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

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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.

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To understand universal features of various nonequilibrium phenomena in nature is still a wide open problem. In spite of considerable interest and effort (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 that 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 Rapid Communication 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 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 motion is a delicate issue that requires 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 ratchetlike 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 light on universal features of nonequilibrium steady states.

Feynman's ratchets may be realized as discrete stochastic models [7] or as continuous models described by a set of Langevin equations [5]. 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 $\boldsymbol{y}$ describing the mechanical interaction between

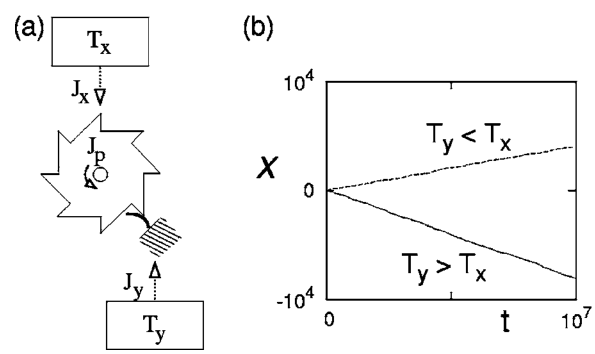

FIG. 1. (a) Schematic figure of Feynman's ratchet composed of a sawtooth-shaped ratchet wheel and a pawl. The system is attached to two heat baths, the wheel to T_x and the pawl to T_y. The temperature difference between T_x and T_y produces the nonvanishing steady rotation J_p, which can be used to execute external work. The variable x denotes the angle of the wheel. There are degenerate stable positions of x corresponding to the ratchet potential wells (there are eight in this figure). Heat flows J_x and J_y are defined as positive when the system absorbs energy from each heat bath. (b) Typical trajectories of x in a NESS. The system exhibits directed motions, i.e., unidirectional rotations on average. The solid lines and the broken lines show the data for the conditions $2T_x=T_y$ and $T_x=2T_y$, respectively, in model II. We clearly see that the direction of the motion depends on the temperature difference.

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the pawl and the ratchet wheel. The degrees x and $\mathbf{y}$ are in contact with heat baths with temperatures 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 (NESSs). The time evolution of the system is described by the set of Langevin equations

$$m_x\ddot{x} = -\gamma_x\dot{x} + \sqrt{2\gamma_x T_x}\xi_x(t) - \partial U(x,\mathbf{y})/\partial x,$$

$$m_y\ddot{\mathbf{y}} = -\gamma_y\dot{\mathbf{y}} + \sqrt{2\gamma_y T_y}\boldsymbol{\xi}_y(t) - \partial U(x,\mathbf{y})/\partial \mathbf{y}, \qquad (1)$$

where the x-asymmetric interaction potential $U(x,\mathbf{y})$ has a translational invariance in x with period $l=1$.[1] Because the potential has stable fixed points in every period, equivalent binding states are aligned periodically in x. γ_x and γ_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 Rapid Communication, 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 [5], which is the simplest case having only two degrees of freedom (x and 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.[2] 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 [8–10]. The particle x and chain sites $\mathbf{y}=\{y_i\}$ are located on a one-dimensional circle. The interaction potential $U(x,\mathbf{y})=\Sigma_i[v(x-y_i)+u_1(y_i-y_{i+1})+u_2(y_i-il)]$ is composed of three parts, namely, an asymmetric nonlinear potential v between the particle and the chain site, a harmonic potential u_1 between the neighboring chain sites, and a harmonic on-site potential u_2.[3] We set $m_x=m_y=1$.

On 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 NESSs. This unbalance generates a directed motion of the particle on 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 steps and that with rightward ones will reveal the hidden heat transfer in equilibrium.

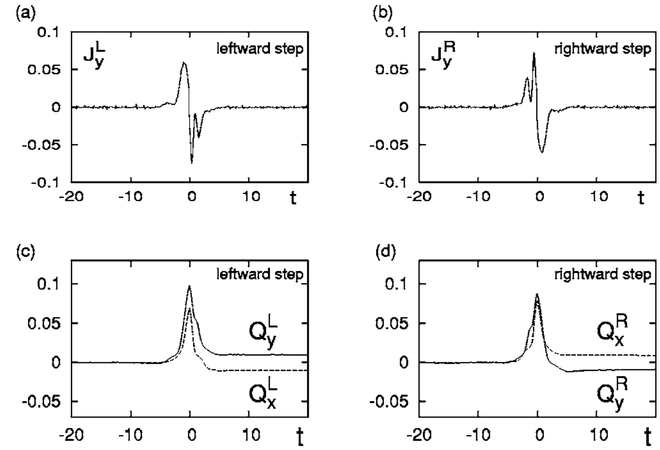

FIG. 2. Time sequences of the averaged heat flow $J_y(t)$ over conditioned ensembles (3.8×10^5 samples) for (a) leftward and (b) rightward step in equilibrium ($T_x=T_y=0.05$) for model II, where the energy barrier height is about $3.1T_x$. For each step, time is shifted so that the particle crosses basin boundaries at $t=0$. Heat transfers $Q_*(t)$ for (c) leftward and (d) rightward steps, respectively, are obtained by the integration of $J_*(t)$ from $t_0=-20$ [see Eq. (3)].

