Dynamical behavior of a thermostated isotropic harmonic oscillator

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Characteristic recurrence phenomena that are strongly dependent on initial conditions but do not depend much on the numbers of degrees of freedom are observed in the study of a system consisting of identical harmonic oscillators coupled with the Nosé-Hoover thermostat. The time evolution of the energy of each oscillator in this system at large Q (Q is a parameter controlling the speed of the response of the thermostat) is composed of a secular periodic motion with frequency of order $1/Q$ and fast fluctuations around it with frequency of order 1. The latter is the natural frequency of oscillators. The secular part depends very sensitively on initial conditions. The dynamical behaviors of the system are analyzed by the perturbation treatment with respect to $1/Q$, and a Hamiltonian $H'=\{\sum_i\sum_j p_i p_j \cos[2(q_i-q_j)]\}/16$, which describes the behavior of the secular part in the original system, is derived of first order in $1/Q$. The coordinate q_i and the conjugated momentum p_i in the Hamiltonian H' are the slowly changing part of the phase ϕ_i of the oscillator and the energy H_i. I found that this Hamiltonian H' is completely integrable and can be solved analytically. The solutions thus obtained describe very well the dynamical behaviors in the original system.

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I. INTRODUCTION

The investigation of completely integrable systems has been an attractive theme in classical mechanics. Only a small number of such systems with two or more degrees of freedom was known before 1967. But the discovery of a new approach to solving nonlinear equations (the inverse scattering method [1]) opened a way for finding new completely integrable systems: the Korteweg–de Vries equation, the Toda lattice [2], etc. The development in this field is compiled in a recent book by Perelomov [3].

I report in this article the finding of characteristic recurrence phenomena in a system consisting of identical harmonic oscillators coupled with the Nosé-Hoover thermostat, that the behavior is very well described by a Hamiltonian system that is derived by a perturbation treatment of the Nosé-Hoover thermostat equations with respect to $1/Q$ (Q is a parameter controlling the speed of response of the thermostat), and that the Hamiltonian is completely integrable and can be solved analytically.

The Nosé-Hoover thermostat [4–7] is one of the constant-temperature molecular-dynamics simulation techniques that can produce the canonical distribution in a classical system. An extended system consisting of a physical system and a degree of freedom corresponding to a heat bath is considered in this formulation.

The rigorous proof that the canonical distribution is really reproduced in the Nosé-Hoover thermostat method is given [4–7]. However, the ergodic behavior in the extended system is always assumed in the proof. Therefore, the canonical distribution is not guaranteed if a system is not ergodic.

Several numerical investigations [8–11] confirm that the ergodic property is attained in many-particle systems if the parameter Q is selected within an appropriate intermediate range. Therefore, the assumption of the ergodic property is justified in a many-particle system in most cases. But in a system with a small number of degrees of freedom, it is not generally guaranteed and should be confirmed separately in each system. A simple counterexample is a single harmonic-oscillator system.

The investigation of a single harmonic oscillator coupled with the Nosé-Hoover thermostat shows the following results [6,12–15]. At large Q, the behavior is regular. The trajectory forms a torus around the unperturbed harmonic oscillation. At small Q less than a critical value, irregular behavior is observed, but there are also many stable periodic orbits at the same Q value. Therefore, the chaotic orbit does not cover the whole region of the phase space. Thus, the single oscillator system coupled with the Nosé-Hoover thermostat is not ergodic.

I extended the study further, to the system with two or more degrees of freedom. One's natural expectation is that the chaotic behavior will be observed more easily in many degrees of freedom than in a single oscillator. And I obtained the expected results when the frequencies of the oscillators were different. The critical Q value shifts considerably to larger values in the case of many oscillators.

However, when all the frequencies are identical (or in an isotropic harmonic oscillator in a high-dimensional space), the critical Q value remains of the same order as in the case of a single oscillator, and the characteristic regular periodic beat of the energy of each oscillator is observed at Q larger than the critical value. The frequency of the beat is of order $1/Q$, which is much slower than a natural frequency in a Nosé-Hoover system of order $(1/Q)^{1/2}$, and the frequency of the oscillators of order 1.

I was interested in this regular behavior and investigated the system more in detail. The frequency of the beat depends drastically on the value of the Q parameter and the initial conditions. Especially, if we set all the differences of phases very small initially, the frequency of the beat becomes quite low. I get several empirical relations from numerical calculations. The following main features do not depend much on the number of oscillators: (i) the sinusoidal beat of the energy, (ii) acceleration of the angular velocity, and (iii) the phase shift of $-\pi$ near the region where the energy of the oscillator takes the minimum value.

The theoretical investigation on this system is carried out with a perturbation calculation with respect to $\epsilon=1/Q$. A Hamiltonian system H' that describes the slow movement of the oscillators with time $\tau=\epsilon t$ is derived from the order-ϵ term of the Nosé-Hoover thermostat equation,

$$H'=\frac{1}{16}\sum_i\sum_j H_{i0}H_{j0}\cos[2(\phi_{i0}-\phi_{j0})] \ . \tag{1.1}$$

H_{i0} and ϕ_{i0} are the slowly changing component of the energy H and the phase ϕ of oscillator i, respectively. I found that the Hamiltonian Eq. (1.1) is completely integrable. The behavior of the slowly changing part of H_i and ϕ_i can be expressed explicitly. The result agrees very well with simulation results.

The Nosé-Hoover thermostat is now routinely employed in molecular-dynamics simulations [16,17] and in the study of the electronic properties [18] combined with the Car-Parrinello technique [19]. The reliability of the method has been questioned by several researchers who do not pay attention to the condition in which the ergodic assumption is justified. This article will give useful information about the nature of the Nosé-Hoover thermostat. A harmonic-oscillator system is one of the typical models of a physical system. Even though the system is simple, the dynamical behaviors change very much depending on the identity of the frequencies. In this article, it will be confirmed that the regular behavior is observed only if all the frequencies are equal. In a general interacting oscillator system, all the normal-mode frequencies are different. This guarantees the reliability of the Nosé-Hoover thermostat in most interacting systems.

In Sec. II, we describe the Nosé-Hoover thermostat and the system in which we are interested. Several properties obtained analytically are also given. The results of the numerical calculations on the system are given in Sec. III.

In Sec. IV, a perturbation calculation is carried out to separate the slowly and rapidly changing parts, and the Hamiltonian Eq. (1.1) will be derived. In Sec. V, the properties of the Hamiltonian Eq. (1.1) are investigated, and it is shown that the reduced Hamiltonian is completely integrable. Several discussions and remarks are given in Sec. VI.

II. NOSÉ-HOOVER THERMOSTAT AND THE SYSTEM IN WHICH WE ARE INTERESTED

The Nosé-Hoover thermostat [4–7] is a method utilized to realize molecular-dynamics simulations at constant-temperature conditions. We consider a classical particle system described by a Hamiltonian $H(\mathbf{p},\mathbf{q})$

$$H(\mathbf{p},\mathbf{q})=\sum_i\frac{\mathbf{p}_i^2}{2m_i}+\Phi(\mathbf{q}) \ , \tag{2.1}$$

where m_i, $\mathbf{p}_i$, $\mathbf{q}_i$ are the mass, the momentum, and the coordinate of the particle i. Φ is the potential energy of the system. The equations of motion in the Nosé-Hoover thermostat formulation are

$$\frac{d\mathbf{q}_i}{dt}=\frac{\partial H}{\partial \mathbf{p}_i}=\frac{\mathbf{p}_i}{m_i} \ , \tag{2.2}$$

$$\frac{d\mathbf{p}_i}{dt}=-\frac{\partial H}{\partial \mathbf{q}_i}-\zeta\mathbf{p}_i=-\frac{\partial \Phi}{\partial \mathbf{q}_i}-\zeta\mathbf{p}_i \ , \tag{2.3}$$

$$\frac{d\zeta}{dt}=\left[\sum_i \mathbf{p}_i\frac{\partial H}{\partial \mathbf{p}_i}-kT\sum_i\frac{\partial \mathbf{p}_i}{\partial \mathbf{p}_i}\right]\Big/Q$$

$$=\left[\sum_i\frac{\mathbf{p}_i^2}{m_i}-gkT\right]\Big/Q \ , \tag{2.4}$$

$$\frac{d\ln s}{dt}=\zeta \ . \tag{2.5}$$

More general extensions of this formulation are discussed by Bulgac and Kusnezov [8,20]. In Eq. (2.3), an additional term similar to a friction force, $-\zeta\mathbf{p}_i$, is added to the ordinary canonical equation. The friction coefficient ζ is not a parameter, but a variable whose time evolution is governed by Eq. (2.4). g is the number of degrees of freedom of a physical system, k is the Boltzmann constant, and T is the temperature. Q is a parameter corresponding to the mass of a heat bath, and controls the speed of response of the heat reservoir.

