

## Features of statistical dynamics in a finite system

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We study features of statistical dynamics in a finite Hamilton system composed of a relevant one degree of freedom coupled to an irrelevant multidegree of freedom system through a weak interaction. Special attention is paid on how the statistical dynamics changes depending on the number of degrees of freedom in the irrelevant system. It is found that the macrolevel statistical aspects are strongly related to an appearance of the microlevel chaotic motion, and a dissipation of the relevant motion is realized passing through three distinct stages: dephasing, statistical relaxation, and equilibrium regimes. It is clarified that the dynamical description and the conventional transport approach provide us with almost the same macrolevel and microlevel mechanisms only for the system with a very large number of irrelevant degrees of freedom. It is also shown that the statistical relaxation in the finite system is an anomalous diffusion and the fluctuation effects have a finite correlation time.

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### I. INTRODUCTION

A dynamic origin of dissipative motion observed in a finite many-body system is a fundamental and challenging problem in various fields of contemporary science [1]. The underlying physics is how the statistical state is realized out of the microscopic deterministic motion, and how the irreversible macrolevel process is generated as a result of the reversible microlevel dynamics.

In the conventional approach in deriving the Fokker-Planck or Langevin equations, the entire system is divided into relevant and irrelevant subsystems intuitively, while the ergodic and irreversible property are assumed for the irrelevant subsystem composed of infinite number of degrees of freedom (DOF), and thermodynamical concepts, such as a thermal heat bath or a time-independent canonical ensemble are introduced by hand. In a *finite* system, however, it is not a trivial discussion whether or not the irrelevant subsystem can be effectively replaced by a statistical object, e.g., a heat bath, even when it shows chaotic behavior and its Lyapunov exponent has a positive value everywhere in the phase space.

In order to explore the microscopic dynamics responsible for the macroscopic transport phenomena, a theory of coupled-master equation has been formulated [2] as a general framework for deriving the transport equation, and for clarifying its underlying assumptions. In order to *self-consistently* and *optimally* divide the finite system into a pair of weakly coupled subsystems, the theory employs the self-consistent collective coordinate (SCC) method [3]. The self-consistent and optimal separation carried out by the SCC method enables us to study the large-amplitude dissipative motion for the relevant subsystem in a reasonable scheme.

It has been clarified [1] that the macroscopic transport equation is obtained from the fully microscopic master equation under the following microscopic conditions.

(i) Effects coming from the irrelevant subsystem on the relevant one are taken into account and mainly expressed by an average effect over the irrelevant distribution function. Namely, the fluctuation effects are considered to be suffi-

ciently small and are able to be treated as a perturbation around the path generated by the average Hamiltonian.

(ii) Irrelevant distribution function has already reached its time-independent stationary state before the main microscopic dynamics responsible for the damping of the relevant motion dominates. According to our previous paper [4], this situation turned out to be well realized even in the two-DOF system.

(iii) Time scale of the irrelevant motion is much shorter than that of the relevant one.

In order to get a full understanding of the dynamical realization of statistical state in a finite system, in our previous paper [5], an evolution process of a simple two-DOF system has been studied by using a general microscopic transport theory [2,4,6]. It has been shown that the nonlinear coupling between different DOF responsible for generating a chaotic motion plays an important role in realizing the statistical state for such a system that is described by a bundle of trajectories (distribution function). For the two-DOF system, however, it is not possible to assign the relevant subsystem or to discuss its transport process, since the chaotic or statistical state can only be realized by a system with at least two DOF. Thus, one needs a system with more than two DOF, which will be allowed to be divided into two weakly coupled subsystems: one is composed of at least two DOF, which is regarded as an irrelevant subsystem and the rest is considered to be a relevant subsystem.

Based on the numerical simulation for a microscopic system composed of the relevant one-DOF system coupled to the irrelevant two-DOF system through a weak interaction, the transport phenomenon was first established theoretically and numerically [1]. It was clarified that the microscopic *dephasing* mechanism caused by the chaoticity of irrelevant subsystem is responsible for the energy transfer from the relevant subsystem to the environment. Although our numerical simulation by employing the Langevin equation was able to reproduce the macrolevel transport phenomenon, it was also clarified that there are substantial differences in the

microlevel mechanism between the fully microscopic description and the Langevin description, and in order to reproduce the same results the parameters used in the Langevin equation do not satisfy the fluctuation-dissipation theorem.

Therefore various questions related to the transport phenomenon realized in the finite system on how to understand the differences between the above-mentioned two descriptions, what kinds of other microscopic mechanisms are there besides the *dephasing*, and when the fluctuation-dissipation theorem comes true, etc., are still remained. In the conventional approaches, e.g., the Fokker-Planck or Langevin type equations, the irrelevant subsystem is always assumed to have a large (even *infinite*) number of DOF and is placed in a canonically equilibrated state. It is then quite natural to ask whether these problems are caused by a limited number (only two) of DOF in the irrelevant subsystem considered in our previous work. In order to fill the gap between two and infinite DOF for the irrelevant subsystem, it is extremely important to study how the microscopic dynamics changes depending on the number of the irrelevant DOF.

For this purpose, in this paper, a Fermi-Pasta-Ulam (FPU) system is adopted for the irrelevant subsystem, as it allows us to change the number of DOF conveniently. It will be shown that although the dephasing mechanism is the main mechanism for a case with a small number of DOF, the diffusion mechanism will start to play a role as the number of DOF becomes large (say, eight or more), and, in general, the energy transport process occurs by passing through three distinct stages, such as, the dephasing, the statistical relaxation, and the equilibrium regimes. By examining a time evolution of a nonextensive entropy [7], an existence of three regimes will be clearly exhibited.

Exploiting an analytical relation, it will be shown that the energy transport process is described by the *generalized* Fokker-Planck and Langevin-type equation, and a phenomenological fluctuation-dissipation relation is satisfied in a case with relatively large DOF system. It will be clarified that the irrelevant subsystem with finite number of DOF can be treated as a heat bath with a finite correlation time, and the statistical relaxation turns out to be an anomalous diffusion, and both the microscopic approach and the conventional phenomenological approach may reach the same microlevel description for the transport phenomena only when the number of irrelevant DOF becomes very large.

The outline of this paper is as follows. In Sec. II, the microscopic model Hamiltonian will be introduced and the most general coupled-master equation will be briefly recapitulated for the sake of self-containedness. In Sec. III, the behavior of energy transfer process will be discussed together with an energy equipartition problem and its dependence on the number of DOF. An evolution process will be examined by using the nonextensive entropy in Sec. IV. In Sec. V, our numerical results will be explored in an analytical way and the Fokker-Planck equation will be derived. The final section will be devoted for discussion and summary.

## II. MICROSCOPIC MODEL

With the aid of the SCC method [3], the whole microscopic system can be optimally divided into the relevant

(collective) and irrelevant (intrinsic) DOF by introducing an optimal canonical coordinate system called the dynamical canonical coordinate (DCC) system for a given trajectory. That is, the total closed system  $\eta \oplus \xi$  is dynamically divided into two subsystems  $\eta$  and  $\xi$ , whose optimal canonical coordinates are expressed as  $\eta_a$ ,  $\eta_a^* : a = 1, \dots$  and  $\xi_\alpha$ ,  $\xi_\alpha^* : \alpha = 1, \dots$ , respectively. The resulting Hamiltonian in the DCC system is expressed as

$$H = H_\eta + H_\xi + H_{coupl}, \quad (1)$$

where  $H_\eta$  depends on the collective,  $H_\xi$  on the intrinsic, and  $H_{coupl}$  on both the collective and intrinsic variables. Time dependence of the collective and intrinsic variables are described by a set of canonical equations of motion given as [1]

$$\begin{aligned} i\dot{\eta}_a &= \frac{\partial H}{\partial \eta_a^*}, & i\dot{\eta}_a^* &= -\frac{\partial H}{\partial \eta_a}, \\ i\dot{\xi}_\alpha &= \frac{\partial H}{\partial \xi_\alpha^*}, & i\dot{\xi}_\alpha^* &= -\frac{\partial H}{\partial \xi_\alpha}. \end{aligned} \quad (2)$$

Here, it is worthwhile mentioning that the SCC method defines the DCC system in such a way that the *linear* coupling between the collective and intrinsic systems is eliminated, i.e., the maximal decoupling condition [2] given by

$$\left. \frac{\partial H_{coupl}}{\partial \eta} \right|_{\xi = \xi^* = 0} = 0 \quad (3)$$

is satisfied. This separation in the DOF has been known to be very important in exploring the energy dissipation process and the nonlinear dynamics between the collective and intrinsic modes of motion.

To deal with an ensemble of trajectories, we start with the Liouville equation for a distribution function

$$\begin{aligned} \dot{\rho}(t) &= -i\mathcal{L}\rho(t), & \mathcal{L} \cdots &\equiv i\{H, \cdots\}_{PB}, \\ \rho(t) &\equiv \rho(\eta(t), \eta(t)^*, \xi(t), \xi(t)^*). \end{aligned} \quad (4)$$

Here the symbol  $\{ \}_{PB}$  denotes the Poisson bracket. Since we are interested in a time evolution of the bundle of trajectories, whose bulk properties ought to be expressed by the collective variables alone, we introduce a pair of reduced distribution functions through

$$\rho_\eta(t) \equiv \text{Tr}_\xi \rho(t), \quad \rho_\xi(t) \equiv \text{Tr}_\eta \rho(t). \quad (5)$$

Here, the total distribution function  $\rho(t)$  is normalized so as to satisfy the relation

$$\text{Tr} \rho(t) = 1, \quad (6)$$

where

$$\begin{aligned} \text{Tr} &\equiv \text{Tr}_\eta \text{Tr}_\xi, \quad \text{Tr}_\eta \equiv \prod_a \int \int d\eta_a d\eta_a^*, \\ \text{Tr}_\xi &\equiv \prod_\alpha \int \int d\xi_\alpha d\xi_\alpha^*. \end{aligned} \quad (7)$$

With the aid of the reduced distribution functions  $\rho_\eta(t)$  and  $\rho_\xi(t)$ , one may decompose the Hamiltonian in Eq. (1) into the following form:

$$\begin{aligned} H &= H_\eta + H_\xi + H_{\text{coupl}} \\ &= H_\eta + H_\eta(t) + H_\xi + H_\xi(t) + H_\Delta(t) - E_0(t), \\ H_\eta(t) &\equiv \text{Tr}_\xi H_{\text{coupl}} \rho_\xi(t), \\ H_\xi(t) &\equiv \text{Tr}_\eta H_{\text{coupl}} \rho_\eta(t), \\ H_{\text{aver}}(t) &\equiv H_\eta(t) + H_\xi(t), \\ E_0(t) &\equiv \text{Tr} H_{\text{coupl}} \rho(t), \\ H_\Delta(t) &\equiv H_{\text{coupl}} - H_{\text{aver}}(t) + E_0(t). \end{aligned} \quad (8)$$

