Entropy and entropy production in simple stochastic models

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Entropy and its production rate play important roles in characterizing nonequilibrium states, which appear in connection with, e.g., stationary transport of matter or heat, a glass transition, and simulated annealing. We derive useful relations between the statistical and the thermodynamic entropies and also derive a Fokker-Planck equation to study fluctuations in the thermodynamic entropy. As simple test systems, we consider Brownian motion in a double-well and a periodic potential. [S1063-651X(98)10702-X]

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I. INTRODUCTION

Recently a lot of attention has been paid to simple stochastic models which are supposed to approximately represent complicated many-body systems. Here the main theoretical interest is centered around the interplay among nonlinearity, noise, and an external perturbation. For example, the so-called stochastic resonance is mainly studied based on models of the Brownian motion in a double-well potential under the action of time-periodic force [1,2]. Similarly, a thermal ratchet is studied with use of a simple stochastic model in which a (nonsymmetric) potential field oscillates in time or nonthermal noise of a non-Markov nature is exerted on a Brownian particle [3,4]. Also of interest is the two-state or double-well model for glass transition in which the temperature of the system is varied in time to realize nonequilibrium states, whose entropies (both thermal and statistical) are the target of theoretical investigations [5,6].

In this paper we discuss entropy and entropy production in nonequilibrium (stationary) states using simple stochastic models, which allow detailed numerical analysis. Furthermore, we formulate (thermal) entropy fluctuations in terms of a Fokker-Planck equation, which can give rise to useful information on stochastic dynamics. Our unified entropy approach would shed some light on rather general stochastic models including those mentioned above.

In Sec. II we derive a simple inequality, which may be interpreted either as monotonic decrease (in time) of the free energy of the system or the distinction between the thermal and statistical entropies. As applications of the results, we consider two types of Brownian motion. First in Sec. III a Brownian particle is put in a space-periodic potential which is inclined due to a uniform field. Here our main concern is with nonequilibrium states with stationary mass transport. In Sec. IV Brownian dynamics in a double-well potential is studied, with temperature of the system varied in time to produce glasslike nonequilibrium states. In Sec. V we conclude this paper with discussions on entropy fluctuations [5] and on ''mechanical'' reservoirs often used to investigate nonequilibrium stationary states [7,8]. The Appendix contains some results for stochastic dynamics governed by a master equation.

II. STOCHASTIC DYNAMICS AND ENTROPY

We consider dynamics of a state variable $\mathbf{x}=(x_1,\ldots,x_n)$ governed by the Langevin equation

$$d\mathbf{x}/dt=-\boldsymbol{\nabla}V(x)+\mathbf{f}(t), \tag{1}$$

with the following fluctuation-dissipation relation:

$$\langle f_i(t)f_j(t')\rangle=2T(t)\delta(t-t')\delta_{i,j}\,. \tag{2}$$

We note that the temperature of the system $T(t)$ is here allowed to be time dependent. The Fokker-Planck equation, which corresponds to Eqs. (1) and (2), is

$$\partial p(\mathbf{x};t)/\partial t=\boldsymbol{\nabla}\cdot[p\boldsymbol{\nabla}V+T(t)\boldsymbol{\nabla}p]. \tag{3}$$

The statistical entropy $S_{\rm st}(t)$ and the internal energy $E(t)$ are defined as follows:

$$S_{\rm st}(t)=-\int d\mathbf{x}\; p(\mathbf{x};t)\ln p(\mathbf{x};t), \tag{4}$$

$$E(t)=\int d\mathbf{x}\; p(\mathbf{x};t)V(\mathbf{x})\equiv\langle V\rangle. \tag{5}$$

With use of Eq. (3) together with partial integration, we notice immediately that

$$dS_{\rm st}(t)/dt=T(t)\langle(\boldsymbol{\nabla}\ \ln p)^2\rangle-\langle\nabla^2V\rangle, \tag{6}$$

$$dE(t)/dt=-\langle(\boldsymbol{\nabla}V)^2\rangle+T(t)\langle\nabla^2V\rangle, \tag{7}$$

from which we derive the inequality of the form

$$dE(t)/dt-T(t)dS_{\rm st}(t)/dt=-\langle(\boldsymbol{\nabla}V+T\boldsymbol{\nabla}\ \ln p)^2\rangle\leq 0. \tag{8}$$