A quantity H^*

$$H^*=\sum_i\frac{\mathbf{p}_i^2}{2m_i}+\Phi(\mathbf{q})+\frac{Q}{2}\zeta^2+gkT\ln s \tag{2.6}$$

is a conserved quantity in a dynamical system described by Eqs. (2.2)–(2.5), and we can consider that the whole system in the Nosé-Hoover thermostat method consists of a physical system $H(\mathbf{p},\mathbf{q})$ and a degree of freedom (s and ζ) corresponding to a heat bath. We shall call this an extended system. H^* in the extended system is conserved but it is not a Hamiltonian of the system. Equations (2.2)–(2.5) cannot be derived from H^* directly. The coupling between the system and the thermostat is expressed via the pseudofriction term. The Hamiltonian Eq. (2.1) is no longer an integral of motion. Equations of motion (2.2)–(2.4) form a closed set of equations in a phase space $\Gamma=(\mathbf{p},\mathbf{q},\zeta)$. The phase-space volume in Γ along a trajectory is not conserved, but it changes proportionally to the inverse of the Boltzmann factor. This non-Hamiltonian nature of the method is the reason why the canonical distribution is realized by the Nosé-Hoover thermostat [7,20]. The ergodic behavior in the extended system is assumed in the proof given in Refs. [4–7]. Therefore the canonical distribution is not guaranteed if a system is not ergodic.

The ergodic property in many-particle systems is confirmed from several numerical investigations [8–11]. But we should be careful in the study in a system with a small number of degrees of freedom.

The typical frequency of variable ζ is analyzed as

$$\omega_1=(2gkT/Q)^{1/2} \tag{2.7}$$

at small Q, and

$$\omega_2=[(2gkT/Q)(gk/2C_V)]^{1/2} \tag{2.8}$$

at large Q, where C_V is the heat capacity. Both formulas (2.7) and (2.8) show $(1/Q)^{1/2}$ dependence of the natural frequency on Q.

Slow peculiar beat behaviors with frequency of order $1/Q$ are observed in the study in an isotropic harmonic-oscillator system. The beat is much slower than the natural frequency of order $(1/Q)^{1/2}$ and the frequency of the oscillators (of order 1). We study the nature of this behavior in this article.

The system in which we are interested is a system consisting of identical harmonic oscillators (or a g-dimensional isotropic oscillator),

$$H(\mathbf{p},\mathbf{q})=\tfrac{1}{2}\sum_i (p_i^2+q_i^2) , \tag{2.9}$$

where we employ reduced units for the coordinate, the time, and the energy, so that $m=1.0$, $\omega=1.0$, and the average value of the energy of an oscillator $kT=1.0$.

The Nosé-Hoover thermostat equations of motion in these reduced units are

$$\frac{dq_i}{dt}=p_i , \tag{2.10}$$

$$\frac{dp_i}{dt}=-q_i-\zeta p_i , \tag{2.11}$$

$$\frac{d\zeta}{dt}=\left[\sum_i p_i^2-g\right]\Big/Q . \tag{2.12}$$

g is the number of the oscillator, and Q is a parameter controlling the speed of response of ζ.

This system possesses a hidden symmetry. Equations (2.10)–(2.12) do not change by any orthogonal transformation S identical in $\mathbf{q}$ and in $\mathbf{p}$ spaces:

$$q_i'=\sum_j S_{ij}q_j , \tag{2.13}$$

$$p_i'=\sum_j S_{ij}p_j . \tag{2.14}$$

The time evolutions starting from initial configurations related by Eqs. (2.13) and (2.14) are not independent, but they always satisfy the relations (2.13) and (2.14).

An action-J_i–angle-ϕ_i variables formulation is more convenient in this problem. The action $J_i=H_i/\omega_i$ is identical with the energy H_i in the isotropic case with $\omega_i=1.0$. H_i and ϕ_i are related to p_i and q_i by a canonical transformation,

$$p_i=\sqrt{2H_i}\cos\phi_i , \tag{2.15}$$

$$q_i=\sqrt{2H_i}\sin\phi_i . \tag{2.16}$$

The equations for H_i,ϕ_i are obtained from Eqs. (2.10)–(2.12) as

$$\frac{dH_i}{dt}=-2\zeta H_i\cos^2\phi_i , \tag{2.17}$$

$$\frac{d\phi_i}{dt}=1+\zeta\sin\phi_i\cos\phi_i , \tag{2.18}$$

$$\frac{d\zeta}{dt}=\left[\sum_i (2H_i\cos^2\phi_i)-g\right]\Big/Q . \tag{2.19}$$

The shift of π in ϕ_i does not change the equations. The phase ϕ can be reduced to $[0,\pi]$ by operation of modulus π.

Consider the difference of two angles ϕ_i and ϕ_j. Subtracting Eq. (2.18) for a phase ϕ_j from that for ϕ_i, an equation describing the difference of two phases $\Delta\phi_{ij}=\phi_i-\phi_j$ is obtained,

$$\begin{aligned}\frac{d}{dt}(\phi_i-\phi_j)&=\zeta(\sin\phi_i\cos\phi_i-\sin\phi_j\cos\phi_j)\\&=\frac{\zeta}{2}(\sin2\phi_i-\sin2\phi_j)\\&=\zeta\cos(\phi_i+\phi_j)\sin(\phi_i-\phi_j) .\end{aligned} \tag{2.20}$$

If $\Delta\phi_{ij}=0$ (mod π) at a certain time, $\Delta\phi_{ij}$ is always 0 (mod π) thereafter. This shows that the phases ϕ_i are ordered, and a phase ϕ_i never gets ahead of another ϕ_j,

$$\phi_1\le\phi_2\le\phi_3\le\cdots\le\phi_g\le\phi_1+\pi . \tag{2.21}$$

The order of phases is determined by initial conditions.

If two or more phases are identical ($\phi_i\equiv\phi_j$ for i and j),

$$\frac{1}{H_i}\frac{dH_i}{dt}-\frac{1}{H_j}\frac{dH_j}{dt}=-2\zeta(\cos^2\phi_i^2-\cos^2\phi_j^2)=0 . \tag{2.22}$$

Therefore, the ratio of the energies is a constant ($H_j=CH_i$). This means that a set of oscillators with the same phase is equivalent to a single oscillator. Especially, if all the phases of oscillators are equal, it behaves as only one oscillator. The number of degrees of freedom is effectively reduced if a phase catches up with another one. However, the overtaking of phases was never observed in numerical calculations. Perhaps it is forbidden in this system.

The thermostat works to keep the total energy around the equipartition value gkT (g in reduced unit). If we set the initial values as $H_i^0=1.0$, $\phi_i^0=i\pi/g+\phi_0$ ($i=1,2,\ldots,g$), and $\zeta^0=0$, the thermostat does not work and all the oscillators behave like a free oscillator, $H_i=1.0$, $\phi_i=t+\phi_i^0$, $\zeta=0$.

III. NUMERICAL CALCULATIONS

The equations of motion of identical harmonic oscillators in energy-angle variables [Eqs. (2.17)–(2.19)] are integrated with the fourth-order Runge-Kutta algorithm. In our calculations, the initial conditions for H_i and ζ are always chosen as $H_i=1$ and $\zeta=0$, and the dependence of dynamical behaviors on the distribution of the initial phases ϕ_i^0, ($i=1,2,\ldots,g$) and on Q are studied. The condition $H_i=1$ may seem to be too strong a restriction, but it is not. We confirmed in preliminary calculations that the dynamical behaviors are always similar if the total energy H is set to the equipartition value g,

$$H=\sum_i H_i=g\ . \qquad (3.1)$$

We will call the condition expressed in Eq. (3.1) the equipartition condition. The total energy of a physical system in Eq. (2.6) already reaches an equilibrium value at the initial stage. Therefore, the energy transfer between the physical system and the thermostat does not occur effectively. The kinetic-energy term of the thermostat is initially set to zero, and it also remains in a small value after that. The thermostat part is considered as a perturbation term of the oscillator system with the equipartition condition. If the total energy H is not equal to g initially, a relaxation process occurs and excess or insufficient energy is taken away or supplied by the thermostat. In both cases, the kinetic-energy term of the thermostat gains considerable energy in this relaxation process, and the term cannot be considered as a perturbation. It is expected that the dynamical behavior becomes more complicated in this situation.

Two typical examples of dynamical behaviors are given in Figs. 1 and 2. The number of oscillators g is 2, Q is 4.0, the integration time step Δt is 0.025, and the initial phases are $\phi_1=0.0$, $\phi_2=5°=\pi/36$ in Fig. 1. $g=5$, $Q=4.0$, $\Delta t=0.025$, and $\phi_i=0.01(i-1)$ $(i=1,2,\ldots 5)$ in Fig. 2. The time evolutions of (a) the energy of each oscillator, (b) the phase $\Delta\phi_i=\phi_i-\omega_i t$, (c) the differences of phases $\phi_i-\phi_1$, and (d) ζ are depicted in both figures, from the top down.