The corresponding Liouvillians are defined as

$$\begin{aligned} \mathcal{L}_\eta \dots &\equiv i\{H_\eta, \dots\}_{PB}, \quad \mathcal{L}_\eta(t) \dots \equiv i\{H_\eta(t), \dots\}_{PB}, \\ \mathcal{L}_\xi \dots &\equiv i\{H_\xi, \dots\}_{PB}, \quad \mathcal{L}_\xi(t) \dots \equiv i\{H_\xi(t), \dots\}_{PB}, \\ \mathcal{L}_{\text{coupl}} \dots &\equiv i\{H_{\text{coupl}}, \dots\}_{PB}, \\ \mathcal{L}_\Delta(t) \dots &\equiv i\{H_\Delta(t), \dots\}_{PB}. \end{aligned} \quad (9)$$

By exploiting the time-dependent projection operator method [2,8], one may decompose the distribution function into a separable part and a correlated one as

$$\begin{aligned} \rho(t) &= \rho_s(t) + \rho_c(t), \\ \rho_s(t) &\equiv P(t)\rho(t) = \rho_\eta(t)\rho_\xi(t), \\ \rho_c(t) &\equiv [1 - P(t)]\rho(t), \end{aligned} \quad (10)$$

where  $P(t)$  is the time-dependent projection operator defined by

$$P(t) \equiv \rho_\eta(t) \text{Tr}_\eta + \rho_\xi(t) \text{Tr}_\xi - \rho_\eta(t) \rho_\xi(t) \text{Tr}_\eta \text{Tr}_\xi. \quad (11)$$

From the Liouville equation (4), one gets

$$\dot{\rho}_s(t) = -iP(t)\mathcal{L}\rho_s(t) - iP(t)\mathcal{L}\rho_c(t), \quad (12)$$

$$\dot{\rho}_c(t) = -i[1 - P(t)]\mathcal{L}\rho_s(t) - i[1 - P(t)]\mathcal{L}\rho_c(t). \quad (13)$$

By introducing a propagator

$$g(t, t') \equiv T \exp \left\{ -i \int_{t'}^t [1 - P(\tau)] \mathcal{L} d\tau \right\}, \quad (14)$$

where  $T$  denotes the time ordering operator, one obtains the master equation for  $\rho_s(t)$  as

$$\begin{aligned} \dot{\rho}_s(t) &= -iP(t)\mathcal{L}\rho_s(t) - iP(t)\mathcal{L}g(t, t_1)\rho_c(t_1) \\ &\quad - \int_{t_1}^t dt' P(t)\mathcal{L}g(t, t')\{1 - P(t')\}\mathcal{L}\rho_s(t'), \end{aligned} \quad (15)$$

where  $t_1$  stands for an initial time. As is easily proved, the Liouvillian  $\mathcal{L}$  appearing inside the time integration in Eq. (15) can be replaced by  $\mathcal{L}_{\text{coupl}}$ . Expressing  $\rho_s(t)$  and  $P(t)$  in terms of  $\rho_\eta(t)$  and  $\rho_\xi(t)$ , and operating  $\text{Tr}_\eta$  and  $\text{Tr}_\xi$  on Eq. (15), one obtains a coupled master equation

$$\begin{aligned} \dot{\rho}_\eta(t) &= -i[\mathcal{L}_\eta + \mathcal{L}_\eta(t)]\rho_\eta(t) - i \text{Tr}_\xi[\mathcal{L}_\eta \\ &\quad + \mathcal{L}_{\text{coupl}}]g(t, t_1)\rho_c(t_1) \\ &\quad - \int_{t_1}^t d\tau \text{Tr}_\xi \mathcal{L}_\Delta(t)g(t, \tau)\mathcal{L}_\Delta(\tau)\rho_\eta(\tau)\rho_\xi(\tau), \end{aligned} \quad (16a)$$

$$\begin{aligned} \dot{\rho}_\xi(t) &= -i[\mathcal{L}_\xi + \mathcal{L}_\xi(t)]\rho_\xi(t) - i \text{Tr}_\eta[\mathcal{L}_\xi \\ &\quad + \mathcal{L}_{\text{coupl}}]g(t, t_1)\rho_c(t_1) \\ &\quad - \int_{t_1}^t d\tau \text{Tr}_\eta \mathcal{L}_\Delta(t)g(t, \tau)\mathcal{L}_\Delta(\tau)\rho_\eta(\tau)\rho_\xi(\tau). \end{aligned} \quad (16b)$$

The coupled master equations (16) are equivalent to the original Liouville equation (4) and can be considered as a general framework for deriving the transport equation and for clarifying its underlying assumptions.

In this paper, the collective system is represented by a harmonic oscillator with a coordinate  $q$ , momentum  $p$ , mass  $M$ , and frequency  $\omega$ , given by

$$H_\eta(q, p) = \frac{p^2}{2M} + \frac{1}{2}M\omega^2 q^2, \quad (17)$$

and the intrinsic system mimicking the environment is described by a  $\beta$ -FPU system (called so because of its quadratic interaction), which was posed in the famous paper [9] and reviewed in [10]

$$\begin{aligned} H_\xi &= \sum_{i=1}^{N_d} \frac{p_i^2}{2} + \sum_{i=2}^{N_d} W(q_i - q_{i-1}) + W(q_{N_d}), \\ W(q) &= \frac{q^4}{4} + \frac{q^2}{2}, \end{aligned} \quad (18)$$

where

$$q = \frac{1}{\sqrt{2}}(\eta + \eta^*), \quad p = \frac{i}{\sqrt{2}}(\eta^* - \eta),$$

$$q_i = \frac{1}{\sqrt{2}}(\xi_i + \xi_i^*), \quad p_i = \frac{i}{\sqrt{2}}(\xi_i^* - \xi_i), \quad (19)$$

and  $N_d$  represents a number of DOF (i.e., a number of nonlinear oscillators). According to the related references [10–12], the dynamics of  $\beta$ -FPU becomes strongly chaotic and relaxation is fast, when the energy per DOF  $\epsilon$  is chosen to be larger than a certain value (called as the critical value [12], say  $\epsilon_c \approx 0.1$ ). In the present paper,  $\epsilon$  is chosen as 10 to guarantee that our irrelevant subsystem can reach fully chaotic situation. Indeed, in this case, the calculated largest Lyapunov exponent  $\sigma(N_d)$  turns out to be positive, for instance,  $\sigma(N_d) = 0.15, 0.11, \text{ and } 0.11$  for  $N_d = 2, 4, \text{ and } 8$ , respectively. Thus, a “fully developed chaos” is expected for the  $\beta$ -FPU system, and an appearance of statistical behavior in its chain of oscillators and an energy equipartition among the modes are expected to be realized.

For the coupling interaction, we use the following nonlinear interaction given by

$$H_{\text{coupl}} = \lambda \{q^2 - q_0^2\} \{q_1^2 - q_{1,0}^2\}. \quad (20)$$

Quantities  $q_0$  and  $q_{1,0}$  in Eq. (20) denote a set of positions of the collective coordinate and the first intrinsic coordinate of a sample trajectory at the time when the interaction is switched on. According to the above form of the coupling,  $q_1$  describing the first oscillator plays a role of doorway variable, through which the intrinsic system exerts its influence on the collective system [11]. Throughout the present study, the coupling strength parameter is chosen as  $\lambda = 0.002$ .

In performing the numerical simulation, the time evolution of the distribution function  $\rho(t)$  is evaluated by using the pseudoparticle method as

$$\rho(t) = \frac{1}{N_p} \sum_{n=1}^{N_p} \prod_{i=1}^{N_d} \delta(q_i - q_{i,n}(t)) \delta(p_i - p_{i,n}(t))$$

$$\times \delta(q - q_n(t)) \delta(p - p_n(t)), \quad (21)$$

where  $N_p$  means a total number of pseudoparticles. The distribution function in Eq. (21) defines an ensemble of systems, each member of which is composed of a collective DOF coupled to a single intrinsic trajectory. The collective coordinates  $q_n(t)$  and  $p_n(t)$ , and the intrinsic coordinates  $q_{i,n}(t)$  and  $p_{i,n}(t)$  ( $i = 1, \dots, N_d$ ) determine a phase-space point of the  $n$ th pseudoparticle at time  $t$ , whose time dependence is described by the canonical equations of motion given by

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}, \quad \{i = 1, \dots, N_d\}$$

$$\dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q}. \quad (22)$$

We use the fourth-order symplectic Runge-Kutta algorithm [13] for integrating the canonical equations of motion and  $N_p$  is chosen to be 10 000.

In our calculation, the coupling interaction is activated after the statistical state has been realized in the intrinsic system, i.e., two subsystems evolve independently at an initial stage. Hereafter  $\tau_{sw}$  denotes a moment when the interaction is switched on. Since our primary aim is to microscopically generate such a transport phenomenon that might be understood in terms of the Langevin-type equation, we have to realize such a microscopic situation where the Conditions (i), (ii), and (iii) discussed in Sec. I are satisfied. To this end, we first let the intrinsic system evolve alone, till the ergodic and irreversible property are well realized *dynamically*. We will show that the above microscopic situation is indeed realized *dynamically* for the intrinsic system.

### III. ENERGY DISSIPATION AND EQUIPARTITION

In Ref. [1], a microscopic dynamical system composed of one collective and two intrinsic DOF was studied, and the dephasing mechanism turned out to be the only mechanism responsible for the energy transfer from the collective system to the environment. It was also shown that the fluctuation-dissipation theorem does not hold, and there is a substantial difference in the microscopic behavior between the dynamical simulations based on the Liouville equation and on the phenomenological Langevin equation, even though these two descriptions provide us with almost the same macroscopic transport phenomenon. Namely, the collective distribution function organized by the former evolves into a ring shape in the collective phase space by approximately keeping its initial collective energy, while that of the latter evolves into a round shape, whose collective energy is ranging from its initial value to zero. In order to understand the above differences, i.e., to clarify a necessary condition where the both descriptions give the same result, and to study a physical situation where the fluctuation-dissipation theorem comes true, it is strongly desired to explore how different microlevel dynamics appears depending on the number of intrinsic DOF.

In our numerical calculation, the used parameters are  $M = 1$ ,  $\omega^2 = 0.2$ . In this case, the collective time scale  $\tau_{col}$  characterized by the harmonic oscillator in Eq. (17) and the intrinsic time scale  $\tau_{in}$  by the harmonic part of the intrinsic Hamiltonian in Eq. (18) satisfies a relation  $\tau_{col} \gg \tau_{in}$ . The switch-on time  $\tau_{sw}$  is set to be  $\tau_{sw} = 100\tau_{col}$ .

