Mechanical and Langevin thermostats: Gulton staircase problem

Toyonori Munakata
Department of Applied Mathematics and Physics, Kyoto University, Kyoto 606, Japan
(Received 14 October 1998)

Dynamics in a Gulton staircase is considered based on a model in which many particles, coupled through an average velocity, are in contact with a Gaussian thermostat. Computer simulation gives information on entropy production, the stationary mass current, and distribution functions of both particle positions and momenta. A Langevin thermostat is also considered for the sake of comparison with a mechanical thermostat. [S1063-651X(99)09105-9]

PACS number(s): 05.20.Gg, 05.40.Fb

Recently a lot of attention has been paid to structures and properties of mechanical thermostats, in connection with nonequilibrium stationary states, nonlinear response, and other (fundamental) problems such as Loschmidt's paradox [1–3]. Dynamics in a Gulton staircase is investigated intensively because of its basic importance and simplicity by Holian and co-workers with use of the Nose-Hoover (NH) thermostat, with special emphasis put on a nonequilibrium stationary state produced by an external force [3–5]. More concretely, time evolution of the system they studied, hereafter to be called the NH model, is described by

$$dq/dt=p, \tag{1}$$

$$dp/dt=F_p(q)+F^{\mathrm{ext}}-\nu zp, \tag{2}$$

$$dz/dt=\nu(p^2/T-1), \tag{3}$$

where we set both mass of a particle and the Boltzmann constant equal to one. In Eq. (2) ν is a parameter controlling coupling strength between a particle and the thermostat and $F_p(q)=-dV_p(q)/dq$ denotes the space-periodic force (with periodicity 2π) derived from the potential $V_p(q)$. Technically, a periodic boundary condition is employed; thus a particle leaving the range $0\leqslant q\leqslant 2\pi$ at $q=2\pi$ enters the range at $q=0$ with the same momentum. z and T denote a dynamic friction and temperature of the system, respectively. The particle moves on average in the direction of the external force F^{ext} and main concern is put around the nonequilibrium stationary state with mass-current and positive entropy production.

Following Holian, Posch, and Hoover, [4] we briefly summarize results obtained for the NH model. Defining the total (the system plus heat bath) energy E by

$$E=p^2/2+V_p(q)+Tz^2/2, \tag{4}$$

it readily follows from Eqs. (1)–(4) that

$$dE/dt=-T\nu z+F^{\mathrm{ext}}p\equiv dQ/dt-dW/dt, \tag{5}$$

where dQ is supposed to represent the heat given to the (total) system and dW denotes the work done by the system. The statistical entropy $S_{\mathrm{sta}}(t)\equiv -\int dp\,dq\,dz\,f(q,p,z;t)\ln f(q,p,z;t)$ changes in time as

$$dS_{\mathrm{sta}}(t)/dt=T^{-1}\langle dQ/dt\rangle=-\nu\langle z\rangle=\langle\Lambda\rangle, \tag{6}$$

where $\langle ...\rangle$ denotes the ensemble average over f, and the rate of expansion Λ of the phase space in Eq. (6) is defined by $\Lambda\equiv\partial(dq/dt)/\partial q+\partial(dp/dt)/\partial p+\partial(dz/dt)/\partial z$. Computer experiment on the NH model showed that [4] (i) the average $\langle z\rangle_{\mathrm{st}}$ in an nonequilibrium stationary state is positive, and (ii) the stationary work $\langle dW/dt\rangle_{\mathrm{st}}=-F^{\mathrm{ext}}\langle p\rangle_{\mathrm{st}}$ coincides with $\langle dQ/dt\rangle_{\mathrm{st}}=-T\nu\langle z\rangle_{\mathrm{st}}$ within a limit of numerical error, coming from the stationarity of the energy $d\langle E\rangle_{\mathrm{st}}/dt=0$.