Equation (8) leads to two important relations, Eqs. (12) and (13) below. To derive from Eq. (8) the inequality (12), observed in Ref. [5(a)], we note that the heat dQ absorbed by the system from the reservoir is given by $dQ(t)=dE(t)$ [see discussions below Eq. (12)]. Then the inequality (8) is expressed as

$$[1/T(t)]dQ(t) \leqslant dS_{\rm st}(t). \tag{9}$$

Here let us consider an experiment in which the system is cooled or heated. In a cooling process from $T_h(t=t_i)$ to $T_l(t=t_f)$, we integrate Eq. (9) in time from t_i to t_f, to obtain

$$S^{\downarrow}_{\rm th}(T_l) \equiv S_{\rm st}(T_h) + \int_{T_h}^{T_l} dQ/T(t) \leqslant S_{\rm st}(T_l), \tag{10}$$

where the thermodynamic entropy $S^{\downarrow}_{\rm th}$ is defined with use of the heat absorbed from the reservoir in a cooling process and we preferred temperature to time in writing Eq. (10). It is noted that if at $T=T_h$ the system relaxes to an equilibrium state rapidly due to strong thermal fluctuations, $S_{\rm st}(T_h)$ on the right-hand side of Eq. (10) is the entropy of an equilibrium state and may be equal to $S_{\rm th}(T_h)$. Similarly by heating the system from T_l to T_h, we have

$$S_{\rm st}(T_l) \leqslant S_{\rm st}(T_h) - \int_{T_l}^{T_h} dQ/T(t) \equiv S^{\uparrow}_{\rm th}(T_l). \tag{11}$$

Combining Eqs. (10) and (11) we are led to the desired inequality

$$S^{\downarrow}_{\rm th}(T_l) \leqslant S_{\rm st}(T_l) \leqslant S^{\uparrow}_{\rm th}(T_l). \tag{12}$$

The physical situation expressed by Eq. (12) is nicely represented by Fig. 1 of Ref. [5(a)]. In passing we note that if we generalize the Langevin dynamics by including momenta $\mathbf{p} = d\mathbf{x}/dt$, we only need to modify Eq. (5) as $E(t) = \langle V + (\mathbf{p}^2/2) \rangle$ to arrive at Eq. (8). This is intuitively understood as follows: By including momentum variables $\mathbf{p}$ (with mass $m=1$) we have $d\mathbf{x}/dt = \mathbf{p}$, $d\mathbf{p}/dt = -\gamma\mathbf{p} - \nabla V + \mathbf{f}$ where γ is the friction constant. The work done on the system by a reservoir is expressed as $(-\gamma\mathbf{p} + \mathbf{f}) \cdot d\mathbf{x} = (d\mathbf{p}/dt + \nabla V) \cdot d\mathbf{x} = d(\mathbf{p}^2/2 + V)$. In the large γ limit we set $d\mathbf{p}/dt = 0$, which is equivalent to Eq. (1) for $\gamma = 1$, to have $dQ = d\langle V \rangle = dE$.

The second interpretation of Eq. (8) is for the case of constant temperature $T(t) = T_0$. Defining the free energy by $F(t) \equiv E(t) - T_0 S_{\rm st}(t)$ we notice from Eq. (8) that it decreases monotonically in time,

$$dF(t)/dt \leqslant 0, \tag{13}$$

until the equilibrium state, represented by $p_{\rm eq}(\mathbf{x}) \propto \exp[-V(\mathbf{x})/T_0]$ is realized. Of course this distribution function should be normalizable if it is to be useful. Thus we cannot use it for the problem in which a constant field is exerted on a system and some stationary transport process is prevailing (see Sec. III). For completeness we consider stochastic processes governed by a master equation and derive an inequality similar to Eq. (8) in the Appendix.

III. MASS TRANSPORT IN A PERIODIC POTENTIAL

In this section we consider one-dimensional Brownian motion on a unit circle described by the Langevin equation

$$d\theta/dt = -dV_p(\theta)/d\theta + F^{\rm ex} + f(t), \tag{14}$$

where the random force $f(t)$ satisfies the relation

$$\langle f(t) f(t') \rangle = 2T_0 \delta(t-t'). \tag{15}$$

The potential $V_p(\theta)$ is periodic $V_p(\theta) = V_p(\theta + 2\pi)$ and $F^{\rm ex}$ denotes the constant external force. The Fokker-Planck equation corresponding to Eq. (14) reads

$$\partial p(\theta,t)/\partial t = -(\partial/\partial\theta)[(F^{\rm ex} - dV_p/d\theta)p - T_0(\partial/\partial\theta)p] \equiv -(\partial/\partial\theta)J(\theta,t). \tag{16}$$