In Figs. 1(a)–1(d), average values of partial Hamiltonians  $\langle H_\eta \rangle_t$ ,  $\langle H_\xi \rangle_t$ , and  $\langle H_{\text{coupl}} \rangle_t$  and of the total Hamiltonian  $\langle H \rangle_t$  defined by

$$\langle X \rangle_t = \int X \rho(t) dq dp \prod_{i=1}^2 dq_i dp_i, \quad (23)$$

as a function of the time are depicted for the cases with  $E_\eta = 30$ ,  $\lambda = 0.002$ , and  $N_d = 2, 4, 8, \text{ and } 16$ , respectively. In order to show clearly how the dissipation of collective energy changes depending on  $N_d$ , the time-dependent average values of collective Hamiltonian  $\langle H_\eta \rangle_t$  are shown in Fig. 2

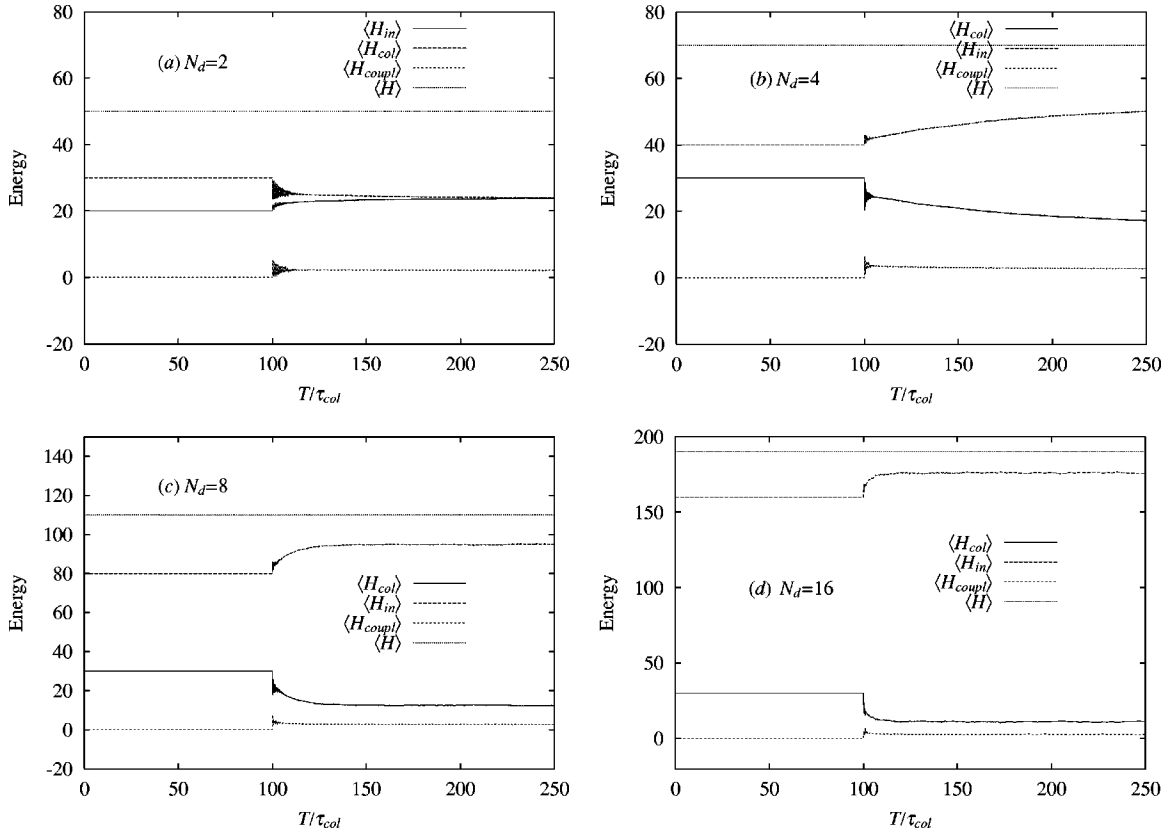


FIG. 1. Time dependence of the average partial Hamiltonian  $\langle H_{\eta} \rangle_t$ ,  $\langle H_{\xi} \rangle_t$ ,  $\langle H_{coupl} \rangle_t$ , and the total Hamiltonian  $\langle H \rangle_t$ , for  $E_\eta = 30$ ,  $\lambda = 0.002$ . (a)  $N_d = 2$ ; (b)  $N_d = 4$ ; (c)  $N_d = 8$ ; and (d)  $N_d = 16$ .

for the cases with  $N_d = 2, 4, 8$ , and  $16$ . In order to understand the final stage of the total system, an asymptotic average energy for each DOF in the intrinsic system is calculated to be 11.92, 12.54, 11.851, and 10.996, and that of the collective system to be 24.03, 17.15, 12.499, and 11.32 for  $N_d = 2, 4, 8$ , and  $16$ , respectively. Considering a boundary effect of the finite  $\beta$ -FPU system, i.e., two end oscillators, one may see that the energy equipartition over every DOF is expected in the saturated stage for the cases with relatively large number of DOF, as  $N_d \geq 8$ .

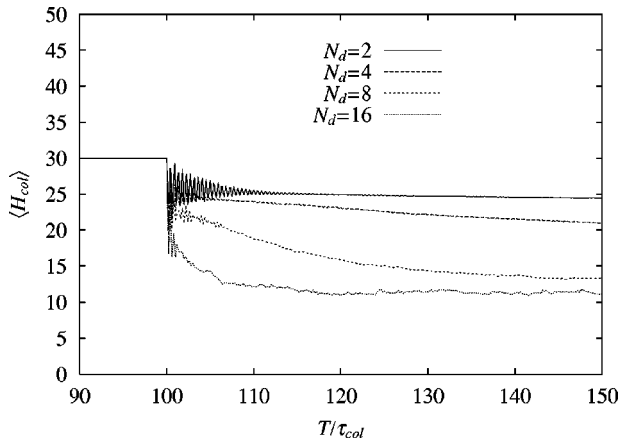


FIG. 2. Time-dependent average value of collective energy  $\langle H_{\eta} \rangle_t$ , for the cases with  $N_d = 2, 4, 8$ , and  $16$ . Parameters are the same as in Fig. 1.

From our numerical calculation, one may clearly see that a very similar result has been obtained for another Hamilton system in the case with  $N_d = 2$  [1]. Namely, the main change occurs in the collective energy as well as the interaction energy, and the main process responsible for this change has been clarified to be the dephasing mechanism. One may also learn from our previous paper [1] that the dissipative-diffusion mechanism plays a crucial role in reducing the oscillation amplitude of collective energy, and in realizing the steady energy flow from the collective system to the environment, when one tries to understand the energy transfer process in terms of the Langevin equation. When  $N_d$  increases, one may clearly learn the following number dependence from Fig. 2: After the dephasing process, the collective energy gradually decreases and finally reaches to a saturated value as the number of intrinsic DOF increases. More precisely, the energy transfer process can be divided into three stages.

(a) *Dephasing regime.* Here the fluctuation interaction reduces a coherence of the collective trajectories and makes the average amplitude of collective motion damped. This regime is the main process for a system with small number of intrinsic DOF (say, two). When the number of intrinsic DOF increases, a lasting time of this regime decreases.

(b) *Nonequilibrium relaxation regime.* This regime will also be called as a thermodynamical regime in the following section. In this regime, the collective energy is irreversibly transferred to the “environment.”

(c) *Saturation regime*. This is an asymptotic regime where the total system reaches to some equilibrium state and the total energy is equally distributed over every DOF realized in the cases with large  $N_d$  (say,  $\geq 8$ ).

A more detailed study on the above three regimes will be discussed in the following sections.

If one sticks to the conventional transport theory and tries to understand the above results from a macroscopic point of view, one may say that a gradually decreasing behavior of the collective energy is due to an irreversible dissipative perturbation coming from the interaction with intrinsic subsystem. In our previous simulation [1], by using the Langevin equation for the case with  $N_d=2$ , it turned out that the fluctuation interaction mainly contributes to a diffusion effect so as to reduce the coherence of collective trajectories, while the irreversible dissipative perturbation (friction force) is much smaller than that predicted by the fluctuation-dissipation theorem. According to a naive picture based on the phenomenological Langevin equation, an appearance of the second regime may be understood to be an increase of the dissipative mechanism, and an asymptotic and saturated behavior may indicate a realization of the conventional fluctuation-dissipation theorem for the cases with  $N_d \geq 8$ . Namely, an effect of the dissipative mechanism is expected to increase as  $N_d$  becomes large. From this phenomenological understanding, the above numerical simulation may provide us with very important information on the mechanism of microscopic dynamics of the dissipative collective motion, which might change depending on the number of intrinsic DOF.

Based on the standard nonequilibrium statistical theory, the nonequilibrium relaxation regime (or called as thermodynamical regime) may be understood within the linear response theory [11,14,15] when the number of intrinsic DOF is sufficiently large. However, we have learned that the dephasing process dominates when the collective system is *nonlinearly* coupled with the intrinsic system composed of a very small number of DOF. For the case with  $N_d=2$ , the dephasing process lasts for a very long time and plays a decisive role in organizing the time evolution of the collective motion. For the case with  $N_d < 8$  where an applicability of the linear response theory is still a question of debate [16,17], the dephasing mechanism may still play an important role in the transport process. When  $N_d$  increases up to 16, the lasting time of the dephasing process becomes very short and the nonequilibrium relaxation process seems to become a dominant mechanism for the energy dissipation. When  $N_d$  becomes large (more than 16), the thermodynamical mechanism seems to become a dominant mechanism and there might be no big differences between the nonlinear and linear response theory.

#### IV. ENTROPY EVOLUTION FOR THE COUPLED SYSTEM

Let us discuss how to understand the three regimes in the transport process discussed in the preceding section. As is shown in Sec. III, the transport, dissipative and damping phenomena in the collective behavior of the ensemble of

trajectories are well realized in our numerical simulation. In the general theory of dynamical system, the order-to-chaos transition is usually regarded as the microscopic origin of an appearance of the statistical state in the finite system. Since one may express the heat bath in terms of the infinite number of *integrable* systems, e.g., the harmonic oscillators whose frequencies have a Debye distribution, it may not be a relevant question whether the chaos plays a decisive role for the dissipation mechanism and for the microscopic generation of the statistical state in a case of the infinite system. In the finite system where the large number limit is not secured, the order-to-chaos transition is expected to play a decisive role in generating some behaviors which are regarded to be statistical. There might be a relation between the generation of the chaotic motion in a single trajectory and the realization of a statistical state for a system described by a bundle of trajectories.

This issue has been studied as a dynamical relation between the Kolmogorov-Sinai (KS) entropy and the physical Boltzmann-Gibbs (BG) entropy in the classical Hamilton system [16], and in the quantum dynamical system [17]. Here, the KS entropy is a single number  $\kappa$  related to an average rate of the exponential divergence of nearby trajectories, whereas the physical BG entropy  $S(t)$  known as an entropy of the second law in the thermodynamics is defined by the distribution function  $\rho(t)$  of a bundle of trajectories as

$$S(t) = - \int \rho(t) \ln \rho(t) dq dp \prod_{i=1}^{N_d} dq_i dp_i, \quad (24)$$

which depends not only on the particular dynamical system, but also on the choice of an initial probability distribution. Therefore, a relation between the KS entropy and physical BG entropy may give an information on the relation between the chaoticity of a single trajectory and the statistical state described by a bundle of trajectories.

It has been concluded [16] that the time evolution of  $S(t)$  in the conserved system goes through three time regimes.

(1) An early regime where  $S(t)$  is heavily dependent on the details of the dynamical system and of the initial distribution. This regime is called as the decoherence regime for the quantum system or the dephasing regime for the classical system. In this regime, there is no generic relation between  $S(t)$  and  $\kappa$ .