Result (i) means that the phase-space volume supporting the distribution function $f(q,p,z;t)$ is continually shrinking, ultimately leading to a fractal support with the statistical entropy going to minus infinity. Also result (ii) shows that the entropy production rate, which is defined to be $-\langle dQ/dt\rangle_{\mathrm{st}}/T=\nu\langle z\rangle$ [6], gives information on transport properties such as stationary mass current or mobility (in the limit $F^{\mathrm{ext}}\to 0$) [7]. With all these interesting properties, the NH model seems to have some problems. First it is remarked that if one expresses momentum as $p=\langle p\rangle+\delta p$, temperature T should be related to the average of fluctuation $(\delta p)^2$, instead of to p^2 as in the NH model. Second, we consider that in discussing thermodynamics of a system in contact with a thermostat, it is more natural to discuss time variation of the internal energy $U\equiv p^2/2+V_p(q)$ rather than the total energy (4), which includes that of a thermostat. For the NH model $dU/dt=F^{\mathrm{ext}}p-\nu zp^2$, which becomes dE/dt only after replacing p^2 by its average T. In our model proposed below, Eq. (4) is replaced by Eq. (12), which precisely represents the first law of thermodynamics [8].

Based on these considerations we propose a model which consists of N particles, each moving under the action of the periodic force $F_p(q)=-dV_p(q)/dq$ and the external force F^{ext} at temperature T. The constraint,

$$\sum (p_i-p_{\mathrm{av}})^2/N=T, \quad \left(p_{\mathrm{av}}\equiv\sum p_i/N\right), \tag{7}$$

can be easily incorporated, with use of the Gauss' principle of least constraint, into equations of motion as [1]

$$dq_i/dt=p_i, \tag{8}$$

$$dp_i/dt=F_p(q_i)+F^{\mathrm{ext}}-z(p_i-p_{\mathrm{av}}), \tag{9}$$

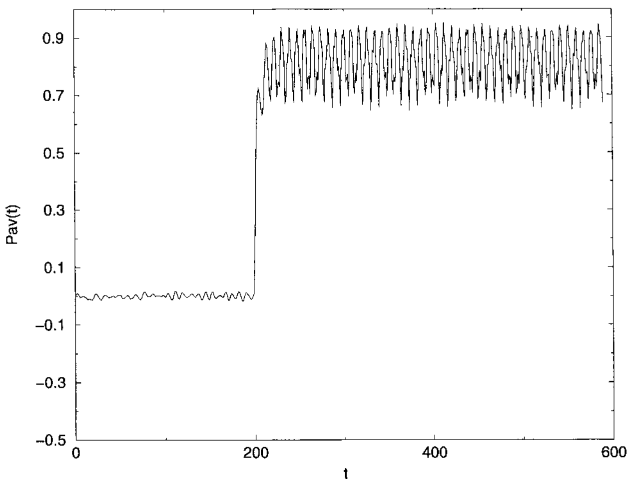

FIG. 1. Time variation of the average momentum $p_{\rm av}(t)$. For $t \geqslant 200$ an external force $F^{\rm ext}=0.3$ is exerted on particles.

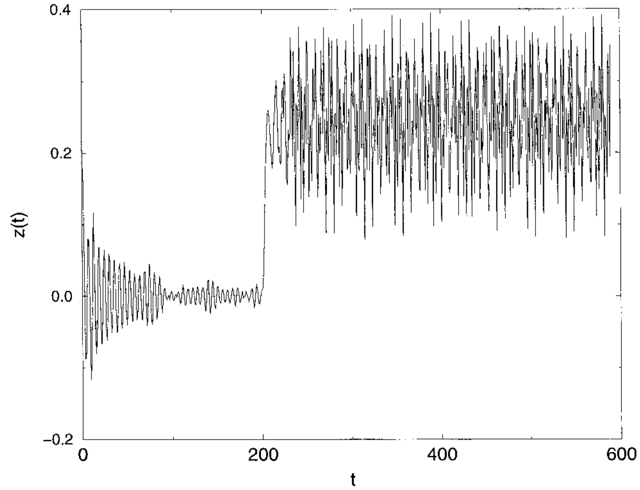

FIG. 2. Time variation of the friction $z(t)$, Eqs. (9) and (10).