The change of the energy [(a) in Figs. 1 and 2] consists

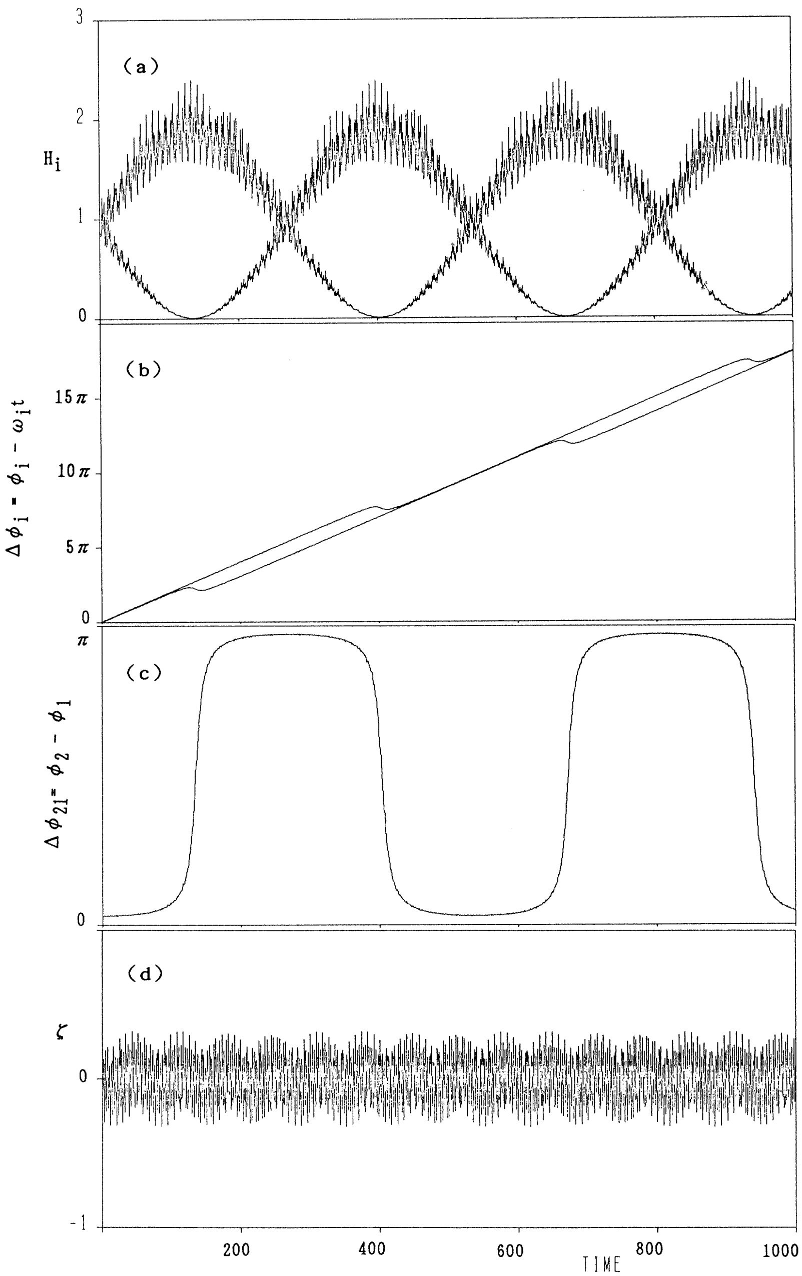

FIG. 1. Time evolution in a two-harmonic-oscillator system: (a) the energy H_i, (b) the angles $\phi_i-\omega_i t$, (c) the difference of angles $\Delta\phi_{i1}=\phi_i-\phi_1$, and (d) the heat-bath variable ζ. The initial condition for this calculation is $H_i^0=1.0$, $\phi_1^0=0$, $\phi_2^0=5°$, $\zeta^0=0$, at $Q=4.0$ with $\Delta t=0.025$.

of two components: a slow oscillation with large amplitude, similar to the beat, and a rapid fluctuation with small amplitude. The slow part of the time evolution is periodic, and it almost returns to the initial condition at about $t=540$ (for $g=2$) and $t=580$ (for $g=5$). This change is very well expressed by a sinusoidal function. The energy of each oscillator takes a very small minimum value, almost zero, during the oscillation.

The time evolution of the phase is also characteristic. In part (b) of Figs. 1 and 2, the deviation of the phase from the unperturbed motion $\Delta\phi_i=\phi_i-\omega_i t$ is depicted. $\Delta\phi_i$ increases linearly in most of one period. This means that the oscillation is accelerated by coupling with a thermostat. $\Delta\phi_i$ decreases in a small region near the minimum of the energy H_i. The absolute value of the slope in this decreasing region is almost equal to that of the linearly increasing part. The total delay of the phase caused by the decreasing region is $-\pi$.

It is clear in Figs. 1 and 2 that the equipartition condition Eq. (3.1) is fairly well satisfied. The main features of the time evolution are common in two and five oscillators. The difference of phases stays near 0 or π in most times, and it changes rapidly in a narrow transition period. The heat-bath variable ζ changes very rapidly and no secular change is detected.

Detailed investigations of the dependence on Q and on the initial configuration are carried out with two oscillators. The dependence on the initial difference of angles is given in Fig. 3. $\Delta\phi=\phi_2^0-\phi_1^0$ is 1°, 2°, 5°, 10°, 30°, 45°, 60° and 75° from the top. The simulation condition is

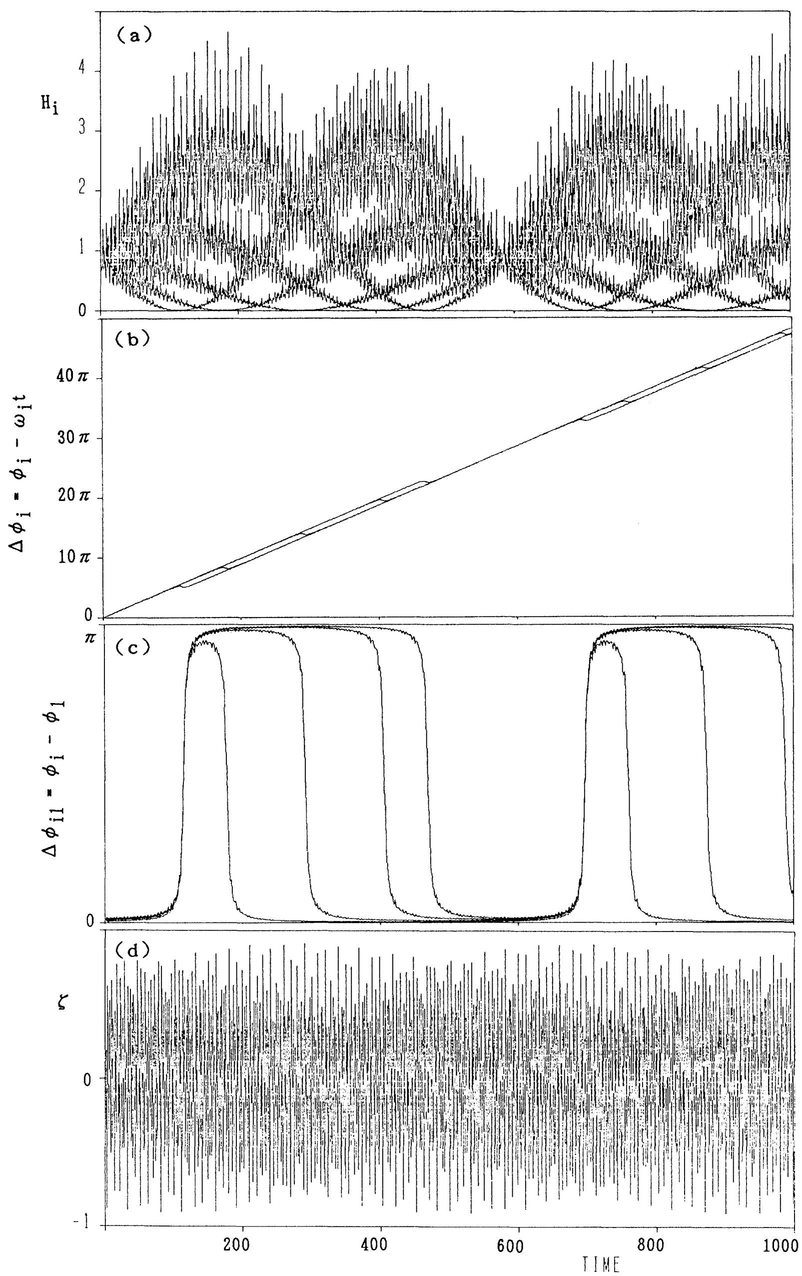

FIG. 2. Time evolution in a five-oscillator system. The quantities are the same as in Fig. 1. The initial angles are selected as $\phi_i^0=0.01(i-1)$.

