Hidden heat transfer in equilibrium states implies directed motion in nonequilibrium states

Teruhisa S. Komatsu
Department of Physics, Gakushuin University, Mejiro, Tokyo 171-8588, Japan

Naoko Nakagawa
Department of Mathematical Sciences, Ibaraki University, Mito 310-8512, Japan

(Dated: March 23, 2022)

We study a class of heat engines including Feynman’s ratchet, which exhibits a directed motion of a particle in nonequilibrium steady states maintained by two heat baths. We measure heat transfer from each heat bath separately, and average them using a careful procedure that reveals the nature of the heat transfer associated with directed steps of the particle. Remarkably we find that steps are associated with nonvanishing heat transfer even in equilibrium, and there is a quantitative relation between this “hidden heat transfer” and the directed motion of the particle. This relation is clearly understood in terms of the “principle of heat transfer enhancement”, which is expected to apply to a large class of highly nonequilibrium systems.

PACS numbers: 05.70.Ln, 05.40.-a, 87.16.Nn, 82.60.Qr

To understand universal features of various nonequilibrium phenomena in nature is still a widely open problem. In spite of considerable interest and efforts (see [1] and references therein), we are still very far from obtaining a universal framework even for nonequilibrium steady states. We thus believe it desirable to study prototypical systems that vividly demonstrate properties which are essential to nonequilibrium states. Heat engines including Feynman’s ratchet [2] of Fig. 1(a), which convert thermal fluctuations into a directed mechanical motion, may be such a prototypical system. These engines have also been investigated as Brownian motors [3]. Although the Curie principle [4] suggests that a spatial asymmetry of the system allows a spatially asymmetric motion of the particle in nonequilibrium, vivid physical pictures of the mechanism of the engines have been missing. The purpose of the present letter is to develop such a universal physical picture.

As is well-known, Feynman’s ratchet consists of a wheel and a pawl attached to separate heat baths, and exhibits a mechanical rotation [2]. Although Feynman introduced this model to illustrate the impossibility of designing a heat engine with the efficiency exceeding the Carnot limit, it has been shown that Feynman’s ratchet cannot attain the Carnot efficiency [5, 6]. In the present study, we focus on a more primitive and hopefully fun physical picture.

The Curie principle [4] suggests that a spatial asymmetry of the systems that vividly demonstrate properties which are essential to nonequilibrium states. Heat engines have also been investigated as Brownian motors [3]. Although the Curie principle [4] suggests that a spatial asymmetry of the system allows a spatially asymmetric motion of the particle in nonequilibrium, vivid physical pictures of the mechanism of the engines have been missing. The purpose of the present letter is to develop such a universal physical picture.

As is well-known, Feynman’s ratchet consists of a wheel and a pawl attached to separate heat baths, and exhibits a mechanical rotation [2]. Although Feynman introduced this model to illustrate the impossibility of designing a heat engine with the efficiency exceeding the Carnot limit, it has been shown that Feynman’s ratchet cannot attain the Carnot efficiency [5, 6]. In the present study, we focus on a more primitive and hopefully fundamental aspect of the ratchet problem, namely, the direction of the rotation. Feynman designed the ratchet so that the wheel is likely to rotate in one direction. But, as Feynman himself pointed out, the wheel can rotate in the opposite direction depending on the temperatures of the baths (see Fig. 1(b)). This fact indicates that the direction of the motion is a delicate issue which requires a careful consideration.

In the present work, we shall reveal that there is a precise statistical quantity that determines the direction of the motion. Such an investigation has a practical importance in higher dimensional ratchet-like problems, where the preferred direction of the motion is far from manifest. We shall point out a deep relation between the directed motion and “hidden heat transfer” that takes place in the equilibrium state. Our main conclusion is summarized in the “principle of heat transfer enhancement”. We believe
that our findings cover a large class of heat engines, and shed new light on universal features of nonequilibrium steady states.