$$z=\sum (p_i-p_{\rm av})F_p(q_i)/(NT). \tag{10}$$

We call Eqs. (8)–(10) the Gauss model. The heat dQ supplied by a thermostat is defined to be the work done by a thermostat, which is expressed as $dQ=-z\Sigma(p_i-p_{\rm av})dq_i$, thus

$$dQ/dt=-NTz=T\Lambda, \tag{11}$$

where the rate of expansion Λ of the phase space is easily calculated for the Gauss model as $-Nz$. Defining the internal energy by $U=\Sigma[p_i^2/2+V_p(q_i)]$, we readily see that

$$dU/dt=Np_{\rm av}F^{\rm ext}-NTz=-dW/dt+dQ/dt, \tag{12}$$

which expresses the first law of thermodynamics. The statistical entropy $S_{\rm sta}(t)$ for the distribution function $f(\{q_i\},\{p_i\};t)$, defined similarly as just above Eq. (6), satisfies

$$dS_{\rm sta}(t)/dt=-N\langle z\rangle=T^{-1}d\langle Q\rangle/dt\equiv dS_{\rm th}(t)/dt, \tag{13}$$

where we have introduced the thermal entropy $S_{\rm th}$ in Eq. (13).

We solved numerically Eqs. (8)–(10) for $V_p(q)=1-\cos(q)$ with use of the Runge-Kutta algorithm. Initially N particles' positions are chosen from a uniform distribution in the range $(0,2\pi)$. On the other hand, N particles' momenta are first taken from a Maxwellian distribution with zero mean at temperature T and then adjusted so as to satisfy the relation (7) (with $p_{\rm av}=0$) exactly. In Figs. 1 and 2 we show $p_{\rm av}(t)$ and $z(t)$ as a function of time for the system with $N=10\,000$ and $T=1$. For $0<t<200$ we put $F^{\rm ext}=0$ and the system attains an equilibrium state around $t=100$. At $t=200$ we switch on an external force $F^{\rm ext}=0.3$. The friction constant z and the average momentum $p_{\rm av}$ rapidly respond to the field. In a nonequilibrium stationary state, the (time) averages $\langle p_{\rm av}\rangle_{\rm st}$ and $\langle z\rangle_{\rm st}$ are 0.8133 and 0.2441, respectively, thus ensuring the overall constancy of the internal energy U [see Eq. (12)]. In Fig. 3 we plot a histogram $H_q(t)$ of position of $N=10\,000$ particles at three time windows, $t=179$ [Fig. 3(a)], 209 [Fig. 3(b)], and 229 [Fig. 3(c)]. For $t=179$ the system is in equilibrium and we observe a broad peak in population around $q=0$ $(=2\pi)$ where $V_p(q)=1-\cos(q)$ is minimum. At $t=209$ the system is under effects of rather strong external force and the distribution has a broad bump around $q=1$. When $F^{\rm ext}>0$, particles are on average moving in the positive direction (Fig. 1) and it is natural that particles pile up in a region where particles are just going to collide with the potential barrier of $V_p(q)$ before jumping over it. This bump is also observed for a stochastic thermostat as will be shown later (Fig. 5). As time still goes on we observe a rather spiky distribution [Fig. 3(c)], meaning that the 10 000 particles are confined to a small area in the configuration space. In fact it is observed that for $t>300$ $H_q(t)$ consists of two spikes, which represent two clusters of particles, one consisting of about 4000 particles, moving with the velocity $v_1\simeq 2$ and the other 6000 particles located near the origin $q=0$ with the velocity $v_2\simeq 0$ (see Fig. 4). We note that this is consistent with Eq. (7) with $T=1$ and $\langle p_{\rm av}\rangle_{\rm st}\simeq 0.8$. As for a histogram $H_p(t)$ in a momentum space we observe quite similar tendency. That is, $H_p(t)$, which is nearly Maxwellian for $t<200$, is shifted to positive direction and becomes very spiky after introduction of an external force. Finally for $t>300$ we observe only two bins which contain weight (see Fig. 4). What is presented here in Fig. 3 together with Fig. 4 shows that the support for the distribution function is shrinking continually, in accordance with the positivity of $\langle z\rangle_{\rm st}$ which is related to the rate of expansion Λ of a phase space via $\Lambda=-Nz$. We remark, however, that the drastic change in the distribution (or histogram) does not have any apparent effects on behavior of observables such as the average momentum $p_{\rm av}(t)$, Fig. 1, as was noted by Holian, Posch, and Hoover [4]. Based on this fact we present the following argument on the entropy production σ. First we decompose entropy change (in time) dS of the system as contribution from heat flow from a reservoir $dS_{\rm th}$ [see Eq. (13)] and the one from irreversibility (dissipation) dS_i, $dS=dS_{\rm th}+dS_i$. Since one may put $dS=0$ in a stationary state, it yields $\sigma=dS_i/dt=-dS_{\rm th}/dt$. For similar argument to obtain the relation $\sigma=-dS_{\rm sta}/dt$, see Ref. [6].