(2) An intermediate time regime where  $S(t)$  increases linearly with slope  $\kappa$ , i.e.,  $|dS(t)/dt| \sim \kappa$ . This stage is called as the Kolmogorov-Sinai regime or thermodynamical regime. In this regime, a transition from dynamics to thermodynamics is expected to occur.

(3) A saturation regime where  $S(t)$  is in equilibrium. In this case,  $\rho(t)$  is uniformly distributed over the whole energetically available area of the phase space. In accordance with a view of Krylov [20], a coarse graining process is required in this regime in dividing the phase space. It should be mentioned that the BG entropy  $S(t)$  in Eq. (24) is unable to deal with a variety of interesting physical problems such as the thermodynamics of self-gravitating systems, some anomalous diffusion phenomena, Lévy flights, etc., among

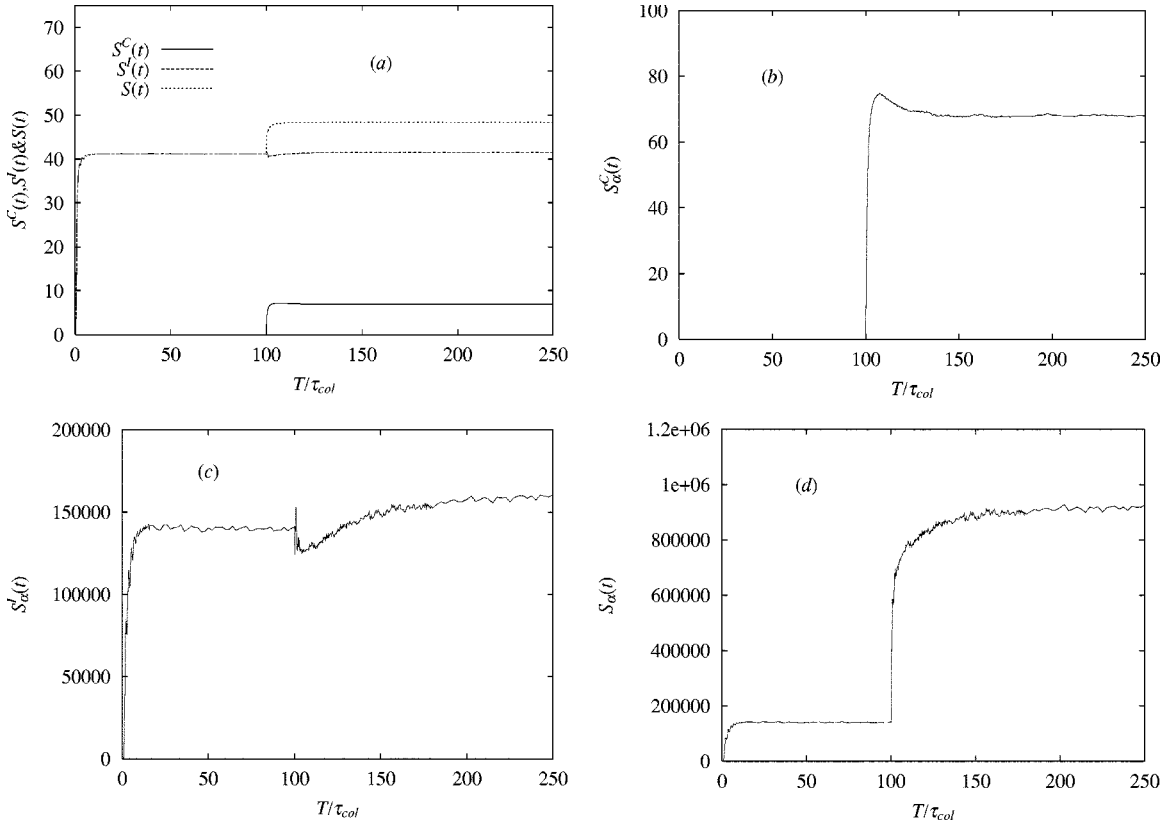


FIG. 3. (a) Physical Boltzmann-Gibbs entropy  $S(t)$ . Nonextensive entropy  $S_\alpha(t)$  for collective (b), intrinsic (c), and total phase space (d) for the case with  $N_d=8$ . Entropic index  $\alpha=0.7$ . Parameters are the same as Fig. 1.

others [21–24]. In order to deal with these difficulties, a generalized, nonextensive entropy is introduced [7]

$$S_\alpha(t) = \frac{1 - \int [\rho(t)]^\alpha dq dp \prod_{i=1}^{N_d} dq_i dp_i}{\alpha - 1}, \quad (25)$$

where  $\alpha$  is called the entropic index characterizing the entropy functional  $S_\alpha(t)$ . When  $\alpha=1$ ,  $S_\alpha(t)$  reduces to the conventional physical BG entropy  $S(t)$ . How to understand a departure of  $\alpha$  from 1 has been discussed in Refs. [21,23]. From a macroscopic point of view, the diversion of  $\alpha$  from 1 measures how the dynamics of the system violates the condition of short-range interaction and correlation, which provides a necessary condition (in the traditional wisdom) in establishing the thermodynamical properties [21]. On the other hand, such deviation can be attributed to the *mixing* (not only ergodicity) property of the phase space. That is, the  $\alpha=1$  and physical BG entropy  $S(t)$  is an adequate hypothesis when the mixing is exponential (strong mixing), whereas the nonextensive entropy should be used [23] when the *mixing* is weak.

It is very interesting to notice that our simulated energy transfer process also shows three regimes as mentioned in Sec. III. Consequently, there arises an inevitable question whether there is some relation between our numerical simulation and the time evolution of  $S(t)$  or  $S_\alpha(t)$ . To this aim, let us introduce the nonextensive entropies

$$S_\alpha^C(t) = \frac{1 - \int [\rho_\eta(t)]^\alpha dq dp}{\alpha - 1}, \quad (26a)$$

$$S_\alpha^I(t) = \frac{1 - \int [\rho_\xi(t)]^\alpha \prod_{i=1}^{N_d} dq_i dp_i}{\alpha - 1}, \quad (26b)$$

where  $\rho_\eta(t)$  and  $\rho_\xi(t)$  are the reduced distribution functions in Eq. (5). For comparison, the physical BG entropies for the collective and intrinsic systems defined as

$$S^C(t) = - \int \rho_\eta(t) \ln \rho_\eta(t) dq dp, \quad (27a)$$

$$S^I(t) = - \int \rho_\xi(t) \ln \rho_\xi(t) \prod_{i=1}^{N_d} dq_i dp_i, \quad (27b)$$

are also introduced.

Time dependence of the physical BG entropy  $S(t)$  is depicted in Fig. 3(a) and that of the nonextensive entropies  $S_\alpha^C(t)$ ,  $S_\alpha^I(t)$ , and  $S_\alpha(t)$  for the collective, intrinsic, and total system are shown in Figs. 3(b)–3(d) for the case with  $N_d=8$ . From this figure, it is recognized that there is no entropy production in the collective system before the coupling interaction is activated. During this time interval, an entropy increasing process in the intrinsic system is obvi-

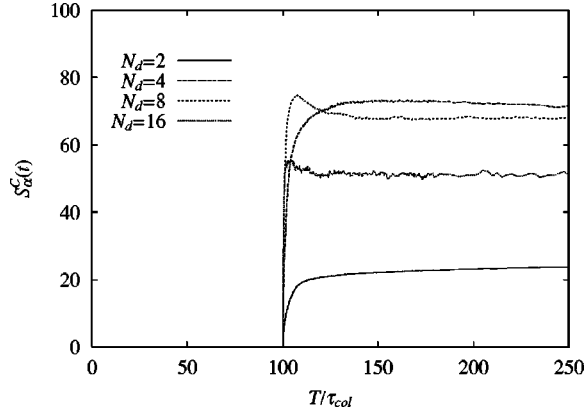


FIG. 4. Comparison of  $S_\alpha^C(t)$  for  $N_d=2, 4, 8,$  and  $16$ . Parameters are the same as in Fig. 3.

ously seen both in the physical BG entropy and in the non-extensive entropy. This means that the intrinsic system ( $\beta$ -FPU system) diffuses far from the equilibrium state to the equilibrium state where trajectories are uniformly distributed in the phase space. This conclusion is consistent with Ref. [11]. After the coupling interaction is switched on, there appear different situation either one uses the physical BG entropy or the nonextensive entropy in evaluating the entropy production of the intrinsic system. As was already shown [1], the intrinsic system is always in a time-independent stationary state even after the switch-on time  $t_{sw}=100\tau_{col}$ , because its time scale is much smaller than the collective one. This point is clearly seen from the present simulation in Fig. 3(a) where no change is observed in  $S^I(t)$  around  $t_{sw}$ . Since there exists an energy transfer process between the collective and intrinsic systems after  $t_{sw}$  [25], there should be a change in the distribution of trajectories in the intrinsic phase space, which is not observed by the BG entropy. Such a change in the distribution can only be observed by means of  $S_\alpha^I(t)$  as shown in Fig. 3(c).

With regard to the collective system, our numerical results for  $S^C(t)$  and  $S_\alpha^C(t)$  are shown in Figs. 3(a) and 3(b), respectively. From Fig. 3(a), one may observe that  $S^C(t)$  increases exponentially to a maximum value just after  $t_{sw}$ . It is not trivial to answer whether or not this maximum value indicates the stationary state for the collective system, because the energy exchange between the collective and intrinsic systems is still going on at this moment as mentioned in the preceding section. This point may be examined by calculating the nonextensive entropy  $S_\alpha^C(t)$  shown in Fig. 3(b). In Fig. 3(b),  $S_\alpha^C(t)$  increases exponentially to a maximal value, and then decreases almost linearly, and finally tends to saturate toward a time-independent value. From the above results, one may say that the time evolution of  $S_\alpha^C(t)$  after  $t_{sw}$  is divided into three stages; exponentially increasing, linearly decreasing, and saturated regimes for  $N_d=8$ .

In order to understand the  $N_d$  dependence of the three-stage transport process,  $S_\alpha^C(t)$  for  $N_d=2, 4, 8,$  and  $16$  are depicted in Fig. 4. For a case with  $N_d=2$ , only an exponentially increasing behavior is observed. Since the dephasing mechanism mainly contributes to the transport process in the case with  $N_d=2$  [1], the *exponentially increasing part* may

correspond to the dephasing regime.

As  $N_d$  increases up to 8, a linearly decreasing process appears in  $S_\alpha^C(t)$  after the exponentially increasing stage. From the discussion in the preceding section, this process may correspond to the nonequilibrium relaxation process in which the collective energy is irreversibly transferred to the “environment.”

Here it should be mentioned why the second regime shows a linearly decreasing, unlike a case discussed by Latora and Baranger [18]. The systems considered by Latora and Baranger and others [19,21,22] are conservative chaotic systems. In our present case, the total system is a conservative system whose entropy is shown in Fig. 3(d), while the intrinsic and collective systems are open systems. Especially, the collective system is a dissipative system after  $t_{sw}$ . In the second regime of energy dissipation, the collective energy irreversibly dissipates into the intrinsic system by making the distribution of collective trajectories in the phase space to shrunk.

