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Temperature of a Hamiltonian system given as the effective temperature of a nonequilibrium steady-state Langevin thermostat

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In nonequilibrium steady states (NESS) far from equilibrium, it is known that the Einstein relation is violated. Then, the ratio of the diffusion coefficient to the mobility is called an effective temperature, and the physical relevance of this effective temperature has been studied in several works. Although the physical relevance is not yet completely clear, it has been found that the role of an effective temperature in NESS is indeed analogous to that of the temperature in equilibrium systems in a number of respects. In this paper, we find further evidence establishing this analogy. We employ a nonequilibrium Langevin system as a thermostat for a Hamiltonian system and find that the kinetic temperature of this Hamiltonian system is equal to the effective temperature of the thermostat.

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Fluctuation-dissipation relations (FDRs) relate dynamical properties of fluctuations in systems under equilibrium conditions to linear transport properties of nonequilibrium systems through the detailed-balance condition [1]. Representative examples of FDRs are the Einstein relation, which relates a diffusion coefficient and a mobility, and the Green-Kubo relation, which relates current fluctuations and the corresponding conductivities.

In recent years, the properties of fluctuations and linear responses to perturbations have been investigated for nonequilibrium states even outside the linear response regime, specifically in steady-state systems [2–4] and in aging systems [5–8]. Although we cannot expect FDRs to be generally valid outside the linear response regime, there have been several relations proposed and investigated recently that represent extensions of FDRs to systems far from equilibrium [9–12].

In Refs. [9,10], the violation of FDRs is studied in the case of a nonequilibrium one-dimensional Langevin system in which a Brownian particle is subject to a spatially constant driving force f and a periodic potential $U(x)$. Explicitly, the system studied there is

$$\gamma\dot{x} = -\frac{\partial U(x)}{\partial x} + f + \xi(t),$$

$$\langle \xi(t)\xi(t')\rangle = 2\gamma T\delta(t-t'), \tag{1}$$

where $x(t)$ is the position of the Brownian particle, $\xi(t)$ is Gaussian noise, γ is the friction coefficient, and T is the temperature of the environment. (The Boltzmann constant is set to unity.) In this model, in the linear response regime, the Einstein relation

$$D = \mu_d T \tag{2}$$

holds, where D is the diffusion coefficient and μ_d is the differential mobility defined as

$$D(f) \equiv \lim_{t\to\infty} \frac{\langle [x(t) - x(0) - v_s(f)t]^2 \rangle}{2t}, \tag{3}$$

$$\mu_d(f) \equiv \frac{dv_s(f)}{df}. \tag{4}$$

Here $v_s(f)$ is the steady-state velocity of the Brownian particle and is known as the Stratonovich formula [9,13]. However, outside the linear response regime, i.e., for large f, the above Einstein relation does not hold. In such situations, as an extension of the concept of temperature, it is natural to define the following quantity:

$$\Theta(f) \equiv \frac{D(f)}{\mu_d(f)}. \tag{5}$$

Then, outside the linear response regime, we have $\Theta \neq T$. Thus, the introduction of Θ allows us to define an extended Einstein relation that applies to nonequilibrium steady states (NESS) far from equilibrium, although this leads to the question of the physical significance of Θ. In Refs. [9,10], in order to elucidate the physical significance of Θ, a large-scale description of the system was derived by applying a perturbation method to the Fokker-Planck equation [9] and by considering a finite time average of the Langevin equation [10]. With these treatments, it was found that Θ plays the role of a temperature in the large-scale description of the nonequilibrium Langevin system (1), and for this reason, it is referred to as an effective temperature.

In this paper, we present a study that further establishes the role of Θ as an effective temperature for NESS. Here, we employ a Langevin system in a NESS as a thermostat for a Hamiltonian system, and we investigate the temperature of the Hamiltonian system established by this thermostat. More precisely, we set out to determine whether the kinetic temperature of the Hamiltonian system is equal to Θ in this situation. We find that, in fact, the kinetic temperature is equal to Θ in the case that the thermostat moves at the speed $v=-v_s(f)$, so that the average velocity of the Brownian particle relative to the Hamiltonian system is zero. (See the schematic in Fig. 1 and *Moving thermostat* for details.)

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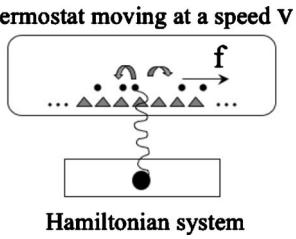

FIG. 1. Schematic depiction of the "moving thermostat." The thermostat moves at a speed v relative to the Hamiltonian system.