Models: Feynman’s ratchet may be realized as discrete stochastic models \[2\] or as continuous models described by a set of Langevin equations \[3\]. We here concentrate on the latter type. The model consists of one translational degree of freedom \(x\) corresponding to the angle of the wheel (in the following we call it the position of a particle) and other degrees of freedom \(y\) describing the mechanical interaction between the pawl and the ratchet wheel. The degrees \(x\) and \(y\) are in contact with heat baths with temperature \(T_x\) and \(T_y\), respectively. By suitably choosing \(T_x\) and \(T_y\), we can study the behavior of the model in equilibrium or in nonequilibrium steady states (NESS). The time evolution of the system is described by the set of Langevin equations,

\[
\begin{align*}
    m_x \ddot{x} &= -\gamma_x \dot{x} + \sqrt{2\gamma_x T_x} \xi_x(t) - \partial U(x, y)/\partial x, \\
    m_y \ddot{y} &= -\gamma_y \dot{y} + \sqrt{2\gamma_y T_y} \xi_y(t) - \partial U(x, y)/\partial y.
\end{align*}
\]

(1)

where the \(x\)-asymmetric interaction potential \(U(x, y)\) has a translational invariance in \(x\) with period \(l = 1\) \[15\]. Because the potential has stable fixed points in every period, equivalent binding states are aligned periodically in \(x\). \(\gamma_x\) and \(\gamma_y\) are the friction coefficients (here we choose \(\gamma_x = \gamma_y = 1\)) and \(\xi(t)\) represent Gaussian white noises with a variance of unity. In this letter, we use two concrete models to demonstrate the results numerically, but the results do not depend on the specific models.

“Model I” is Sekimoto’s version of Feynman’s ratchet \[3\] which is the simplest case having only two degrees of freedom \((x, y)\). The potential is given by \(U(x, y) = \exp(-y + \phi(x)) + y^2/2\), where \(\phi(x)\) is a sawtooth shaped periodic function of \(x\) \[13\]. The inertia terms are neglected \((m_x = m_y = 0)\).

“Model II” has higher degrees of freedom, and was introduced as a toy model for molecular motors \[2, 3, 10\]. The particle \(x\) and each site \(y_i\) is located on a one-dimensional circle. The interaction potential \(U(x, y) = \sum_i [v(x - y_i) + u_1(y_i - y_{i+1}) + u_2(y_i - y_{i-1})]\) is composed of three parts, namely, as asymmetric nonlinear potential \(v\) between the particle and the chain site, harmonic potential \(u_1\) between the neighboring sites, and harmonic on-site potential \(u_2\) \[17\]. We set \(m_x = m_y = 1\).

Hidden heat transfer in equilibrium: In shorter time scales, the particle (the angle of the wheel) is mostly bound to one of the binding states of the potential well, and from time to time exhibits sudden jumps (steps) to neighboring binding states due to thermal activation. The probabilities of rightward and leftward steps must be identical in equilibrium, but are in general different in NESS. This unbalance generates a directed motion of the particle in longer time scales.

The thermally activated step is an elementary process of the system. During a single step (i.e., a jump of the particle from a binding state to a neighboring state), the system first absorbs some amount of energy (heat) from the heat baths and returns it afterward. A close investigation comparing the heat transfer associated with leftward and rightward steps and that with rightward ones will reveal the hidden heat transfer in equilibrium.

In order to examine the heat transfers from respective heat baths, let us define the time-dependent heat flows \(\dot{J}_x(t)\) and \(\dot{J}_y(t)\) (energy absorbed into the system per unit time) for each trajectory by using the stochastic energetics method \[3, 11\] as

\[
\begin{align*}
    \dot{J}_x(t) &= -\gamma_x \dot{x} + \sqrt{2\gamma_x T_x} \xi_x(t) \circ \dot{x}, \\
    \dot{J}_y(t) &= -\gamma_y \dot{y} + \sqrt{2\gamma_y T_y} \xi_y(t) \circ \dot{y},
\end{align*}
\]

(2)

which should be time integrated with the Stratonovich interpretation.

The heat flows \(\dot{J}_x(t)\) and \(\dot{J}_y(t)\) exhibit large fluctuation and hardly allow any physical interpretation as they are. In order to detect the heat transfers associated with the thermally activated step, we introduce a carefully conditioned ensemble average as follows. For each step, we shift the time variable so that at time \(t = 0\) the particle moves from the basin of a binding state to the basin of a neighboring state. Then we perform ensemble averaging of \(\dot{J}_x(t)\) and \(\dot{J}_y(t)\), separately for rightward steps and leftward steps. The averaged quantities are denoted as \(\dot{J}^R_x(t)\), \(\dot{J}^L_x(t)\), \(\dot{J}^R_y(t)\), and \(\dot{J}^L_y(t)\), where \(\dot{J}^R_x(t)\) is the heat flow from \(T_x\) associated with rightward steps, and so on.

