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# Efficiency of Brownian heat engines

Imre Derényi and R. Dean Astumian
*Department of Surgery, MC 6035, University of Chicago, 5841 South Maryland Avenue, Chicago, Illinois 60637*
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We study the efficiency of one-dimensional thermally driven Brownian ratchets or heat engines. We identify and compare the three basic setups characterized by the type of the connection between the Brownian particle and the two heat reservoirs: (i) simultaneous, (ii) alternating in time, and (iii) position dependent. We make a clear distinction between the heat flow via the kinetic and the potential energy of the particle, and show that the former is always irreversible and it is only the third setup where the latter is reversible when the engine works quasistatically. We also show that in the third setup the heat flow via the kinetic energy can be reduced arbitrarily, proving that even for microscopic heat engines there is no fundamental limit of the efficiency lower than that of a Carnot cycle. [S1063-651X(99)50106-2]

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Brownian ratchets are spatially asymmetric but periodic structures in which transport of Brownian particles is induced by some nonequilibrium process [1,2], such as external modulation of the underlying potential or a nonequilibrium chemical reaction coupled to a change of the potential, or contact with reservoirs at different temperatures. The most intensively studied quantity has been the velocity of the transported particle. However, another important quantity is the *efficiency* of the energy conversion characterizing the operation of the system when the transported particle does work (e.g., advances against an external force). The system parameters at maximum efficiency can be significantly different from those at maximum velocity. The efficiency of some externally and chemically driven ratchet systems has been studied in Refs. [2–6]. Here we investigate the efficiency of thermally driven Brownian ratchets or *Brownian heat engines*. Two major issues are (i) what the possible sources of irreversibility, and (ii) whether the irreversibility can be suppressed such that the efficiency approaches that of a Carnot cycle.

There are three basic setups for one-dimensional Brownian heat engines, which differ only in the type of the connection between the Brownian particle and two reservoirs at temperatures $T_A$ and $T_B$. In the first, exemplified by Feynman's ''ratchet and pawl'' engine [7], the particle is in contact with the two reservoirs *simultaneously*. Feynman estimated the efficiency to approach that of a Carnot cycle. However, detailed analysis by Parrondo and Español [8], and by Sekimoto [9] revealed that Feynman's estimation contained some inconsistencies: the engine can never work in a reversible way, and therefore, can never approach the Carnot efficiency. This is because a particle in contact simultaneously with two reservoirs at different temperatures cannot be in thermal equilibrium. The warmer reservoir continually tends to increase the particle's (kinetic and potential) energy while the colder reservoir tends to decrease it. In other words, the energy of each ''thermal kick'' coming from either reservoir is finally dissipated in both reservoirs. This continuous and irreversible heat flow from the warmer reservoir to the colder one is proportional to the inverse of the mass of the particle ($1/m$) [8] and goes to infinity in the overdamped limit ($m \rightarrow 0$). It is important to note that if the system is extended to two spatial dimensions, such that either coordinate is in contact with only one of the reservoirs and the coordinates are coupled elastically, the coupling constant also controls the heat flow, which remains finite even in the overdamped limit [8,9].

In a second setup [10,11] the temperature is homogeneous in space, but alternates in time between $T_A$ and $T_B$, i.e., the

 