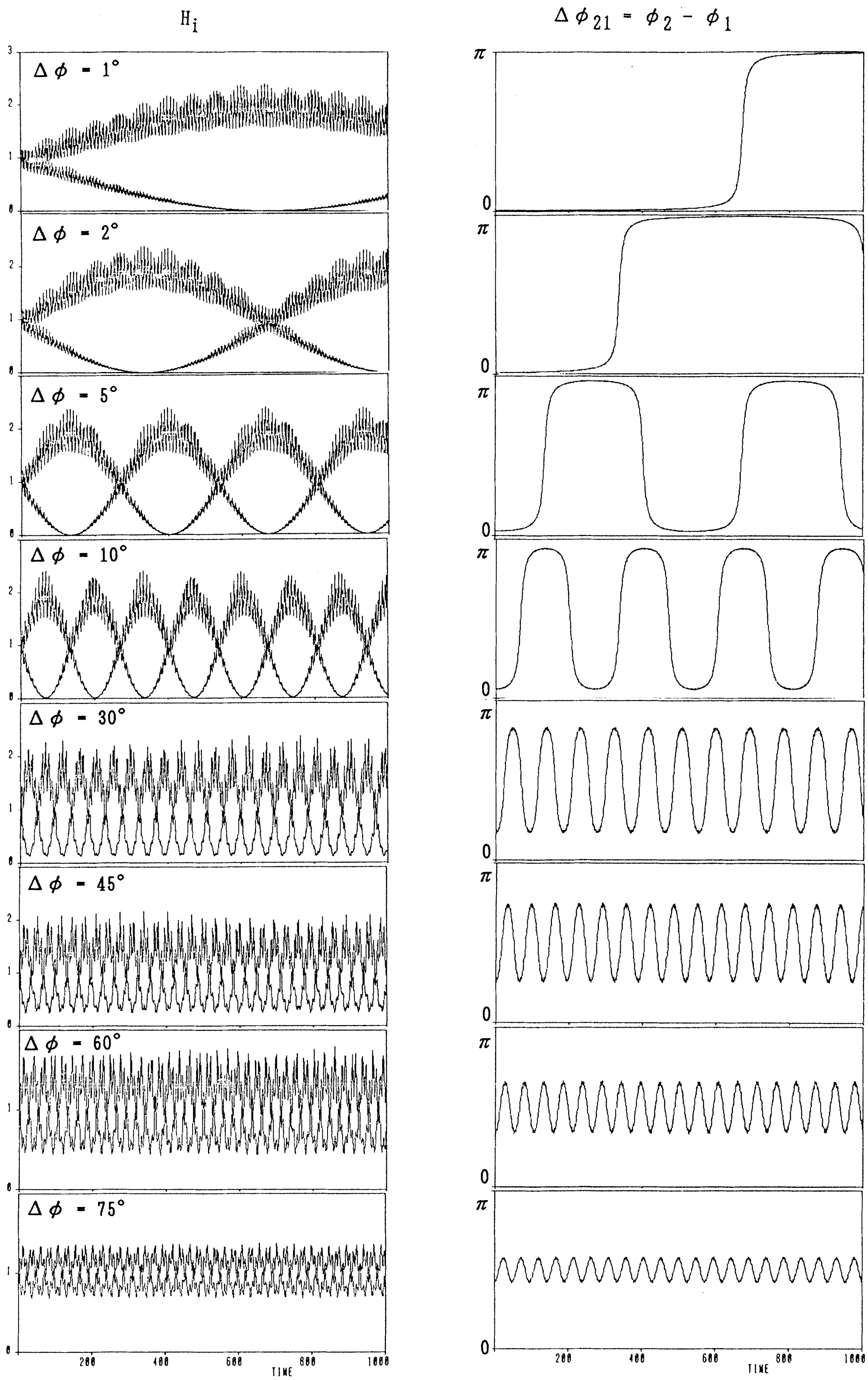

FIG. 3. Dependence on the initial condition at $g=2$, $Q=4$, and $\Delta t=0.05$. The column on the left is the energy H_i, and the difference of the two angles $\Delta\phi_{21}$ is on the right. The initial differences between angles are 1°, 2°, 5°, 10°, 30°, 45°, 60°, and 75°, from the top down.

$Q=4.0$, $\Delta t=0.05$, $H_i^0=1.0$, $\zeta^0=0.0$. The left-hand side in Fig. 3 is the time evolution of the energy of the oscillator, and the right-hand side is the difference of angles $\Delta\phi_{21}=\phi_2-\phi_1$. The beat frequency increases with $\Delta\phi$. At large $\Delta\phi$, the separation of the rapidly and slowly changing components is not so clear in energy, but in the difference between two phases the slow component is easily recognized even in such conditions. $\Delta\phi$ dependence of the beat frequency is very well expressed by

$$\Omega \sim A'\sin\Delta\phi \tag{3.2}$$

(see Fig. 4). The value of the constant A' determined from the data in Fig. 3 ($Q=4.0$, $g=2$) is 0.136. The minimum of the energy differs clearly from 0 in the region $\Delta\phi \geq 30°$. The range of the energy beat is limited to

$$1-\cos\Delta\phi \leq H_i \leq 1+\cos\Delta\phi\ . \tag{3.3}$$

The change of $\Delta\phi_{21}=\phi_2-\phi_1$ is limited in the range

$$\Delta\phi \leq \Delta\phi_{21} \leq \pi-\Delta\phi\ . \tag{3.4}$$

The Q dependence with $\Delta\phi=5°$ is given in Fig. 5. The results at $Q=1$, 2, 4, and 8 are depicted. At large Q, the behavior is regular. The frequency decreases in proportion to $\epsilon=1/Q$ at large Q (Fig. 6). However, at $Q=1$, the time evolution exhibits some kind of irregularity.

Empirical relations deduced from the numerical calculations are expressed as

$$H_i=1+\cos\Delta\phi\sin\left[A\frac{\sin\Delta\phi}{Q}t+\beta_i\right], \tag{3.5}$$

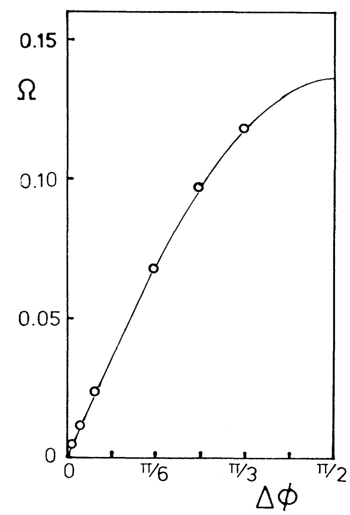

FIG. 4. Relation between the frequency of the beat Ω and the initial difference $\Delta\phi$. Circles indicate data points shown in Fig. 3. The solid curve is a sine function $A'\sin\Delta\phi$, with the best-fitted parameter $A'=0.136$.

where $\Delta\phi$ is the initial difference of phases, and A and β_i are constants. The amplitude of the beat is proportional to $\cos\Delta\phi$ and is independent of Q, and the frequency of the beat is proportional to $\sin\Delta\phi$ and $1/Q$. The slope of $\Delta\phi_i$ is proportional to $1/Q$, but is almost independent of $\Delta\phi$. The amplitude of the ζ fluctuation is smaller than $1/\sqrt{Q}$, which is expected in the equipartition law.

