Classical small systems coupled to finite baths

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We have studied the properties of a classical \( N_S \)-body system coupled to a bath containing \( N_B \)-body harmonic oscillators, employing an \((N_S + N_B)\) model that is different from most of the existing models with \( N_S = 1 \). We have performed simulations for \( N_S \)-oscillator systems, solving \( 2(N_S + N_B) \) first-order differential equations with \( N_S \gtrsim 1–10 \) and \( N_B \gtrsim 10–1000 \), in order to calculate the time-dependent energy exchange between the system and the bath. The calculated energy in the system rapidly changes while its envelope has a much slower time dependence. Detailed calculations of the stationary energy distribution of the system \( f_S(u) \) (an energy per particle in the system) have shown that its properties are mainly determined by \( N_B \) but weakly depend on \( N_S \). The calculated \( f_S(u) \) is analyzed with the use of the \( \Gamma \) and \( q-\Gamma \) distributions: the latter is derived with the superstatistical approach (SSA) and microcanonical approach (MCA) to the nonextensive statistics, where \( q \) stands for the entropic index. Based on analyses of our simulation results, a critical comparison is made between the SSA and MCA. Simulations have been performed also for the \( N_S \)-body ideal-gas system. The effect of the coupling between oscillators in the bath has been examined by additional \((N_S + N_B)\) models that include baths consisting of coupled linear chains with periodic and fixed-end boundary conditions.

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I. INTRODUCTION

The study of open systems is one of the important areas in classical and quantum statistics [1]. In the theory of open systems, the deterministic dynamics of particles in the system is replaced by the stochastic Langevin equation in the classical limit. The problem has been investigated with the use of various models in which a single particle (the system) is attached at the center (or edge) of a linear chain [2,3], or it is coupled to a bath consisting of a collection of harmonic oscillators [4–13]. Many studies have been made for open systems by using the Caldeira-Leggett (CL) model given by [4–6]

\[
H_{CL} = \frac{p^2}{2M} + V(Q) + \sum_{n=1}^{N_B} \left[ \frac{p_n^2}{2m} + \frac{m\omega_n^2}{2} (q_n - c_n/m\omega_n^2 Q)^2 \right],
\]

where \( M \) (\( m \)), \( P \) (\( p_n \)), and \( Q \) (\( q_n \)) denote the mass, momentum, and coordinate of a particle in a system (bath), \( V(Q) \) the potential in the system, \( \omega_n \) the frequency of the \( n \)th oscillator in the \( N_B \)-body bath, and \( c_n \) the coupling constant between the system and bath. The CL model was originally introduced for infinite bath (\( N_B \rightarrow \infty \)). In recent years, the CL model has been employed for a study of properties of a small system coupled to a finite bath [9–10]. A thermalization of a particle (the system) coupled to a finite bath has been investigated [9,10]. It has been shown that a complete thermalization of the particle requires some conditions for relative ranges of oscillating frequencies in the system and bath [9,10]. The specific heat of a single oscillator (the system) coupled to a finite bath has been studied with the use of two different evaluation methods [11,12]. The energy exchange between particles in a ratchet potential (the system) and finite bath (\( N_B = 1-500 \)) also has been investigated [13].

Ford and Kac proposed the model given by [7]

\[
H_{FK} = \frac{p^2}{2M} + V(Q) + \sum_{n=1}^{N_B} \left[ \frac{p_n^2}{2m} + \frac{m\omega_n^2}{2} (q_n - Q)^2 \right],
\]

which is referred to as the FK model. The CL and FK models are formally equivalent [7] because Eq. (2) may be derived from Eq. (1) with \( c_n = m\omega_n^2 \). However, the physical meanings of the coupling term in the CL and FK models are not the same. The CL model was initially introduced such that we take into account a linear coupling of \( -Q \sum_n c_n q_n \) between system and bath [4], and then the counterterm of \( c_n^2 Q^2/m\omega_n^2 \) was included for a compensation of the renormalization in the oscillating frequency by the introduced interaction. In contrast, the interaction term in Eq. (2) of the FK model clearly expresses the quadratic potential of springs between \( Q \) and \( q_n \). It is evident that the interaction term of the FK model in Eq. (2) preserves the translational invariance whereas that of the CL model in Eq. (1) does not in a strict sense [14–16] except for \( c_n = m\omega_n^2 \), for which the CL model reduces to the FK model as has been mentioned. The importance of the translational invariance in the system plus bath models has been discussed in Refs. [14–16].

In existing models that have been proposed for open systems [5–13], the number of particles in a systems is taken to be unity (\( N_S = 1 \)) while a generic open system may contain any number of particles. It is necessary to develop an \((N_S + N_B)\) model including a \( N_S \)-body system (\( N_S \geq 1 \)) coupled to an \( N_B \)-body bath with which we may investigate the properties of generic small systems. Extending the FK model, we will propose in this paper three types of \((N_S + N_B)\) models (referred to as A, B, and C). In model A a bath consists of uncoupled oscillators, and in models B and C baths contain coupled oscillators with the periodic and fixed-end boundary conditions, respectively. They are adopted for a study on effects of couplings in bath oscillators.
In the last decade, many studies have been made for nonextensive statistics initially proposed by Tsallis [17–20]. In nonextensive systems, the probability distribution generally does not follow the Gaussian, but it is well described by the \( q \)-exponential distribution,

\[
p(u) \propto e^{(1-q)\beta_0 u} = [1 - (1-q)\beta_0 u]^{1/(1-q)},
\]

where an inverse of the effective temperature \( \beta_0 \) and the entropic index \( q \) are fitting parameters, and the \( q \)-exponential function \( e_q \) is defined by [17–20]

\[
e_q^x = [1 + (1-q)x]^{1/(1-q)},
\]

with \( [\gamma]_+ = \max(\gamma,0) \). In the limit of \( q \to 1.0 \), \( e_q^x \) reduces to the exponential function \( e^x \). In a seminal paper [17], the \( q \)-exponential distribution was first derived by the maximum-entropy method with the use of the so-called Tsallis entropy. Later superstatistical [21,22] and microcanonical methods [23,24] have been proposed as alternative approaches to nonextensive statistics. A recent development has shown that small systems belong to nonextensive systems [20].

Nonextensive statistics initially proposed by Tsallis [17–20].

The probability distribution of the nonextensive statistics is generally different from that of the conventional statistics. Here \( f_S(u) \) is defined by [17–20]

\[
f_S(u) = \frac{1}{\Gamma(1-q)/(1-q)\beta_0} \frac{\partial}{\partial u} \left[ e^{(1-q)\beta_0 u} \right],
\]

where \( \Gamma(\cdot) \) is the gamma function. In nonextensive systems, the probability distribution generally does not follow the Gaussian, but it is well described by the \( q \)-exponential distribution. However, the \( q \)-distribution is not a good approximation of the Gaussian distribution for small values of \( q \). The \( q \)-exponential distribution is more appropriate for describing systems with small sizes or systems in which the number of particles is small.

The present paper is twofold: to develop the \( (N_S + N_B) \) model with the system containing independent \( N_S \) oscillators (model A), we have calculated the stationary distribution of \( f_S(u) \) for the energy per particle \( u \) (= \( E_S/N_S \), \( E_S \): the system energy). The calculated distribution is well described by the \( q \)-\( \Gamma \) distribution given by

\[
f_S(u) \propto u^{a-1} e^{bu},
\]

where \( a, b \), and \( q \) are fitting parameters. It is easy to see that in the limit of \( q \to 1.0 \), the \( q \)-\( \Gamma \) distribution reduces to the conventional \( \Gamma \) distribution. As will be shown in Sec. III, a superstatistical approach (SSA) [21,22] and a microcanonical approach (MCA) [23–29] lead to the equivalent expressions for \( f_S(u) \) given by Eq. (5) with \( a = N_S \) and \( b = \beta_0 N_S \), but with different expressions for the entropic index \( q \):

\[
q = \begin{cases} 1 + \frac{\alpha}{(N_S-1)} & \text{in the SSA}, \\ 1 - \frac{\alpha}{(N_S-1)} & \text{in the MCA}. \end{cases}
\]

The entropic index in the SSA is expressed in terms of a system parameter \( N_S \), while that in the MCA is expressed in terms of a bath parameter \( N_B \). This difference is serious from the physical viewpoint of small open systems. The purpose of the present paper is twofold: to develop the \( (N_S + N_B) \) model in which an open system contains finite \( N_S \) particles, and to investigate the validity of the stationary distribution functions derived in the SSA [21,22] and MCA [23–29]. This is the first study on open systems with finite \( N_S \geq 1 \) as far as we are aware.