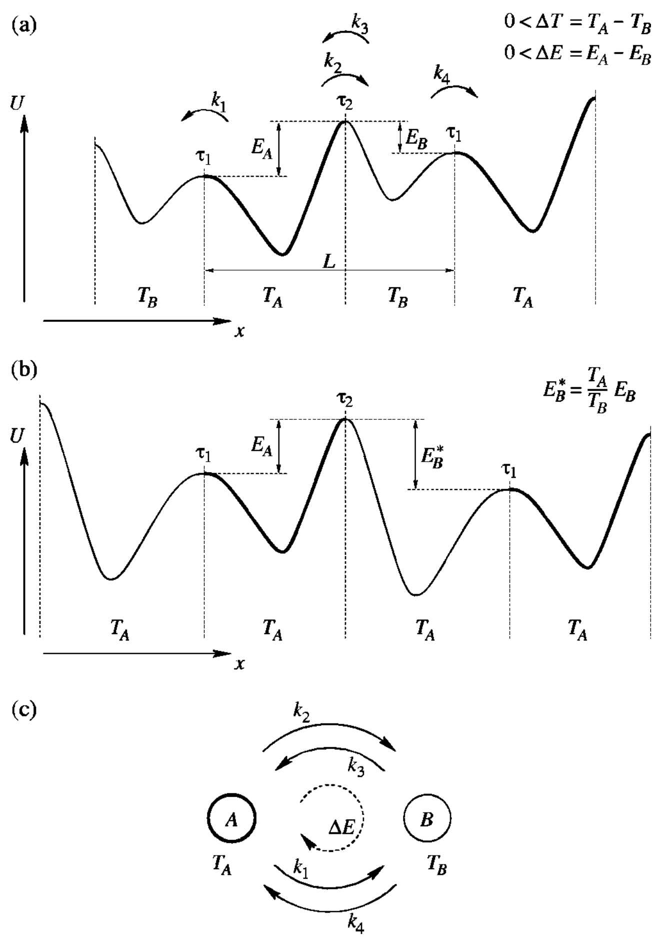


FIG. 1. (a) A ratchet potential with two wells at different temperatures ($T_A$ and $T_B$) in each period (of length $L$), superimposed on a linear potential (with steepness $\Delta E/L$). The kinetic rate constants over the barriers are $k_i$ ($i=1,\ldots,4$). $\tau_1$ and $\tau_2$ are the transmission coefficients (see the text). (b) The potential after applying the transformation (2) with $\kappa=T_A/T_B$ for the segments at temperature $T_B$. (c) The potential can be mapped to a two-state kinetic model.

particle is in contact with the two reservoirs *alternately*. The efficiency of such engines was studied in Ref. [11] via a discrete three-state model with thermally activated transitions (a two-state model would have been enough [12]). The analysis focused on the potential energy of the particle, and revealed that there is an irreversible heat flow from the warmer reservoir to the colder one, which prevents the efficiency from approaching that of a Carnot cycle. Indeed, contact with the warmer reservoir raises the average potential energy of the particle, and then contact with the colder reservoir lowers it, dissipating the excess energy to the colder reservoir. The irreversible nature of this heat flow is the most conspicuous when the engine works quasistatically (approaching zero velocity) and, therefore, the useful work approaches zero. Further, the kinetic energy (not considered in the discrete model of Ref. [11]) also results in an irreversible heat flow of $k_B\Delta T/2$ per cycle. Consequently, this type of heat engine is also inherently irreversible because, similar to the first setup, there is an irreversible heat flow between the two reservoirs via both the kinetic and the potential energy of the particle.

In this paper we give a detailed analysis of a third setup, the Büttiker-Landauer model [13], where the temperature distribution along the ratchet potential is constant in time, but inhomogeneous in space, i.e., the particle is in contact with different reservoirs at different *positions*. We show that in such systems the heat transfer via the potential energy of the particle is reversible when the engine works quasistatically and, in some cases, the irreversible heat flow via the kinetic energy can be small enough that the efficiency approaches that of a Carnot cycle.

Consider the motion of a Brownian particle with mass $m$ and viscous drag coefficient $\gamma$ in a potential $U(x)$. The potential [such as the one in Fig. 1(a)] consists of a periodic ratchet potential (that is flat on average) with period $L$, plus a linear potential, which rises by $\Delta E(>0)$ on each period. The linear part corresponds to the external homogeneous force $-\Delta E/L$ against which the particle advances and does "useful work." The temperature $T(x)$ along the potential with values $T_A$ and $T_B$ (where $0<\Delta T=T_A-T_B$) is also periodic with period $L$. Note that Fig. 1(a) shows a specific example but, in general, the periodic ratchet potential can have an arbitrary shape with an arbitrary number of transitions between $T_A$ and $T_B$. Let us denote the sum of the net potential changes on those segments of a period where $T(x)=T_A$ by $E_A$ and, similarly, that for $T(x)=T_B$ by $-E_B$ (thus $\Delta E=E_A-E_B$).

