Heat Flow and Efficiency in a Microscopic Engine

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Abstract

We study the energetics of a thermal motor driven by temperature differences, which consists of Brownian particles moving in a sawtooth potential with an external load where the viscous medium is alternately in contact with hot and cold heat reservoir along space coordinate. The motor can work as a heat engine or a refrigerator under different conditions. The heat flow via both potential and kinetic energy are considered. The former is reversible when the engine works quasistatically and the latter is always irreversible. The efficiency of the heat engine (Coefficient Of Performance (COP) of a refrigerator) can never approach Carnot efficiency (COP).
INTRODUCTION

Recently, Brownian ratchets (motors) have attracted considerable attention simulated by research on molecular motors \[1, 2\]. A Brownian ratchet, which appeared in Feynman's famous textbook for the first time as a thermal ratchet \[3\], is a machine which can rectify thermal fluctuation and produce a directed current. These subjects are motivated by the challenge to understand molecular motors \[4\], nanoscale friction \[5\], surface smoothening \[6\], coupled Josephson junctions \[7\], optical ratchets and directed motion of laser cooled atoms \[8\], and mass separation and trapping schemes at the microscale \[9\].

The Brownian ratchet are spatially asymmetric but periodic structure in which transport of Brownian particles is induced by some nonequilibrium processes \[10, 11, 12, 13\], such as external modulation of the underling 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 on the velocity of the transport particle. However, another important quantity is efficiency of energy conversion characteristic the operation of the system when the transported particle does work.

How efficiency can Brownian ratchets work? This question is important not only for the construction of theory of molecular motors \[14\] but also for foundation of non-equilibrium statistical physics. Like Carnot cycle, Brownian heat engine can extract work from the temperature difference of the heat baths, where Brownian working material operates as a transducer of thermal energy into work. The study of the energetics of Brownian ratchets is relevant for several reasons \[15\]. Firstly, highly efficient motors are desirable in order to decrease the energy consumption or to decrease the heat dissipation. Secondly, Brownian motors are related to fundamental problems of thermodynamics and statistical mechanics, such as the Maxwell demon and the trade-off between entropy and information. Thirdly, many models proposed in the literature are based on nonequilibrium fluctuations without specifying their source. On the other hand, the study of the energetics of such models required a more precise formulation, since one has to determine the physical nature of the external agent and verify that the motor is consistent with the second law of thermodynamics.

Recently, Sekimoto has been unambiguously defined the concept of the heat at mesoscopic scales in terms of Langevin equation \[16\]. He refers to the formalism providing this definition
as stochastic energetics. The essential point of this formalism is that the heat transferred
to the system is nothing but the microscopic work done by both friction force and the
random force in the Langevin equation. Stochastic energetics has been applied to the study
of thermodynamic processes. Derenyi and Astumian \[17\] have studied the efficiency of one-
dimensional thermally driven Brownian engines. They identify and compare the three basic
setups characterized by the type of the connection between the Brownian particle and the
two reservoirs: (1) simultaneous \[3\], (2) alternating in time \[18\], and (3) position dependent
\[19\]. Parrondo and Cisneros \[15\] has reviewed the literature the energetics of Brownian
motors, distinguishing between forced ratchet, chemical motors-driven out of equilibrium by
difference of chemical potential, and thermal motors-driven by temperature differences. In
this paper we give a detailed study of the last motors-thermal motors.

Energetics of the thermal motors-driven by temperature differences are investigated by
some previous works \[20, 21\]. Asfaw \[20\] et al. have explored the performance of the mo-
tors under various conditions of practical interest such as maximum power and optimized
efficiency. They found that the efficiency can approach the Carnot efficiency under the
quasistatic limit. The same results are also obtained in Matsuo and Sasa’s work \[21\] by
stochastic energetics theory. The previous works are limited to case of heat flow via poten-
tial. The present work extends the study to case of heat flow via both potential and kinetics
energy. The motor can work as a heat engine or a refrigerator under various conditions.
The efficiency of heat engine (COP of refrigerator) is different from the results of previous
works and can never approach the Carnot efficiency (COP). The heat flow via potential is
reversible when the engine works at quasistatic limit. The heat flow via the kinetic is always
irreversible in nature.