The paper is organized as follows. In Sec. II, we propose model A described earlier, for which we perform DS of \( 2(N_S + N_B) \) differential equations for the \( N_S \)-oscillator system in order to calculate the time-dependent energy exchange between the system and bath. We present detailed calculations of \( f_S(u) \), changing model parameters such as \( N_S \), \( N_B \), frequency distribution, mass of oscillators in the bath, and coupling strength between the system and bath. In Sec. III, we analyze the calculated \( f_S(u) \) by using the \( \Gamma \) distribution [Eq. (36)] and the \( q \)-\( \Gamma \) distribution [Eq. (5) or (45)]. The former is derived based on the Boltzmann-Gibbs statistics, and the latter is obtained with the SSA [21,22] and MCA [23–29] of the nonextensive statistics. DS has been made also for the system consisting of \( N_B \)-body ideal gases, whose results are compared to those of oscillators. We introduce models B and C, whose DS for the oscillator systems will be reported. A comparison is made among Langevin equations derived in various models for open systems. The final Sec. IV is devoted to our conclusion.

II. ADOPTED \((N_S + N_B)\) MODEL

A. A system with bath containing uncoupled oscillators

We consider a system \( (H_S) \) and a bath \( (H_B) \) consisting of independent \( N_S \) and \( N_B \) one-dimensional oscillators, respectively, that are coupled by the interaction \( (H_I) \). We assume that the total Hamiltonian is given by

\[
H = H_S + H_B + H_I,
\]

with

\[
H_S = \sum_{k=1}^{N_S} \left[ \frac{p_k^2}{2M} + V(Q_k) \right] - f(t) \sum_{k=1}^{N_S} Q_k,
\]

\[
H_B = \sum_{n=1}^{N_B} \left[ \frac{p_n^2}{2m} + v(q_n) \right],
\]

\[
H_I = \frac{1}{2} \sum_{k=1}^{N_S} \sum_{n=1}^{N_B} c_{kn} (Q_k - q_n)^2.
\]

\[
v(q_n) = \frac{b_n}{2} q_n^2 = \frac{m \omega_n^2}{2} q_n^2 \quad \text{(model A)},
\]

which is referred to as model A. Here \( M \) (\( m \)) denotes the mass, \( p_k \) (\( p_n \)) the momentum, \( Q_k \) (\( q_n \)) the position of the oscillator, \( V(Q_k) \) \( v(q_n) \) the potential in the system (bath). \( c_{nk} \) the coupling constant, \( b_n \) and \( \omega_n \) the spring constant and frequency in the bath, respectively, and \( f(t) \) an external force. A simple generalization of the FK model [Eq. (2)] yields the model Hamiltonian given by Eq. (7) with \( H_S \) given by Eq. (8),

\[
H_B = \sum_{n=1}^{N_B} \frac{p_n^2}{2m} \quad \text{and} \quad H_I = \sum_{k=1}^{N_S} \sum_{n=1}^{N_B} (m \omega_n^2/2)(Q_k - q_n)^2.
\]

In our model Hamiltonian, we have added \( v(q_n) \) in \( H_B \) such that the Hamiltonian is symmetric with respect to an exchange of system ↔ bath [for \( f(t) = 0 \)] and such that we may discuss the coupled oscillators in baths (models B and C). Furthermore, we have included coupling \( c_{kn} \) in place of \( m \omega_n^2 \) in \( H_I \) of the generalized FK model in order to study the effect of system-bath couplings. We note that \( H_I \) in Eq. (10) may be rewritten as

\[
H_I = \frac{1}{2} \sum_{k=1}^{N_S} \left( \sum_{n=1}^{N_B} c_{kn} Q_k^2 \right) + \frac{1}{2} \sum_{n=1}^{N_B} \left( \sum_{k=1}^{N_S} c_{kn} \right) q_n^2
\]

\[
- \sum_{k=1}^{N_S} \sum_{n=1}^{N_B} c_{kn} Q_k q_n.
\]

Absorbing the first and second terms in Eq. (12) to \( H_S \) and \( H_B \), respectively, we may regard the last term as the interaction. Such a model Hamiltonian with a linear coupling of \( - \sum_{k} \sum_{n} c_{kn} Q_k q_n \) corresponds to the generalized CL model for finite \( N_S \).
From Eqs. (7)–(11), we obtain $2(N_S + N_B)$ first-order differential equations,

$$\dot{Q}_k = \frac{P_k}{M},$$  \hspace{1cm} (13)

$$\dot{P}_k = -V'(Q_k) - \sum_{n=1}^{N_S} c_{kn}(Q_k - q_n) + f(t),$$  \hspace{1cm} (14)

$$\dot{q}_n = \frac{p_n}{m},$$  \hspace{1cm} (15)

$$\dot{p}_n = -m\omega_n^2 q_n - \sum_{k=1}^{N_S} c_{kn}(q_n - Q_k),$$  \hspace{1cm} (16)

which yield

$$M \ddot{Q}_k = -V'(Q_k) - \sum_{n=1}^{N_S} c_{kn}(Q_k - q_n) + f(t),$$  \hspace{1cm} (17)

$$m \ddot{q}_n = -m\omega_n^2 q_n - \sum_{k=1}^{N_S} c_{kn}(q_n - Q_k),$$  \hspace{1cm} (18)

with prime (') and dot (·) denoting derivatives with respect to the argument and time, respectively.

A formal solution of Eq. (18) for $q_n(t)$ is given by

$$q_n(t) = q_n(0) \cos \tilde{\omega}_n t + \frac{\dot{q}_n(0)}{\tilde{\omega}_n} \sin \tilde{\omega}_n t$$

$$+ \sum_{\ell=1}^{N_S} \frac{c_{kn}}{m \tilde{\omega}_n} \int_0^t \sin \tilde{\omega}_n (t - \tau) Q_\ell(\tau) d\tau,$$  \hspace{1cm} (19)

with

$$\tilde{\omega}_n^2 = \frac{b_n}{m} + \sum_{k=1}^{N_S} \frac{c_{kn}^2}{m} = \omega_n^2 + \sum_{k=1}^{N_S} c_{kn}/m.$$  \hspace{1cm} (20)

Substituting Eq. (19) into Eq. (17), we obtain the Langevin equation given by

$$M \ddot{Q}_k = -V'(Q_k) - M \sum_{\ell=1}^{N_S} \xi_{k\ell} \dot{Q}_\ell(t)$$

$$- \sum_{\ell=1}^{N_S} \int_0^t \gamma_{k\ell}(t - \tau) \dot{Q}_\ell(\tau) d\tau'$$

$$- \sum_{\ell=1}^{N_S} \gamma_{k\ell}(t) Q_\ell(0) + \zeta_k(t) + f(t)$$

$$\quad (k = 1 \text{ to } N_S),$$  \hspace{1cm} (21)

with

$$M \xi_{k\ell} = \sum_{n=1}^{N_B} \left( c_{kn} \delta_{k\ell} - \frac{c_{kn} c_{\ell n}}{m \tilde{\omega}_n^2} \right),$$  \hspace{1cm} (22)

$$\gamma_{k\ell}(t) = \sum_{n=1}^{N_S} \left( \frac{c_{kn} c_{\ell n}}{m \tilde{\omega}_n^2} \right) \cos \tilde{\omega}_n t,$$  \hspace{1cm} (23)

$$\zeta_k(t) = \sum_{n=1}^{N_S} c_{kn} \left[ q_n(0) \cos \tilde{\omega}_n t + \frac{\dot{q}_n(0)}{\tilde{\omega}_n} \sin \tilde{\omega}_n t \right].$$  \hspace{1cm} (24)

where $\xi_{k\ell}$ denotes the additional interaction between $k$ and $\ell$th particles in the system induced by couplings $\{c_{kn}\}$, $\gamma_{k\ell}(t)$ the memory kernel, and $\xi_k$ the stochastic force.

