $\mathcal{E}_{\text{out}}$ (or power output $\mathcal{P}_{\text{out}}$) of an engine as the *minimum* energy input $\mathcal{E}_{\text{in}}^{\text{min}}$ (or minimum power input $\mathcal{P}_{\text{in}}^{\text{min}}$) required to accomplish the same *task* as the engine. In other words, the energy output is the minimum energy cost of completing a task. If we pay more input energy $\mathcal{E}_{\text{in}}$ (or input power $\mathcal{P}_{\text{in}}$) than the necessary minimum, the efficiency $\eta = \mathcal{E}_{\text{out}}/\mathcal{E}_{\text{in}} \equiv \mathcal{E}_{\text{in}}^{\text{min}}/\mathcal{E}_{\text{in}}$ is smaller than 1. The efficiency approaches 1 only if the task is completed in the energetically most favorable way. If the task is simply to charge a battery or lift a weight, the energy output reduces back to its conventional definition. However, with our new concept any task in any system can be translated into energy language and can be treated energetically.

Let us apply this now for molecular motors moving through a viscous medium at a constant temperature $T(x,t) = T$. In general, faster motion requires more energy over a fixed distance. But for $F_{\text{ext}} = 0$ all of this energy ends up heating the medium via friction and it is not recoverable afterwards. It is, however, not right to say that the energy is not being used to do useful work. In the design of motor proteins, for instance, we can assume evolution to have worked toward a compromise between fast transport and its energy cost. Consequently, for molecular motors, the task is not only to *translocate* the motor over a distance L, but also to do this during a given time τ, i.e., with a given *average velocity* $v = L/\tau$. Since the dissipation via friction ($\int_0^L \gamma\dot{x}\,dx = \gamma \int_0^\tau \dot{x}^2\,dt$) is minimal when the motor is moving uniformly [$\dot{x}(t) = v$], the power output, i.e., the minimum necessary power to

maintain a motion with an average velocity v against an opposing external force $F_{\rm ext}$, is

$$\mathcal{P}_{\rm out} \equiv \mathcal{P}_{\rm in}^{\rm min} = F_{\rm ext} v + \gamma v^2. \quad (2)$$

Our generalized efficiency $\eta = \mathcal{P}_{\rm out}/\mathcal{P}_{\rm in}$, with the above power output, makes it possible to compare and characterize the operation of molecular motors in various situations (even when $F_{\rm ext}$ is zero [7]).

The conventional definition ($F_{\rm ext} v/\mathcal{P}_{\rm in}$) is not too informative. If we plot it as a function of $F_{\rm ext}$, it starts linearly from 0, reaches a maximum, and then drops to 0 at the stall force (where $v = 0$ but $\mathcal{P}_{\rm in}$ is usually still greater than 0). In contrast, our generalized efficiency gives useful information even for small $F_{\rm ext}$. It starts from a nonzero value and may or may not exhibit a local maximum before it reaches 0 at the stall force. The maximum (which is always at a lower $F_{\rm ext}$ than the maximum of the conventional definition) marks out the optimal load of the motor. This optimal load is very useful to determine whether the motor is designed to pull big loads or to perform fast transport of small loads.

As a nontrivial example let us look at the chemical engine (or information ratchet [8]) depicted in Fig. 1a for $F_{\rm ext} = 0$, where the net motion of a Brownian particle is generated purely by rectifying its diffusion. On both potentials the particle moves diffusively between two reflecting barriers. As it hits the right (left) reflecting barrier a chemical transition with rate constant α (β) can take the particle to the other potential. More precisely, the transition rate constants are delta functions at the reflecting barriers with integrated values α and β. When the particle advances one period ($2l$) to the right it consumes $\Delta G = 2k_{\rm B}T \ln(\alpha/\beta)$ free energy. Consequently, for $\Delta G > 0$ there will be a net flux, j, from left to right. To determine the particle's average velocity, $v = 2lj$, we analyze the system in terms of probability densities. Because of the symmetry of the system, at steady state we can denote the probability density by P_- at the left end and by P_+ at the right end of each accessible interval on both potentials. Since the potentials are flat between the reflecting barriers, the probability density changes linearly along the intervals. We can write for the flux

$$j = \alpha P_+ - \beta P_-, \quad (3)$$

$$j = D(P_- - P_+)/l, \quad (4)$$

and for the normalization over one period

$$2l \frac{P_- + P_+}{2} = 1. \quad (5)$$

Eliminating P_- and P_+ from the three equations we get

$$j = \frac{D}{l} \frac{\alpha - \beta}{2D + (\alpha + \beta)l} < \frac{D}{l^2} \frac{\alpha - \beta}{\alpha + \beta} = \frac{D}{l^2} \tanh\left(\frac{\Delta G}{4k_{\rm B}T}\right). \quad (6)$$