Thus far we considered effects of some mechanical thermostats (the Nose-Hoover and Gaussian thermostats), for which it turned out that the statistical entropy $S_{\rm sta}(t)$ de-

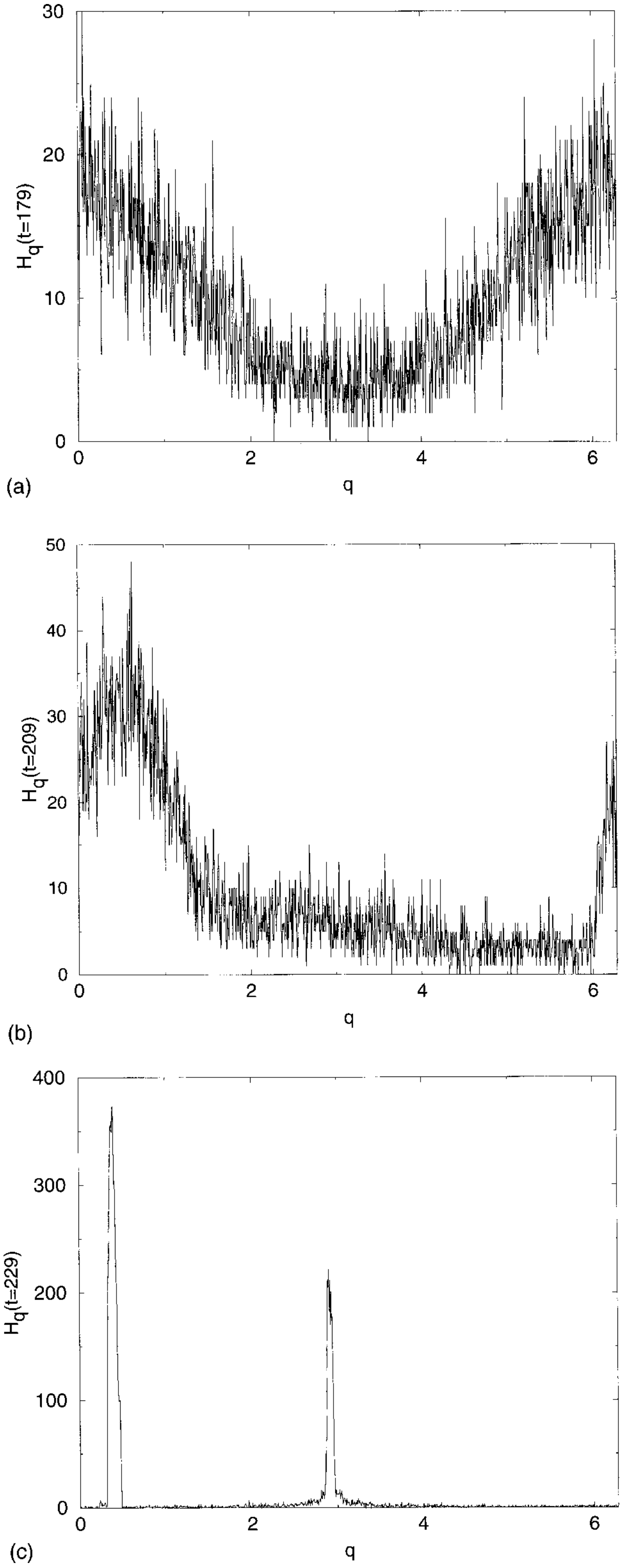

FIG. 3. The histogram $H_q(t)$ of position of $N=10\,000$ particles at several time windows, $t=179$ (a), 209 (b), and 229 (c).

creased in time like $-\sigma t$ in a nonequilibrium stationary state. Below we briefly consider the Gulton staircase in contact with the Langevin thermostat in order to contrast mechanical thermostats to stochastic thermostats [9]. The Langevin equation for a particle in a Gulton staircase is given by

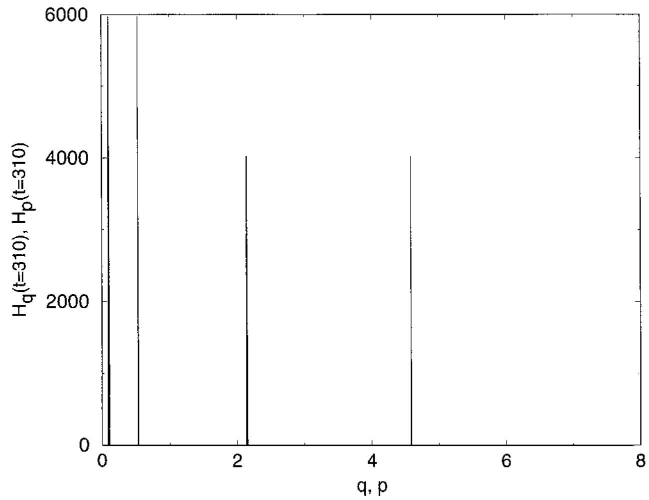

FIG. 4. The histogram $H_q(t)$ (thin curve) and $H_p(t)$ (thick curve) at $t=310$.

$$dq/dt=p, \tag{14}$$

$$dp/dt=F_p(q)+F^{\rm ext}-zp+R(t), \tag{15}$$

with the following fluctuation-dissipation relation:

$$\langle R(t)R(t')\rangle = 2zT\delta(t-t'). \tag{16}$$

The Fokker-Planck equation for the Langevin model, Eqs. (14)–(16), is

$$\partial f(q,p;t)/\partial t = -\partial(pf)/\partial q - \partial([-zp+F_p(q)+F^{\rm ext}]f)/\partial p + zT\partial^2 f/\partial p^2. \tag{17}$$

Heat flow from the Langevin thermostat to a particle is defined, as for the Gauss model, to be $dQ=[-zp+R(t)]dq$, which is expressed from Eq. (15) as

$$dQ=d(p^2/2+V_p(q))-F^{\rm ext}dq \equiv dU+dW, \tag{18}$$

where dU denotes the increment in the internal energy and dW denotes the work done by the system. For the statistical entropy $S_{\rm sta}(t)$, we can derive from Eq. (17),

$$\begin{aligned} &dS_{\rm sta}(t)/dt-(1/T)[d\langle U\rangle(t)/dt+d\langle W\rangle(t)/dt] \\ &\quad \equiv dS_{\rm sta}/dt-dS_{\rm th}/dt \\ &\quad =(z/T)\int dp\,dq[T(\partial f/\partial p)/\sqrt{f}+p\sqrt{f}]^2 \geqslant 0. \end{aligned} \tag{19}$$