If the equipartition relation is realized in initial values of $q_n(0)$ and $\dot{q}_n(0)$,

$$\langle m \dot{q}_n^2 q_n(0)^2 \rangle_B = \langle m \dot{q}_n(0)^2 \rangle_B = k_B T,$$  \hspace{1cm} (25)

we obtain the fluctuation-dissipation relation:

$$\langle \xi_k(t) \xi_k(t') \rangle_B = k_B T \delta(t - t'),$$  \hspace{1cm} (26)

where $\langle \cdot \rangle_B$ stands for the average over variables in the bath.

In the case of $N_B \to \infty$, summations in Eqs. (22)–(24) are replaced by integrals. When the density of states $[D(\omega) = \int_0^{\infty} \delta(\omega - \omega_n)]$ is given by the Debye form, $D(\omega) \propto \omega^2$ for $0 \leq \omega < \omega_D$, the kernel becomes

$$\gamma(t) \propto \frac{\sin \omega_D t}{\pi t} \propto \delta(t),$$  \hspace{1cm} (27)

which leads to the Markovian Langevin equation.

In the case of $N_S = 1$, we obtain $\xi$ and $\gamma$ in Eqs. (22) and (23), where the subscripts $k$ and $\ell$ are dropped (e.g., $c_{kn} = c_n$),

$$M \xi(t) = \sum_{n=1}^{N_B} c_n \left( 1 - \frac{c_n}{m \tilde{\omega}_n^2} \right),$$  \hspace{1cm} (28)

$$\gamma(t) = \sum_{n=1}^{N_B} \left( \frac{c_n^2}{m \tilde{\omega}_n^2} \right) \cos \tilde{\omega}_n t.$$  \hspace{1cm} (29)

The additional interaction vanishes ($\xi = 0$) if we choose $c_n = m \tilde{\omega}_n^2$ in Eq. (28).

In the case of $N_S \neq 1$, however, it is impossible to choose $\{c_{kn}\}$ such that $\xi_{k\ell} = 0$ is realized for all pairs of $(k, \ell)$ in Eq. (22). Then $Q_k$ is inevitably coupled to $Q_\ell$ for $\ell \neq k$ with the superexchange-type interaction of antiferromagnets:

$$- \sum_{n=1}^{N_S} c_{kn} c_{\ell n} / m \tilde{\omega}_n^2$$

in Eq. (22).

B. Model calculations for oscillator systems

It is easier to solve $2(N_S + N_B)$ first-order differential equations given by Eqs. (13)–(16) than to solve the $N_S$ Langevin equations given by Eqs. (21)–(24) although the latter provide us with clearer physical insight than the former. We have performed DS, solving the differential equations for the oscillator system with $V(Q_k) = M \Omega_k^2 Q_k^2 / 2$ in Eq. (8) for $f(t) = 0$, $M = m = 1.0$, and $\Omega_k = \omega_0 = 1.0$ otherwise noticed with the use of the fourth-order Runge-Kutta method with the time step 0.01. In order to study the $N_S$ and $N_B$ dependences of various physical quantities, we have assumed the coupling given by

$$c_{kn} = \frac{c_0}{N_S N_B},$$  \hspace{1cm} (30)

because the interaction term includes summations of $\sum_{k=1}^{N_S}$ and $\sum_{n=1}^{N_B}$ in Eq. (10). We have chosen $c_0 = 10.0$ (see Sec. III B 3). It is noted that with our choice of $c_{kn}$, the interaction contribution is finite even in the thermodynamical limit $N_B \to \infty$ because the summation over $n$ runs from 1 to
For means and unit variances. Simulations have been performed neglecting a contribution from the interaction term \( H_I \), which is valid for the weak interaction although a treatment of the finite interaction is ambiguous and controversial \[11,12\]. Figures 1(a) and 1(b) show the time dependence of \( u_{\eta}(t) \) in the system \((\eta = S)\) and the bath \((\eta = B)\) are given by

\[
\begin{align*}
  u_S &= \frac{1}{N_S} \sum_{k=1}^{N_S} \left( \frac{p_k^2}{2M} + \frac{M\Omega^2 Q_k^2}{2} \right), \\
  u_B &= \frac{1}{N_B} \sum_{n=1}^{N_B} \left( \frac{p_n^2}{2m} + \frac{m\omega_n^2 q_n^2}{2} \right),
\end{align*}
\]

(31)

(32)

(33)

neglecting a contribution from the interaction term \( H_I \), which is valid for the weak interaction although a treatment of the finite interaction is ambiguous and controversial \[11,12\]. Figures 1(a) and 1(b) show the time dependence of \( u_{\eta}(t) \) for \( N_S = 1 \) and 10, respectively, with \( N_B = 1000 \) of a single DS run. We note that although \( u_{\eta}(t) \) rapidly oscillates, its envelope has much slower time dependence. Periods for rapid oscillations are about 0.95 and 2.22 for \( N_S = 1 \) and 10, respectively. The latter value is larger than the former because of a larger renormalization effect due to couplings [the \( \xi_{t} \) term in Eq. (22)]. Magnitudes of time variations in \( u_{\eta}(t) \) are larger than those in \( u_{\eta}(t) \) because \( N_S \ll N_B \). The width of variation in \( u_{\eta}(t) \) for \( N_S = 1 \) in Fig. 1(a) is larger than that for \( N_S = 10 \) in Fig. 1(b). Even when the energy of the system is once decreased flowing into the bath, later it returns back to the system within the finite time \[31\]. Then the dissipative energy transfer from the system to the bath or vice versa does not occur on a long timescale in Fig. 1. This is in contrast with the result of Ref. \[13\], which has reported a transition from non-dissipative to dissipative energy transfer at \( N_B \sim 300 \) \( \sim 400 \) with \( N_S = 1 \).

In the following, we will show calculations of the stationary distributions of the system and bath, changing \( N_S, N_B \), interaction strength \( (c_0) \), the distribution of \( \omega_n \), and the ratio of \( m/M \). Hereafter the argument \( u \) in the stationary distributions of \( f_S(u) \) and \( f_B(u) \) expresses \( u = u_S \) and \( u = u_B \), respectively.

1. Effect of \( N_S \)

First we study the effect of \( N_S \). Dashed, dotted, chain, and solid curves in Fig. 2(a) show the stationary distribution of the system \( f_S(u) \) for \( N_S = 1, 2, 5, \) and 10, respectively, with \( N_B = 100 \). \( f_S(u) \) for \( N_S = 1 \) shows an exponential-like behavior, while \( f_S(u) \) for \( N_S > 1 \) has a structure with a peak near the center of the stationary distribution of the bath \( f_B(u) \). Distributions of \( f_B(u) \) for \( N_S = 1, 2, 5, \) and 10 with \( N_B = 100 \) are plotted by dashed, dotted, chain, and solid curves, respectively, in Fig. 2(b), which is nearly independent of \( N_S \). More detailed discussion on the \( N_S \) dependence will be given in Sec. III A.

2. Effect of \( N_B \)

Calculated distributions of \( f_S(u) \) for \( N_S = 1 \) with \( N_B = 10, 100, \) and 1000 are plotted by solid, dashed, and chain curves, respectively, in Fig. 3(a). Similar results of \( f_B(u) \) are shown.
in Fig. 3(b). Profiles of $f_S(u)$ showing an exponential-like behavior are almost independent of $N_B$ while those of $f_B(u)$ change: Its width becomes narrower for larger $N_B$. Solid, dashed, and chain curves in Fig. 4(a) [Fig. 4(b)] show $f_S(u)$ [$f_B(u)$] for $N_B = 10, 100, \text{and } 1000$, respectively, with $N_S = 10$. Again $f_S(u)$ of $N_S = 10$ is nearly independent of $N_B$. In particular, for $N_S = N_B = 10$, we obtain $f_S(u) = f_B(u)$ because the system and bath are equivalent. $f_B(u)$ for $N_S = 10$ in Fig. 4(b) is indistinguishable to that for $N_S = 1$ in Fig. 3(b).

3. Effect of $c_0$

We change the coupling strength of $c_0$ in $c_{kn} = c_0/n_S N_B$. Figures 5(a), 5(b), and 5(c) show distributions of $f_S(u)$ and $f_B(u)$ for $c_0 = 1.0, 10.0, \text{and } 100.0$, respectively, with $N_S = 1$ and $N_S = 10$ for $N_B = 100$. Results for $c_0 = 1.0$ [Fig. 5(a)] and $c_0 = 10.0$ [Fig. 5(b)] are almost identical. When $c_0$ is increased to 100.0, distribution of $f_S(u)$ becomes much wider than those in Figs. 5(a) and 5(b). At the same time, $f_B(u)$ is modified by the stronger coupling. We have decided to adopt $c_0 = 10.0$ in our DS; the related discussion is given in Sec. III A.