\section*{THERMAL MOTOR WORKS AS A HEAT ENGINE}

The model (shown in Fig. 1) consists of Brownian particles moving in a sawtooth potential
with an external load where the medium is alternately in contact with hot and cold heat
reservoirs along the space coordinate. Let \( E \) be the barrier height of the potential. \( L_1, L_2 \)
are the length of the left part and the right part of the ratchet, respectively. \( E + FL_1 \) is
the energy needed for a forward jump, while \( E - FL_2 \) is the energy required for a backward
jump. The left part of a period ratchet is at temperature \( T_H \) (hot reservoir) and the right
one is at temperature $T_C$ (cold reservoir). We can assume that the rates of both forward and backward jumps are proportional to the corresponding Arrhenius’ factor $[22]$, such that

\[ \dot{N}_+ = \frac{1}{t} \exp \left[ -\frac{E + FL_1}{k_B T_H} \right], \]

\[ \dot{N}_- = \frac{1}{t} \exp \left[ -\frac{E - FL_2}{k_B T_C} \right], \]

are the number of forward and backward jumps per unit time, respectively, $k_B$ the Boltzmann constant, $t$ a proportionality constant with dimensions of time.

If $\dot{N}_+ > \dot{N}_-$, the ratchet works as a two-reservoir heat engine shown in Fig. 2. The rate of heat flow from hot reservoir to the heat engine via potential is given by

\[ \dot{Q}_{pot}^H = (\dot{N}_+ - \dot{N}_-)(E + FL_1). \]

The rate of heat flow from the engine to the cold reservoir via potential is

\[ \dot{Q}_{pot}^C = (\dot{N}_+ - \dot{N}_-)(E - FL_2). \]

The heat flow via the kinetic energy of the particle is much more complicated to determined $[15]$. Whenever a particle stay at a hot segment (temperature $T_H$) it absorbs $\frac{1}{2}k_B T_H$ energy on average from the hot reservoir. It can pick up $\frac{1}{2}k_B T_C$ energy on average from the
FIG. 2: The engine acts as a heat engine. Heat flows via both potential energy and kinetic energy in a thermal motor in contact with two thermal baths at temperatures $T_H > T_C$, $W$ is power output, heat flows via potential energy is reversible, heat flows via kinetic energy is irreversible.

cold reservoir when the particle stay at a cold segment. It is obvious that when a particle leaves from a hot segment to a cold segment and then returns to the hot segment, the hot reservoir will lose $\frac{1}{2}(k_B T_H - k_B T_C)$ energy on average, the lost energy is released to the colder reservoir and never to the hot reservoir or to the particle’s potential energy, which indicates the inherently irreversible nature of this heat flow. On the other hand, if a particle goes out from a hot segment to a cold segment and never returns to the hot segment, the hot reservoir will lose $\frac{1}{2}k_B T_H$ energy on average. Therefore the rate of net heat flow via kinetic energy from the hot reservoir to the cold reservoir is given by

$$\dot{Q}^{\text{kin}} = \frac{1}{2} \dot{N}_+ k_B T_H - \frac{1}{2} \dot{N}_- k_B T_C. \quad (5)$$

Therefore, the rate of total heat transferred from the hot reservoir is given by

$$\dot{Q}_H = \dot{Q}^{\text{plot}}_H + \dot{Q}^{\text{kin}},$$

$$= (\dot{N}_+ - \dot{N}_-)(E + FL_1) + \frac{1}{2} \dot{N}_+ k_B T_H - \frac{1}{2} \dot{N}_- k_B T_C. \quad (6)$$

The rate of total heat transferred to the cold reservoir is

$$\dot{Q}_C = \dot{Q}^{\text{plot}}_C + \dot{Q}^{\text{kin}}$$

$$= (\dot{N}_+ - \dot{N}_-)(E - FL_2) + \frac{1}{2} \dot{N}_+ k_B T_H - \frac{1}{2} \dot{N}_- k_B T_C. \quad (7)$$