For simplicity, we absorb the Boltzmann coefficient in the temperature and measure the temperature in the units of energy. Then the motion of the particle is described by the Langevin equation

$$m\ddot{x}(t)=-\gamma\dot{x}(t)-U'(x)+\sqrt{2\gamma T(x)}\xi(t), \tag{1}$$

where $x$ denotes the position of the particle and $\xi(t)$ is a Gaussian white noise with the autocorrelation function $\langle\xi(t)\xi(t')\rangle=\delta(t-t')$. Since the Langevin equation is invariant under the transformation

$$\{T,U,x\}\rightarrow\{\kappa T,\kappa U,\sqrt{\kappa}x\}, \tag{2}$$

one can easily get rid of the space dependence of the temperature by applying this transformation with $\kappa=T_A/T_B$ only to those segments where $T(x)=T_B$, as illustrated in Fig. 1(b). Thus, $E_B$ transforms to $E_B^*=E_BT_A/T_B$, and the potential change on each period of the transformed potential becomes $E_A-E_B^*$. Since this transformation results in a sudden change of the velocity at the borders of the segments, it is valid only for strongly damped systems, i.e., where the thermal length scale [14] (the maximal value of $\sqrt{mT(x)/\gamma}$), on which the particle's velocity is thermalized, is much shorter than any other length scale of the system [such as the length of the segments or the minimal value of $\sqrt{T(x)/U''(x)}$]. This condition also means that the particle's kinetic energy can be considered to be adapted to the local temperature at every instant. In the following we confine ourselves to such strongly damped systems. Thus, the condition to get a positive net particle current $J$ and, therefore, positive power output,

$$J_W=J\Delta E, \tag{3}$$

can be determined trivially; the transformed potential must be descending ($E_A-E_B^*<0$), i.e.,

$$0<\alpha=\frac{E_B}{T_B}-\frac{E_A}{T_A}=\frac{\Delta T\, E_A-T_A\,\Delta E}{T_A\,T_B}. \tag{4}$$

Note that the above transformation can be applied for strongly damped systems even with continuously changing temperature, $T(x)$. In this case, if the transformed temperature is chosen to be unity, the potential drop of the transformed system over one period is $\alpha=-\int_0^L[U'(x)/T(x)]dx$. This allows us to directly compare thermally and chemically driven motors because, for the latter, similar transformation to an effective tilted potential is also possible [15].

To calculate the efficiency $\eta$ of the heat engine we also have to determine the input power, which is equivalent to the heat flow $J_Q$ out of the warmer reservoir. This can be divided into two terms:

$$J_Q=J_Q^{\mathrm{kin}}+J_Q^{\mathrm{pot}}, \tag{5}$$

where $J_Q^{\mathrm{pot}}=JE_A$ is the heat flow via the potential energy of the particle, because each time the particle advances one period to the right it gains $E_A$ potential energy from the warmer reservoir, and when the particle happens to go back one period it releases $E_A$ from its potential energy to the warmer reservoir. The heat flow $J_Q^{\mathrm{kin}}$ via the kinetic energy of the particle is much more complicated to determine. Whenever the particle enters a segment at temperature $T_A$ it picks up $\Delta T/2$ energy on average from the warmer reservoir to raise its average kinetic energy from $T_B/2$ to $T_A/2$, but when it leaves this excess $\Delta T/2$ kinetic energy is always released to the colder reservoir and never to the warmer reservoir or to the particle's potential energy, indicating the inherently irreversible nature of this heat flow. The number of times the particle crosses the borders between $T_A$ and $T_B$ depends on the system parameters very sensitively (see below). Thus, the efficiency can be written as

$$\eta=\frac{J_W}{J_Q}=\frac{1}{1+\Theta}\,\eta_{\mathrm{pot}}, \tag{6}$$

where

$$\Theta=\frac{J_Q^{\mathrm{kin}}}{J_Q^{\mathrm{pot}}},\quad \text{and} \quad \eta_{\mathrm{pot}}=\frac{J_W}{J_Q^{\mathrm{pot}}}=\frac{\Delta E}{E_A} \tag{7}$$

is the efficiency if $J_Q^{\mathrm{kin}}$ is omitted. Comparing $\eta_{\mathrm{pot}}$ to the Carnot efficiency $\eta_{\mathrm{Carnot}}=\Delta T/T_A$, we get

$$\frac{\eta_{\mathrm{pot}}}{\eta_{\mathrm{Carnot}}}=\frac{T_A\Delta E}{\Delta T E_A}=1-\frac{T_A T_B}{\Delta T E_A}\alpha, \tag{8}$$

where we substituted $T_A\Delta E$ by $\Delta TE_A+T_AT_B\alpha$, in accordance with Eq. (4). This is one of the main results of the paper, clearly showing that when the engine works quasistatically ($\alpha\to 0$ or $E_A\to\infty$), the heat transfer via the potential energy of the particle is *reversible*, because $\eta_{\mathrm{pot}}$ approaches the Carnot efficiency, independently of all other properties of the system. Notice the difference between the two static limit. In the $E_A\to\infty$ limit the particle is essentially unable to move, because it cannot overcome the infinitely high energy barriers, while in the $\alpha\to 0$ limit the particle can move, but with a zero average velocity, because the transformed potential is flat on average.