In order to explore this situation more deeply, a time development of the collective distribution function  $\rho_\eta(t)$  in the collective  $(p,q)$ -phase space and a probability distribution function of collective trajectories defined as

$$P_\eta(\epsilon) = \int \rho_\eta(t) |_{H_\eta(q,p)=\epsilon} dq dp, \quad (28)$$

are shown in Fig. 5 at various times for  $N_d=8$ . These figures illustrate how a shape of the distribution function  $\rho_\eta(t)$  disperses depending on time. Dynamic process of the damping ought to be observed when a peak location of the distribution function changes from the outside (higher collective energy) region to the inside (lower collective energy) region, and the dissipative diffusion mechanism is studied by observing how strongly a distribution function initially (at  $t=\tau_{sw}$ ) located at a tiny region of the collective phase space disperses depending on time.

One may see that in the period shortly after the coupling interaction is switched on, i.e., from  $t_{sw}=100\tau_{col}$  to  $110\tau_{col}$ ,  $\rho_\eta(t)$  quickly disperses and tends to cover a ring shape in the collective phase space by approximately keeping its initial collective energy. When the distribution function tends to expand over the whole ring shape, the relevant part of the bundle of trajectories does not have the same time dependence. Some trajectories have an advanced phase, whereas other trajectories have a retarded phase in comparison with the average motion over the bundle of trajectories. This dephasing mechanism is considered to be the microscopic origin of the entropy production in the exponential regime.

A more interesting situation appears from  $T=110\tau_{col}$  through  $140\tau_{col}$ . One may see that the distribution function gradually invades into a central region. A peak of the distribution gradually moves to the center, and the distribution tends to have the Boltzmann distribution as

$$P_\eta(\epsilon) \sim e^{-\beta\epsilon}, \quad (29)$$



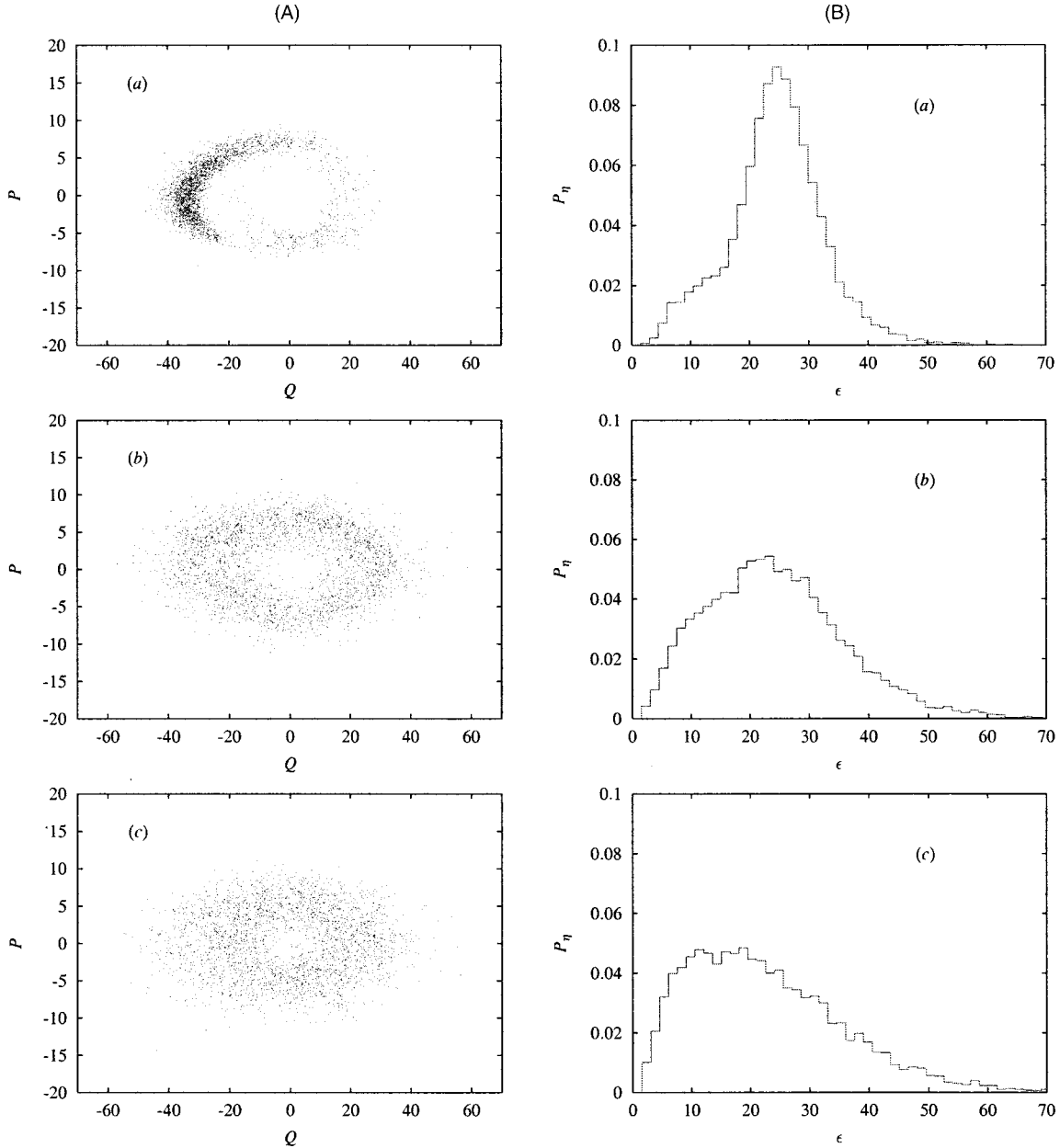


FIG. 5. (A) parts (a)–(f) Collective distribution function in  $(p, q)$  space; (B) parts (a)–(f) probability distribution function  $P_\eta(\epsilon)$  of collective trajectories at  $T = 102.5\tau_{col}$ ,  $110\tau_{col}$ ,  $120\tau_{col}$ ,  $140\tau_{col}$ ,  $160\tau_{col}$ , and  $240\tau_{col}$  for  $E_\eta = 30$  and  $\lambda = 0.002$ .

which is clearly seen from subfigures (d), (e), and (f) of Part (B) of Fig. 5. After  $T = 160\tau_{col}$  to  $240\tau_{col}$ , the distribution function does not practically change anymore, which corresponds to the saturated regime. Comparing the distribution in subfigure (f) of Part (A) of Fig. 5 with the one obtained by the phenomenological transport equation (such as the Langevin equation) in our previous paper [1], one may see that the final stationary distribution is consistent with the results simulated by the Langevin equation. From the above discussion, a transition from dynamics to thermodynamics is indeed realized numerically, and the collective system is regarded to reach to the equilibrium state finally.

Here it is worthwhile to clarify a relation between an anomalous diffusion and the above-mentioned nonextensive entropy expressed by the time evolution of the subsystems

with  $\alpha < 1$ , because the nonequilibrium relaxation regime is characterized not by the physical BG entropy, but by the nonextensive entropy with  $\alpha < 1$ . Generally, the diffusion process is characterized by the average square displacement or its variance as

$$\sigma^2(t) \sim t^\mu. \quad (30)$$

For normal diffusion  $\mu = 1$ . All processes with  $\mu \neq 1$  are termed as an anomalous diffusion, namely, subdiffusion for  $0 < \mu < 1$  and superdiffusion for  $1 < \mu < 2$ .

We calculate a time-dependent variance of collective coordinate  $\sigma_q^2(t) = \langle q^2 - \langle q \rangle_t^2 \rangle_t$  for the case with  $N_d = 8$  as depicted in Fig. 6, which also clearly shows the three stages as

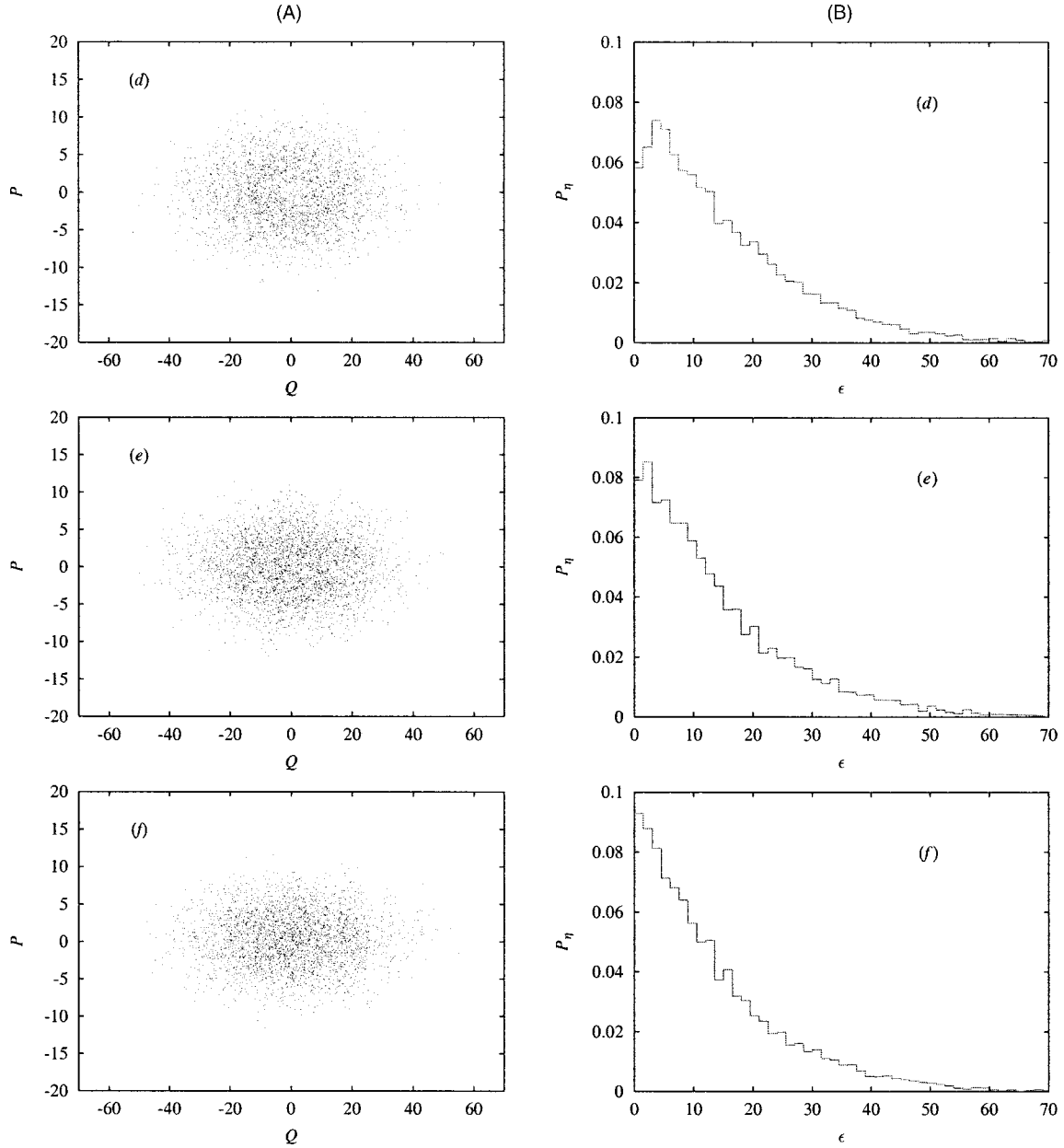


FIG. 5. (Continued).

discussed above. The result of  $\sigma_q^2(t)$  in nonequilibrium relaxation regime can be characterized by the expression

$$\sigma_q^2(t) = \sigma_q^2(t_0) - D(t - t_0)^{\mu_q}, \quad (31)$$

where  $t_0 = 110\tau_{col}$  is a moment when the dephasing regime has finished, and  $\sigma_q^2(t_0) = 335.0$  the value of  $\sigma_q^2(t)$  at time  $t_0$ . We fit the diffusion coefficient  $D$  and diffusion exponent  $\mu_q$  in Eq. (31) for the non-equilibrium relaxation regime as plotted in Fig 7. The resultant values are  $D = 15.5$  and  $\mu_q = 0.58$ , which suggest that the nonequilibrium relaxation process of a finite system correspond to an *anomalous* diffusion process.