The power output is

$$\dot{W} = \dot{Q}_H - \dot{Q}_C = (\dot{N}_+ - \dot{N}_-)FL. \quad (8)$$
It is easy to obtain the efficiency of the heat engine

\[ \eta = \frac{\dot{W}}{Q_H}. \]  

(9)

If the heat flow via the kinetic energy is not considered, the efficiency is given by

\[ \eta^{pot} = \frac{\dot{W}}{Q_H^{pot}}. \]  

(10)

In order to discuss simply, we can rewrite Eq. (5-10) in a dimensionless form, then we get

\[ q_H = \frac{\dot{Q}_{Ht}}{k_B T_H} = e^{-\epsilon/\tau}\left[ (\epsilon + \frac{1}{2} + \mu f) e^{f_0 - \mu f} - (\epsilon + \frac{1}{2} \tau + \mu f) e^{(1-\mu)f/\tau}\right], \]  

(11)

\[ q_C = e^{-\epsilon/\tau}\left[ (\epsilon + \frac{1}{2} + \mu f - f) e^{f_0 - \mu f} - (\epsilon + \frac{1}{2} \tau + \mu f - f) e^{(1-\mu)f/\tau}\right], \]  

(12)

\[ q^{kin} = \frac{\dot{Q}_{kin}}{k_B T_H} = \frac{1}{2} e^{-\epsilon/\tau}\left[ e^{f_0 - \mu f} - \tau e^{(1-\mu)f/\tau}\right], \]  

(13)

\[ w = \frac{\dot{W}t}{k_B T_H} = e^{-\epsilon/\tau}\left[ e^{f_0 - \mu f} - e^{(1-\mu)f/\tau}\right], \]  

(14)

\[ \eta = \frac{\left[ e^{f_0 - \mu f} - e^{(1-\mu)f/\tau}\right]}{\epsilon + \mu f + f_0 - \left[ e^{f_0 - \mu f} - e^{(1-\mu)f/\tau}\right]}, \]  

(15)

\[ \eta^{pot} = \frac{f}{\epsilon + \mu f}, \]  

(16)

where

\[ f = \frac{FL}{k_B T_H}, \epsilon = \frac{E}{k_B T_H}, \tau = \frac{T_C}{T_H}, \mu = \frac{L_1}{L}, f_0 = \frac{(1-\tau)\epsilon}{\tau}. \]  

(17)

From the above equations, one has \( \epsilon \geq 0, 0 \leq \tau \leq 1, 0 \leq \mu \leq 1. \) Since the motor acts as a heat engine, the power output can not be negative, namely, \( w \geq 0. \) one can also obtain the value range of \( f, \) \( 0 \leq f \leq f_m, \) where

\[ f_m = \frac{(1-\tau)\epsilon}{(\tau-1)\mu + 1}. \]  

(18)

Therefore, it is easy to obtain

\[ \eta^{pot} = \frac{f}{\epsilon + \mu f} \leq \frac{f_m}{\epsilon + \mu f_m} = 1 - \tau = 1 - \frac{T_C}{T_H} = \eta_C, \]  

(19)

where \( \eta_C \) is Carnot efficiency. However, \( \eta^{pot} \) attains the Carnot efficiency, namely, \( f = f_m \) which indicates that the power output is zero. From Eq. (15) and Eq. (16), it obvious that \( \eta \) is always less than \( \eta^{pot}. \) The results are given by Fig. 3-10.
FIG. 3: Dimensionless heat flow $q_H, q_C$ and power output $w$ vs the load $f$ at $\tau = 0.1, \epsilon = 2.0, \mu = 0.1$.

Figure 3 shows that the heat flow $q_H, q_C$ and power output $w$ as a function of the load $f$. When $f = 0$, namely, the engine runs without a load, $q_H$ is equal to $q_C$, which indicates that the heat that absorbs from the hot reservoir releases to the cold reservoir entirely and no power output is obtained. When $f$ increases, $q_H$ and $q_C$ decreases. when $f \to 0$, no power output is obtained ($w=0$). When $f \to f_m$, no currents occur, the ratchet can’t give any power output. So the power output $w$ has a maximum value at certain value of $f$ which depends on $\tau$, $\epsilon$ and $\mu$.