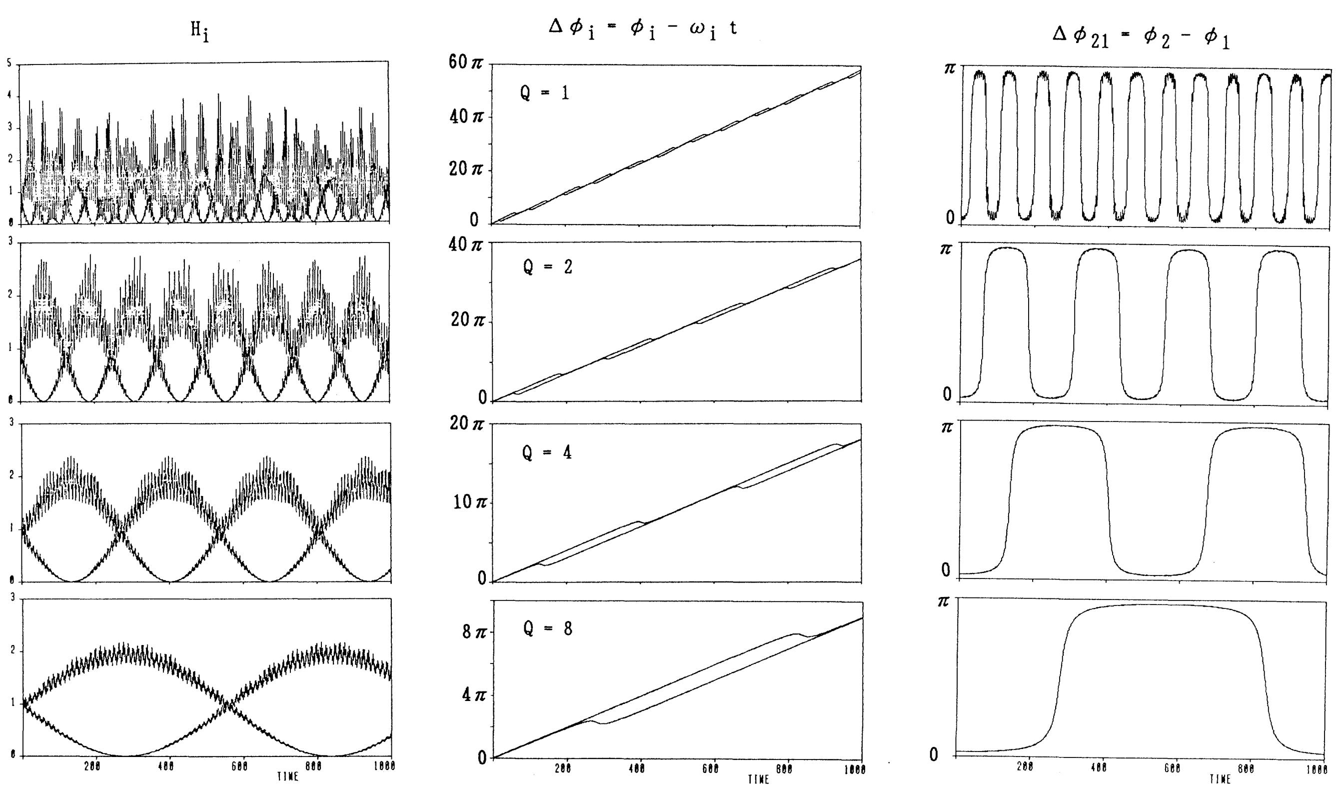

FIG. 5. Dependence on the parameter Q. The columns show the results of the energy, the angles, and the difference of angles, from the left. The parameter Q is 1, 2, 4, and 8, from the top down ($\Delta\phi=5°$, $\Delta t=0.05$).

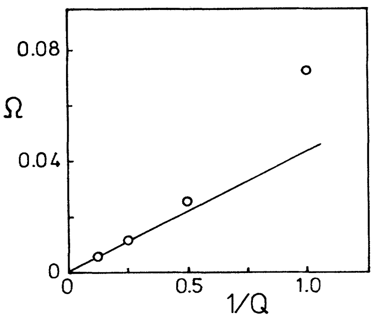

FIG. 6. Q dependence of the beat frequency Ω. The solid line expresses the theoretical relation $\Omega=(\sin\Delta\phi)/2Q$ at large Q.

Therefore, the thermodynamical equilibrium in the extended system is not attained at large Q in these calculations.

The typical beat with large amplitude appears with small $\Delta\phi$. When $\Delta\phi$ is near $\pi/2$, the fluctuation of the energy is very small. This is the behavior mentioned already in the final part of Sec. II.

We found that the dynamical evolution is periodic in the isotropic harmonic oscillator. This suggests the existence of integrals of motion. We also studied the anisotropic oscillator. The dynamical behavior is very different from that in the isotropic case. No systematic dependence on $\Delta\phi$ is detected in the anisotropic case, because the passing of the phases must occur. Also the regularity of the time evolution is lost at larger Q values. In Fig. 7, two time evolutions of the energy H_2 with $\omega_1=1.0$ and $\omega_2=\sqrt{3}$ at $Q=4$, started from the same initial configuration, are shown. The only difference is the length of the integration time step Δt: (a) 0.006 25 and (b) 0.001 562 5. The time evolution depends significantly on the integration time length Δt at the same Q ($Q=4$) as in Figs. 1 and 2. During a short period, they behave similarly, but a small difference caused by the different accuracy in the integration grows very rapidly, and after about $t=200$, the two time evolutions are quite different. This detailed dependence on initial or simulation conditions is an indication of chaotic behavior. The sensitive dependence on the length of the integration time step has never occurred in the isotropic case.

IV. SEPARATION OF RAPIDLY AND SLOWLY CHANGING COMPONENTS

The numerical calculations given in Sec. III suggest the regular behavior of the thermostated isotropic oscillator at large Q. We study the dynamical behaviors in a system described by Eqs. (2.17)–(2.19) by a perturbation analysis with respect to $\epsilon=1/Q$. This perturbation parameter is suggested from the Q dependence of the frequency, Eq. (3.5). When the equipartition condition, Eq. (3.1), is satisfied, the energy of the thermostat part in Eq. (2.6) is very small. We could consider this term as a per-

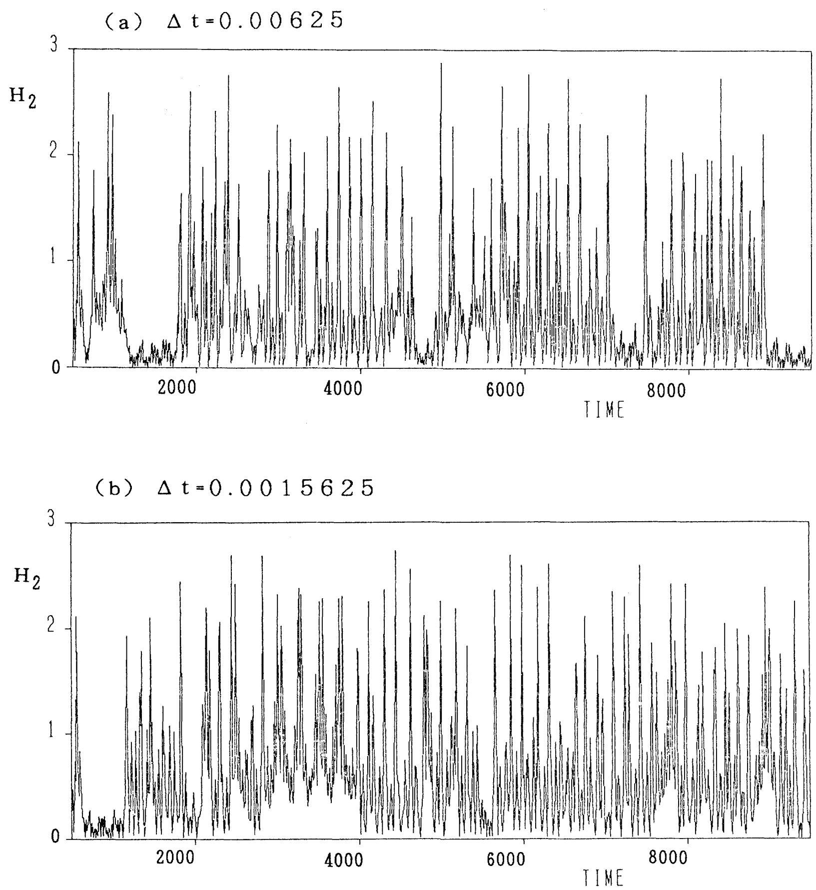

FIG. 7. Time evolution with irrational frequency ratio, $\omega_1=1$, $\omega_2=\sqrt{3}$. The two time evolutions of the energy of the second oscillator H_2 are depicted with (a) $\Delta t=0.006\,25$ and (b) $\Delta t=0.001\,562\,5$. The two evolutions deviate considerably after $t=200$.

turbation that may cause the coupling between harmonic oscillators. ζ is proportional to $1/Q$ in Eq. (2.19). If we scale ζ as

$$\zeta=\epsilon\zeta_1 , \tag{4.1}$$

the kinetic-energy term of the thermostat $Q\zeta^2/2$ is $\epsilon\zeta_1^2/2$ and becomes of order ϵ.

We rewrite Eqs. (2.17)–(2.19) explicitly with ϵ as

$$\frac{dH_i}{dt}=-2\epsilon\zeta_1 H_i\cos^2\phi_i , \tag{4.2}$$

$$\frac{d\phi_i}{dt}=1+\epsilon\zeta_1\sin\phi_i\cos\phi_i , \tag{4.3}$$

$$\epsilon\frac{d\zeta_1}{dt}=\epsilon\left[\sum_j (2H_j\cos^2\phi_j)-g\right] . \tag{4.4}$$

The solution of zeroth order is clearly the unperturbed motion of the oscillator:

$$H_i=H_{i0} , \tag{4.5}$$

$$\phi_i=t+\phi_{i0} , \tag{4.6}$$

where H_{i0} and ϕ_{i0} are constants.