At the end of this section, one may come to the following conclusions.

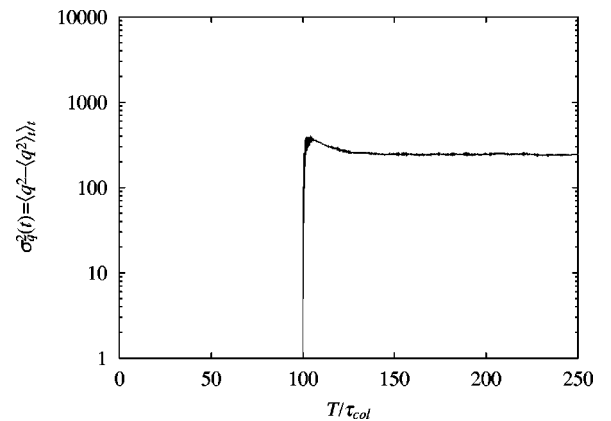


FIG. 6. Time-dependent variance  $\sigma_q^2(t)$  with  $N_d = 8$ . Parameters are the same as in Fig. 1.

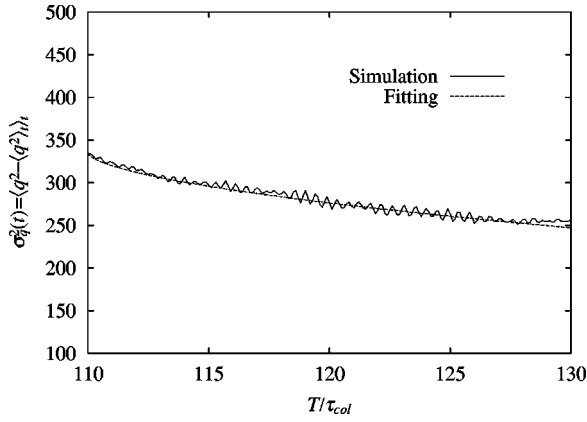


FIG. 7. Time-dependent variance  $\sigma_q^2(t)$  for the case with  $N_d = 8$ . Solid line refers to the result of dynamical simulation as shown in Fig. 6; long dashed line refers to the fitting result of Eq. (31) with parameters  $D = 15.5$  and  $\mu_q = 0.58$ .

(i) When the physical BG entropy is used to evaluate the entropy production for the system considered in this work, the three characteristic regimes cannot be detected in the collective system. When the nonextensive entropy is used with  $\alpha < 1.0$ , the three dynamical stages, i.e., the dephasing regime, nonequilibrium relaxation regime and equilibrium regime appear for a relatively large number of intrinsic DOF as  $N_d \geq 8$ . The second regime may disappear for a small number of DOF case, e.g.,  $N_d = 2$ .

(ii) Since the collective system is a dissipative system whose distribution function varies nonuniformly in the non-equilibrium relaxation regime, one has to use the entropy index  $\alpha$  different from 1.

(iii) As is shown by the  $\sigma_q^2(t)$  and by  $\alpha < 1$ , the nonequilibrium relaxation process of a finite system considered in this paper corresponds to the anomalous diffusion process.

(iv) The final regime is consistent with the simulation obtained by the phenomenological transport equation. Namely, the statistical state is actually realized dynamically in a finite system, which is composed by the collective and intrinsic systems coupled with the nonlinear interaction.

## V. FLUCTUATION-DISSIPATION RELATION OF COLLECTIVE MOTION

We are now in a position to analytically understand why and how the second regime, i.e., the thermodynamical regime appears when  $N_d$  increases. Since the intrinsic DOF is regarded to be in the fully developed chaotic situation in the second regime, it is reasonable to assume that the effects on the collective system coming from the intrinsic one are mainly expressed by an average effect. Namely, the effects arising from the fluctuation  $H_{\Delta}(t)$  are assumed to be much smaller than those coming from  $H_{\eta} + H_{\eta}(t)$ , and are able to be treated as a perturbation around the path determined by the *mean-field* [26] Hamiltonian  $H_{\eta} + H_{\eta}(t)$ . In the previous paper [1], a phenomenological Langevin equation given by

$$M\ddot{q} + \frac{\partial U^{mf}(q)}{\partial q} + \gamma\dot{q} = f(t), \quad q = \frac{\eta + \eta^*}{\sqrt{2}}, \quad (32)$$

was used in reproducing our simulated results phenomenologically. Here  $U^{mf}(q)$  denotes the potential part of  $H_{\eta} + H_{\eta}(t)$ ,  $\gamma$  the friction parameter, and  $f(t)$  the Gaussian white noise with an appropriate temperature. Since our present main concern is to make clear a relation between the macrolevel dynamics organized by the phenomenological equation, e.g., Eq. (32) [or Fokker-Planck equation (55) or the macrolevel Eq. (60) discussed in the following] and the microlevel dynamics by Eq. (16) one step further, we start with the Hamiltonian given by

$$H_{\eta}^T = H_{\eta} + H_{\eta}(t) + \lambda H_{\Delta, \eta}(t), \quad (33)$$

where  $H_{\eta}$  and  $H_{\eta}(t)$  are defined in Eqs. (17) and (8), respectively. An explicit form of  $H_{\Delta, \eta}(t)$  will be discussed in Eq. (35). The main differences between Eq. (32) and Eq. (33) are (i)  $\gamma$  and  $f(t)$  in Eq. (32) are given by hand and (ii)  $\rho_{\xi}(t)$  specifying the fluctuation effects  $H_{\Delta, \eta}(t)$  in Eq. (33) is determined microscopically from Eq. (16). What we are going to discuss in the following is to understand a change of phenomenological parameters in Eqs. (32), (55), or (60) in terms of the fluctuation  $H_{\Delta, \eta}(t)$  associated with the microscopic dynamics  $\rho_{\xi}(t)$  determined by Eq. (16).

In terms of Eq. (20), the coupling interaction is expressed as

$$H_{coupl}(\eta, \xi) = \lambda A(\eta)B(\xi). \quad (34)$$

The fluctuation Hamiltonian  $H_{\Delta, \eta}(t)$  in Eq. (33) is then expressed as

$$H_{\Delta, \eta}(t) = \phi'(t)A(\eta), \quad \phi'(t) = B(\xi) - \langle B(\xi) \rangle_t. \quad (35)$$

With the aid of the Hamiltonian (33), the collective distribution function  $\rho_{\eta}(t)$  determined by Eq. (16) may be explored by using the Liouville equation given by

$$\dot{\rho}_{\eta}(t) = -i\mathcal{L}_{\eta}^T \rho_{\eta}(t) = -i[\mathcal{L}_{\eta} + \mathcal{L}_{\eta}(t) + \lambda \mathcal{L}_{\Delta, \eta}(t)]\rho_{\eta}(t), \quad (36)$$

where  $\mathcal{L}_{\eta}^T$  and  $\mathcal{L}_{\Delta, \eta}(t)$  are defined as

$$\mathcal{L}_{\eta}^T \cdots \equiv i\{H_{\eta}^T, \cdots\}_{PB}, \quad \mathcal{L}_{\Delta, \eta}(t) \cdots \equiv i\{H_{\Delta, \eta}(t), \cdots\}_{PB}. \quad (37)$$

Here  $\{, \}_{PB}$  denotes a Poisson bracket with respect to the collective variables. Although  $H_{\Delta, \eta}(t)$  contains the intrinsic variables, in the present formulation, the fluctuation  $H_{\Delta, \eta}(t)$  should be considered to be a time-dependent stochastic force expressed as  $\phi'(t)$  in Eq. (35), and a stochastic average is obtained by taking the integration over the intrinsic variables with a weight function  $\rho_{\xi}(t)$ . Here it should be noticed that the Liouville equation (36) is an approximation to Eq. (16). Since our present aim is to explore how the effects on the collective system coming from the intrinsic fluctuation  $\phi'(t)$  change depending on the number of intrinsic DOF as simple as possible, we start with Eq. (36) rather than Eq. (16). Namely, the collective fluctuation effects originated from  $A(\eta) - \text{Tr}_{\eta} A(\eta)\rho_{\eta}$  on the intrinsic system ought to be disregarded, because we are now studying the average dynamics of collective motion. It should be also noticed that the

Liouville equation (36) will not be used to determine  $\rho_\eta(t)$ , but it will be used only to understand what happens in the collective distribution function  $\rho_\eta(t)$ , which is numerically obtained by integrating the canonical equations of motion (22) with the Hamiltonian in Eq. (1).

Let us start our discussion just after the dephasing process has finished. When the stochastic term is regarded as a perturbation, it is convenient to introduce the *mean-field* propagator

$$G_\eta(t, t') = T \exp \left\{ -i \int_{t'}^t [\mathcal{L}_\eta + \mathcal{L}_\eta(\tau)] d\tau \right\}, \quad (38)$$

which describes an average time evolution of the collective system. Using the *mean-field* propagator  $G_\eta(t, t')$  and taking the stochastic average over  $\rho_\xi(t)$ , one may obtain the following master equation for  $\rho_\eta(t)$  from Eq. (36) as

$$\begin{aligned} \dot{\rho}_\eta(t) = & -i \{ \mathcal{L}_\eta + \mathcal{L}_\eta(t) \} \rho_\eta(t) - \lambda^2 \int_0^\infty d\tau \langle \langle \mathcal{L}_{\Delta, \eta}(t) \\ & \times G_\eta(t, t-\tau) \mathcal{L}_{\Delta, \eta}(t-\tau) \rangle \rangle_t \rho_\eta(t-\tau), \end{aligned} \quad (39)$$

where a symbol  $\langle \langle \dots \rangle \rangle_t$  denotes a cumulant related to the average  $\langle * \rangle_t = \text{Tr}_\xi^* \rho_\xi(t)$ , and a derivation of Eq. (39) is given in the Appendix. In getting Eq. (39) from Eq. (A10), the collective distribution function  $\rho_\eta(t)$  is assumed [27] to evolve through the mean-field Hamiltonian  $H_\eta + H_\eta(t)$  from  $t$  to  $t-\tau$ . This is because the fluctuation effects are so small as to be treated as a perturbation around the path generated by the mean-field Hamiltonian  $H_\eta + H_\eta(t)$ , and are sufficient to be retained up to the second order in  $\lambda$  in Eq. (39). Under the assumption of a weak coupling interaction and of a finite correlation time  $\tau_c$ , i.e.,

$$\langle \langle \phi'(t) \phi'(t') \rangle \rangle_t = 0 \quad \text{for} \quad |t-t'| > \tau_c,$$

an upper limit in the time integration in Eq. (39) is extended to  $\infty$ .