In order to examine the heat transfers from the respective heat baths, let us define the time-dependent heat flows $\hat{J}_x(t)$ and $\hat{J}_y(t)$ (energy absorbed into the system per unit time) for each trajectory by using the stochastic energetics method [5,11] as

$$\hat{J}_x(t) = [-\gamma_x\dot{x} + \sqrt{2\gamma_x T_x}\xi_x(t)]\circ\dot{x},$$

$$\hat{J}_y(t) = [-\gamma_y\dot{\mathbf{y}} + \sqrt{2\gamma_y T_y}\boldsymbol{\xi}_y(t)]\circ\dot{\mathbf{y}}, \qquad (2)$$

which should be time integrated with the Stratonovich interpretation.

The heat flows $\hat{J}_x(t)$ and $\hat{J}_y(t)$ exhibit large fluctuations 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 $\hat{J}_x(t)$ and $\hat{J}_y(t)$, separately for rightward steps and leftward steps. The averaged quantities are denoted as $J_x^R(t)$, $J_x^L(t)$, $J_y^R(t)$, and $J_y^L(t)$, where $J_x^R(t)$ is the heat flow from T_x associated with rightward steps, and so on.

Figures 2(a) and 2(b) show these averaged heat flow profiles in the 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

[1]To be precise, the translational invariance means $U(x+l,\mathrm{R}_l\mathbf{y})=U(x,\mathbf{y})$. Here R_l is the operator that translates $\mathbf{y}$ by l along the wheel. In the case of model I, $\mathrm{R}_l y=y$. In the case of model II, $(\mathrm{R}_l\mathbf{y})_i=y_{i-1}+l$.

[2]Here the smooth function $\phi(x)=-\sin(2\pi x)/2-\sin(4\pi x)/12+1/2$ is used for convenience of numerical calculations.

[3]The magnitude of u_1 and u_2 determines the stiffness of the system, which is a control parameter used for exploring model space. Please refer to [8,9] for the explicit form of the potential functions and to [10] for the method to determine the basin boundary.

$$Q_x^{\mathrm{R}}(t) \equiv \int_{t_0}^{t} dt' J_x^{\mathrm{R}}(t'), \tag{3}$$

where $t_0<0$ is chosen so that $J_x^{\mathrm{R}}(t)$ is negligible for $t\le t_0$. The quantities $Q_x^{\mathrm{L}}(t)$, $Q_y^{\mathrm{R}}(t)$, and $Q_y^{\mathrm{L}}(t)$ are defined similarly. Figures 2(c) and 2(d) show the heat transfer in the 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 any of the thermodynamics laws.[4] The nonvanishing heat transfer is observed only when we treat rightward and leftward steps separately. The words "hidden heat transfer" denote such heat transfer. Of course, when averaged over all steps in both directions, there is no heat transfer in equilibrium.

In the following, we denote by q^{eq} the hidden heat transfer from T_x to T_y in equilibrium associated with rightward steps. Note that we have

$$q^{\mathrm{eq}} \equiv Q_x^{\mathrm{R}}(\infty) = -Q_x^{\mathrm{L}}(\infty) = -Q_y^{\mathrm{R}}(\infty) = Q_y^{\mathrm{L}}(\infty) \tag{4}$$

as is seen in Figs. 2(c) and 2(d). The nonvanishing hidden heat transfer q^{eq} in equilibrium comes from the asymmetry of the interaction potential $U(x,\boldsymbol{y})$ 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.

The hidden heat transfer in equilibrium explored in the above determines the direction of the particle motion in NESSs as we shall now discuss. Let us define the response coefficient χ_{p} of the particle flow to the temperature difference as

$$\chi_{\mathrm{p}} = \lim_{\Delta\beta\to 0} J_{\mathrm{p}}(\beta-\Delta\beta/2,\beta+\Delta\beta/2)/\Delta\beta, \tag{5}$$

where $J_{\mathrm{p}}(\beta_x,\beta_y)=\langle \dot{x}_{\mathrm{p}}\rangle$ 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 $J_{\mathrm{p}}(\beta,\beta)=0$. From the sign of χ_{p}, the direction of the particle flow is specified. For example, when $\chi_{\mathrm{p}}>0$ 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 χ_{p} and the hidden heat transfer q^{eq},

$$q^{\mathrm{eq}} = \frac{l\chi_{\mathrm{p}}}{D_{\mathrm{p}}^{\mathrm{eq}}}, \tag{6}$$

where $D_{\mathrm{p}}^{\mathrm{eq}}$ is the diffusion constant of the particle in equilibrium states and l is the period of the interaction potential in x. The relation (6) not only relates the directions of particle motion and hidden heat transfer, but shows that these two are related in a quantitative manner. In 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 χ_{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 $(\hat{J}_x-\hat{J}_y)/2$ at equilibrium. Evaluating this expression under the assumption that each step occurs independently, we can derive Eq. (6) [13].