The stationary state (SS) with a constant flow $J_{\rm SS}$ is obtained by solving the equation $(F^{\rm ex} - dV/d\theta)p_{\rm SS} - T_0(d/d\theta)p_{\rm SS} = J_{\rm SS}$ to be

$$p_{\rm SS}(\theta) = G(\theta)\left((-J_{\rm ss}/T_0) \int_0^{\theta} d\theta'/G(\theta') + C \right), \tag{17}$$

where $G(\theta) \equiv \exp\int_0^{\theta} d\theta' [F^{\rm ex} - dV_p(\theta')/d\theta']/T_0$. Two unknown constants, C and $J_{\rm SS}$, are determined from the normalization $\int_0^{2\pi} d\theta\, p_{\rm SS} = 1$ and the periodicity $p_{\rm SS}(0) = p_{\rm SS}(2\pi)$ to obtain

$$J_{\rm SS}/T_0 = -\left(G(2\pi) \int_0^{2\pi} d\theta G(\theta)/[1 - G(2\pi)] \times \int_0^{2\pi} d\theta/G(\theta) + \int_0^{2\pi} d\theta G(\theta) \int_0^{\theta} d\theta'/G(\theta') \right)^{-1}.$$

We take $V_p(\theta) = [1 + \cos(2\theta)]/2$ and $T_0 = 0.5$. In Fig. 1 is plotted $p_{\rm SS}(\theta)$ for some values of the external force $F^{\rm ex}$ together with the equilibrium state ($\propto \exp[-V_p(\theta)/T_0]$) for $F^{\rm ex} = 0$. It is observed that the nonequilibrium SS distribution becomes less sharp as $F^{\rm ex}$ becomes larger. The SS current $J_{\rm SS}$ turns out to be a simple increasing function of $F^{\rm ex}$ as expected.

Next we consider how our system approaches the stationary state $p_{\rm SS}(\theta)$. First we note that the potential V in Eq. (5), which takes the form $V = V_p(\theta) - F^{\rm ex}\theta$, is not periodic in θ and we must consider θ in the extended range $-\infty < \theta < \infty$ when we calculate the energy $E(t) = \langle V \rangle$. However, reflecting the fact that we used partial integration to derive Eq. (8), it contains only ∇V and the argument θ of $p(\theta,t)$ in Eq. (8) is restricted to the range $0 \leqslant \theta < 2\pi$. Thus it holds that

$$dF(t)/dt = dE(t)/dt - T_0 dS_{\rm st}(t)/dt \to -2\pi J_{\rm SS} F^{\rm ex} \quad (t \to \infty). \tag{18}$$

Since $S_{\rm st}(t)$ goes to a constant $-\int d\theta p_{\rm SS} \ln p_{\rm SS}$ as $t \to \infty$, we see from Eq. (18) that the energy goes to $-\infty$ due to circular motion of the Brownian particle in the direction of $F^{\rm ex}$.

In terms of the thermal entropy $dS_{\rm th}(t) = dE(t)/T_0$, this fact is expressed as

$$\sigma \equiv -dS_{\rm th}(t)/dt \to 2\pi J_{\rm SS} F^{\rm ex}/T_0 \quad (t \to \infty), \tag{19}$$

where σ denotes the entropy production (rate), since the Brownian particle gives energy $2\pi J_{\rm SS} F^{\rm ex}$ per unit time to the reservoir with temperature T_0.

In order to calculate σ and $dF(t)/dt$ one must obtain $p(\theta;t)$ by solving the Smoluchowski equation (16) numerically. For this purpose we employ an implicit scheme, which