FIG. 4: $\eta_C, \eta_{pot}$ and $\eta$ vs the load $f$ at $\tau = 0.1, \epsilon = 2.0, \mu = 0.1$.

Figure 4 shows the variation of the efficiency $\eta_C$, $\eta_{pot}$, $\eta$ with the load $f$. If the heat flow via kinetic energy is ignored, the efficiency $\eta_{pot}$ increases with the load $f$, it approaches the Carnot efficiency $\eta_C$ at quasistatic condition ($f = f_m$). The result is also presented in Asfaw’s
work \cite{20}. When the heat flow via kinetic energy are considered, the curve of the efficiency $\eta$ is observed to be bell-shaped, a feature of resonance. The efficiency $\eta$ is always less than $\eta_{pot}$ and never approaches Carnot efficiency $\eta_{C}$. It is obvious that the heat flow via kinetic energy is always irreversible and energy leakage is inevitable, so the efficiency is less than $\eta_{pot}$ and can’t approach Carnot efficiency.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5.png}
\caption{(a)Dimensionless heat flow $q^{\text{kin}}$ vs the load $f$ ($\tau = 0.5, \epsilon = 2.0, \mu = 0.5$); (b)Dimensionless heat flow $q^{\text{kin}}$ vs barrier height $\epsilon$ for different values of $f = 0.4, 1.0$ at $\tau = 0.5, \mu = 0.5$.}
\end{figure}

Figure 5a shows the heat flow $q^{\text{kin}}$ out of hot reservoir via kinetic energy as a function of the load $f$. When $f < f_{m}$, $q^{\text{kin}}$ is positive. When $f > f_{m}$, $q^{\text{kin}}$ is negative. No heat flow occurs at $f = f_{m}$. It is found that the heat flow via kinetic is dependant on the current of the ratchet. Figure 5b shows the heat flow out of the hot reservoir via kinetic energy as a function of barrier height $\epsilon$. The curve is bell-shaped. Therefore, there is an optimized value of $\epsilon$ at which $q^{\text{kin}}$ takes its maximum value.

Figure 6 shows the power output $w$ as a function of the load $f$ for different values of $\mu = 0.1, 0.5, 0.8$. From the figure, we can see that the power output has a maximum value at certain value of $f$. The maximum load $f_{m}$ of the engine changes with the parameter $\mu$ of asymmetry in potential. In other word, the structure of the potential determines the maximum load capability of the engine.

Figure 7 shows the variation of the efficiency $\eta$ with the load $f$ for different values of $\mu = 0.0, 0.5, 0.8$. The maximum value of $\eta$ increases with $\mu$. However, the maximum value of $\eta$ can’t approach the Carnot efficiency.

Figure 8 shows the power output $w$ as a function of the barrier height $\epsilon$ for different
FIG. 6: Dimensionless power output $w$ vs the load $f$ for different values of $\mu = 0.1, 0.5, 0.8$ at $\tau = 0.1, \epsilon = 1.0$.

FIG. 7: Efficiency $\eta$ vs the load $f$ for different values of $\mu = 0.1, 0.5, 0.8$ at $\tau = 0.1, \epsilon = 1.0$.

values of the load $f = 0.1, 0.2, 0.5$. When $\epsilon \to 0$, the effect of ratchet disappears, the power output tends to zero. When $\epsilon \to +\infty$ so that the particle can’t pass the barrier, the power output $w$ goes to zero, too. The power output $w$ has a maximum value at certain value of $\epsilon$ which is dependant on $\tau$, $\mu$ and $f$. On the other hand, the minimum height of the barrier for working as a heat engine increases with the load $f$.

Figure 9 shows the efficiency $\eta_C$, $\eta_{pot}$ and $\eta$ as a function of the barrier height. The efficiency $\eta_{pot}$ without the heat flow via kinetic energy approaches the Carnot efficiency at $\epsilon = \epsilon_m$, at which no power output occurs. The efficiency $\eta$ is a peaked function of the barrier height $\epsilon$ which is dependant on values of $\tau$, $f$ and $\mu$. 
FIG. 8: Dimensionless power output $w$ vs barrier height $\epsilon$ for different values of $f=0.1, 0.2, 0.5$ at $\tau = 0.1, \mu = 0.1$.

