Computer Experiments on Ergodic Problems in Anharmonic Lattice Vibrations

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Various computer experiments based on the numerical integration of dynamical equation of motion are reviewed and their importance is emphasized in connection with ergodic theory. To do this a short review of the present status of the ergodic theories is also given and the interrelations among various results of ergodic theories are clarified. The induction period discovered in the previous papers (H. Hirooka and N. Saitô, J. Phys. Soc. Japan **26** (1969), 624; N. Ooyama, H. Hirooka and N. Saitô, J. Phys. Soc. Japan **27** (1969), 815) is further examined in one-dimensional anharmonic lattices including exponential lattices. The apparent randomness which the system exhibits after elapsing the induction period is, strictly speaking, quasi-stochastic in the sence that the process is described completely as deterministic. The "true" stochasticity which seems required in the thermodynamical state will be realized in the thermodynamical limit.

§1. Introduction

The ergodic theory is regarded as most fundamental in statistical mechanics. Since the age of Boltzmann various discussions were given to this problem. The development is mainly done by mathematicians, and especially important results were obtained by Birkhoff, Von Neumann, Hopf, Khinchine and others. The theories, however, were not necessarily satisfactory for physicists, since one can say nothing about ergodicity in real physical systems. The fundamental postulates of thermodynamics and statistical mechanics, such as the zeroth law of thermodynamics or ergodicity etc., are introduced from *passive* experiences or from purely theoretical requirements. The theoretical investigation of elucidating these postulates from mechanical point of view is an important task of theoretical physics. But there was devised no *active* experiment to clarify the essential aspects of these problems. This is quite peculiar compared with other branches of theoretical physics. The unsatisfactory stage of mathematical theory of ergodicity, and the lack of experiments which are seductive to theorists may be the reason why many physicists have been almost indifferent to ergodic theory.

However in 1950's two epochmaking progresses which opened the new ways were made. One is the mathematical studies done by Kolmogorov and his school and the other is the numerical experiments on computer carried

out by Fermi and others. These are reviewed in later sections, but it is to be emphasized that the progress of computer has made possible the experiments which were impossible in the usual procedures of experiments on ordinary materials.

The purpose of the present article is to give a review of computer experiments on anharmonic lattices related to the problem of ergodicity. In §2, computer experiments for obtaining macroscopic properties by means of numerical calculation are reviewed. This kind of molecular dynamics is of course related to ergodicity, but no special intention is payed for elucidating ergodic problems. In §3 problems initiated by Fermi, Pasta and Ulam and excited thereby are discussed. Section 4 is devoted to a short review of the ergodic theory, with special emphasis of recent achievements by Kolmogorov and others,*) in connection with the existence of the invariant tori in weak anharmonic vibrations. The relations among the results obtained by various ergodic theories are summarized in Figs. 1 and 2. In §5, computer experiments on various mechanical models are given to show the isolating integrals as well as the unstable regions. These studies are related to the invariant tori discussed in §4. Section 6 is the main part of the present article and presents the computer experiments made in our laboratory. Especially the induction period is investigated in further detail, and the approach to equilibrium is discussed. Section 7 is the conclusion and the meaning of stochasticity is discussed.

§2. Molecular dynamics

In the last two decades many computer experiments have been carried out in various fields of statirtical mechanics including equilibrium and non-equilibrium problems. In these studies we notice two different approaches. The one is the probabilistic method, based on Gibbs' statistics or stochastic equations. In equilibrium problems canonical averages are sometimes calculated by the Monte Carlo method.[1] As an example of time-dependent problems we refer to the work of Ogita et al.[2] on the study of the dynamical property of an Ising system by simulating it on computer as a stochastic process.

In the present article, however, we pay particular attention to another one, i.e. the method of integrating directly the equation of motion without recourse to partition functions or other stochastic methods. For example, Alder et al.[3] carried out the experiments of the interaction of hard spheres moving in a vessel to investigate the phase transition and transport phenomena in this system. Similarly Köhler and Bellemans[4] verified that the system of weakly coupled electric dipoles on a rigid lattice reaches an equilibrium state and the relaxation time of fourth moment of angular momentum distribution is inversely proportional to the eighth power of the dipole moment, as ex-

*) Excellent reviews are also found in references 12) and 35).

pected from statistical mechanical theory. Rahman[5] and Verlet[6] simulated on computer the molecular dynamics of liquid argon using a system of 864 particles interacting through a Lennard-Jones potential and obtained the time-relaxed pair-correlation function and the constant of self-diffusion as well as several equilibrium quantities, which agree well with real experiments on argon. Further Harp and Berne[7] studied the linear- and angular-momentum correlation functions in liquid CO. On the other hand, Visscher et al.[8] discussed the lattice thermal conductivity in disordered harmonic and anharmonic crystal models. The thermal conductivity obtained shows the expected dependence on the composition of the impurity atoms, but, except nearly monatomic lattices, the computer experiments yield larger heat conductivities in anharmonic lattices than in harmonic ones. In connection with these results, Hirooka et al.[9] studied the effect of anharmonicity on the localization of modes in disordered lattices.

Thus the computer-simulated molecular dynamics gives interesting and useful information about macroscopic properties of a system of large number of interacting particles.