In the perturbation of the first order with ϵ, we must take into consideration the slow change of the constants H_{i0} and ϕ_{i0}, because their time derivatives become the same order as those of H_{i1} and ϕ_{i1}. The time variable appropriate for these variables is

$$\tau=\epsilon t . \tag{4.7}$$

Therefore, proper expansions of the variables to order ϵ are

$$H_i=H_{i0}(\epsilon t)+\epsilon H_{i1}(t)+\cdots , \tag{4.8}$$

$$\phi_i=t+\phi_{i0}(\epsilon t)+\epsilon\phi_{i1}(t)+\cdots , \tag{4.9}$$

$$\zeta=\epsilon\zeta_1(t)+\cdots . \tag{4.10}$$

The equations of first order with ϵ are obtained as

$$\frac{dH_{i0}}{d\tau}+\frac{dH_{i1}}{dt}=-2\zeta_1 H_{i0}\cos^2(t+\phi_{i0}) , \tag{4.11}$$

$$\frac{d\phi_{i0}}{d\tau}+\frac{d\phi_{i1}}{dt}=\zeta_1\sin(t+\phi_{i0})\cos(t+\phi_{i0}) , \tag{4.12}$$

$$\frac{d\zeta_1}{dt}=\sum_j 2H_{j0}\cos^2(t+\phi_{j0})-g = \left[\sum_j H_{j0}-g\right]+\sum_j H_{j0}\cos[2(t+\phi_{j0})] . \tag{4.13}$$

We assume that the equipartition condition, Eq. (3.1), is always satisfied. As already mentioned in Sec. III, the conservation of the total energy of the oscillator system is a plausible assumption. Then the first term of Eq. (4.13) vanishes and Eq. (4.13) becomes

$$\frac{d\zeta_1}{dt}=\sum_j H_{j0}\cos[2(t+\phi_{j0})] . \tag{4.14}$$

The only rapidly changing part in the right-hand side of Eq. (4.14) is the time t in the cosine function. Therefore, this equation can be integrated in zeroth order as

$$\zeta_1=\sum_j \frac{H_{j0}}{2}\sin[2(t+\phi_{j0})] . \tag{4.15}$$

A possible additional constant to Eq. (4.15) is 0, because the average of ζ_1 should vanish. ζ_1 in Eq. (4.11) is replaced by Eq. (4.15),

$$\begin{aligned}\frac{dH_{i0}}{d\tau}+\frac{dH_{i1}}{dt}&=-2H_{i0}\left[\sum_j \frac{H_{j0}}{2}\sin[2(t+\phi_{j0})]\right]\frac{1+\cos[2(t+\phi_{i0})]}{2}\\&=-\tfrac{1}{2}H_{i0}\sum_j H_{j0}\sin[2(t+\phi_{j0})]-\tfrac{1}{2}H_{i0}\sum_j H_{j0}\sin[2(t+\phi_{j0})]\cos[2(t+\phi_{i0})]\\&=-\tfrac{1}{2}H_{i0}\sum_j H_{j0}\sin[2(t+\phi_{j0})]-\tfrac{1}{4}H_{i0}\sum_j H_{j0}\{\sin(4t+2\phi_{i0}+2\phi_{j0})+\sin[2(\phi_{j0}-\phi_{i0})]\} .\end{aligned} \tag{4.16}$$

We can separate the slowly and rapidly changing components of the equation. The slowly changing part is

$$\frac{dH_{i0}}{d\tau}=-\tfrac{1}{4}H_{i0}\sum_j H_{j0}\sin[2(\phi_{j0}-\phi_{i0})] , \tag{4.17}$$

and the rapidly changing part is

$$\frac{dH_{i1}}{dt}=-\tfrac{1}{2}H_{i0}\sum_j H_{j0}\sin(2t+2\phi_{j0}) -\tfrac{1}{4}H_{i0}\sum_j H_{j0}\sin(4t+2\phi_{j0}+2\phi_{i0}) . \tag{4.18}$$

Equation (4.18) can be integrated in zeroth order as

$$H_{i1}(t)=\tfrac{1}{4}H_{i0}\sum_j H_{j0}\cos(2t+2\phi_{j0}) +\tfrac{1}{16}H_{i0}\sum_j H_{j0}\cos(4t+2\phi_{j0}+2\phi_{i0}) . \tag{4.19}$$

The equation for ϕ_i is obtained in the same way as for H_i,

$$\begin{aligned}\frac{d\phi_{i0}}{d\tau}+\frac{d\phi_{j0}}{dt}&=\tfrac{1}{2}\sin(2t+2\phi_{i0})\sum_j \tfrac{1}{2}H_{j0}\sin(2t+2\phi_{j0})\\&=-\tfrac{1}{8}\sum_j H_{j0}\{\cos(4t+2\phi_{i0}+2\phi_{j0})-\cos[2(\phi_{i0}-\phi_{j0})]\} .\end{aligned} \tag{4.20}$$

The slowly changing part of ϕ_i is

$$\frac{d\phi_{i0}}{d\tau}=\tfrac{1}{8}\sum_j H_{j0}\cos[2(\phi_{i0}-\phi_{j0})]\ , \tag{4.21}$$

and the rapidly changing part is

$$\frac{d\phi_{i1}}{dt}=-\tfrac{1}{8}\sum_j H_{j0}\cos(4t+2\phi_{i0}+2\phi_{j0})\ . \tag{4.22}$$

ϕ_{i1} is obtained in zeroth order as

$$\phi_{i1}(t)=-\tfrac{1}{32}\sum_j H_{j0}\sin(4t+2\phi_{i0}+2\phi_{j0})\ . \tag{4.23}$$

We derived the equations of motion governing the slowly changing part, Eqs. (4.17) and (4.21). If we reinterpret H_{i0} as a momentum p_i, and ϕ_{i0} as a coordinate q_i, and $\tau=\epsilon t$ as the time, the equations become a canonical form,

$$\frac{dq_i}{d\tau}=\tfrac{1}{8}\sum_j p_j\cos[2(q_i-q_j)]\ , \tag{4.24}$$

$$\frac{dp_i}{d\tau}=\tfrac{1}{4}p_i\sum_j p_j\sin[2(q_i-q_j)]\ , \tag{4.25}$$

and they can be derived from a Hamiltonian H',

$$H'=\tfrac{1}{16}\sum_i\sum_j p_ip_j\cos[2(q_i-q_j)]\ . \tag{4.26}$$

V. THE INTEGRATION OF THE REDUCED EQUATIONS OF MOTION

We will show in this section that the Hamiltonian Eq. (4.26), describing the slow change of the thermostated oscillators, is completely integrable. A key property is that the Hamiltonian can be factorized as

$$\begin{aligned}H'&=\tfrac{1}{16}\sum_i\sum_j p_ip_j\cos[2(q_i-q_j)]\\&=\tfrac{1}{16}\left[\sum_i p_ie^{2iq_i}\right]\left[\sum_j p_je^{-2iq_j}\right]\\&=\tfrac{1}{16}XX^*\ ,\end{aligned} \tag{5.1}$$

where the factor X is defined as

$$X=\sum_i p_ie^{2iq_i}\ . \tag{5.2}$$

X^* is the complex conjugate of X. Equations (4.24) and (4.25) are expressed in a simple form with X and X^*

$$\frac{dq_i}{d\tau}=\tfrac{1}{16}(e^{2iq_i}X^*+e^{-2iq_i}X)\ , \tag{5.3}$$

$$\frac{dp_i}{d\tau}=-\frac{i}{8}p_i(e^{2iq_i}X^*-e^{-2iq_i}X)\ . \tag{5.4}$$

The interactions with other oscillators occur only via common factors X and X^*.

The total momentum P

$$P=\sum_i p_i \tag{5.5}$$

(or the total energy in the original system) is a constant of motion. It can be shown easily as

$$\frac{dP}{d\tau}=\sum_i\frac{dp_i}{d\tau}=\tfrac{1}{4}\sum_i\sum_j p_ip_j\sin[2(q_i-q_j)]=0\ . \tag{5.6}$$

The last equality holds because the sine function is an odd function of q_i-q_j. The conservation of P is consistent with the equipartition condition, Eq. (3.1), assumed in the process of derivation of the reduced Hamiltonian, Eq. (5.1). We define a quantity H''

$$H''=\frac{16}{P^2}H'\ , \tag{5.7}$$

so that the solution of p_i and q_i can be expressed in a simple form.