FIG. 9: $\eta_C$, $\eta_{pot}$ and $\eta$ vs the barrier height $\epsilon$ at $\tau = 0.1, f = 0.4, \mu = 0.1$.

FIG. 10: Dimensionless heat flow $q_H$, $q_C$ and power output $w$ vs $\tau$ at $f = 0.9$, $\epsilon = 1.0$, $\mu = 0.5$. 
Figure 10 shows plot of $w$, $q_H$ and $\eta$ versus $\tau$. From the figure, we can see that $w$, $q_H$ and $\eta$ change very slowly at small $\tau$ and they decreases drastically near $\tau = \tau_m$.

When the load $f$ is less than the maximum load $f_m$, the motor works as a heat engine. The power output is a peaked function of the load $f$ and the barrier height $\epsilon$. The efficiency $\eta$ is less than the efficiency $\eta_{\text{pot}}$ and can never approach the Carnot efficiency $\eta_C$. The heat flow via kinetic energy causes the energy leakage unavoidably and reduces the efficiency of the heat engine.

**THERMAL MOTOR WORKS AS A REFRIGERATOR**

If the load is large enough along with appropriately chosen other quantities, the motor will run in the reverse direction $\dot{N}_+ \leq \dot{N}_-$. The motor will absorb the heat from the cold reservoir and release it to the hot reservoir. Under this condition, the thermal motor acts as a refrigerator shown in Fig. 11.

\[ \dot{Q}_C = \dot{Q}_{\text{pot}}^C + \dot{Q}_{\text{kin}}^C = (\dot{N}_- - \dot{N}_+)(E - FL_2) - \frac{1}{2}k_B(\dot{N}_+T_H - \dot{N}_- T_C). \quad (21) \]

\[ \dot{W} = (\dot{N}_- - \dot{N}_+)FL. \quad (22) \]
The above equations can also be rewritten in a dimensionless form with Eq. (17)

\[
q_H = \frac{\dot{Q}_H}{k_B T_H} = e^{-\epsilon/\tau}[\epsilon + \frac{1}{2} + \mu f] e^{(1-\mu)f/\tau} - (\epsilon + \frac{1}{2} + \mu f) e^{f_0-\mu f},
\]

(23)

\[
q_C = \frac{\dot{Q}_C}{k_B T_H} = e^{-\epsilon/\tau}[\epsilon + \frac{1}{2} + \mu f - f] e^{(1-\mu)f/\tau} - (\epsilon + \frac{1}{2} + \mu f - f) e^{f_0-\mu f},
\]

(24)

\[
w = \frac{\dot{W}}{k_B T_H} = e^{-\epsilon/\tau}[\epsilon e^{(1-\mu)f/\tau} - e^{f_0-\mu f}] f.
\]

(25)

For a refrigerator, \(\dot{N}_+ \leq \dot{N}_-\), one can get \(f \geq f_m\). The heat flow from cold reservoir must not be negative (\(q_C \geq 0\)), which is important feature of a refrigerator.

As for a refrigerator, its generalized COP is most important, which is given by

\[
P = \frac{q_C}{w} = \frac{(\epsilon + \frac{1}{2} + \mu x - x) e^{(1-\mu)x/\tau} - (\epsilon + \frac{1}{2} + \mu x - x) e^{x_0-\mu x}}{[e^{(1-\mu)x/\tau} - e^{x_0-\mu x}]}.
\]

(26)

If the heat flow via the kinetic energy is not considered, the COP is given by

\[
P_{pot} = \frac{\epsilon + \mu - 1}{f_m} + \mu - 1 = \frac{\tau}{1 - \tau} = P_C
\]

(27)

where \(P_C\) is COP of a Carnot refrigerator. When \(P_{pot}\) attains the \(P_C\), namely, \(f = f_m\), the power input is zero. The results are shown in Fig. 12-14.

FIG. 12: Dimensionless heat flow \(P\), \(q_C\) and power input \(w\) vs the load \(f\) at \(\tau = 0.9\), \(\epsilon = 2.0\), \(\mu = 0.5\).