Since the power input is $\mathcal{P}_{\rm in} = j\Delta G$, we get

$$\eta = \frac{\gamma(2lj)^2}{j\Delta G} < \frac{\tanh[\Delta G/(4k_{\rm B}T)]}{\Delta G/(4k_{\rm B}T)} \quad (7)$$

for the engine's efficiency. The last expression is always smaller than 1, goes to zero as $\Delta G \to \infty$, and approaches 1 as $\Delta G \to 0$.

An interesting consequence of Eq. (7) is that in the optimal situation (when η approaches 1) the average velocity, $v = 2lj$, approaches $\Delta G/(2l\gamma)$, i.e., the particle behaves as if a constant $\Delta G/(2l)$ force were pulling it. To see how a rectified diffusion (where ΔG free energy is liberated in each period of length $2l$) can be converted to a uniform motion with a constant pulling force $\Delta G/(2l)$, we map the system of Fig. 1a to the staircase potential of Fig. 1b with kinetic barriers at the step edges. If the transition rate constants are fast enough ($2D/l < \alpha + \beta$), the kinetic barriers can be neglected, and the Brownian particle is basically moving on a monotonic staircase potential. Since the motion along a potential with an average slope $\Delta G/(2l)$ is fastest if the potential is a straight slope, the maximum average velocity of the particle is indeed $\Delta G/(2l\gamma)$. This velocity can be approached only when the stepwise nature of the potential vanishes in the thermal noise, i.e., when $\Delta G \ll k_{\rm B}T$, in agreement with Eq. (7). Similar arguments hold for other chemical engines, indicating the reliability and usefulness of our generalized definition of the efficiency. In particular, recent experiments [4] on the stepping motion of the F_1-ATPase motor have revealed that, for $F_{\rm ext} = 0$ and for different values of γ, the quantity $\gamma v L$ (where L is the step size) approaches the free energy of ATP (adenosine 5′-triphosphate) hydrolysis, i.e., the generalized efficiency of this motor approaches unity in the load-free case. Further investigation of the generalized efficiency in the presence of external loads could provide more information about the operation of

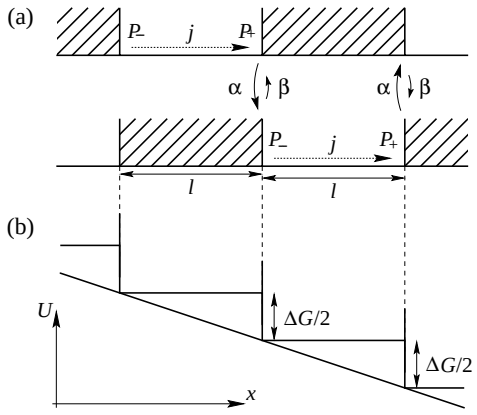

FIG. 1. (a) A chemical engine, where a Brownian particle moves diffusively in the unshaded regions of both potentials, and a chemical transition at the reflecting barriers of the unshaded intervals takes the particle from one potential to the other. (b) The system can be mapped to a staircase potential with step heights $\Delta G/(2l)$ and with kinetic barriers at the step edges.

the motor. Note that the chemical engine of Fig. 1a is a special case of Huxley's model [9] for the actomyosin system with zero spring constant and delta function transition rates.

Let us now consider a thermally driven motor or heat engine (such as the one in Fig. 2a), where the temperature $T(x)$ along the periodic potential is constant in time, but inhomogeneous in space [10,11]. For part of each period, the Brownian particle is in contact with a cold reservoir at temperature T_c, while everywhere else it is in contact with a hot reservoir at temperature T_h. For isothermal motors we reported that the energy dissipated via friction is not recoverable. For nonisothermal motors, however, this is not necessarily true. Any heat that is dissipated into the hot reservoir "charges up" the heat engine, and therefore can partially be recovered.