Now let us examine how $J_Q^{\mathrm{kin}}$ affects the engine's efficiency. It is clear from Eq. (6) that, via the parameter $\Theta$, this heat flow always decreases the efficiency, indicating again its inherently irreversible nature.

First we give an estimation for the magnitude of this heat flow. The (unidirectional) particle flow from a segment at temperature $T_B$ to the neighboring segment at $T_A$ is proportional to the particle's probability density at the border and also to the average velocity of the particle in the desired direction. The average velocity, supposing equilibrium (Maxwell) velocity distribution, is $\sqrt{2T_B/(\pi m)}$. Thus, $J_Q^{\mathrm{kin}}$ and $\Theta$ are proportional to $1/\sqrt{m}$ and, for small $m$, the efficiency is proportional to $\sqrt{m}$. In the overdamped limit ($m\to 0$) the heat flow goes to infinity and the efficiency goes to zero. However, as $m$ increases from zero the efficiency rises very quickly, with an initially infinite derivative. The above arguments are independent of the details of the system (and hold even for continuously changing temperature).

To minimize the heat flow via the kinetic energy of the particle let us consider the specific example depicted in Fig. 1(a), where the irreversible heat exchange occurs at the most rarely visited parts of the potential – the top of the barriers. Another reason for choosing this system is that it can be readily mapped to a two-state kinetic model [12] as shown in Fig. 1(c).

Then, the stationary probabilities that the particle can be found in the wells at temperatures $T_A$ and $T_B$ are

$$P_A=\frac{k_3+k_4}{\sum_{i=1}^{4}k_i}\quad \text{and} \quad P_B=\frac{k_1+k_2}{\sum_{i=1}^{4}k_i}, \tag{9}$$

respectively ($P_A+P_B=1$). This two-state kinetic description is valid if the relaxation time of the probability density in each well is much shorter than any inverse rate constant $k_i^{-1}$. The net particle current in its most symmetric form is

$$J=\frac{P_A(k_2-k_1)+P_B(k_4-k_3)}{2}. \tag{10}$$

A certain fraction of $J_Q^{\mathrm{kin}}$, which comes from the jumping events from the potential wells at temperature $T_B$ to the neighboring wells at $T_A$ by omitting the recrossing of the top of the barriers,

$$J_{Q,\min}^{\mathrm{kin}}=\frac{1}{2}\Delta TP_B(k_3+k_4)=\frac{1}{2}\Delta TP_AP_B\sum_{i=1}^{4}k_i, \tag{11}$$

is always and inevitably present in the system, yielding a minimum value for the parameter $\Theta$:

$$\Theta_{\min}=\frac{J_{Q,\min}^{\mathrm{kin}}}{J_Q^{\mathrm{pot}}}=\frac{\Delta T}{E_A}\left(\frac{k_2-k_1}{k_2+k_1}+\frac{k_4-k_3}{k_4+k_3}\right)^{-1}. \tag{12}$$

The question is how to construct a system to avoid additional irreversible heat flow due to recrossing events. Here we show one simple possibility by introducing some gating mechanism at the top of the barriers.

Usually after a particle crosses the top of a barrier ($j=1,2$ indexes the barriers) it spends some time ($t_j^{\mathrm{dwell}}\approx\gamma/|U_j''|$) near the top, recrossing many times before it reaches the basin of attraction of one of the wells. The number of recrosses is proportional to $1/\sqrt{m}$ in a strongly damped system. However, after crossing the top of a barrier there is a characteristic time ($t_j^{\rm char}=m/\gamma$) necessary for the particle to lose its velocity and return to the top. Thus, by introducing a gating mechanism at the top of the barriers, such that the gates are never open for a longer time than $t_j^{\rm char}$, and are always closed for a longer time than $t_j^{\rm dwell}$, the recrossing can be almost completely excluded, $J_{Q,\min}^{\rm kin}$ can be well approached, and, also, the system can be well described in terms of the two-state kinetic model of Fig. 1(c). (Note that in two-dimensional systems the gating mechanism can be replaced by applying narrow windows at the tops of the barriers.)