Figure 12 shows \(P\), \(q_C\) and \(w\) as a function of the input force \(f\). The power input \(w\) increases with the input force \(f\). The heat \(q_C\) that absorbs from the cold reservoir has a
maximum value at certain value of input force $f$. The COP $P$ of the refrigerator takes its maximum value at which the power input tends to zero.

Figure 13 gives the plot of COP $P_C$, $P_{pot}$ and $P$ versus the input force $f$. When the heat flow via kinetic energy is ignored, the COP of the refrigerator $P_{pot}$ decreases with increasing of $f$ and it approaches the Carnot COP at $f = f_m$. When the heat flow via kinetic energy is considered, the curve of COP $P$ is bell-shaped and it can never approach the Carnot COP $P_C$. The COP $P$ without the heat flow via kinetic energy is less than $P_{pot}$ when $f_m < f < f_C$, larger than $P_{pot}$ when $f > f_C$ and equal to $P_{pot}$ at $f = f_C$. However, $P$ can never approach the Carnot COP $P_C$.

FIG. 14: The COP $P$ vs the input force $f$ for different values of $\tau = 0.4, 0.6, 0.8, 0.9$ at $\epsilon = 0.1$, $\mu = 0.5$. 
Figure 14 shows the variation of the COP $P$ with the input force $f$ for different values of the $\tau = 0.4, 0.6, 0.8, 0.9$. From the figure, it is easy to see that the COP $P$ increases with the value of $\tau$ and the minimum input force $f_m$ increases with the decreasing of the value of $\tau$. In another word, when temperature difference is small, for example, $\tau = 0.9$, the heat leakage is small, so the COP $P$ is large. On the contrary, when the minimum input force is large, the temperature difference is large, for example, $\tau = 0.4$.

When $f$ is so large that the motor runs reversibly, $f$ becomes the input force, so the motor works as a refrigerator. The COP $P$ is a peaked function of input force $f$ which indicates the the COP can not obtain a maximum value at quasi-static limit. The COP of refrigerator can never approach the Carnot COP $P_C$ because of the heat flow via kinetic energy.

**CONCLUDING REMARKS**

In present work, we study the energestic of a thermal motor which consists of Brownian particles moving a sawtooth potential with an external load where the viscous medium is alternately in contact with hot and cold reservoirs along the space coordinate. The thermal motor can works as both a heat engine and a refrigerator. 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 the latter may be reversible when the engine works quasistatically.

When the external load is not enough, the thermal motor can work as a heat engine. The power output has a maximum value at certain value of the load $f$ which dependant on the others parameters. If only the heat flow via potential is considered, the efficiency $\eta_{pot}$ increases with the load $f$ and approaches the Carnot efficiency $\eta_C$ under quasistatic condition, which agrees with the previous work. When the heat flow via kinetic energy is also considered, the efficiency $\eta$ is less than $\eta_{pot}$ and can never approach the Carnot efficiency $\eta_C$. It is also found that the structure of the potential decides the maximum load capability of the heat engine. The heat flow via potential is reversible, while the heat flow via kinetic energy is irreversible. The heat flow via kinetic energy reduces the heat engine efficiency.

When the external load is so large that the motor moves reversely, the thermal motor can work as a refrigerator. When the heat flow via kinetic energy is ignored, the COP $P_{pot}$
decreases with increasing of the input force $f$ and can approach the Carnot COP $P_C$. When the heat flow via both potential and kinetic energy are considered, the COP $P$ is less than $P_{pot}$ when $f_m < f < f_C$, larger than $P_{pot}$ when $f > f_C$ and equal to $P_{pot}$ at $f = f_C$. However, $P$ can never approach the Carnot COP $P_C$.

The thermal motor was initially proposed in an attempt of describing molecular motors in biological systems. The heat flow via energy is irreversible, so the efficiency (COP) can not approach the the Carnot efficiency (COP) at a quasistatic condition. However, Molecular motors are known to operator efficiency \[23, 24, 25, 26, 27\]. They can convert molecular scale chemical energy into macroscopic mechanical work with high efficiency in water at room temperatures, where the effect of thermal fluctuation is unavoidable. Thus, the next challenging question would be ” How to reduce the heat flow via kinetic energy ? ”

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