4. Effect of distributions of $\omega_n$

Although we have so far assumed $\omega_n = 1.0$ in the bath, we will examine additional two types of distribution ranges for $\omega_n$: uniform distributions in $[0.5, 1.5]$ and $[2.0, 3.0]$ with a fixed $\Omega_k = 1.0$ in the system. Calculated $f_S(u)$ and $f_B(u)$ for $\omega_n \in [0.5, 1.5]$ in Fig. 6(b) are almost the same as those for $\omega_n = 1.0$ in Figs. 6(a). In Fig. 6(c), where distribution of $\omega_n \in [2.0, 3.0]$ in the bath does not have an overlap with those of $\Omega_k = 1.0$ in the system, $f_S(u)$ is nearly the same as those in Figs. 6(a) and 6(b) in which the frequency ranges of the bath overlap those of the system. In contrast, $f_B(u)$ in Fig. 6(c) is quite different from those in Figs. 6(a) and 6(b) as expected. Our results shown in Figs. 6(a), 6(b), and 6(c) suggest that $f_S(u)$ is not so sensitive to the position of frequency ranges of the bath relative to that of the system. This is in contrast with the result for $N_S = 1$ in Ref. [9], which shows that for a thermalization of the system, the relative position between the oscillating frequency range of the system and that of the bath is very important.

5. Effect of $m/M$

Finally we will change a value of $m$ that has been so far assumed to be $m = M = 1.0$. Figures 7(a) and 7(b) show $f_S(u)$ for $N_S = 1$ and $N_S = 10$, respectively, with
III. DISCUSSION

A. Analysis of DS results for oscillator systems

1. Boltzmann-Gibbs statistics

We may theoretically evaluate the distribution of $f_S(u)$ as follows. First, we calculate the distribution for a set of variables of $(Q_k, V_k)$ $(V_k = \tilde{Q}_k)$ with the Boltzmann-Gibbs statistics for the infinite bath characterized by the inverse temperature $\beta$ (see Appendix A),

$$f(Q, V) dQdV \propto \exp \left[ -\beta \sum_{k=1}^{N_b} \left( \frac{MV_k^2}{2} + \frac{M\Omega_k^2Q_k^2}{2} \right) \right] \times \prod_{k=1}^{N_b} dQ_k dV_k, \quad (34)$$

$$\propto E_{S}^{-N_{S}^{-1}} e^{-\beta E_{S}} dE_{S}, \quad (35)$$

where $E_S$ denotes the energy in the system: $E_S = \sum_{k=1}^{N_S/2} (MV_k^2/2 + M\Omega_k^2Q_k^2/2)$. From Eq. (35), the distribution of the system for $u (=E_S/N_S)$ becomes

$$f_S(u) = \frac{1}{Z} a^{u-1} e^{-a u} \equiv g_1(u), \quad (36)$$

with

$$a = N_{S}, \quad b = N_{S} \beta, \quad (37)$$

$$Z = \frac{\Gamma(a)}{b^a}. \quad (38)$$

Equation (39) expresses the equipartition relation. The distribution $f_B(u)$ of the bath for $u (=E_B/N_B)$ may be obtainable in a similar way, where $E_B$ signifies the bath energy.

Our DS in the preceding section has shown that the most influential parameter on the properties of the system is $N_s$. We now pay our attention to the $N_S$ dependence of calculated means ($\mu_B$) and root-mean-square (RMS) ($\sigma_B$) of the system ($\eta = S$) and bath ($\eta = B$). Figure 8 shows $\mu_S$ and $\sigma_S$ as a function of $N_S$ with $N_B = 100$ obtained by DS: filled (open) circles denote $\mu_S$ ($\sigma_S$) of the system; filled (open) squares stand for $\mu_B$ ($\sigma_B$) of the bath. We obtain $(\mu_S, \sigma_S) = (2.84, 3.77)$, $(1.97, 2.12)$, $(1.302, 0.755)$, and $(1.097, 0.393)$ for $N_S = 1, 2, 5$, and 10, respectively. With decreasing $N_S$ from $N_S = 10$, $\mu_S$ and $\sigma_S$ are increased. In contrast, $\mu_B$ and $\sigma_B$ are almost independent of $N_S$. An increase in $\mu_S$ with decreasing $N_S$ is attributed to an increase in the effective frequency of the system given by [Eqs. (22) and (30)]

$$\Omega_{kk}^2 = \Omega_{kk}^2 + \frac{1}{M} \left[ \frac{c_0}{N_S} - \frac{c_0^2}{N_S^2(N_B\omega^2 + c_0/m)} \right].$$

An increase in $\sigma_S$ with decreasing $N_S$ is due to an increase in $\xi_S$ given by Eq. (24), which is proportional to $c_0/N_S$. When we adopt a smaller value of $c_0$, these increases are reduced. For

\[ \text{FIG. 6. (Color online) Stationary distributions of } f_s(u) \text{ (solid curves) and } f_B(u) \text{ (dashed curves) for (a) } \omega_n = 1.0, \text{ (b) } \omega_n \in [0.5, 1.5], \text{ and (c) } \omega_n \in [2.0, 3.0] \text{ with } N_b = 10 \text{ and } N_B = 100, f_B(u) \text{ being divided by a factor of two.} \]

\[ \text{FIG. 7. (Color online) Stationary distributions of } f_s(u) \text{ for (a) } N_S = 1 \text{ and (b) } N_S = 10 \text{ with } N_B = 100 \text{ for various } m/M: m/M = 1.0 \text{ (solid curves), 0.1 (dashed curves), and 0.01 (chain curves).} \]
example, \( \mu_S (\sigma_S) \) calculated with a smaller \( c_0 = 1.0 \) are plotted by filled (open) triangles in Fig. 8, which shows \( (\mu_S, \sigma_S) = (1.12, 1.24), (1.02, 0.78), (0.97, 0.45), \) and \( (0.97, 0.31) \) for \( N_S = 1, 2, 5, \) and 10, respectively. Related distributions for \( N_S = 1 \) and 10 are plotted in Fig. 5(a). For this choice of \( c_0 = 1.0 \), the energy exchange between system and bath is considerably decreased.

We have performed DS by using also an alternative choice of couplings of \( c_{\text{DS}} = c_0 / \sqrt{N_SN_B} \) given by Eq. (31). Filled and open diamonds in Fig. 8 show \( \mu_S \) and \( \sigma_S \), respectively, calculated with \( c_0 = 1.0 \) and \( c_0 = 0.01 \) as Eq. (30) for \( N_S = 10 \) and \( N_B = 100 \). For \( N_S = 1, 2, 5, \) and 10, we obtain \( (\mu_S, \sigma_S) = (1.61, 2.10), (1.35, 1.25), (1.18, 0.58), \) and \( (1.097, 0.393) \), respectively. With decreasing \( N_S \), both \( \mu_S \) and \( \sigma_S \) are increased, which are qualitatively similar to those obtained with couplings given by Eq. (30).

Next we examine the profiles of \( N_S \)-dependent \( f_S(u) \). By using the relation between parameters \( a \) and \( b \) in the \( \Gamma \) distribution with its average and variance given by Eqs. (39) and (40), we may determine \( a \) and \( b \) by \( a = (\mu^2 / \sigma^2) \) and \( b = \mu / \sigma^2 \). With the use of the calculated \( \mu_S \) and \( \sigma_S \), we obtain \( (a, b) = (0.565, 0.199), (0.861, 0.437), (2.98, 2.28), \) and \( (7.78, 7.11) \) for \( N_S = 1, 2, 5, \) and 10, respectively. Unfortunately, these values of \( a \) are not in agreement with the theoretical value of \( a = N_S \) given by Eq. (37). We have employed the \( \Gamma \) distribution given by Eq. (36) with the parameters \( a \) and \( b \) determined earlier for our analysis of \( f_S(u) \) shown in Fig. 2(a). Dashed curves in Figs. 9(a)–9(d) show the calculated \( \Gamma \) distribution, while solid curves express DS results. We note in Figs. 9(c) and 9(d) that the \( \Gamma \) distributions for \( N_S = 5 \) and 10 are ostensibly in good agreement with calculated \( f_S(u) \) although the calculated \( a \) disagrees with the theoretical value of \( a = N_S \) as we have mentioned. Furthermore, an agreement becomes poor for results of smaller \( N_S = 1 \) and 2, whose analyses will be discussed next with the use of the nonextensive statistics.