Equation (12) contains only the ratios of the kinetic rate constants, which can easily be expressed as

$$\frac{k_2}{k_1}=\frac{\tau_2}{\tau_1}\exp\left(-\frac{E_A}{T_A}\right) \quad \text{and} \quad \frac{k_4}{k_3}=\frac{\tau_1}{\tau_2}\exp\left(\frac{E_B}{T_B}\right), \tag{13}$$

where $\tau_j=t_j^{\rm open}/(t_j^{\rm open}+t_j^{\rm closed})$ are the transmission coefficients, and $t_j^{\rm open}$ and $t_j^{\rm closed}$ are the characteristic times for keeping the gates open and closed, respectively. Note that, analogous to the chemically driven motors, the thermodynamic driving force of this process is $\ln[k_2k_4/(k_1k_3)]=\alpha$, which characterizes the average slope of the transformed potential. Inserting Eqs. (13) into Eq. (12) with the notation $\lambda=\ln(\tau_2/\tau_1)$, we get

$$\Theta_{\min}=\frac{\Delta T/E_A}{\tanh\left(\frac{E_A}{2T_A}-\frac{\lambda}{2}+\frac{\alpha}{2}\right)-\tanh\left(\frac{E_A}{2T_A}-\frac{\lambda}{2}\right)}. \tag{14}$$

The smallest possible value of $\Theta_{\min}$ can be achieved by setting the transmission coefficients, such that $\lambda=E_A/T_A+\alpha/2$, leading to $\Theta_{\min}\approx 2\Delta T/(\alpha E_A)$ for small values of $\alpha$. Inserting this into Eqs. (6) and (8), we get

$$\frac{\eta}{\eta_{\rm Carnot}}\approx\left(1-\frac{T_AT_B}{\Delta T E_A}\alpha\right)\Bigg/\left(1+\frac{2\Delta T}{\alpha E_A}\right), \tag{15}$$

which approaches one in the quasistatic limit $E_A\to\infty$ with all of the other parameters ($T_A$, $T_B$, and $\alpha$) fixed. This result shows that in certain situations the inherently irreversible heat flow $J_Q^{\rm kin}$ can be suppressed relative to the heat flow $J_Q^{\rm pot}$, such that the efficiency of the Brownian heat engine approaches that of a Carnot cycle.

The irreversible heat flow via the kinetic energy of the particle is always present in any Brownian heat engine. However, it is only the third type of setup (with spatially inhomogeneous temperature) where the motion and the temperature change are completely coupled, allowing the heat flow via the potential energy of the particle to be reversible when the engine works quasistatically. In these systems the heat flow via the kinetic energy can be made small compared to the heat flow via the potential energy, thus the efficiency of the heat engine can approach that of a Carnot cycle.

Numerous authors have examined models of microscopic motors that are inherently irreversible and have very small efficiency [3,4,6,8,9,11]. This suggests that microscopic engines, for which diffusion is an essential element in the production of useful work, are intrinsically less efficient than motors based on macroscopic deterministic principles. In this paper, by presenting an explicit example where the efficiency approaches that of a Carnot cycle, we have demonstrated that there does not exist any fundamental lower limit for microscopic heat engines.

The immediate significance of our work lies in the virtual explosion of experimental results both on biomolecular engines and chemically synthesized molecular motors [16]. Although biomolecular motors operate isothermally, it is not difficult to imagine a constructed microscopic motor that could be immobilized near a heated surface, such that part of the working cycle takes place near the relatively hot surface and another part takes place further in the cooler bulk. But an explicit realization of the Büttiker-Landauer model [13] is possible even with biomolecular engines, whose dipole moment, $\mathbf{P}(x)$, varies with the reaction coordinate, $x$, and interacts with a fluctuating electric field, $\mathbf{E}(t)$. If $\mathbf{E}(t)$ can be well approximated with a Gaussian white noise, the term $\mathbf{E}(t)d\mathbf{P}/dx$, which should be added to the Langevin Eq. (1), corresponds to an effective, position dependent temperature.

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