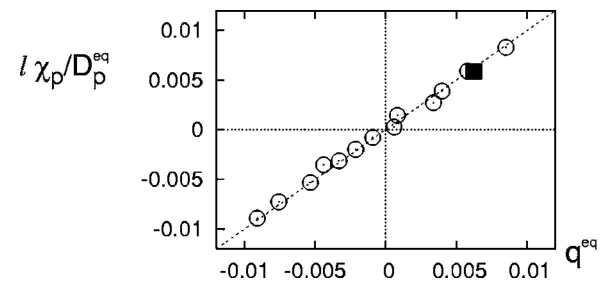

FIG. 3. Hidden heat transfer q^{eq} at equilibrium and $l\chi_{\mathrm{p}}/D_{\mathrm{p}}^{\mathrm{eq}}$. This reveals that there is a nontrivial relation (6) between the motion of the particle in NESSs and hidden heat transfer in equilibrium. Results for the two models, model I (filled square) at $\beta=3$ and model II (open circles) at $\beta=20$, are shown. For the latter model, the stiffness parameter of the model is varied to explore the model space broadly so that we have many points for the same temperature conditions.

Equation (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 $\chi_{\mathrm{p}}>0$ and $T_x>T_y$, the particle flows toward the right from the definition (5). At the same time, Eq. (6) implies $q^{\mathrm{eq}}>0$, 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 as to enhance the heat transfer between the two baths. This principle of heat transfer enhancement may look quite natural and reasonable.

Let us proceed to the observation of heat transfer far from equilibrium. Because there is net steady heat transfer, we consider the *excess* heat transfer associated with steps in NESSs defined as

$$Q_{x,\mathrm{ex}}^{\mathrm{R}}(t) \equiv \int_{t_0}^{t} dt[J_x^{\mathrm{R}}(t) - \bar{J}_x]. \tag{7}$$

The quantities $Q_{x,\mathrm{ex}}^{\mathrm{L}}(t)$, $Q_{y,\mathrm{ex}}^{\mathrm{R}}(t)$, and $Q_{y,\mathrm{ex}}^{\mathrm{L}}(t)$ are defined similarly. Here $J_x^{\mathrm{R}}(t)$ is the conditioned ensemble average of the heat flow and the contributions from the steady heat flow, $\bar{J}_x$ and $\bar{J}_y$, satisfying $\bar{J}_y=-\bar{J}_x$, are subtracted; the overbar means the long-time average. Note that we have $\lim_{t\to\pm\infty} J_x^{\mathrm{R}}(t)=\bar{J}_x$, etc.

Figure 4 shows the excess heat transfers in NESSs. Note that, in the figure, the excess heat transfers associated with rightward and leftward steps have the same direction,

[4]Comparing the profiles for rightward and leftward steps, we can find that the equalities $J_y^{\mathrm{R}}(t)=-J_y^{\mathrm{L}}(-t), J_x^{\mathrm{R}}(t)=-J_x^{\mathrm{L}}(-t)$ hold. We also find that rightward and leftward steps occur with exactly the same probability in equilibrium. Indeed these properties are necessary consequences of the reversibility of equilibrium states. That we have confirmed these properties can be regarded as a sign of reliability of our numerical calculations.

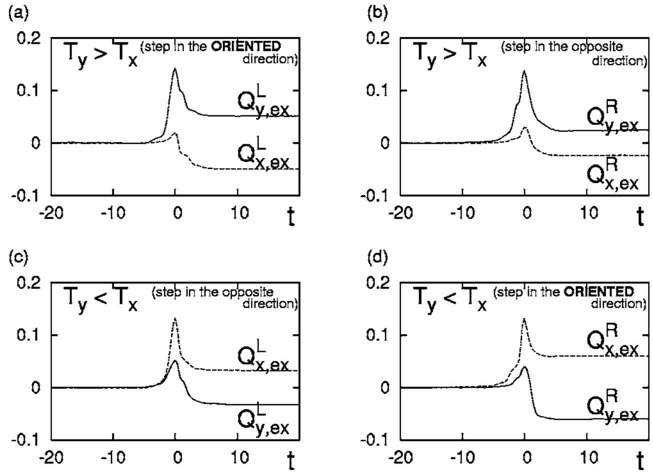

FIG. 4. Profile of excess heat transfer in the NESS of model II. In the upper figures with $T_y = 2T_x$, particle flow is leftward. In the lower figures with $2T_y = T_x$, particle flow is rightward.

namely, from the hotter bath to the colder. However, the amounts of heat transfer are different for the rightward and leftward steps, and we again find that the direction which enhances the net heat transfer is selected. We conclude that the principle of heat transfer enhancement holds also in systems far from equilibrium.

We have investigated a class of heat engines including Feynman's ratchet and found a clear relation between the directed motion in NESSs and hidden heat transfer in the equilibrium state. The relation (6), 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^{eq}. 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 quantum 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 [7,14]. 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 universal viewpoint for studying NESS, and will lead to a better understanding of nonequilibrium physics in general.

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