2. Nonextensive statistics

a. Superstatistical approach. A disagreement between theoretical results and DS ones might arise from a use of the Boltzmann-Gibbs statistics. We will analyze the calculated results by using the nonextensive statistics [17–20]. Wilk and Włodarcz [21] and Beck [22] have pointed out that the observed non-Gaussian distribution may be accounted for if we assume that the Gaussian distribution \( e^{-\beta u} \) is averaged over the \( \Gamma \) distribution of \( g(\beta) \) for fluctuating inverse temperature \( \beta \).

\[
p(u) \propto e^{-\beta u} g(\beta) d\beta, \tag{41}
\]

with

\[
g(\beta) = \frac{1}{\Gamma(n/2)} \left( \frac{n}{2\beta_0} \right)^{n/2} \beta^{n/2 - 1} e^{-n\beta/2\beta_0}. \tag{42}
\]

Here \( n \) denotes the number of independent Gaussian \( X_i \) contributions to the \( \chi^2 \) distribution of \( \beta = \sum_{i=1}^{N} X_i^2 \) [22], and \( \beta_0 \) stands for the mean of \( \beta: \beta_0 = \langle \beta \rangle \), and variance is given by \( \langle \beta^2 \rangle - \beta_0^2 = (2/n)\beta_0^2 \). Equations (41) and (42) express the superstatistics whose concept may be understood such that complex nonextensive systems are in the nonequilibrium states with temporarily and spatially fluctuating inverse temperature.

In order to more accurately account for our calculated \( f_S(u) \), we employ the concept of the superstatistics. We assume that the \( \Gamma \) distribution \( f(u) \) given by Eq. (36) is averaged over the distribution \( g(\beta) \) given by Eq. (42) with \( n = 2N_S \),

\[
f_S(u) \propto \int_0^u u^{N_S - 1} e^{-\beta N_S u} g(\beta) d\beta, \tag{43}
\]

\[
\propto \frac{u^{N_S - 1}}{(1 + \beta_0 u)^{N_S}}. \tag{44}
\]

With the normalization factor, \( f_S(u) \) is expressed by the \( q-\Gamma \) distribution \( g_q(u) \),

\[
f_S(u) = \frac{1}{Z_q} u^{1-q} e^{-bu} \equiv g_q(u), \tag{45}
\]
are given by

\[ q = 1 + \frac{1}{N_S} \quad (46) \]

\[ a = N_S \quad (47) \]

\[ b = N_S \beta_0 \quad (48) \]

\[
Z_q = \begin{cases} 
\frac{1}{b^q} \frac{\Gamma(a)\Gamma\left(\frac{1}{q} - a\right)}{\Gamma\left(\frac{1}{q}\right)} & \text{for } q > 1.0, \\
\frac{\Gamma(a)\Gamma(q-1)}{b^{q-1}} & \text{for } q = 1.0, \\
\frac{1}{b^q} \frac{\Gamma(a)\Gamma\left(\frac{1}{q} - a\right)}{\Gamma\left(\frac{1}{q}\right)} & \text{for } q < 1.0.
\end{cases}
\]

(49)

It is easy to see that in the limit of \( q \to 1.0 \), the \( q \)-\( \Gamma \) distribution \( g_q(u) \) given by Eq. (45) reduces to the \( \Gamma \) distribution \( g_1(u) \) given by Eq. (36). Average and variance of the \( q \)-\( \Gamma \) distribution are given by

\[
\mu_q = \frac{a}{b[1 - (q - 1)(a + 1)]},
\]

(50)

\[
\sigma_q^2 = \frac{a(2 - q)}{b^2[1 - (q - 1)(a + 2)][1 - (q - 1)(a + 1)]^2}
\]

for \( q > 1.0 \),

(51)

which reduce to \( \mu_1 = a/b \) and \( \sigma_1^2 = a/b^2 \) for \( q = 1.0 \). In agreement with Eqs. (39) and (40). The \( q \)-\( \Gamma \) distribution \( g_q(u) \) has a maximum at

\[
u = u_m = \frac{(a - 1)}{b[1 - (q - 1)(a + 1)]} \quad \text{for } a > 1.0.
\]

(52)

The \( u \) dependence of \( g_q(u) \) for typical parameters is shown in Appendix A (Fig. 15).

b. Microcanonical approach I. Next we mention the MCA in regard to the nonextensive statistics [23–29]. We consider microcanonical ensembles of \( N \) particles with the energy \( E \), which is divided into two subsystems 1 and 2. A probability for subsystem 1 containing \( N_1 \) particles to have energy \( E_1 \) is given by [23,27]

\[
f_{N_1}(E_1) = \frac{\Omega_1(E_1)\Omega_2(E_2)}{\Omega_{N_1,E_1}(E)},
\]

(53)

where the structure function \( \Omega_k(E) (k = 1,2,1 + 2) \) expresses the number of states with the energy \( E \). We assume that \( \Omega_k(E) \) is given by [23,27]

\[
\Omega_k(E) = Km_k E^{m_k-1},
\]

(54)

where \( K \) is a constant and \( m_k \) the degrees of freedom of variables in subsystem \( k \). Equation (54) is valid for ideal gases and harmonic oscillators with \( m_k \gg 1 \).

Interpreting subsystems 1 and 2 as a system and a bath, respectively, we apply the MCA to the oscillator system under consideration for which \( m_S = N_S \) and \( m_B = N_B \). For \( 1 < N_S \ll N_B \) and \( E_S \ll E_B \), Eqs. (53) and (54) yield

\[
f_{S}(E_S) \propto E_S^{N_S-1} \left(1 - \frac{E_S}{E}\right)^{N_S-1},
\]

(55)

\[
= E_S^{N_S-1} \left[1 - (1 - \frac{E}{E_S})^\beta E_S\right]^1/(1-\beta),
\]

(56)

\[
= E_S^{N_S-1} e^{-\frac{E}{E_S} E_S},
\]

(57)

with

\[
\hat{q} = 1 - \frac{1}{(N_B - 1)},
\]

(58)

\[
\hat{\beta} = \frac{N_B}{E},
\]

(59)

where we attach “hats” for quantities in the MCA to distinguish them from counterparts in the SSA. Equation (57) is equivalent to the \( q \)-\( \Gamma \) distribution given by Eq. (45) if we read \( E_S = N_S\mu \) and \( \hat{\beta} = \beta_0 \). Similarly, we obtain the distribution defined by [23,27]

\[
p_S(E_S) = \frac{\Omega_B(E - E_S)}{\Omega_{S+B}(E)} \equiv e^{-\frac{\hat{\beta} E_S}{E}},
\]

(60)

\[
\times \frac{\Omega_B(E - E_S)}{\Omega_{S+B}(E)} e^{-\frac{\hat{\beta} E_S}{E}}.
\]

(61)

In the limit of \( N_B \to \infty \), Eqs. (57) and (61) reduce to

\[
f_{S}(E_S) \propto E_S^{N_S-1} e^{-\hat{\beta} E_S},
\]

(62)

\[
p_S(E_S) \propto e^{-\hat{\beta} E_S},
\]

(63)

with

\[
\hat{\beta} = \frac{N_B}{E} = \frac{1}{k_B T}.
\]

(64)

where the equipartition relation is employed for \( E_B \gg E_S \). From Eqs. (53) and (60), a relation between \( f_{S}(E_S) \) and \( p_S(E_S) \) is given by

\[
f_{S}(E_S) = \frac{\Omega_S(E_S) p_S(E_S)}{\Omega_S(E_S) p_S(E_S)}.
\]

(65)

With increasing \( E_S \), \( p_S(E_S) \) is decreased whereas \( \Omega_S(E_S) \propto E_S^{N_S-1} \), and then \( f_{S}(E_S) \) has a maximum at \( E_S = (N_S - 1)/\hat{\beta}[1 - (q - 1)(N_S - 1)] \) for \( N_S > 1 \).

It should be noted that the \( q \)-exponential function adopted in Refs. [24–29] is defined by

\[
e^q \hat{\beta} = [1 + (q' - 1)x]^{1/(q'-1)} \quad \text{for } q' > 1,
\]

(66)

which is different from that given by Eq. (4) proposed in Ref. [17]. The relation between \( q' \) and \( q \) is \( q' = 1 - q \), with which Eq. (58) becomes \( q' = 1 + 1/(N_B - 1) \gg 1.0 \).