Equations (18) and (19) may be regarded as the first and the second law of thermodynamics for the Langevin model. Equation (19) [also Eq. (21) below] should be compared with Eq. (13), which states that $S_{\rm sta}$ is the same with $S_{\rm th}$. For the Langevin thermostat we have $dS_{\rm sta}(t)/dt=0$ in a stationary state, because the distribution function $f(q,p;t)$ approaches a nonfractal stationary one $f_{\rm st}(q,p)$. From Eqs. (18) and (19) we see thus $dS_{\rm sta}(t)/dt\to 0$, $d\langle U\rangle(t)/dt\to 0$ and $-d\langle W\rangle(t)/dt=F^{\rm ext}\langle p\rangle_{\rm st}>0$. This means that the thermal entropy behaves like $-\sigma t$ for a stochastic thermostat.

In the overdamped limit $z \gg 1$, to be called the Smoluchowski model for the reason stated below, we put $dp/dt = 0$ in Eq. (15) and have a Smoluchowski equation,

$$\partial f(q;t)/\partial t = -z^{-1}\{\partial([F_p(q)+F^{\mathrm{ext}}]f)/\partial q - T\partial^2 f/\partial q^2\}$$
$$= -\partial j(q;t)/\partial q. \tag{20}$$

If we absorb z in Eq. (20) in a new time scale, we have Eq. (16) of Ref. [9]. We have from Eq. (20),

$$dS_{\mathrm{sta}}(t)/dt - (1/T)d[\langle U\rangle(t) + \langle W\rangle(t)]/dt$$
$$= (zT)^{-1}\langle [dV_t(q)/dq + Td\ln f/dq]^2\rangle, \tag{21}$$

where the internal energy U is now defined by $U = V_p(q)$ and $V_t \equiv V_p - F^{\mathrm{ext}}q$ as before [10].

From the above it is seen that as for the thermal entropy $S_{\mathrm{th}}(t)$ the stochastic and mechanical reservoirs give the same asymptotic behavior as $t\to\infty$. However for the statistical entropy, we have $S_{\mathrm{st}}(t) \sim -\sigma t$ as $t\to\infty$ for the mechanical reservoir and $dS_{\mathrm{st}}(t)/dt \to 0$ as $t\to\infty$ for the stochastic reservoir. Finally we show in Fig. 5 the stationary distribution $f(q,t\to\infty)$ which is obtained by solving the equation $j = \mathrm{const}$ with j defined by Eq. (20) [9]. As was seen in Fig. 3(b) for the Gauss model, we see a bump in the region where particles are just in front of the potential barrier whose center is located at $q=\pi$. This becomes more salient as the temperature goes down. Thus the piling up of particles in the Gulton staircase is seen to be a rather general aspects of dynamics.