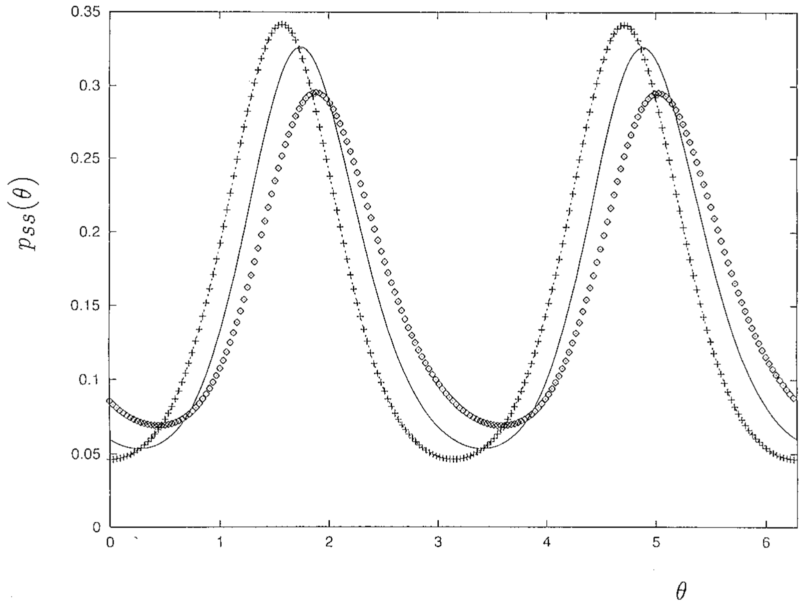

FIG. 1. Stationary distribution $p_{SS}(\theta)$ for $F^{ex}=0$ (equilibrium) (denoted by a dashed line with $+$), 0.5 (denoted by a solid line), and 1.0 (denoted by $\diamond$) for $T_0=0.5$.

we require to conserve the probability to at least 10^{-3}. It turns out that this conservation condition is achieved so long as the constant $T_0\Delta t/\Delta\theta^2$ is made smaller than 0.1 where Δt and $\Delta\theta$ are the time and space increments in our difference sheme [9]. In Fig. 2 we depict $T_0\sigma$ and $-dF(t)/dt$ for $F^{ex}=0.5$, where the initial condition $p(\theta;t=0)$ is taken to be uniform on $0\leqslant\theta<2\pi$. The rate σ is seen to decrease monotonically and achieves the SS of minimum entropy production.

IV. BROWNIAN MOTION IN A DOUBLE-WELL POTENTIAL

As an application of the formalism developed in Sec. II, we next consider Langevin dynamics in a one-dimensional double-well potential

$$V(x)=\begin{cases} x^2(x-2)^2 & (x<1) \\ x^2(x-2)^2+0.6(x-1)^3 & (x\geqslant 1) \end{cases}, \tag{20}$$

which is shown in Fig. 3.

Here our interest is centered around the nonequilibrium distribution $p(x;t)$ and two kinds of entropies $S_{th}(t)$ and $S_{st}(t)$ associated with time variation of temperature $T(t)$ in Eq. (3). We consider the following experiment: The system is kept in equilibrium at temperature $T_0(=1)$ for $t<0$, thus $p(x,t<0)\propto\exp[-V(x)/T_0]$. In the cooling process $0<t<t_M$, $T(t)$ is chosen to be a stepwise function, which changes by $\delta T(=0.01)$ at time t_i $(i=1,2,\ldots,M-1)$ with $t_1=0$, $T(t_i<t\leqslant t_{i+1})=T_0-i\,\delta T$. The time t_i is determined from the relation $f(t_{i+1})=T_0-i\,\delta T$ with $f(t)$ given by

$$f(t)=T_0/[1+rt]. \tag{21}$$

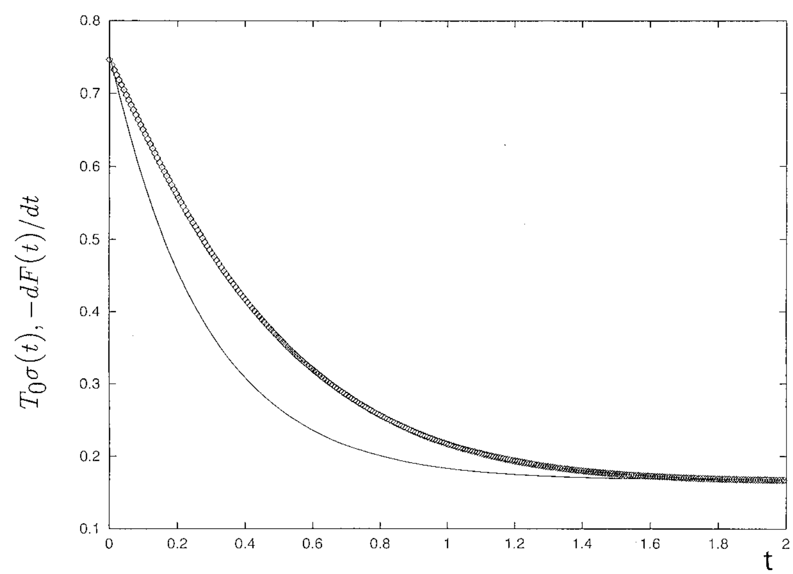

FIG. 2. $T_0\sigma(t)$ (denoted by $\diamond$) and $-dF(t)/dt$ (denoted by a solid line) for $F^{ex}=0.5$.