Stationary thermostat. In Fig. 1, we present a schematic depiction of the model we study. In this section, we consider a combined system consisting of a Hamiltonian system in contact with a Langevin thermostat in the case that the two are relatively at rest, i.e., $v=0$.

The Langevin thermostat consists of N Brownian particles ($N=20$) which are confined to move along a single direction, say the x direction. Because there is no interaction between the Brownian particles, the statistical properties of each are the same as those in the model (1), studied in Refs. [9,10]. Each Brownian particle is subject to a constant driving force f and a periodic potential $U(x_i)=(U_0/T)\sin(2\pi x_i/\ell)$, where x_i represents the position of the ith particle. The size of the thermostat is chosen as 20ℓ $(-10\ell \leqslant x_i \leqslant 10\ell)$, and periodic boundary conditions are imposed on the Brownian particles.

The Hamiltonian system we consider is a one-dimensional system consisting of a single particle. Each Brownian particle in the Langevin system interacts with this Hamiltonian particle through the potential $U_{\rm int}=\varepsilon(x_i-x^H)^2/2$ for $|x_i-x^H|<r_c$ and $U_{\rm int}=0$ otherwise, where x^H is the position of the Hamiltonian particle, and r_c is the cutoff length of the interaction. This particle is confined to the region $-5\ell \leqslant x^H \leqslant 5\ell$ by wall potentials of the forms $U_L(x^H)=(x^H+5\ell)^{-4}$ and $U_R(x^H)=(x^H-5\ell)^{-4}$.

The time evolution of the ith Brownian particle is described by the one-dimensional Langevin equation

$$\gamma\dot{x}_i = -\frac{\partial U(x_i)}{\partial x_i} + f - \frac{\partial U_{\rm int}(x_i - x^H)}{\partial x_i} + \xi_i(t),$$

$$\langle \xi_i(t)\xi_j(t')\rangle = 2\gamma T\delta(t-t')\delta_{i,j}, \tag{6}$$

and that of the Hamiltonian particle is described by

$$m\dot{v}^H = -\sum_{i=1}^{N}\frac{\partial U_{\rm int}(x_i - x^H)}{\partial x^H} - \frac{\partial U_L(x^H)}{\partial x^H} - \frac{\partial U_R(x^H)}{\partial x^H},$$

$$\dot{x}^H = v^H. \tag{7}$$

In our numerical simulation, the velocity Verlet method was adopted to integrate the equation of motion (7) with a time step $\Delta t=5\times10^{-5}$, and we used the parameter values $T=1$, $\gamma=1$, $\ell=1$, $U_0=3$, $\varepsilon=1$, $m=1$, $r_c=4$, and $0\leqslant f\leqslant 25$. As to an initial condition, $x^H(0)=0$, $x_i(0)=i/2-10$ $(i=1,2,\ldots,20)$, and $v^H(0)$ was chosen randomly according to a Gaussian distribution.

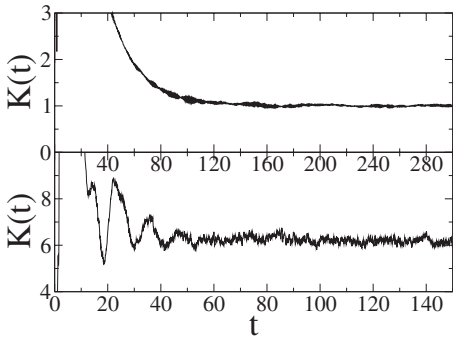

FIG. 2. $K(t)$ obtained using a stationary thermostat as a function of time in the cases $f=0$ (upper) and $f=10$ (lower). These results were obtained from 5000 samples.

We define the velocity fluctuation of the Hamiltonian particle as

$$K(t) \equiv m\{\langle v^H(t)^2\rangle - \langle v^H(t)\rangle^2\}. \tag{8}$$

In Fig. 2, we plot $K(t)$ as a function of time for $f=0$ and $f=10$ in the case of a stationary thermostat. Next, we define the kinetic temperature as

$$\bar{K} \equiv \lim_{t\to\infty} K(t). \tag{9}$$

In the case $f=0$, we find that $\bar{K}=1.00\pm0.016$, which is equal to the temperature of the environment ($T=1$). In the case $f=10$, because the Brownian particles exhibit a nonzero average velocity maintained by f, significantly more heat flows into the Hamiltonian system than in the case $f=0$. But in this case, as in the $f=0$ case, as t increases, $K(t)$ approaches a constant value, with a kind of stationary behavior being established between the Hamiltonian system and the thermostat. In this case, we find $\bar{K}=6.22\pm0.22$. (We obtain $\bar{K}$ by averaging $K(t)$ over the intervals $t\in[60,150]$ and $t\in[200,300]$ for $f=10$ and $f=0$, respectively.)