The schematic diagram in Fig. 2c represents a heat engine operating between two reservoirs: W useful work is extracted while Q heat is transferred from the hot reservoir to the cold one (solid gray arrows). Normally, the heat engine is recharged by supplying the hot reservoir with $Q + W$ heat. However, if we use W to do some job, during which part of W is dissipated into the hot reservoir, less than $Q + W$ heat is enough to recharge the engine. In the optimal situation, all of the W work is eventually dissipated into the hot reservoir (dashed gray arrow), reducing the necessary heat to recharge the engine to only Q.

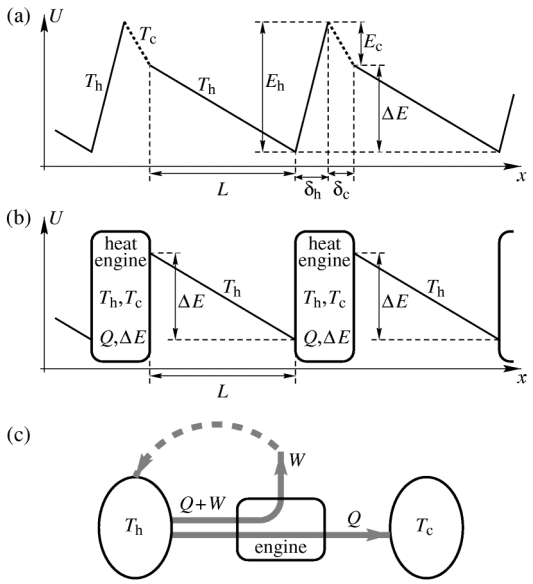

FIG. 2. (a) Schematic picture of a thermally driven Brownian motor. Since the system is cooled down on a descending part of the potential, the motion of the particle becomes rectified to the right. (b) The system can be viewed as a periodic array of heat engines (which raise the particle's potential energy by ΔE while transferring heat Q to the cold reservoir) connected by downslides (along which the particle dissipates the ΔE energy back into the hot reservoir). (c) The diagram illustrates a heat engine. An amount of energy $Q + W$ is extracted from the hot reservoir. Q immediately goes into the cold reservoir and W is transduced into useful work, which eventually can be dissipated back into the hot reservoir.

This optimal case is realized by the system in Fig. 2b, which consists of a periodic array of heat engines connected by downslides of length L at temperature T_h. Each engine raises the particle's potential energy by $W \equiv \Delta E$ while transferring some heat Q to the cold reservoir, and the particle dissipates this ΔE energy back into the hot reservoir along its way down to the next engine. If the heat engines are much smaller than L and operate much faster than the average duration of a downslide, the particle experiences a uniform motion with an average velocity $v = \Delta E/(L\gamma)$. We will see later how the parameters of Fig. 2a should be chosen to get a system that matches the above description.

For simplicity, we first consider the load-free case. To calculate the power output (i.e., the minimum power input) we suppose that the heat engines operate reversibly, i.e., the entropy production is zero:

$$\frac{Q + \Delta E}{T_h} = \frac{Q}{T_c}, \text{ from which } Q = \frac{T_c}{T_h - T_c}\,\Delta E\,. \quad (8)$$

To keep the power input minimal, the engines have to be recharged in the energetically most favorable way, i.e., the hot reservoir has to be supplied with heat Q (and not $Q + \Delta E$) by operating a heat pump between the two reservoirs reversibly: $Q/T_h = (Q - \mathcal{E}_{in}^{min})/T_c$. From this equation the minimum energy input per period can be expressed as

$$\mathcal{E}_{in}^{min} = \frac{T_h - T_c}{T_h}\,Q = \frac{T_c}{T_h}\,\Delta E\,, \quad (9)$$

and the minimum power input is

$$\mathcal{P}_{in}^{min} = \frac{v}{l}\,\mathcal{E}_{in}^{min} = \frac{T_c}{T_h}\,\gamma v^2. \quad (10)$$

A very interesting and counterintuitive consequence of this result is that for a fixed power input a thermally driven molecular motor can achieve larger velocity than any isothermal motor by a factor of $\sqrt{T_h/T_c}$. This also means that, while the velocity of an isothermal motor is limited by the power input, the velocity of a thermally driven motor has no such limit and can be increased arbitrarily by increasing T_h.