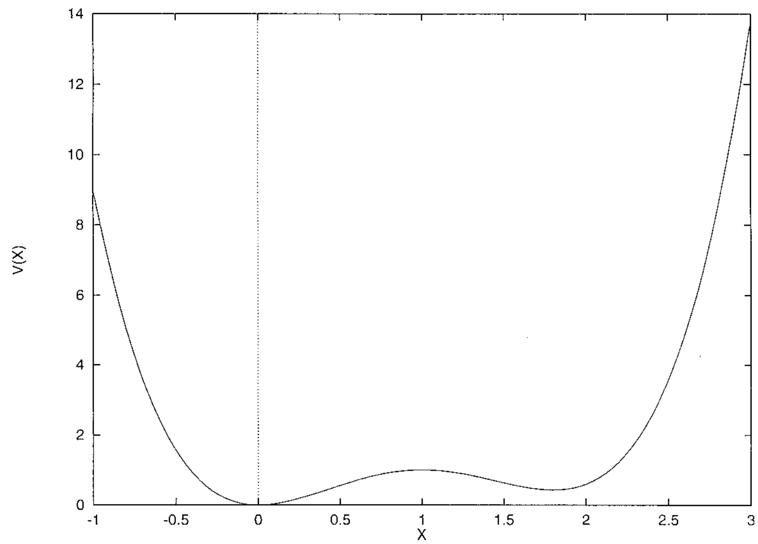

FIG. 3. Double-well potential Eq. (20).

The r in Eq. (21) controls the cooling (or heating) rate. In the heating process $t_M < t < \infty$ we proceed precisely in the reversed way coming back to T_0 at time $t = 2t_M$. For $t > 2t_M$ the system is kept at $T = T_0$, relaxing to an equilibrium state in which it was at time $t < 0$. The Smoluchowski equation (3) with the potential Eq. (20) is solved numerically with a similar difference sheme as used in Sec. III.

In Fig. 4 we depict $p(x,t_i)$ with $i = 1$ and $2M$ for the case $M = 91$ and the rate $r = 0.5$. Both distribution functions correspond to temperature $T = T_0$, with $p(x;t_1)$ representing the equilibrium one and the difference shows the nonequilibrium effects. In the cooling process $(0 < t < t_M)$ the weight around the first (second) peak $x \simeq 0$ $(x \simeq 1.7)$ increases (decreases) and in the heating process $(t_M < t < t_{2M})$ the distribution tends to recover its original shape. However, since the system is out of equilibrium due to the finite rate r, the recovery is not enough and we observe more (less) weight around the first (second) peak in the nonequilibrium distribution $p(x:t_{2M})$. Of course this tendency becomes weaker as r becomes small and almost indiscernible for $r = 0.01$ in the scale of this figure.

In Fig. 5 we show $S_{\rm th}^{\uparrow}(T_M)$, $S_{\rm th}^{\downarrow}(T_M)$, and $S_{\rm st}(T_M)$ for $T_M = T_0 - 0.05I\,[I = 1,2,\ldots,18]$. For calculation of these three entropies for each T_M, we consider the temperature loop $T_0 \to T_M \to T_0$ mentioned before. The inequality (12) is clearly confirmed from Fig. 5. We note that in the heating process the contribution to $S_{\rm th}^{\uparrow}(T_M)$ from the heat absorbed by the system during equilibration process $\infty > t > t_{2M}$ should be included. The thermal entropy as depicted in Fig. 5 may be called an average thermal entropy because there are many thermal processes corresponding to each realization of the random processes $f(t)$ in Eq. (1) and $S_{\rm th}$ is an average over these realizations. In Sec. V fluctuations of thermal entropy are formulated.