The mean-field propagator  $G_\eta(t, t-\tau)$  provides a solution of the unperturbed equation. That is, there holds a relation

$$f(\eta, t) = G_\eta(t, t-\tau) f(\eta, t-\tau), \quad (40)$$

provided  $f(\eta, t)$  satisfies a relation

$$\frac{\partial f(\eta, t)}{\partial t} = -i [\mathcal{L}_\eta + \mathcal{L}_\eta(t)] f(\eta, t). \quad (41)$$

Since the Liouville equation (41) is equivalent to the canonical equation of motion given by

$$i \dot{\eta}_a = \frac{\partial (H_\eta + H_\eta(t))}{\partial \eta_a^*}, \quad (42)$$

$$i \dot{\eta}_a^* = - \frac{\partial (H_\eta + H_\eta(t))}{\partial \eta_a}, \quad (43)$$

there holds a relation

$$f(\eta, t) = f(\eta^{t-\tau}, t-\tau) \left| \frac{d\eta^{t-\tau}}{d\eta} \right| = G_\eta(t, t-\tau) f(\eta, t-\tau), \quad (44)$$

$|d\eta^{t-\tau}/d\eta|$  being a Jacobian determinant.

Using the above relation, Eq. (39) is simplified as

$$\begin{aligned} \dot{\rho}_\eta(t) = & -i \{ \mathcal{L}_\eta + \mathcal{L}_\eta(t) \} \rho_\eta(t) - \lambda^2 \int_0^\infty d\tau \left| \frac{d\eta^{t-\tau}}{d\eta} \right| \\ & \times \langle \langle \mathcal{L}_{\Delta, \eta}(t) \mathcal{L}_{\Delta, \eta}^{-\tau}(t-\tau) \rangle \rangle_t \left| \frac{d\eta}{d\eta^{t-\tau}} \right| \rho_\eta(t), \end{aligned} \quad (45)$$

where

$$\mathcal{L}_{\Delta, \eta}(t) \dots \equiv i \phi'(t) \{ A(\eta), \dots \}, \quad (46)$$

$$\mathcal{L}_{\Delta, \eta}^{-\tau}(t-\tau) \dots \equiv i \phi'(t-\tau) \{ A(\eta^{t-\tau}), \dots \}. \quad (47)$$

With the Hamiltonians  $H_\eta$  and  $H_\eta(t)$  defined in Eqs. (17) and (8), one may easily get an analytic form of mapping  $\eta \rightarrow \eta^\tau$  by solving the unperturbed Eqs. (42) and (43) as

$$q(\tau) = q \cos \omega' \tau + \frac{p}{M \omega'} \sin \omega' \tau, \quad (48)$$

$$p(\tau) = -q M \omega' \sin \omega' \tau + p \cos \omega' \tau, \quad (49)$$

with

$$\omega'^2 \equiv \omega^2 + \frac{2\lambda \langle \{ q_1^2 - q_{1,0}^2 \} \rangle_t}{M},$$

where Eq. (19) is used. The Jacobian determinant of this mapping reads

$$\left| \frac{d\eta^{-\tau}}{d\eta} \right| = \left| \frac{d\eta}{d\eta^{-\tau}} \right| = 1, \quad (50)$$

because  $\omega'$  does not practically depend on time. In terms of the coupling interaction (20), the fluctuation Hamiltonian  $H_{\Delta, \eta}(t)$  in Eq. (35) can be explicitly written as

$$H_{\Delta, \eta}(t) = \phi'(t) \{ q^2 - q_0^2 \}, \quad (51)$$

$$\phi'(t) = \{ q_1^2 - q_{1,0}^2 \} - \langle \{ q_1^2 - q_{1,0}^2 \} \rangle_t. \quad (52)$$

With the aid of Eq. (51), the cumulant in Eq. (45) is expressed as

$$\begin{aligned} \langle\langle \mathcal{L}_{\Delta,\eta}(t) \mathcal{L}_{\Delta,\eta}^{-\tau}(t-\tau) \rangle\rangle_t &= -\langle\langle \phi(t) \phi(t-\tau) \rangle\rangle_t q \frac{\partial}{\partial p} \\ &\times q(t-\tau) \frac{\partial}{\partial p(t-\tau)}, \end{aligned} \quad (53)$$

where  $\phi(t) = 2\phi'(t)$ . Considering  $(\eta^{-\tau})^\tau = \eta$  and using Eqs. (48) and (49), one gets

$$\begin{aligned} q(t-\tau) \frac{\partial}{\partial p(t-\tau)} &= \left( q \frac{\sin \omega' \tau \cos \omega' \tau}{M \omega'} - p \frac{\sin^2 \omega' \tau}{M^2 \omega'^2} \right) \frac{\partial}{\partial q} \\ &+ \left( q \cos^2 \omega' \tau - p \frac{\sin \omega' \tau \cos \omega' \tau}{M \omega'} \right) \frac{\partial}{\partial p}. \end{aligned} \quad (54)$$

Finally, Eq. (45) is explicitly written as

$$\begin{aligned} \frac{\partial \rho_\eta(t)}{\partial t} &= \left\{ \mathcal{L}_{eff} + \lambda^2 \left[ \beta_1 q \frac{\partial}{\partial p} \left( q \frac{\partial}{\partial q} - p \frac{\partial}{\partial p} \right) + \beta_2 q^2 \frac{\partial}{\partial p^2} \right. \right. \\ &\left. \left. - \beta_3 q \frac{\partial}{\partial p} p \frac{\partial}{\partial q} \right] \right\} \rho_\eta(t), \end{aligned} \quad (55)$$

where

$$\mathcal{L}_{eff} = -\frac{p}{M} \frac{\partial}{\partial q} + (M \omega'^2 + \lambda \beta_0) q \frac{\partial}{\partial p}$$

is an effective unperturbed (mean-field) Liouvillian of the collective system. The parameters  $\beta_0$ ,  $\beta_1$ ,  $\beta_2$ , and  $\beta_3$  are expressed as Fourier transformations of the correlation functions of intrinsic system

$$\beta_0 = \langle \phi(t) \rangle_t, \quad (56a)$$

$$\beta_1 = \frac{1}{M \omega'} \int_0^\infty d\tau \langle \langle \phi(t) \phi(t-\tau) \rangle \rangle_t \cos \omega' \tau \sin \omega' \tau, \quad (56b)$$

$$\beta_2 = \int_0^\infty d\tau \langle \langle \phi(t) \phi(t-\tau) \rangle \rangle_t \cos^2 \omega' \tau, \quad (56c)$$

$$\beta_3 = \frac{1}{M^2 \omega'^2} \int_0^\infty d\tau \langle \langle \phi(t) \phi(t-\tau) \rangle \rangle_t \sin^2 \omega' \tau. \quad (56d)$$

Equation (55) is a two-dimensional Fokker-Planck equation. The first term on the right-hand side of Eq. (55) represents the contribution from the mean-field part  $H_\eta + H_\eta(t)$ , and the last three terms represent contributions from the dynamical fluctuation effects  $H_{\Delta,\eta}$ . The parameters  $\beta_0$ ,  $\beta_1$ ,  $\beta_2$ , and  $\beta_3$  establish the connection between the macrolevel dynamical evolution of collective system and the microlevel fluctuation of intrinsic one.

A time derivative of the average collective quantity is calculated as

$$\frac{d\langle X \rangle}{dt} = \int X \frac{d\rho_\eta(t)}{dt} dq dp \quad (57)$$

for any collective variable  $X$  which does not explicitly depend on time. When one inserts Eq. (55) into Eq. (57), and evaluates the individual term by observing the standard rule

$$\int A \{B, C\}_{PB} dq dp = \int \{A, B\}_{PB} C dq dp, \quad (58)$$

one obtains the equation for the first moment

$$\frac{d\langle q \rangle}{dt} = \frac{\langle p \rangle}{M},$$

$$\frac{d\langle p \rangle}{dt} = -\frac{\lambda \beta_3}{M} \langle p \rangle - \left[ M \omega'^2 + \lambda \beta_0 - \lambda^2 \frac{\beta_1}{M} \right] \langle q \rangle, \quad (59)$$

or in a compact way as

$$M \langle \ddot{q} \rangle + \gamma \langle \dot{q} \rangle + \left[ M \omega'^2 + \lambda \beta_0 - \lambda^2 \frac{\beta_1}{M} \right] \langle q \rangle = 0, \quad (60)$$

$$\gamma = \frac{\lambda \beta_3}{M}. \quad (61)$$

Here  $\beta_3$  (or  $\gamma$ ) represents the damping effects on collective motion coming from the fluctuation interaction, which originates from the chaoticity of intrinsic system. Equation (61) is regarded as a fluctuation-dissipation relation, and the damping factor (described by  $\beta_3$  or  $\gamma$ ) implies an irreversible energy dissipation from the collective system to the intrinsic one.

Applying similar procedures as in obtaining Eq. (60), one may derive an equation of motion for the second moments as

$$\frac{d}{dt} \begin{bmatrix} \langle qq \rangle \\ \langle pp \rangle \\ \langle qp \rangle \end{bmatrix} = \begin{bmatrix} 0 & 0 & \frac{2}{M} \\ 4\lambda^2 M^2 \omega'^2 \beta_3 + 2\lambda^2 \beta_2 & -4\lambda^2 \beta_3 & -2M \omega'^2 - 2\lambda \beta_0 \\ -M^2 \omega'^2 - \lambda \beta_0 + 2\lambda^2 \beta_1 & \frac{1}{M} & -4\lambda^2 \beta_3 \end{bmatrix} \begin{bmatrix} \langle qq \rangle \\ \langle pp \rangle \\ \langle qp \rangle \end{bmatrix}. \quad (62)$$

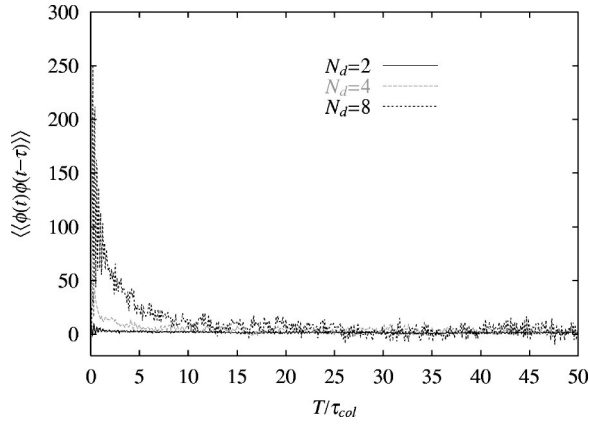


FIG. 8. Correlation function at  $t=120\tau_{col}$  for the cases with  $N_d=2, 4,$  and  $8$ . Parameters are the same as in Fig. 1.