By differentiating X with respect to the time τ, we obtain a simple closed relation,

$$\begin{aligned}\frac{dX}{d\tau}&=\frac{d}{d\tau}\left[\sum_i p_ie^{2iq_i}\right]=\sum_i e^{2iq_i}\left[\frac{dp_i}{d\tau}+2ip_i\frac{dq_i}{d\tau}\right]\\&=\sum_i e^{2iq_i}\left[-\frac{i}{8}p_i(e^{2iq_i}X^*-e^{-2iq_i}X)+2ip_i\tfrac{1}{16}(e^{2iq_i}X^*+e^{-2iq_i}X)\right]\\&=\frac{i}{4}\left[\sum_i p_i\right]X=\frac{i}{4}PX\ .\end{aligned} \tag{5.8}$$

Because P is an integral of the motion, the time evolution of the factor X can be obtained as

$$X=Ce^{(i/4)P\tau}\ . \tag{5.9}$$

The constant C is determined to satisfy Eq. (5.1),

$$C=4(H')^{1/2}e^{2i\alpha}\ , \tag{5.10}$$

where α is a constant. Now that the factors X and X^* are obtained as functions of the time τ, the equations of motion, Eqs. (5.3) and (5.4), can be separated in each degree of freedom and can be integrated independently.

At first, we consider the equation for q_i,

$$\frac{dq_i}{d\tau}=\tfrac{1}{16}(e^{2iq_i}X^*+e^{-2iq_i}X)$$
$$=\frac{(H')^{1/2}}{4}(e^{i[2q_i-(P/4)\tau-2\alpha]}+e^{-i[2q_i-(P/4)\tau-2\alpha]})$$
$$=\frac{(H')^{1/2}}{2}\cos\left[2q_i-\frac{P}{4}\tau-2\alpha\right] . \qquad (5.11)$$

We define a new variable ψ_i as

$$\psi_i=q_i-\frac{P}{8}\tau-\alpha . \qquad (5.12)$$

The equation for ψ_i becomes

$$\frac{d\psi_i}{d\tau}=\frac{dq_i}{d\tau}-\frac{P}{8}=\frac{(H')^{1/2}}{2}\cos 2\psi_i-\frac{P}{8} . \qquad (5.13)$$

This equation can be integrated as

$$-\frac{8}{P}(1-H'')^{-1/2}\tan^{-1}\left[\left[\frac{1+(H'')^{1/2}}{1-(H'')^{1/2}}\right]^{1/2}\tan\psi_i\right]=\tau+\beta_i' . \qquad (5.14)$$

Thus

$$\psi_i=-\tan^{-1}\left[\left[\frac{1-(H'')^{1/2}}{1+(H'')^{1/2}}\right]^{1/2}\tan\left[\frac{P}{8}(1-H'')^{1/2}\tau+\frac{\beta_i}{2}\right]\right] . \qquad (5.15)$$

An appropriate branch of the $\tan^{-1}$ function should be chosen so that ψ_i is a continuous function of the time τ. Therefore, the slow component of the angle $\phi_{i0}=q_i$ is obtained as

$$\phi_{i0}(\tau)=q_i=\frac{P}{8}\tau+\alpha-\tan^{-1}\left[\left[\frac{1-(H'')^{1/2}}{1+(H'')^{1/2}}\right]^{1/2}\tan\left[\frac{P}{8}(1-H'')^{1/2}\tau+\frac{\beta_i}{2}\right]\right] . \qquad (5.16)$$

Equation (5.16) consists of a linearly increasing term and a periodically decreasing term. The frequency Ω in the periodic term is

$$\Omega=\frac{P}{4}(1-H'')^{1/2} \qquad (5.17)$$

in reduced units. In the original problem, the frequency in the g oscillator system Ω_g is expressed as

$$\Omega_g=\frac{g}{4Q}\left[1-\frac{16}{g^2}H'\right]^{1/2} , \qquad (5.18)$$

where $P=g$ by Eq. (3.1).

ϕ_{i0} increases linearly with slope $P/8$ in most of one period. ϕ_{i0} decreases near the point $\tau=\tau_0$, where

$$\Omega\tau_0+\beta_i=\pi+2n\pi . \qquad (5.19)$$

The slope of ϕ_{i0} at τ_0 is negative

$$\left.\frac{d\phi_{i0}}{d\tau}\right|_{\tau=\tau_0}=\frac{P}{8}\{1-[1+(H'')^{1/2}]\}=-\tfrac{1}{2}(H')^{1/2} . \qquad (5.20)$$

When the initial q_i are selected from a narrow region, H' is nearly $g^2/16$, and Eq. (5.20) gives $-P/8$, whose absolute value is almost equal to the slope in the linearly increasing region.

Next, we consider the equation for p_i,

$$\frac{dp_i}{d\tau}=-\frac{i}{8}p_i(e^{2iq_i}X^*-e^{-2iq_i}X)$$
$$=p_i(H')^{1/2}\sin\left[2q_i-\frac{P}{4}\tau-2\alpha\right]$$
$$=p_i(H')^{1/2}\sin 2\psi_i . \qquad (5.21)$$

We have already obtained the expression for ψ_i. The equation can be transformed to an integrable form,

$$\frac{d\ln p_i}{d\tau}=(H')^{1/2}\sin 2\psi_i=-\frac{P}{4}(H'')^{1/2}\sin\left\{2\tan^{-1}\left[\left[\frac{1-(H'')^{1/2}}{1+(H'')^{1/2}}\right]^{1/2}\tan[(\Omega\tau+\beta_i)/2]\right]\right\}$$
$$=-(H'')^{1/2}\Omega\frac{\sin(\Omega\tau+\beta_i)}{1+(H'')^{1/2}\cos(\Omega\tau+\beta_i)}$$
$$=\frac{d}{d\tau}\ln[1+(H'')^{1/2}\cos(\Omega\tau+\beta_i)] . \qquad (5.22)$$

Thus, p_i or H_{i0}, the slow component of the energy change, is also obtained in a closed form,

$$H_{i0}(\tau)=p_i=C_i[1+(H'')^{1/2}\cos(\Omega\tau+\beta_i)]=C_i\left\{1+\frac{4}{P}(H')^{1/2}\cos\left[\frac{P}{4}\left[1-\frac{16}{P^2}H'\right]^{1/2}\tau+\beta_i\right]\right\} . \qquad (5.23)$$

The change of $H_{i0}(\tau)$ is described by a sinusoidal function and the functional form does not depend on the number of oscillators. This agrees well with the numerical calculations given in Figs. 1 and 2.

Equations (5.16) and (5.23) are the complete solution of the reduced Hamiltonian Eq. (5.1) that describes the slowly changing part of the thermostated oscillators. The constants α, β_i, and C_i are determined in the following steps. Only α, out of these constants, appears in the expression of the factor X,

$$X=\sum_i p_i e^{2iq_i}=4(H')^{1/2}e^{i[(P/4)\tau+2\alpha]} . \tag{5.24}$$

Thus α is determined from the relation

$$\tan 2\alpha=\frac{\sum_i p_i^0 \sin 2q_i^0}{\sum_i p_i^0 \cos 2q_i^0} . \tag{5.25}$$

p_i^0 and q_i^0 are the initial values of p_i and q_i. α and β_i appear in Eq. (5.16). At $\tau=0$, it becomes

$$q_i^0=\alpha-\tan^{-1}\left[\left[\frac{1-(H'')^{1/2}}{1+(H'')^{1/2}}\right]^{1/2}\tan(\beta_i/2)\right] . \tag{5.26}$$

Thus the constant β_i is determined as

$$\beta_i=2\tan^{-1}\left[\left[\frac{1+(H'')^{1/2}}{1-(H'')^{1/2}}\right]^{1/2}\tan(\alpha-q_i^0)\right] . \tag{5.27}$$

Finally, the C_i is determined from Eq. (5.23),

$$C_i=\frac{p_i^0}{1+(H'')^{1/2}\cos\beta_i}=\frac{p_i^0}{1-H''}\{1-(H'')^{1/2}\cos[2(\alpha-q_i^0)]\} . \tag{5.28}$$

Conserved quantities of the reduced Hamiltonian are the Hamiltonian H', the total momentum P, and J_i ($i=1,2,\ldots,g$), which is equivalent to the coefficient C_i, Eq. (5.28):

$$J_i=p_i\left[P-\sum_j p_j\cos[2(q_i-q_j)]\right]=p_i\sum_j p_j\{1-\cos[2(q_i-q_j)]\}=2p_i\sum_j p_j\sin^2(q_i-q_j) . \tag{5.29}$$

The number of integrals is $g+2$, but they are not independent. The Hamiltonian H' can be expressed by P and J_i as

$$H'=\frac{1}{16}\left[P^2-\sum_i J_i\right] . \tag{5.30}$$

Also, all J_i is not independent. With $g=2$, clearly $J_1=J_2$, and the independent conserved quantities are $P=p_1+p_2$ and $J=2p_ip_2\sin^2(q_1-q_2)$.