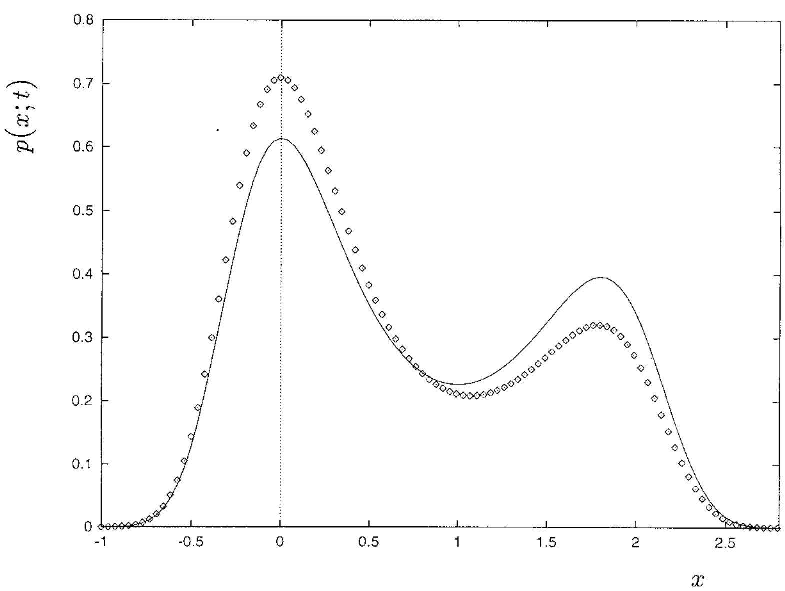

FIG. 4. Equilibrium and nonequilibrium distributions, $p(x;t_1)$ (denoted by a solid line) and $p(x;t_{2M})$ (denoted by $\diamond$) for $M = 91$.

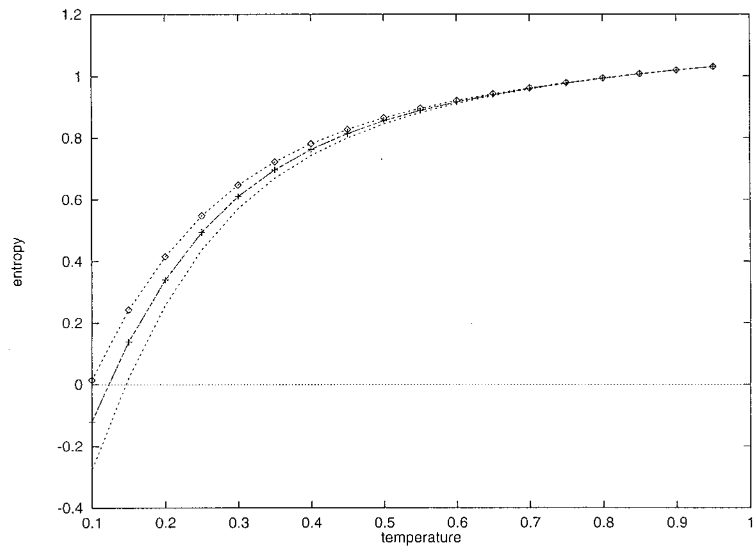

FIG. 5. $S_{\rm th}^{\uparrow}(T_M)$ (denoted by a dotted line), $S_{\rm th}^{\downarrow}(T_M)$ (denoted by a line with $\diamond$), and $S_{\rm st}(T_M)$ (denoted by a line with $+$) for $T_M=T_0-0.05I$ $[I=1,2,\ldots,18]$.

Here we note that temporal variation of temperature $T(t)$ was recently discussed by Reimann *et al.* [10] in relation to directed Brownian motion, based on the one-dimensional version of Eqs. (1) and (2). Two differences from our model in this section are first $T(t)$ is cyclic with a *finite* period and secondly the periodic potential $V(x)$ has broken symmetry (ratchet [3,4]) in Ref. [10]. Although the general inequality (8), the main result in this paper, has no direct relevance to directed diffusion, our numerical approach based on the Smoluchowski equation as developed in Secs. III and IV is expected to yield useful information not only on stationary particle current but also on transient behaviors before establishing the stationary current.

V. SOME REMARKS

In this paper we derive an inequality Eq. (8), based on which two types of Brownian motion are studied [11]. One is related to a nonequilibrium stationary state, especially an entropy production $\sigma\equiv-dS_{\rm th}/dt$ associated with mass transport in an external field. The other is the entropy of nonequilibrium states, which are produced by cooling or heating processes.

One of the motivations for our study of the stationary state (Sec. III) is to contrast the *stochastic* reservoir used here with the reversible or *mechanical* reservoir of the Nose-Hoover or Gauss type [12], because the nonequilibrium stationary states produced by these reservoirs gather considerable interest [7,8]. We take a particle in a periodic potential $V_p(q)$ in contact with the Nose-Hoover reservoir [7]. The system is expressed by

$$dq/dt=p, \tag{22}$$

$$dp/dt=-dV_p(q)/dq-\eta p+F^{\rm ex}, \tag{23}$$

$$d\eta/dt=(p^2/T_0-1), \tag{24}$$

where η denotes a friction coefficient. $V_p(q)$, T_0, and $F^{\rm ex}$ have the same meaning as in Eq. (14). Holian, Posch, and Hoover numerically studied the system Eqs. (22)–(24) and their results are summarized as follows [7].