Moving thermostat. Next, we consider the case of a moving thermostat. Specifically, we study the situation in which the thermostat moves at a constant speed of $v=-v_s(f)$ relative to the Hamiltonian system, where $v_s(f)$ is the steady-state velocity of the Brownian particles [9]. With such a moving thermostat, the average velocity of each Brownian particle measured with respect to the spatial coordinate of the Hamiltonian system vanishes. Defining $y_i \equiv x_i - v_s(f)t$, we can realize such a system by simply replacing $U_{\rm int}(x_i-x^H)$ with $U_{\rm int}(y_i-x^H)$ in Eqs. (6) and (7).

In Fig. 3, we plot $K(t)$ as a function of time in the cases $f=5$, 10, and 15. Note that in order to obtain these results for $K(t)$, we use the analytical solutions of $v_s(f)$ for the model (1) [14]. From the data plotted in the graphs of Fig. 3, we find $\bar{K}=1.25\pm0.05$ in the case $f=5$, $\bar{K}=1.54\pm0.03$ in the case $f=10$, and $\bar{K}=1.68\pm0.06$ in the case $f=15$. Comparing the middle graph of Fig. 3 with the lower graph of Fig. 2, both corresponding to the case $f=10$, we find that the value

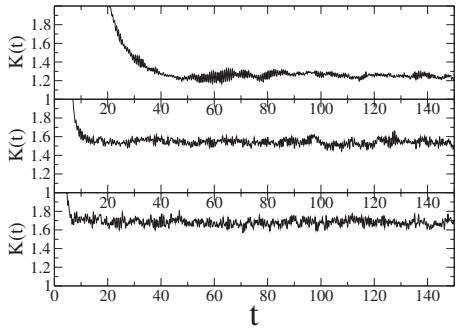

FIG. 3. $K(t)$ obtained using a moving thermostat as a function of time in the cases $f=5$ (upper), $f=10$ (middle), and $f=15$ (lower). These results were obtained from 5000 samples.

of $\bar{K}$ obtained when using the moving thermostat differs significantly from that obtained when using the stationary thermostat.

Now, let us compare the above results for $\bar{K}$ with the values of Θ for the thermostat. In Ref. [9], from calculations of $D(f)$ and $\mu_d(f)$, it was found that $D/\mu_d=1.24$ in the case $f=5$, $D/\mu_d=1.52$ in the case $f=10$, and $D/\mu_d=1.67$ in the case $f=15$ for the model (1). Because $T=1$, these values of D/μ_d indicate that the Einstein relation (2) does not hold for $f\geqslant 5$. Comparing these values with the values of $\bar{K}$ computed presently, we find that the relation $\bar{K}=D/\mu_d$ holds when ε, which represents the strength of the interaction between the thermostat and the Hamiltonian system, is sufficiently small [15]. This implies that the kinetic temperature of the Hamiltonian system is equal to the effective temperature Θ given by Eq. (5) in the case that the Hamiltonian system is in contact with the moving thermostat. In Fig. 4, we compare $\bar{K}$ with Θ $(\equiv D/\mu_d)$ for various values of f. It is seen that the relation

$$\bar{K}=\Theta \tag{10}$$

holds, to the precision of the numerical computations.

Interpretation of Eq. (10). In Ref. [9], a large-scale description of the probability density for the model (1) was derived using a perturbation method, and it was found that Θ

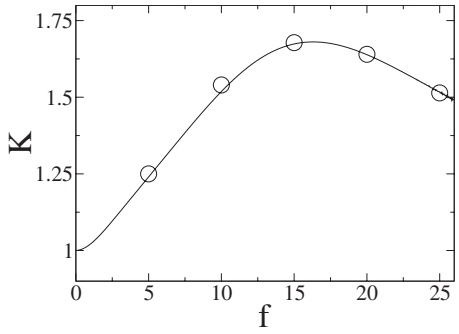

FIG. 4. The kinetic temperature $\bar{K}$ obtained using a moving thermostat as a function of f (circles). The solid curve denotes the analytical solution of $\Theta(f)$ $[\equiv D(f)/\mu_d(f)]$ for the model (1) [9].