We have tried to apply the \( q \)-\( \Gamma \) distribution given by Eqs. (45)–(49) to an analysis of profiles of \( f_{S}(u) \) in Fig. 9, but we could not obtain satisfactory results. Rather we have phenomenologically adopted the \( q \)-\( \Gamma \) distribution, choosing its parameters \( a, b, q \) such as to provide results in fairly good agreement with \( f_{S}(u) \) in Fig. 9 and satisfying Eqs. (50) and (51). Chain curves in Figs. 9(a) and 9(b) express \( g_q(u) \) with \( (a,b,q) = (1.0,1.31,1.30) \) and \( (1.64,1.36,1.09) \), respectively, for \( N_S = 1 \) and \( 2 \), which have been tentatively determined by a cut and try method. It is noted that \( f_{S}(u) \) of DS is finite at \( u = 0.0 \) for \( N_S = 1 \), which requires \( a > 1.0 \). These chain curves are in better agreement with the calculated \( f_{S}(u) \) than dashed curves expressing the \( \Gamma \) distribution.

c. Microcanonical approach II. We will derive the stationary distribution with the alternative MCA (MCA II). We again consider a collection of \( N \) particles with the energy \( E = m\epsilon_0 \), where \( \epsilon_0 \) denotes an appropriate energy unit. A
the probability for its subsystem 1 containing \( N_1 \) particles to have energy \( E_1 = (M_1, \epsilon_0) \) is given by

\[
  f_{N1}(M_1) = \frac{w_{N_1}(M_1) w_{N-N_1}(M-M_1)}{w_N(M)},
\]

(67)

with

\[
  w_N(M) = \frac{(M+N-1)!}{(N-1)! M!}.
\]

(68)

We apply Eq. (67) to a system plus bath without using the condition \( 1 \ll N_1 \ll N \), which is employed in the MCA I. We assume that \( M \) and \( M_1 \) are real as given by

\[
  N = N_S + N_B, \quad N_1 = N_S, \quad M = E_S + E_B, \quad M_1 = \frac{E_S}{\epsilon_0},
\]

(69)

where \( E_S \) (\( E_B \)) denotes an energy in the system (bath). Then the probability for \( u = (E_S/N_S) \) in the system is given by

\[
  f_{S}(u) \propto \frac{w_{N1}(M_1) w_{N-N_1}(M-M_1)}{w_{N+S}(M)},
\]

(70)

with

\[
  k_B T = \frac{1}{\beta} = \frac{E_B}{N_B} = \mu_B,
\]

(71)

where \( \mu_B \) is the mean energy in the bath and \( w_N(M) \) is given by Eq. (68) with a replacement of \( n! \rightarrow \Gamma(n+1), \Gamma(x) \) being the \( \Gamma \) function.

We have calculated \( f_S(u) \) with the MCA II by using Eqs. (69)–(71), whose results with \( \epsilon_0 = 1.0 \) (dashed curves), 0.1 (dotted curves), and 0.01 (chain curves) are shown in Figs. 10(a)–10(d). With decreasing \( \epsilon_0 \), results of MCA II are expected to approach the classical limit. Although a general trend is accounted for by MCA II calculations, their agreement with DS results is not so good.

**B. Comparison with ideal-gas systems**

Our model A given by Eqs. (7)–(11) may be applied to ideal gases (the system) coupled to a finite bath, for which we set \( V(Q_b) = 0 \). We have performed DS with the same model parameters (except for \( \Omega_2 = 0 \)) as in the case of oscillator systems mentioned in Sec. II. Solid curves in Figs. 11(a), 11(b), 11(c), and 11(d) show calculated \( f_S(u) \) of \( N_S \)-body ideal gases for \( N_S = 1, 2, 5, \) and 10, respectively, with \( N_B = 100 \) for a comparison, we show by dotted curves, the corresponding results for oscillators having been plotted in Fig. 2(a). The energy distributions of a bath, \( f_B(u) \), for ideal-gas systems are almost the same as those for oscillator systems shown in Fig. 2(b). Comparing solid curves to dotted curves, we note that the distribution of \( f_S(u) \) for ideal gases has larger magnitude at small \( u \) than that for oscillators. This yields the smaller average energy in ideal gases than that in oscillators, which is related with the fact the former has a smaller degree of freedom than the latter, as expressed in the equipartition relation.

Figure 12 shows the \( N_S \) dependence of \( \mu_\eta \) and \( \sigma_\eta = S,B \): Filled (open) circles show \( \mu_S \) (\( \sigma_S \)), and filled (open) squares denote \( \mu_B \) (\( \sigma_B \)). Although \( \mu_S \) in Fig. 12 has similar \( N_S \) dependence to that in Fig. 8 for oscillator systems,
magnitudes of the former are smaller than the latter. The ratio of $\mu_s/(G/\mu_s(O_{SC})$ approaches 0.5 with increasing $N_S$, although the ratio is increased for $N_S \to 1$.

We have analyzed calculated $f_5(a)$ in Figs. 11(a)–11(d) by using the $\Gamma$ distribution given by Eq. (36) with

$$a = \frac{N_S}{2}, \quad b = N_S \beta,$$

which lead to

$$\mu = \frac{a}{b} = \frac{1}{2\beta},$$

$$\sigma^2 = \frac{a}{b^2} = \frac{1}{2N_S \beta^2}.$$  

Equation (73) expresses the equipartition relation of ideal gases. Simulations shown in Fig. 11 yield $(\mu,\sigma)$ = (2.59, 3.62), (1.50, 1.76), (0.716, 0.504), and (0.469, 0.222) for $N_S$ = 1, 2, 5, and 10, respectively, from which we obtain $(a,b) = (0.514, 0.198), (0.733, 0.487), (2.02, 2.82)$, and (4.47 9.54). Dashed curves in Figs. 11(a)–11(d) express the $\Gamma$ distribution calculated with the use of $a$ and $b$ thus obtained. They are in good agreement with the DS results for $N_S$ = 5 and 10, but not for $N_S$ = 1 and 2. Chain curves express the $q$-$\Gamma$ distributions obtained with $(a,b,q) = (0.61,0.38,1.18)$ and (1.0,0.85,1.09) for $N_S$ = 1 and 2, respectively, which have been determined by a cut-and-try method. The results of the $q$-$\Gamma$ distribution are in better agreement with DS than those of the $\Gamma$ distribution. This situation is the same as in the case of oscillator systems as discussed in Sec. III A.

### C. Bath containing coupled oscillators

In most of existing models for open systems [5–13], baths are assumed to be consisting of uncoupled oscillators. In order to study the effect of couplings of oscillators in a bath, we consider models B and C in which baths consist of coupled oscillators with the periodic and fixed-end boundary conditions, respectively.

#### 1. Model B

In model B, we assume that the Hamiltonian is given by Eqs. (7)–(10) with $v(q_n)$,

$$v(q_n) = \frac{b}{2}(q_n - q_{n+1})^2 \quad \text{(model B)},$$

under the periodic boundary condition:

$$q_{N_B+n} = q_n, \quad p_{N_B+n} = p_n,$$  

where $b$ denotes the spring constant between neighboring sites in the bath and $N_B$ is assumed even without a loss of generality. Equations of motion for $Q_k$ and $q_n$ are given by

$$M \ddot{Q}_k = -V(Q_k) - \sum_{n=-N_S/2}^{N_S/2-1} c(Q_k - q_n) + f(t),$$

$$m \ddot{q}_n = -b(2q_n - q_{n-1} - q_{n+1}) - \sum_{k=1}^{N_S} c(q_n - Q_k).$$  

By using a transformation mentioned in Appendix B, we obtain the Langevin equation for $Q_k(t)$ given by Eq. (21) with

$$M \ddot{Q}_k = cN_B \beta_k - \frac{c^2 N_B}{m \tilde{\omega}_0^2},$$

$$\gamma_k(t) = \left(\frac{c^2 N_B}{m \tilde{\omega}_0^2}\right) \cos \tilde{\omega}_0 t,$$

$$\zeta_k(t) = c \sqrt{\gamma_k} \left[ \tilde{q}_0(0) \cos \tilde{\omega}_0 t + \frac{\tilde{q}_0(0)}{\tilde{\omega}_0} \sin \tilde{\omega}_0 t \right].$$