(a) The external force $F^{\rm ex}$ produces mass current $\overline{p}(>0)$ where the bar means time average.

(b) The expansion rate of phase space $\Lambda\equiv\partial\dot{q}/\partial q+\partial\dot{p}/\partial p+\partial\dot{\eta}/\partial\eta=-\eta$ takes negative value on average or $\overline{\Lambda}=-\overline{\eta}<0$, meaning that the support of the distribution function $p(p,q,\eta;t)$ shrinks in time and it reduces to a fractal set in the limit $t\to\infty$. From the definition (4) and Eqs. (22)–(24),

$$dS_{\rm st}(t)/dt=-\int dp\ dq\ d\eta\ p(p,q,\eta,t)\,\eta\equiv-\langle\eta\rangle. \tag{25}$$

From the above the statistical entropy behaves as $S_{\rm st}(t)\sim-\overline{\eta}t$ as $t\to\infty$.

(c) The heat transferred to the system (p,q) from the reservoir is expressed as $-\eta p\ dq$ [see the lines just below Eq. (12)], which is rewritten as $d[p^2/2+V_p(q)-F^{\rm ex}q]$, thus leading to our result $dQ=dE$ derived in Sec. II. If we take time average of $T_0dS_{\rm th}/dt=dQ/dt=dE/dt$, we have $T_0\overline{dS_{\rm th}/dt}\to-F^{\rm ex}\overline{p}$ [cf. Eq. (19)]. This was *numerically* found to be equal to $-\overline{\eta}T_0$.

As for the thermal entropy $S_{\rm th}(t)$ the stochastic and mechanical reservoirs give the same asymptotic behavior as $t\to\infty$. However, for the statistical entropy, we have $S_{\rm st}(t)\sim-\overline{\eta}t$ as $t\to\infty$ for the mechanical reservoir and $dS_{\rm st}(t)/dt\to0$ as $t\to\infty$ for the stochastic reservoir. The most subtle point about the mechanical reservoir is that the time average $\overline{\eta}$ becomes positive and at the moment we do not know where this result comes from. Intuitively this may come from the fact that the stochastic reservoir may be regarded as a system with infinitely many degrees of freedom, while the mechanical one consists of at most a few degrees of freedom. However, it must be noted that p defined by Eq. (22) should be expressed as $\overline{p}+\delta p$ for large t and δp should be related to temperature T_0 in Eq. (24). This point is also important for the Gauss reservoir [8] and is currently under study.

Thermal entropy defined in Sec. II is an average over an ensemble of many sample trajectories and its fluctuations can give useful information on relaxational properties, especially when the temperature of the system $T(t)$ is controlled as discussed in Ref. [5] for the case of the (discrete) two-level system. We now formulate entropy fluctuations based on the Fokker-Planck equation for the model of continuous variables $\mathbf{x}$. First we rewrite Eq. (1) as

$$d\mathbf{x}(t)=-\boldsymbol{\nabla}V(\mathbf{x})dt+\sqrt{2T(t)}d\mathbf{W}, \qquad (26)$$

where $\mathbf{W}(t)=(W_1(t),\ldots,W_n(t))$ denotes the n-dimensional Wiener process [13], which satisfies

$$\langle W_i(t)\rangle=0 \quad \text{and} \quad \langle dW_i(t)dW_j(t)\rangle=dt\,\delta_{i,j}. \qquad (27)$$

The heat absorbed from the reservoir $dQ(t)\equiv V(\mathbf{x}+d\mathbf{x})-V(\mathbf{x})$ [14] is calculated from Eq. (26) as

$$dQ(t)=[-(\boldsymbol{\nabla}V)^2+T(t)\nabla^2V]dt+\sqrt{2T(t)}\boldsymbol{\nabla}V\cdot d\mathbf{W}, \qquad (28)$$