Fig. \(2(a)(b)\) shows these averaged heat flow profiles in equilibrium state. The system absorbs energy from the heat baths before the step \((t < 0)\), and dissipates it after the step \((t > 0)\). The heat flow rapidly converges to zero sufficiently after or before the step, and net heat flow appears only around the step.

The heat transfer, i.e., time integrated heat flow, is defined as

\[
\dot{Q}^R_x(t) \equiv \int_{t_0}^t dt' \dot{J}^R_x(t'),
\]

(3)

where \(t_0 < 0\) is chosen so that \(\dot{J}^R_x(t)\) is negligible for \(t \leq t_0\). The quantities \(\dot{Q}^L_x(t)\), \(\dot{Q}^R_y(t)\), and \(\dot{Q}^L_y(t)\) are defined similarly. Fig. \(2(c)(d)\) shows the heat transfer in equilibrium state. We here notice the significant fact that energy absorbed from one heat bath before the step is not returned to the same heat bath after the step. This implies that, even in equilibrium, each step carries heat from one heat bath to the other. Although the existence of such heat transfer may look surprising, it does not contradict with any of the thermodynamics laws \[18\]. The nonvanishing heat transfer is observed only when we treat rightward and leftward steps separately. The word “hidden heat transfer” denotes such heat transfer. Of course, when averaged over all steps in both the directions, there is no heat transfer in equilibrium.

In the following, we denote by \(q^n\) the hidden heat transfer from \(T_x\) to \(T_y\) in equilibrium associated with
where explored in the above determines the direction of the par-

The “hidden heat transfer in equilibrium” ex-

pect that similar nonvanishing hidden heat transfer in

the temperature difference as

boundaries at $t = 0$. Heat transfers $Q_x(t)$ for (c) leftward and (d) rightward steps respectively, which is obtained by the integration of $J_x(t)$ from $t_0 = -20$ (see Eq.(3)).

rightward steps. Note that we have

$$q_{eq} \equiv Q_x^R(\infty) = Q_x^L(\infty) = Q_y^L(\infty)$$

as is seen in Fig.2(c)(d). The nonvanishing hidden heat transfer $q_{eq}$ in equilibrium comes from the asymmetry of the interaction potential $U(x,y)$ and the resulting dynamics. Since such an asymmetry is not a special feature of the present models but a rather generic one, we expect that similar nonvanishing hidden heat transfer in equilibrium states is found in a wider class of systems.

Heat transfer and directed motion in NESS near equilibrium: The “hidden heat transfer in equilibrium” explored in the above determines the direction of the particle motion in NESS as we shall now discuss. Let us define the response coefficient $\chi_p$ of the particle flow to the temperature difference as

$$\chi_p = \lim_{\Delta \beta \to 0} J_p(\beta - \Delta \beta/2, \beta + \Delta \beta/2)/\Delta \beta,$$

where $J_p(\beta_x, \beta_y) = \langle \dot{x}_p \rangle$ is the particle current for $T_x = 1/\beta_x$ and $T_y = 1/\beta_y$ (where $\Delta \beta = 1/T_y - 1/T_x$ and $2\beta = 1/T_y + 1/T_x$). One of course has $J_p(\beta, \beta) = 0$.

From the sign of $\chi_p$, the direction of the particle flow is specified. For example, when $\chi_p > 0$ right-oriented flow appears for $\Delta \beta > 0$, i.e., $T_x > T_y$.

As shown in Fig.3, we found a remarkable relation between $\chi_p$ and the hidden heat transfer $q_{eq}$,

$$q_{eq} = \frac{l \chi_p}{D_p^{eq}}$$

where $D_p^{eq}$ is the diffusion constant of the particle in equilibrium states and $l$ is the period of the interaction potential in $x$. The relation (6) does not only relate the directions of particle motion and “hidden heat transfer”, but shows that these two are related in a quantitative manner. In the systems of heat engines, the directed particle flow is induced by a “field” associated with temperature differences. Based on linear response theory [12], the quantity $\chi_p$, which is the particle flow divided by a temperature gradient, is expressed in terms of a time correlation function between the particle flow $\dot{x}$ and the heat flow $(J_x - J_y)/2$ at equilibrium. Evaluating this expression under the assumption that each step occurs independently, we can derive Eq. (6).