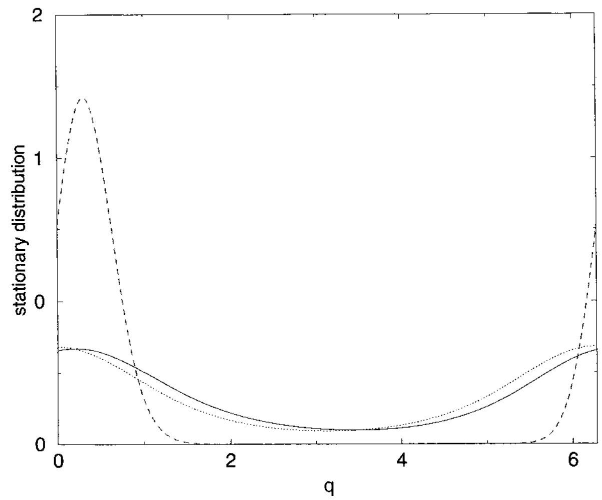

FIG. 5. Stationary distribution function $f_{\mathrm{st}}(q)$ obtained from the Smoluchowski equation (20). The dotted curve represents the equilibrium (canonical) distribution for $F^{\mathrm{ext}}=0$ and the solid curve represents the nonequilibrium distribution for $F^{\mathrm{ext}}=0.3$ at $T=1$. The dashed curve is for the case $F^{\mathrm{ext}}=0.3$ but at lower temzperature $T=0.1$.

Summarizing this paper, we have proposed the Gauss model, Eqs. (7)–(10), as a mechanical thermostat for the Gulton staircase and compared it with the Langevin thermostat. The Gauss model enables us to properly introduce temperature T and formulate the law of thermodynamics consistently. As expected we observed from numerical simulations positive average friction $\langle z\rangle_{\mathrm{st}}$ (Fig. 1) and the mass current (Fig. 2). We found that the phase space shrinks in the course of time very rapidly leading finally to only two clusters each composed of many particles (see Fig. 4). At this stage of time evolution, the whole dynamics is reduced to a problem of a few or several degrees of freedom. As for the entropy production rate σ, it is defined, for both a mechanical and a Langevin thermostat, in terms of the heat dQ absorbed by the system as $\sigma = -T^{-1}dQ/dt \equiv -dS_{\mathrm{th}}/dt$. For a mechanical model, σ is also given in terms of the statistical entropy S_{sta} from Eq. (13). Finally it is remarked that the clustering phenomenon mentioned above, which has gathered lots of attention recently in connection with synchronization or more generally with population dynamics of coupled oscillators [11], shows that apparently a rather complex-looking problem turns out to be simple at the nonequilibrium stationary state, on which current interest is concentrated [6]. In contrast with stochastic thermostats, studies on properties of mechanical thermostats may be said to have just begun and many fundamental insights on statistical mechanics are expected to be revealed in the near future.

We have benefited greatly from discussions with K. Kitahara at an early stage of this study. This paper was supported by the Japanese Grant-in-Aid for Science Research Fund from the Ministry of Education, Science, and Culture.

[1] D. J. Evans and G. P. Morriss, *Statistical Mechanics of Nonequilibrium Liquids* (Academic, New York, 1990).
[2] W. G. Hoover, *Computational Statistical Mechanics* (Elsevier, Amsterdam, 1991).
[3] B. L. Holian, W. G. Hoover, and H. A. Posch, Phys. Rev. Lett. **59**, 10 (1987).
[4] B. L. Holian, H. A. Posch, and W. G. Hoover, Phys. Rev. A **42**, 3196 (1990).
[5] W. G. Hoover, H. A. Posch, B. L. Holian, M. J. Gillan, M. Mareschal, and C. Massobrio, Mol. Simul. **1**, 79 (1987).
[6] D. Ruelle, J. Stat. Phys. **85**, 1 (1996); G. Gallaavotti and E. G. D. Cohen, *ibid.* **80**, 831 (1995).
[7] D. J. Evans, E. G. D. Cohen, and G. P. Morriss, Phys. Rev. A **42**, 5990 (1990).
[8] For the heat dQ absorbed by the system, see Eq. (11) for a Gaussian thermostat and Eq. (18) for a Langevin thermostat.
[9] T. Munakata, A. Igarashi, and T. Shiotani, Phys. Rev. E **57**, 1403 (1998).
[10] We note that the work $dW = -F^{\mathrm{ext}}dq$ done by the system was included in the energy $dE = dU + dW$ in Ref. [9]. Of course, discussions on entropy production developed there is intact.
[11] Y. Nakamura, F. Tominaga, and T. Munakata, Phys. Rev. E **49**, 4849 (1994), and the references cited therein.