where $\boldsymbol{\nabla}V\cdot\mathbf{W}$ is interpreted as an Ito-type stochastic integral [13]. From the definition $dS_{\mathrm{th}}=dQ/T(t)$ [14] and taking into account the relations $\langle(dS_{\mathrm{th}})^2\rangle/dt=2(\boldsymbol{\nabla}V)^2/T(t)$ and $\langle d\mathbf{x}\,dS_{\mathrm{th}}\rangle/dt=2\boldsymbol{\nabla}V$, we have the Fokker-Planck equation for the distribution function $p(\mathbf{x},S_{\mathrm{th}};t)$,

$$\partial p/\partial t=\boldsymbol{\nabla}\cdot[p\boldsymbol{\nabla}V]-A\partial p/\partial S_{\mathrm{th}}+T\nabla^2p+2\boldsymbol{\nabla}\cdot\partial(p\boldsymbol{\nabla}V)/\partial S_{\mathrm{th}}+[(\boldsymbol{\nabla}V)^2/T]\partial^2p/\partial S_{\mathrm{th}}^2, \qquad (29)$$

where $A=A(\mathbf{x};t)\equiv\nabla^2V-(\boldsymbol{\nabla}V)^2/T(t)$. It is noted that integration of Eq. (29) over S_{th} yields Eq. (3) as it should. If we solve Eq. (29) under the initial condition

$$p(\mathbf{x},S_{\mathrm{th}};t=0)=\delta(\mathbf{x}-\mathbf{x}_0)\,\delta(S_{\mathrm{th}}-S_0), \qquad (30)$$

$p(S_{\mathrm{th}};t)=\int d\mathbf{x}\;p(\mathbf{x},S_{\mathrm{th}};t)$ gives us the (thermodynamic) entropy distribution at time t due to noise and temperature variation $T(t)$.

A stationary solution to Eq. (29) for the case $T(t)=T_0$ can be found if one notes that the distribution of $\mathbf{x}$ approaches $p_{\mathrm{eq}}(\mathbf{x})\propto\exp[-V(\mathbf{x})/T_0]$ and $S_{\mathrm{th}}=[V(\mathbf{x})-V(\mathbf{x}_0)]/T_0+S_0$. It is easily confirmed that $p_{\mathrm{eq}}^1(\mathbf{x},S_{\mathrm{th}})\equiv p_{\mathrm{eq}}(\mathbf{x})\,\delta\{S_{\mathrm{th}}-[V(\mathbf{x})-V(\mathbf{x}_0)]/T_0-S_0\}$ gives one stationary solution to Eq. (29). More generally, introducing a distribution $p(S_0)$ for the initial entropy value, $p_{\mathrm{eq}}^2\equiv\int dS_0p_{\mathrm{eq}}^1p(S_0)=p_{\mathrm{eq}}(\mathbf{x})p\{S_{\mathrm{th}}-[V(\mathbf{x})-V(\mathbf{x}_0)]/T_0\}$ also gives a stationary solution to Eq. (29). These arguments give partial support to the validity of Eq. (29). Numerical studies on Eq. (29) for a time-dependent temperature are in progress and will be reported elsewhere.

APPENDIX: ENTROPY IN MASTER EQUATION DYNAMICS

We consider the master equation for the probability density $p(\mathbf{x};t)$,

$$\partial p(\mathbf{x};t)/\partial t=\int d\mathbf{y}[W(\mathbf{y}\to\mathbf{x})p(\mathbf{y};t)-W(\mathbf{x}\to\mathbf{y})p(\mathbf{x};t)]\equiv\int d\mathbf{y}[A-B], \qquad (A1)$$

where we assume the detailed balance relation

$$W(\mathbf{x}\to\mathbf{y})/W(\mathbf{y}\to\mathbf{x})=\exp\{[V(\mathbf{x})-V(\mathbf{y})]/T(t)\}. \qquad (A2)$$

With use of definitions (4) and (5), we readily see that

$$d\langle V\rangle(t)/dt-T(t)dS_{\mathrm{st}}(t)/dt=\int d\mathbf{x}\int d\mathbf{y}[A-B][V(\mathbf{x})+T(t)\ln p(\mathbf{x};t)]. \qquad (A3)$$

By interchanging $\mathbf{x}$ and $\mathbf{y}$ in the integrand of Eq. (29) we see that

$$d\langle V\rangle(t)/dt-T(t)dS_{\mathrm{st}}(t)/dt=[T(t)/2]\int d\mathbf{x}\int d\mathbf{y}[A-B]\ln(B/A)\leqslant 0. \qquad (A4)$$

Following the same argument as before we see that the relation (12) also holds for the master equation dynamics. It goes without saying that the state variable $\mathbf{x}$, which is dealt here as continuous, can be discrete.

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