Another way of deriving the factor T_h/T_c is as follows. Since the useful work is finally dissipated into the hot reservoir (see Fig. 2c), the $q = (T_h - T_c)/T_h$ part of it can be recovered for later use. But, because the q part of this part can be recovered again, we end up with a geometric series with quotient q. The sum of this series, $1/(1 - q) = T_h/T_c$, tells us how many times the input energy can eventually be used to do some work, if during the work the energy is completely dissipated back to the hot reservoir.

Thus, according to our definition for the generalized power output, we have to modify Eq. (2) to include

the possible reuse of the dissipated energy if the motor operates in a nonisothermal environment:

$$\mathcal{P}_{\text{out}} = F_{\text{ext}} v + \frac{T_c}{T_h} \gamma v^2. \quad (11)$$

In general, T_h and T_c denote the two extremes of the temperature. Since $F_{\text{ext}} v$ goes into the potential energy of the external load, it is not dissipated, and therefore it must not be multiplied by T_c/T_h.

Finally, let us see how the system in Fig. 2b can be realized with the setup of Fig. 2a. Since the Langevin equation (1) is invariant under the transformation $\{T, U, x\} \to \{\kappa T, \kappa U, \sqrt{\kappa}\, x\}$, one can get rid of the space dependence of the temperature by applying this transformation with $\kappa = T_h/T_c$ to the segments at temperature T_c. This changes the length of these segments to $\delta_c^* = \delta_c \sqrt{T_h/T_c}$, but most importantly it also changes their height to $E_c^* = E_c T_h/T_c$. If we choose the parameters such that $E_h = E_c^*$, and both δ_h and δ_c go to zero, the barriers of the transformed potential disappear and the downslides line up as one straight slope. The unidirectional motion of the particle along this slope is driven by the temperature difference between neighboring δ_h and δ_c segments, which, therefore, can be viewed as small "heat engines." To calculate the heat transfer Q to the cold reservoir by these heat engines, let us look at the potential energy of the particle. Whenever the particle goes through the cold segment from left to right (right to left) it dissipates (picks up) E_c potential energy to (from) the cold reservoir; therefore Q is identical to E_c. An interesting consequence of this identity is that the condition $(E_h = E_c^*)$ for aligning the downslides of the transformed potential, which can also be written as $(Q + \Delta E)/T_h = Q/T_c$, is equivalent to the condition for zero entropy production (8). Note that in general there is an additional heat transfer via the kinetic energy of the particle due to the recrossing of the boundary between the segments at different temperatures, but this heat transfer is very sensitive to the parameters of the system, and in certain situations can be negligibly small compared to the heat transfer via the potential energy [11].

In this paper we have generalized the definition of the energy output of an engine, as the minimum energy input required to accomplish the same task as the engine, allowing us to measure the efficiency of any physical process. This generalized efficiency can never be greater than 1, approaches unity only if the task is completed in the energetically most favorable way, and reduces back to the conventional definition if the task is simply charging a battery. Applying this new concept to microscopic motors gives us a very useful tool for either comparing and characterizing the operation of molecular motors in different situations (without the necessity of attaching any external load to them) or designing nanoscale motors for various purposes. We have illustrated this new concept via a simple and nontrivial example of a chemical engine, and showed that even a rectified diffusion can approach 100% efficiency, i.e., mimic the effect of a constant pulling force. We have extended our analysis to thermally driven motors, and obtained some very surprising results due to the fact that the heat dissipated into the hot reservoir can be partially recovered. For a given power input a thermally driven motor can go faster than any isothermal motor; its velocity is not limited by the power input, and it can be increased arbitrarily by increasing the temperature of the hot reservoir. This effect is incorporated into Eq. (11), leading to a sensible and consistent measure of the efficiency of molecular motors driven by any source of energy.

We have already mentioned that there was one experiment [4] on molecular motors, where the power output was measured as γv^2. Although this choice seemed natural and reasonable without any theoretical finding, it is our investigation of the thermally driven ratchets that shows the subtlety of the correct definition of the generalized efficiency. The blind use of γv^2 could lead to an efficiency that is larger than unity. Fortunately, our rigorous theoretical finding justifies that for isothermal motors the above choice was indeed correct and provides a solid basis for the application of Eqs. (2) and (11) for other biological and man-made molecular motors.

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