with

$$\tilde{\omega}_0^2 = \frac{cN_S}{m}.$$  

#### 2. Model C

In model C, we assume that the Hamiltonian is given by Eqs. (7)–(11) with $v(q_n)$,

$$v(q_n) = \frac{b}{2}(q_n - q_{n+1})^2 \quad \text{(model C)},$$

under the fixed-end boundary condition given by

$$q_0 = q_{N_B+1} = 0, \quad p_0 = p_{N_B+1} = 0.$$  

Equations of motion for $Q_k$ and $q_n$ are given by

$$M \ddot{Q}_k = -V(Q_k) - \sum_{n=0}^{N_S} c(Q_k - q_n) + f(t),$$

$$m \ddot{q}_n = -b(2q_n - q_{n-1} - q_{n+1}) - \sum_{k=1}^{N_S} c(q_n - Q_k).$$

By using a transformation mentioned in Appendix C, we obtain the Langevin equation given by Eq. (21) with

$$M \ddot{Q}_k = c(N_B + 2) \beta_k - \sum_{s=1}^{N_S} c^2 a_s^2 \frac{m \tilde{\omega}_s^2}{\omega_s^2},$$

$$\gamma_k(t) = \sum_{s=1}^{N_S} \left( \frac{c^2 a_s^2}{m \omega_s^2} \right) \cos \omega_s t,$$

$$\zeta_k(t) = \sum_{s=1}^{N_S} c a_s \left[ \tilde{q}_s(0) \cos \omega_s t + \frac{\tilde{q}_s(0)}{\omega_s} \sin \omega_s t \right],$$

where $\omega_s$ and $a_s$ are expressed by

$$\omega_s^2 = \omega_0^2 + \frac{(N_s + 2)^2}{m},$$

$$a_s = \sqrt{\frac{1}{2(N_B+1)}} \left\{ \cos \frac{\pi s}{2} - \left( \frac{N_B + 2 + \pi s}{2(N_B + 1)} \right) \cos \left( \frac{\pi s}{2} + \frac{N_B + 2 + \pi s}{2(N_B + 1)} \right) \right\}.$$

DS calculations for models B and C have been performed for oscillator systems with the same parameters as in Sec. II in addition to $b = 1.0$. Dashed and solid curves in Fig. 13(a)
D. Comparisons among various models

Table I summarizes comparisons among elements of $\xi_{kn}$, $\gamma_{kn}$, and $\zeta_k$ in Langevin equation derived from various models for open systems including CL [5] and FK models [7] and models A, B, and C, which are proposed in Secs. II and III. Additional interactions $\xi_{kn}$ induced by introduced couplings between the system and bath remain finite in models A, B, and C, although they vanish in the CL and FK models for $N_B = 1$. We note that functional forms of $\xi_{k\ell}$ in the CL and FK models are similar. This is the reason why properties of $f_S(u)$ and $f_B(u)$ in Figs. 2, 13, and 14 are similar. We note, however, that the kernel $\xi_{k\ell}$ of the model B is oscillating and not dissipative even for $N_B \to \infty$, which arises from the translational symmetry in the bath.

![Image of Fig. 13](https://example.com/fig13.png)

**FIG. 13.** (Color online) Stationary distributions of (a) $f_S(u)$ and (b) $f_B(u)$ of model B for $N_S = 1$ (dashed curves) and 10 (solid curves) with $N_B = 100$.

![Image of Fig. 14](https://example.com/fig14.png)

**FIG. 14.** (Color online) Stationary distributions of (a) $f_S(u)$ and (b) $f_B(u)$ of model C for $N_S = 1$ (dashed curves) and 10 (solid curves) with $N_B = 100$.

**TABLE I.** Terms of $\xi_{k\ell}$, $\gamma_{k\ell}$, and $\zeta_k$ in the Langevin equation, $M \dot{Q}_k(t) = -V'(Q_k) - M \sum_i \xi_{k\ell} Q_i(t) - \sum_i \gamma_{k\ell}(t-t') Q_i(t') dt' - \sum \gamma_{k\ell}(t) Q_i(0) + \zeta_k(t)$, calculated by various models: (1) CL model [Eq. (1)]; (2) FK model [Eq. (2)]; (3) model A [Eq. (11)]; (4) model B [Eq. (75)]; (5) model C [Eq. (83)]. The CL and FK models are for $N_S = 1$ for which subscripts $k, \ell$ are dropped.

<table>
<thead>
<tr>
<th>Model</th>
<th>$M \xi_{k\ell}$</th>
<th>$\gamma_{k\ell}$</th>
<th>$\zeta_k$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CL$^{(1)}$ ($N_S = 1$)</td>
<td>0</td>
<td>$\sum_n \left( \frac{\omega_n^2}{m^2 \omega_s^2} \right) \cos \omega_n t$</td>
<td>$\sum_n c_n \left[ q_n(0) \cos \omega_n t + \left( \frac{\omega_n}{m \omega_s} \right) \sin \omega_n t \right]$</td>
</tr>
<tr>
<td>FK$^{(2)}$ ($N_S = 1$)</td>
<td>0</td>
<td>$\sum_n m^2 \omega_n^2 \cos \omega_n t$</td>
<td>$\sum_n m^2 \omega_n^2 \left[ q_n(0) \cos \omega_n t + \left( \frac{\omega_n}{m \omega_s} \right) \sin \omega_n t \right]$</td>
</tr>
<tr>
<td>A$^{(3)}$</td>
<td>$\sum_n \left( c_n \delta_{k\ell} - \frac{c_{kn} q_n}{m \omega_s} \right)$</td>
<td>$\sum_n \left( \frac{c_n q_n}{m \omega_s} \right) \cos \omega n t$</td>
<td>$\sum_n c_n \left[ q_n(0) \cos \omega_n t + \left( \frac{\omega_n}{m \omega_s} \right) \sin \omega_n t \right]$</td>
</tr>
<tr>
<td>B$^{(4)}$</td>
<td>$c N_B \delta_{k\ell} - \sum_n \frac{c_{n}^2}{m \omega_s^2}$</td>
<td>$\sum_n \left( \frac{c_n q_n}{m \omega_s} \right) \cos \omega n t$</td>
<td>$c \sqrt{N_B} \left[ q_n(0) \cos \omega_n t + \left( \frac{\omega_n}{m \omega_s} \right) \sin \omega_n t \right]$</td>
</tr>
<tr>
<td>C$^{(5)}$</td>
<td>$c(N_B + 2) \delta_{k\ell} - \sum_n \frac{c_{n}^2}{m \omega_s^2}$</td>
<td>$\sum_n \left( \frac{c_n q_n}{m \omega_s} \right) \cos \omega n t$</td>
<td>$\sum_n c_n \left[ \dot{q}_n(0) \cos \omega_n t + \left( \frac{\omega_n}{m \omega_s} \right) \sin \omega_n t \right]$</td>
</tr>
</tbody>
</table>
(N_S + N_B) models A, B and C, in which an N_S-body system is coupled to an N_B-body bath. Simulations for oscillator and ideal-gas systems have shown the following:

(i) The energy of the system oscillates rapidly although its envelope has much slower time dependence.

(ii) The dissipation of the system energy is not observed in our DS with N_S ~ 1–10 and N_B ~ 10–1000.

(iii) The stationary energy distribution of the system f_S(u) for N_S > 1 has a peak at about the average energy of the bath, although f_S(u) for N_S = 1 has an exponential-like distribution decreasing monotonously with increasing u.

(iv) Calculated f_S(u), whose properties depend mainly on N_S but only weakly on N_B, may be phenomenologically described by the $\Gamma$ or q-$\Gamma$ distribution [Eq. (45)].

(v) The coupling among oscillators in the bath yields little effect in classical systems.

Item (i) is consistent with a previous study for N_S = 1 in Ref. [13]. Item (ii) suggests that for the energy dissipation of system, we might need to adopt a much larger N_B ($\gg$ 1000) [31]. The thermalized state reported in Refs. [9,10] corresponds to our state for N_S = 1 with the exponential-like distribution, in agreement with item (iii). Item (iv) is favorable to the SSA but not to the MCA, although either of them cannot quantitatively explain the DS results. Item (v) is consistent with the classical specific heat of harmonic oscillators for which both Einstein and Debye models yield the same results.