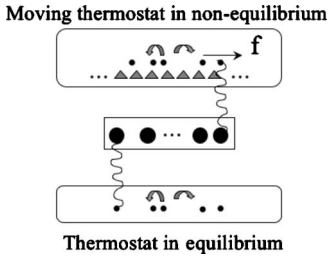

FIG. 5. Schematic depiction of the heat conduction system using the effective temperature.

appears as a temperature in a Fokker-Planck equation of the coarse-grained probability density. Then, in order to further investigate the physical properties of Θ, in Ref. [10], a coarse-grained description of the motion of a Brownian particle was derived by computing a finite time average of the Langevin equation, rather than analyzing the probability density. This coarse-grained description is given by the equations $\Gamma(X_{n+1}-X_n)/\delta t=F+\Xi_n$ and $\langle \Xi_n \Xi_m \rangle \delta t=2\Gamma\Theta\delta_{m,n}$, where we have $F\equiv\Gamma v_s$, $X_n\equiv x(t_n)$, and $t_n\equiv n\delta t$ $(n=0,1,2,\ldots)$, and the time interval δt is chosen to be sufficiently longer than the characteristic time of the system. Here, Γ and F are uniquely determined as functions of the parameters that appear in the model (1) [10]. Then, using the moving coordinates $Y_n\equiv X_n-v_s t_n$, we can describe the large-scale motion of a Brownian particle by the equilibrium-form Langevin equation

$$\Gamma\frac{Y_{n+1}-Y_n}{\delta t}=\Xi_n. \tag{11}$$

In the present investigation, choosing the cutoff length of the interaction between the Brownian particles and the Hamiltonian particle, r_c, to be sufficiently large, we considered the change in behavior of the system as we increase the number of the Brownian particles that interact with the Hamiltonian particle. In the case that there are many Brownian particles, the Hamiltonian particle moves slowly enough that its characteristic time is larger than δt. Because in this case, when we use the moving thermostat, the motion of each Brownian particle is described by Eq. (11), we obtain the result (10).

Heat conduction. As an application of the moving Langevin thermostat, we study the heat conduction system described below (see the schematic depiction in Fig. 5). Here, a one-dimensional Hamiltonian system consisting of ten particles is in contact with two thermostats: a moving, nonequilibrium thermostat of the type described above and an equilibrium thermostat. Although the temperatures of the environments of both thermostats are set to $T=1$, it is expected that a nonzero heat flux will be observed in the Hamiltonian system because Θ (which differs from T) plays the role of the temperature in the moving thermostat.

Let x_j^H be the position of the jth Hamiltonian particle $(j=1,\ldots,10)$. In our model, the jth particle interacts only with its neighbors (the $j\pm 1$th particles) through the potential $U_{\rm int}^H(x_j^H-x_{j\pm1}^H)=(1/2)(x_j^H-x_{j\pm1}^H)^2+(10/4)(x_j^H-x_{j\pm1}^H)^4$. Then,

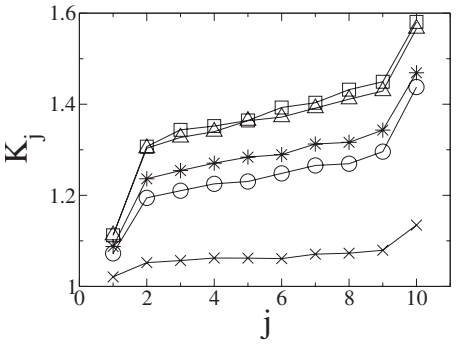

FIG. 6. $\bar{K}_j$ as a function of j in the cases $f=5$ (pluses), $f=10$ (circles), $f=15$ (squares), $f=20$ (triangles), and $f=25$ (asterisks).

only the first Hamiltonian particle is in contact with the equilibrium thermostat, and only the tenth Hamiltonian particle is in contact with the moving thermostat.

Defining $\bar{K}_j$ as the kinetic temperature of the jth Hamiltonian particle, in Fig. 6, we plot $\bar{K}_j$. It is seen that $K_j < K_{j+1}$. This is due to the relation $\Theta > T$. Although $\Theta > T$ in our model, it has been reported that the case $\Theta < T$ can also be realized with an appropriate choice of the periodic potential $U(x_i)$ [16]. This implies that we could control the direction of the heat flux by altering the functional form of $U(x_i)$.

Conclusion. In this paper, we have investigated the use of a Langevin system in a NESS as a thermostat to establish the kinetic temperature of a Hamiltonian system. Our main results consist of the relation (10) and the data plotted in Fig. 6, both obtained with the use of the moving Langevin thermostat. Because the physical relevance of effective temperatures in NESS [9,10], glassy systems [5–7], and biomolecules [8] is not yet fully clarified, we hope that our study sheds more light on it.

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