Eq. (6) implies that a step in the direction of the particle flow enhances heat transfer from the hotter to the colder heat bath. For example, considering the case $\chi_p > 0$ and $T_x > T_y$, the particle flows toward right from the definition (6). At the same time, Eq. (6) implies $q_{eq} > 0$, which means that rightward steps carry heat $q_{eq}$ from $T_x$ to $T_y$, i.e., from hotter to colder, while leftward steps carry the same amount of heat in the opposite direction. We conclude that the direction of the particle motion is chosen so that to enhance the heat transfer between the two baths. This “principle of heat transfer enhancement” may look quite natural and reasonable.

Heat transfer and directed motion in NESS far from equilibrium: Let us proceed to the observation of heat transfer far from equilibrium. Because there is not steady heat transfer, we consider the excess heat transfer associated with steps in NESS defined as

$$Q_{x,ex}(t) = \int_{t_0}^t dt[J_x^R(t) - J_x].$$

The quantities $Q_{x,ex}^L(t)$, $Q_x^R(t)$ and $Q_{x,ex}^L(t)$ are defined similarly. Here $J_x^R(t)$ is the conditioned ensemble average of the heat flow and the contributions from the steady heat flow, $J_x$ and $J_y$ satisfying $J_x = -J_y$, are subtracted, where “bar” means the long time average. Note that we have $\lim_{t \to \pm \infty} J_x^R(t) = J_x$, etc.
We conclude that the “principle of heat transfer enhancement” holds also in systems far from equilibrium.

Discussion: We have investigated a class of heat engines including Feynman’s ratchet and found a clear relation between the directed motion in NESS and hidden heat transfer in the equilibrium state. The relation (10), which universally holds for the present class, can be derived from the cross correlation between the fluctuation of the heat flow and that of the particle flow. By focusing on thermally activated steps, we were able to characterize this correlation in terms of the hidden heat transfer $q^\text{hid}$. The notion of the hidden heat transfer provides us with a vivid picture for the elementary process of the heat engine, namely, each directional step carries a heat quanta depending on its direction. Heat transfers separately measured for each heat bath would be useful quantities for the investigation of other systems with multiple heat baths. It is also interesting to explore other models of heat engine suitable for theoretical treatments [10-14].

The fact that the principle of heat transfer enhancement holds even in NESS far from equilibrium suggests that there can be a universal characterization of NESS. This remains as a future problem. We believe that our findings offer a novel universal view point for studying NESS, and will lead to a better understanding of nonequilibrium physics in general.

We are grateful to H. Tasaki for a critical reading of this manuscript.

[1] Y. Oono and M. Paniconi: Prog. Theor. Phys. Suppl. 130 (1998) 29.
[2] R. P. Feynman: Lectures in Physics, Vol.I (Addison-Wesley Publishing Co., 1963).
[3] P. Reimann: Physics Reports 361 (2002) 57.
[4] P. Curie: J. Phys. III 3 (1894) 393.
[5] K. Sekimoto: J. Phys. Soc. Jpn. 66 (1997) 1234.
[6] J. M. R. Parrondo and P. Espanol Am. J. Phys. 64 (1996) 1125.
[7] C. Jarzynski and O. Mazonka Phys. Rev. E 59 (1999) 6448.
[8] N. Nakagawa and K. Kaneko: Phys. Rev. E 67 (2003) 040901(R).
[9] N. Nakagawa and T. S. Komatsu: J. Phys. Soc. Jpn. 74 (2005) 1653.
[10] N. Nakagawa and T. S. Komatsu: Physica A 361 (2006) 216.
[11] K. Sekimoto, F. Takagi and T. Hondou: Phys. Rev. E 62 (2000) 7759.
[12] R. Kubo, M. Toda and N. Hashitsume: Statistical Physics II: Nonequilibrium Stastical Mechanics (Springer-Verlag, Berlin, 1991).
[13] N. Nakagawa and T. S. Komatsu: cond-mat/0603228, to appear in Eur. Phys. Lett..
[14] C. Van den Broeck, P. Meus and R. Kawai: New J. Phys. 7 (2005) 10.