A real eigenvalue of the matrix in the above equation indicates an instability of collective trajectory, which is caused by the chaoticity of intrinsic trajectory through fluctuation Hamiltonian  $H_{\Delta,\eta}$  [10]. Equations (55), (60), and (62) set up the relations among the microlevel properties of the intrinsic system and the macrolevel time evolution of the collective system through the microscopic correlation functions.

Employing the numerical simulation for Eq. (22), we calculate the correlation function  $\langle\langle\phi(t)\phi(t-\tau)\rangle\rangle_t$  at  $t=120\tau_{col}$  for the cases with  $N_d=2, 4,$  and  $8$  as shown in Fig. 8. Generally speaking, the correlation function  $\langle\langle\phi(t)\phi(t-\tau)\rangle\rangle_t$  as well as the parameters  $\beta_0, \beta_1, \beta_2,$  and  $\beta_3$  may have a strong time dependence, when the intrinsic system undergoes a drastic change as in the dephasing regime. In the present context, in understanding why the second regime, i.e., thermodynamical regime appears when the number of intrinsic DOF increases from  $N_d=2$  to larger one as  $N_d=8$ , it is reasonable to select a time just after the dephasing process has finished. From Figs. 1–5, it can be seen that  $t=120\tau_{col}$  just corresponds to such a moment.

From Fig. 8, one can see that the correlation function for  $N_d=2$  is very weak and oscillates around  $\langle\langle\phi(t)\phi(t-\tau)\rangle\rangle_t=0$ . In this case, the main influence of the intrinsic system on the collective one has taken place in the dephasing regime, and has finished before  $t=120\tau_{col}$ . As  $N_d$  increases, the magnitude of the correlation function becomes large and behaves similar to a “colored noise” with finite correlation time  $\tau_c$

$$\langle\langle\phi(t)\phi(t-\tau)\rangle\rangle_t \sim e^{-\tau/\tau_c}.$$

From this calculation, the correlation function seems to reach a  $\delta$  function representing a “white noise” when  $N_d$  increases to infinity. This results verify our understanding as discussed in Secs. III and IV.

(1) The dephasing regime is the main mechanism for the small number of DOF (say, two) case.

(2) Both the dynamical description and conventional transport approach may provide us with almost the same macrolevel and microlevel mechanisms only for the system with a very large number of DOF, say  $N_d > 8$ . For the finite

TABLE I. Calculated values of  $\beta_3$  at  $t=120\tau_{col}$  for the case with  $N_d=2, 4, 8,$  and  $16$ , respectively.

$N_d$	2	4	8	16
$\beta_3$	0.201	0.530	0.820	1.773

system, however, the statistical relaxation is anomalous diffusion and the fluctuation effects have finite correlation time.

Using the correlation function, we calculate the parameter  $\beta_3$  as shown in Table I. As is obviously seen, the damping effects on the collective motion will increase when the number of intrinsic DOF increases. For the case with small number of intrinsic DOF, the damping effects are too small to make the second regime realized. For the case with a larger number of DOF as  $N_d=8$ , the damping effects become appreciable and make the collective system relaxed thermodynamically to an equilibrium state.

At the end of this section, we discuss the fluctuation-dissipation relation of the collective motion. As mentioned in Sec. III, the energy equipartition among every DOF is expected in the final regime for the case with relatively large number of DOF, as  $N_d=8$ . This situation just corresponds to a case where the conventional transport equation is applied and the fluctuation-dissipation relation of the collective motion is expected. Since the collective energy is given by

$$\langle E \rangle = \frac{\langle p^2 \rangle}{2M} + \frac{1}{2} m \omega^3 \langle q^2 \rangle, \quad (63)$$

which is derived from Eq. (17), one may evaluate a rate of collective energy change as

$$\frac{d\langle E \rangle}{dt} = \left[ \frac{4\lambda^2 M^2 \omega'^2 \beta_3 + 2\lambda^2 \beta_2}{2M} \langle qq \rangle - \frac{4\lambda^2 \beta_3}{2M} \langle pp \rangle \right] \quad (64)$$

by using Eq. (62). Since the energy interchange between two systems is supposed to have finished on average in the third regime, the relation  $d\langle E \rangle/dt=0$ , i.e.,

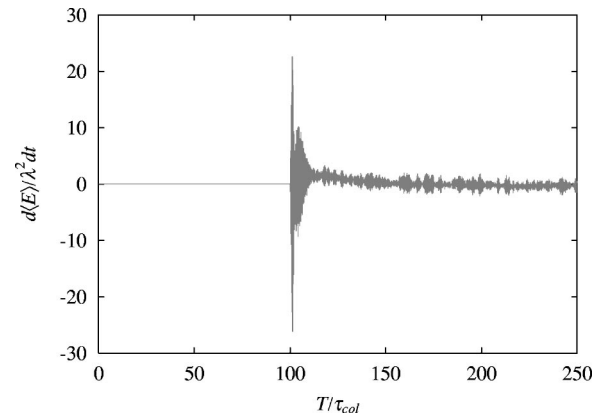


FIG. 9. Rate of collective energy change in Eq. (64). Correlation function is calculated at  $t=240\tau_{col}$  for  $N_d=8$ . Parameters are the same as in Fig. 1.

$$[(2M^2\omega'^2\beta_3 + \beta_2)\langle qq \rangle - 2\beta_3\langle pp \rangle] = 0 \quad (65)$$

must be satisfied. Figure 9 shows numerical results of the right-hand side (rhs) of Eq. (64). It is clearly seen that a relation (65) is actually satisfied on the third regime.

To summarize this section, one may get the following conclusions. The damping mechanism caused by the fluctuation interaction is the main reason for the appearance of the thermodynamical process. When the number of intrinsic DOF becomes relatively large (as  $N_d=8$ ), the damping mechanism generates the thermodynamical process and the saturated situation. In this case, the traditional Fokker-Planck equation is safely used in describing the thermodynamical process, and a fluctuation-dissipation relation is well realized.

## VI. DISCUSSION

In this paper, we have systematically studied the nonequilibrium process of a microscopic Hamilton system with finite DOF without introducing any statistical ansatz. A macroscopic transport equation has been derived from the master equation, which describes a microscopic system composed of the one collective DOF coupled to a finite intrinsic DOF through a weak interaction.

It has been shown that for the case with small number of intrinsic DOF (say, two), the dephasing mechanism is the dominant process for the dissipation of collective energy. When the number of intrinsic DOF becomes large (say, eight or more), the energy transport process can be divided into three regimes, i.e., the dephasing, nonequilibrium relaxation, and saturation regimes. We have shown that the energy transport process is safely described by the Fokker-Planck- and Langevin-type equation, when the number of intrinsic DOF is relatively large. In this case, the intrinsic system exhibits very interesting property, such as a finite *heat bath*, and the fluctuation has the finite correlation time (as colored noise). Only when the number of intrinsic DOF is infinite, the intrinsic system may be treated as a statistical heat bath with white noise.

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## APPENDIX

In this appendix, a derivation of the master equation (39) is discussed. The mean-field propagator  $G_\eta(t, t')$  defined in Eq. (38) satisfies the following relations:

$$\frac{dG_\eta(t, t')}{dt} = -i\lambda[\mathcal{L}_\eta + \mathcal{L}_\eta(t)]G_\eta(t, t'), \quad (A1)$$

$$G_\eta(t, t_1)G_\eta(t_1, t') = G_\eta(t, t'),$$

$$G_\eta^{-1}(t, t') = G_\eta(t', t), \quad (A2)$$

where  $G_\eta^{-1}(t, t')$  is the inverse propagator of  $G_\eta(t, t')$ .

With the aid of the mean-field propagator, one may introduce the interaction representation  $\rho'_\eta(t)$  through

$$\rho_\eta(t) = G_\eta(t, 0)\rho'_\eta(t). \quad (A3)$$

Taking a time derivative of Eq. (A3), and using the relation (A1), one gets the following relation from Eq. (36):

$$\dot{\rho}'_\eta(t) = -i\lambda\mathcal{L}'_{\Delta, \eta}(t)\rho'_\eta(t), \quad (A4)$$

where

$$\mathcal{L}'_{\Delta, \eta}(t) = G_\eta^{-1}(t, 0)\mathcal{L}_{\Delta, \eta}(t)G_\eta(t, 0). \quad (A5)$$

Equation (A4) is a linear stochastic differential equation. Integrating Eq. (A4) iteratively, one gets

$$\rho'_\eta(t) = T \exp\left\{-i\lambda \int_0^t \mathcal{L}'_{\Delta, \eta}(\tau) d\tau\right\} \rho'_\eta(0). \quad (A6)$$

Taking the average over the intrinsic distribution function  $\rho_\xi(t)$  at  $t$  in Eq. (A6), one may evaluate stochastic effects coming from the irrelevant DOF. Applying the cumulant expansion [16] in the rhs of the resulting equation, one gets

$$\begin{aligned} \dot{\rho}'_\eta(t) &= -i\lambda \langle \langle \mathcal{L}'_{\Delta, \eta}(t) \rangle \rangle_t \rho'_\eta(t) \\ &\quad - \lambda^2 \int_0^t d\tau \langle \langle \mathcal{L}'_{\Delta, \eta}(t) \mathcal{L}'_{\Delta, \eta}(\tau) \rangle \rangle_t \rho'_\eta(\tau), \end{aligned} \quad (A7)$$

where  $\langle \langle \dots \rangle \rangle_t$  denotes a cumulant at time  $t$  related to the average over the intrinsic degrees of freedom  $\langle \dots \rangle_t \equiv \text{Tr}_\xi \dots \rho_\xi(t)$  at time  $t$ . Equation (A7) is valid upto the second order in  $\lambda$ . According to the definition of the fluctuation Hamiltonian  $H_{\Delta, \eta}(t)$  in Eq. (35), the first-order term in Eq. (A7) is zero, since there holds a relation

$$\langle \langle \mathcal{L}'_{\Delta, \eta}(t) \rangle \rangle_t \sim \langle \langle \phi'(t) \rangle \rangle_t = \langle \phi'(t) \rangle_t = 0. \quad (A8)$$

One thus obtains

$$\dot{\rho}'_\eta(t) = -\lambda^2 \int_0^t d\tau \langle \langle \mathcal{L}'_{\Delta, \eta}(t) \mathcal{L}'_{\Delta, \eta}(\tau) \rangle \rangle_t \rho'_\eta(\tau). \quad (A9)$$

Going back to the original representation, one has

$$\begin{aligned} \dot{\rho}_\eta(t) &= -i\lambda[\mathcal{L}_\eta + \mathcal{L}_\eta(t)]\rho_\eta(t) - \lambda^2 \\ &\quad \times \int_0^t d\tau \langle \langle \mathcal{L}_{\Delta, \eta}(t) G_\eta(t, \tau) \mathcal{L}_{\Delta, \eta}(\tau) \rangle \rangle_t G_\eta(\tau, t) \rho_\eta(\tau). \end{aligned} \quad (A10)$$

Making the variable transformation  $\tau \rightarrow t - \tau$ , one finally gets Eq. (39).

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