VI. DISCUSSION

We have shown that the dynamical behavior of the thermostated isotropic harmonic oscillator is completely regular and the system is integrable at large Q limit. The solution H_{i0} [Eq. (5.23)] and ϕ_{i0} [Eq. (5.16)] explains the characteristic behaviors obtained in numerical simulations.

At first we consider solutions for $g=2$, where detailed investigations are carried out in Sec. III. Parameters C_i and β_i should satisfy

$$C_1=C_2=1.0 , \tag{6.1}$$

$$\beta_2=\beta_1+\pi , \tag{6.2}$$

in this case. The general solutions for $g=2$ are

$$H_{10}(\tau)=1+(H'')^{1/2}\cos(\Omega\tau+\beta_1) , \tag{6.3}$$

$$H_{20}(\tau)=1-(H'')^{1/2}\cos(\Omega\tau+\beta_1) , \tag{6.4}$$

$$\phi_{10}(\tau)=\tfrac{1}{4}\tau+\alpha-\tan^{-1}\left[\left[\frac{1-(H'')^{1/2}}{1+(H'')^{1/2}}\right]^{1/2}\tan[(\Omega\tau+\beta_1)/2]\right] , \tag{6.5}$$

$$\phi_{20}(\tau)=\tfrac{1}{4}\tau+\alpha+\tan^{-1}\left[\left[\frac{1-(H'')^{1/2}}{1+(H'')^{1/2}}\right]^{1/2}\Big/\tan[(\Omega\tau+\beta_1)/2]\right] , \tag{6.6}$$

where the total energy of the oscillator system H'' is

$$H''=4H'=1-H_1^0H_2^0\sin^2(\phi_1^0-\phi_2^0) , \tag{6.7}$$

the frequency is

$$\Omega=\tfrac{1}{2}(1-H'')^{1/2}=\tfrac{1}{2}(H_1^0H_2^0)^{1/2}\sin|\phi_1^0-\phi_2^0| . \tag{6.8}$$

and the remaining parameters α and β_1 are determined as

$$\alpha=\tfrac{1}{2}\tan^{-1}\left[\frac{H_1^0\sin 2\phi_1^0+H_2^0\sin 2\phi_2^0}{H_1^0\cos 2\phi_1^0+H_2^0\cos 2\phi_2^0}\right] , \tag{6.9}$$

$$\beta_1=\cos^{-1}\left[\frac{H_1^0-H_2^0}{2(H'')^{1/2}}\right] . \tag{6.10}$$

For special cases $H_1^0=H_2^0=1.0$, and $\phi_2^0=\Delta\phi$, $\phi_1^0=0$ depicted in Figs. 1, 3, and 5, the parameters in Eqs. (6.7)–(6.10) are further simplified as

$H''=1-\sin^2\Delta\phi=\cos^2\Delta\phi$, $\alpha=\Delta\phi/2$, $\beta_1=\pi/2$. Thus the frequency for $g=2$ obtained in Fig. 3 should satisfy the relation

$$\Omega_2=\frac{1}{2Q}(1-\cos^2\Delta\phi)^{1/2}=\frac{1}{2Q}\sin\Delta\phi \ . \tag{6.11}$$

This is the same form as that deduced from the numerical calculations [Eq. (3.5)]. The coefficient A appearing in the expression of beat frequency in Eq. (3.5) is 0.545, with $g=2$ and at $Q=4.0$. This value is close to the theoretical value 0.5 [see Eq. (6.11)]. Better agreement is expected at larger Q. The frequency Ω deviates to a larger value at small Q from Eq. (5.18) (see Fig. 6). The effects of higher-order terms should be included to explain this Q dependence.

The difference of angles is a periodic function

$$\cot(\phi_{20}-\phi_{10})=\cot(\Delta\phi)\cos\left[\frac{\sin\Delta\phi}{2Q}t\right] . \tag{6.12}$$

This function describes very well the behavior given in Figs. 1, 3, and 5.

The frequency Ω [Eq. (5.17)] and the amplitude H_{i0} [Eq. (5.23)] of the beat depend drastically on the value of the reduced Hamiltonian, Eq. (5.1). When $H''=16H'/g^2$ is close to 1, a slow beat with large amplitude is expected. This condition is fulfilled when all the differences of angles are very small. If the angles distribute randomly in a many-oscillator system, the value of H'' is about $1/g$, which is considerably smaller than 1, and the beat is not so apparent in this case.

We will study a typical beat behavior. Solutions for the initial configurations $H_i^0=1.0$ and $\phi_k^0=(k-1)\Delta\phi$, where the angles are distributed with equal distances, are obtained as follows at small $\Delta\phi$ limit:

$$\begin{aligned} H'' &\simeq 1-\frac{1}{g^2}\sum_{k=1}^{g-1}(g-k)k^2(\Delta\phi)^2 \\ &=1-\tfrac{1}{3}(g^2-1)(\Delta\phi)^2 , \end{aligned} \tag{6.13}$$

$$C_k=\tfrac{1}{2}+\tfrac{3}{2}\frac{(2k-g-1)^2}{g^2-1} , \tag{6.14}$$

$$\beta_k=2\tan^{-1}\left[\left[\frac{12}{g^2-1}\right]^{1/2}\left[\frac{g+1}{2}-k\right]\right] . \tag{6.15}$$

C_k and β_k do not depend on $\Delta\phi$ at the small $\Delta\phi$ limit.

Especially for the case given in Fig. 2 ($g=5$), $C_1=C_5=\frac{3}{2}$, $C_2=C_4=\frac{3}{4}$, $C_3=\frac{1}{2}$, $\beta_1=-\beta_5=2\tan^{-1}\sqrt{2}=\theta_t=109.47°$, $\beta_2=-\beta_4=2\tan^{-1}(1/\sqrt{2})=\pi-\theta_t=70.53°$, and $\beta_3=0$, where θ_t is the tetrahedral angle.

We do not notice any reference describing the Hamiltonian, Eq. (5.1). But it belongs to a type of Hamiltonian [21]

$$H=\tfrac{1}{2}\sum_i\sum_j a_{ij}(q)p_ip_j , \tag{6.16}$$

which describes the geodesic flow in a curved space. The metric tensor g_{ij} in this space is the inverse matrix to a_{ij}. Especially, a Hamiltonian [22]

$$H=\tfrac{1}{2}\left[\sum_i p_i^2\right]\left[\sum_j q_j^2\right] \tag{6.17}$$

has a close relation with Eq. (5.1). A complex canonical transformation, Eq. (6.18)

$$\begin{aligned} P_i &=-i\sqrt{p_i}e^{-iq_i} , \\ Q_i &=\sqrt{p_i}e^{iq_i} , \end{aligned} \tag{6.18}$$

changes Eq. (5.1) into

$$H'=-\tfrac{1}{16}\left[\sum_i P_i^2\right]\left[\sum_j Q_j^2\right] . \tag{6.19}$$

The reduced Hamiltonian is factorized as in Eq. (5.1) or Eq. (6.19). The separation of the phase space into subspaces consisting of each degree of freedom is realized by this factorization. The factors X and X^* express a common global coupling between oscillators. In a system of this type, the mean-field approximation holds exactly, and this is the major reason that we can solve Eqs. (4.17) and (4.21).

Equation (5.11) and the solution [Eq. (5.16)] are the same as those obtained from the coupled rotator model [23] at a global coupling limit. The change of the phase of rotator i in this model is determined by

$$\frac{d\phi_i}{dt}=\omega_i+\sum_j\Gamma_{ji}(\phi_i-\phi_j) . \tag{6.20}$$

Γ_{ji} is a function of the difference between two phases ϕ_i and ϕ_j. At a global coupling limit, it becomes

$$\Gamma_{ji}(x)=K\sin x , \tag{6.21}$$

for all (i,j) pairs. Then the equation in this case is

$$\frac{d\phi_i}{dt}=\omega_i+K\sum_j\sin(\phi_i-\phi_j) . \tag{6.22}$$

The mean-field approximation is exact in Eq. (6.22), and the equations for each ϕ_i can be separated. This has the same functional form as Eq. (5.11). One must remark that the coupled rotator model is a phenomenological model and that it is not a Hamiltonian system. On the other hand, our Eqs. (4.17) and (4.21), derived by a perturbation treatment, are a Hamiltonian system.

VII. CONCLUSIONS

A harmonic oscillator system coupled with the Nosé-Hoover thermostat exhibits regular periodic beat behaviors at large Q (Q is the parameter controlling the speed of the response of the thermostat). The equations of motion describing the slowly changing part of the thermostated oscillators are obtained from a perturbation analysis with respect to $1/Q$. The equations can be associated with a Hamiltonian, and the system is completely integrable, irrespective of the number of the oscillators. The change of the energy is expressed by a sinusoidal function. The frequency of the beat becomes quite low when all the differences of the phases are very small.

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