Our model A given by Eqs. (7)–(11) is expected to have a wide applicability to classical small systems: for example, for studies on a system with various potentials $V$ . ACKNOWLEDGMENT

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APPENDIX: A. q-$\chi^2$ AND q-$\Gamma$ DISTRIBUTIONS

1. The q-$\chi^2$ distribution

We will show that if $n$ independent variables of \{x_i\} follow the q-Gaussian distribution, a variable defined by $Y = \sum_{i=1}^{n} x_i^q$ follows the q-$\chi^2$ distribution with rank $n$ defined by

$$P(Y) = \frac{1}{Z} \epsilon_q^{-Y} Y^{n/2-1}, \quad (A1)$$

where $Z$ stands for the normalization factor.

In order to derive Eq. (A1), we first define a new variable of $X^2 = \sum_{i=1}^{n} x_i^2$, for which we obtain

$$p(x)dx \propto \epsilon_q^{-\sum_{i=1}^{n} x_i^2} \prod_{i=1}^{n} dx_i, \propto \epsilon_q^{-X^2} X^{n-1} dX,$$

$$\propto \epsilon_q^{-Y} Y^{(n-1)/2} Y^{-1/2} dY, = \epsilon_q^{-Y} Y^{n/2-1} dY, \quad (A2)$$

leading to the q-deformed $\chi^2$ distribution given by Eq. (A1).

FIG. 15. (Color online) The q-$\Gamma$ distribution $g_q(u)$ [Eq. (A4)] for (a) $a = 0.5$, (b) 1.0, (c) 1.5, (d) 2.0, (e) 3.0, and (f) 4.0 with $b = 1.0$: $q = 0.9$ (chain curves), 1.0 (dashed curves), and 1.1 (solid curves).

It is noted that the factorization is not satisfied for the q-exponential function [17,32],

$$\epsilon_q^{-\sum_{i=1}^{n} x_i^q} \neq \prod_{i=1}^{n} \epsilon_q^{-x_i^q}, \quad (A3)$$

except for $q = 1$ or $n = 1$. Then we cannot employ the method of the characteristic function by which the $\chi^2$-function is conventionally derived from $n$ independent Gaussians.

2. The q-$\Gamma$ distribution

When generalizing n/2 in Eq. (A1) to a real number $a$, we obtain the q-$\Gamma$ distribution,

$$g_q(u) = \frac{1}{Z_q} u^{-a} \epsilon_q^{-b/u}, \quad (A4)$$

where $Z_q$ is given by Eq. (49). Some numerical examples of $g_q(u)$ are shown in Fig. 15. The q-$\Gamma$ distribution for $q > 1.0$ has a larger magnitude than the $\Gamma$ distribution ($q = 1.0$) at large $u$ because of the flat-tail properties of the q-exponential function [17]. In contrast, the q-$\Gamma$ distribution for $q < 1.0$ has a compact structure because of cutoff properties of the q-exponential function with no magnitudes for $u \geq 1/(1 - q)b$.

APPENDIX: B. LANGEVIN EQUATION IN MODEL B

We will explain a derivation of the Langevin equation in model B given by Eqs. (7)–(10), (75), and (76). By using the transformation given by [3,33]

$$q_n = \frac{1}{\sqrt{N_B}} \sum_{i=1}^{N_B} e^{i(2\pi ns/N_B)} \tilde{q}_n, \quad (B1)$$

leading to the q-deformed $\chi^2$ distribution given by Eq. (A1).
we obtain the diagonalized $H_B$,

$$H_B = \sum_{s=-N_B/2}^{N_B/2-1} \left( \frac{1}{2m} \tilde{p}_s^2 + \frac{m \omega_s^2}{2} \tilde{q}_s^2 \right), \quad (B3)$$

with

$$\omega_s^2 = \left( \frac{4b}{m} \right) \sin^2 \left( \frac{\pi s}{N_B} \right) \quad (s = -N_B/2, \ldots, N_B/2 - 1). \quad (B4)$$

Substituting Eqs. (B1) and (B2) into Eq. (10) leads to

$$H_I = \frac{cN_B}{2} \sum_{k=1}^{N_B} \tilde{q}_k^2 + \frac{cN_S}{2} \sum_{s=-N_B/2}^{N_B/2-1} \tilde{q}_s^2 - c\sqrt{N_B} \tilde{q}_0 \sum_{k=1}^{N_S} Q_k. \quad (B5)$$

Then equations of motion become

$$M \ddot{Q}_k = -V'(Q_k) - cN_B \dot{Q}_s + c\sqrt{N_B} \tilde{q}_0 + F(t), \quad (B6)$$

$$m \ddot{q}_s = -m \omega_s^2 \dot{q}_s + c\sqrt{N_B} \sum_{k=1}^{N_S} Q_k \delta_{sk}. \quad (B7)$$

with

$$\omega_s^2 = \omega_s^2 + \frac{cN_S}{m}. \quad (B8)$$

Note that the third term of Eq. (B6) and the second term of Eq. (B7) include only the $s = 0$ component. Substituting a formal solution of $\tilde{q}_s$ to Eq. (B6), we obtain the Langevin equation given by Eqs. (21) and (79)–(82).

APPENDIX: C. LANGEVIN EQUATION IN THE MODEL C

A derivation of the Langevin equation in the model C given by Eqs. (7)–(10), (83), and (84) will be explained. A transformation given by [3,33]

$$q_n = \sqrt{\frac{2}{N_B + 1}} \sum_{s=1}^{N_B} \sin \left( \frac{\pi ns}{N_B + 1} \right) \tilde{q}_s, \quad (C1)$$

$$p_n = \sqrt{\frac{2}{N_B + 1}} \sum_{s=1}^{N_B} \sin \left( \frac{\pi ns}{N_B + 1} \right) \tilde{p}_s, \quad (C2)$$

yields the diagonalized $H_B$,

$$H_B = \sum_{s=1}^{N_B} \left( \tilde{p}_s^2 + \frac{m \omega_s^2 \tilde{q}_s^2}{2} \right), \quad (C3)$$

with

$$\omega_s^2 = \left( \frac{4b}{m} \right) \sin^2 \left( \frac{\pi s}{2(N_B+1)} \right) \quad (s = 1, 2, \ldots, N_B). \quad (C4)$$

From a transformation given by Eqs. (C1) and (C2), we obtain $H_I$ given by

$$H_I = \frac{(N_B + 2)c}{2} \sum_{k=1}^{N_B} \tilde{q}_k^2 + \frac{(N_S + 2)c}{2} \sum_{s=1}^{N_S} \tilde{q}_s^2 - c\sum_{k=1}^{N_S} \sum_{s=1}^{N_S} a_s \tilde{q}_s, \quad (C5)$$

with

$$a_s = \sqrt{\frac{2}{N_B + 1}} \sum_{s=0}^{N_B+1} \sin \left( \frac{\pi ns}{N_B + 1} \right). \quad (C6)$$

Then equations of motion for $Q_k$ and $\tilde{q}_s$ become

$$M \ddot{Q}_k = -V'(Q_k) - c(N_B + 2) \dot{Q}_s + c\sum_{s=1}^{N_S} a_s \tilde{q}_s + F(t), \quad (C7)$$

$$m \ddot{q}_s = -m \omega_s^2 \dot{q}_s + c\sum_{k=1}^{N_S} Q_k \delta_{sk}, \quad (C8)$$

with

$$m \omega_s^2 = m \omega_s^2 + c(N_S + 2). \quad (C9)$$

Substituting a formal solution of $\tilde{q}_s$ to Eq. (C7), we obtain the Langevin equation given by Eqs. (21) and (87)–(89).

The $s$ dependence of $a_s$ given by Eq. (C6) or (91) is plotted in Fig. 16, showing the zigzag structure whose magnitude decreases rapidly with increasing $s$.
[30] In the CL model ($N_S = 1$), we assume $c_n = a/\sqrt{N_B}$ ($a$: constant) because the kernel $\gamma(t)$ includes the $c_n^2$ term as given by $\gamma(t) = \sum_{n=1}^{N_B} c_n^2 (\cos \omega_n t/m_\omega^2)$, which becomes $\gamma(t) = \int D(\omega) (\cos \omega t/m_\omega^2) d\omega \propto \delta(t)$ in the limit of $N_B \to \infty$, $D(\omega)$ denoting the density of states (see Table 1).