§3. FPU problem

Notwithstanding the success of the works mentioned above of molecular dynamics since 1960, we have to make mention of the study of Fermi, Pasta and Ulam[10] early in 1950's, which seems the most important computer experiment, although the earliest.

FPU observed on computer how the energy is transfered to higher normal modes on exciting the lowest mode initially in one-dimensional anharmonic lattices where the nonlinear forces considered are quadratic, cubic and broken linear ones. Here the normal modes are defined as those of the system in the absence of nonlinear forces. They expected that the presence of anharmonicity gave rise to the energy sharing among normal modes required for the establishment of an equilibrium state. Unexpectedly, however, they failed to show the appreciable energy transfer to higher modes, but rather they found a recurrence phenomenon. This surprising result seems to be in contradiction to the zeroth law of thermodynamics.

A similar phenomenon was also observed by Saitô and Hirooka,[11] who showed that a one-dimensional anharmonic lattice does not have a tendency to reach a new equilibrium state which is characterized by a Maxwell distribution of particle velocities, when a constant force is applied to the system which is initially in mechanical equilibrium. Since the work of Fermi et al., many investigations followed to explain the FPU results. In particular Ford[12] and Jackson[13] emphasized the resonance condition for energy exchange among normal modes. Northcote and Potts[14] considered a lattice of harmonically

bound particles, but introduced an additional potential of rigid-sphere type between nearest particles. This system, which is regarded as a limiting case of large anharmonicity, was shown to reach an equilibrium state when one excites the lowest mode. The existence of stable and stochastic regions in anharmonic vibrations was pointed out by Israilievand Chirikov[15] and by Zaslavski and Sagdeev.[16] They have given qualitative arguments from the approximate treatments of nonlinear vibration.

On the other hand Zabusky,[17] observing that the anharmonic lattice vibration is approximately described by Korteweg-de Vries (KdV) equation, studied the properties of solitons in this case by computer experiments and found the recurrence phenomenon which is similar to FPU case. Toda[18),19] also found analytically the wave train solution and the solitary wave solution (lattice soliton) in a special example of coupled nonlinear oscillators. The recurrence phenomenon and the existence of stable solitons in anharmonic lattices or in KdV equations show nonergodic property of these systems. The stability of lattice solitons is discussed elsewhere in this issue by Ooyama and Saitô.[18]

The ergodic property of anharmonic lattice vibrations will be discussed in the present paper, but before doing this, it would be appropriate to make a short review of ergodic theory.

§4. Short review of ergodic theories of classical mechanics

The term ergodic is sometimes used with confusion. Boltzmann assumed that most physical systems are ergodic, in the sense that a representative point in Γ-space passes through every point of the energy surface corresponding to the initial condition. One also says that a system is ergodic, if the long time average $\overline{f}$ of any dynamical quantity expressed as a phase space function f of the system is equal to its ensemble average f^*. These two ways of use have different meanings. We retain the term ergodic for the latter meaning, and we use the term "ergodic in Boltzmann's meaning" for the original meaning introduced by Boltzmann. It is recognized that ergodic systems in Boltzmann's meaning would never exist, since the crossing of the path in phase space cannot occur and thus the constant-energy surface of dimension larger than 2 cannot be filled by an essentially one-dimensional orbit. Thus one expects that most physical systems would be quasi-ergodic, in the sence that an orbit in phase space covers the energy surface everywhere densely.

In 1931, Birkhoff[21] proved that the dynamical system is ergodic if and only if the surface of constant energy in phase space is metrically indecomposable. But it is not necessarily trivial to determine in Birkhoff's theorem whether or not a real system is indecomposable. Many mathematical models are proposed to show that there exist the transformations which ensure the metric transitivity. Especially Oxtoby and Ulam[22] proved that homeomorphism

on a quite general class of surfaces are metrically indecomposable. In this connection mention must be made of the theorems due to Burns and Poincaré found in the last century. Burns[23] showed that in the problem of three bodies no algebraic integral exists other than ten well-known integrals, namely the six integrals of motion of the center of gravity, three integrals of angular momentum and the integral of energy. Further Poincaré[24] showed that a canonical normal system does not have a family of integrals other than that of energy which are analytic and uniform in a certain domain and for small range of parameter μ. A canonical normal system is defined as the conservative system which is described by a set of coordinates y_i, x_i, $(i=1, 2, \cdots, n)$, in such a way that the Hamiltonian H can be expanded as

$$H=H_0+\mu H_1+\mu^2 H_2+\cdots \tag{1}$$

with respect to a small parameter μ, where H_0 is independent of x_i's and, H and H_i's are periodic in x_i's. In 1923, Fermi[25] proved by generalizing Poincaré's theorem that a canonical normal system for $n\geq 2$ does not have a uniform integral aside from the energy integral, and thus the system is quasi-ergodic. A system of anharmonic oscillators belongs to this class of canonical normal systems. Van Hove,[26] however, claimed that a quasi-ergodic system is not always metrically transitive. Furthermore, if an isolating integral exists (§5), the non-existence of uniform integrals does not lead to quasi-ergodicity. An important result was obtained in 1954 by Kolmogorov.[27] Kolmogorov, Arnold and Moser (KAM)[27] proved that almost all the systems with invariant multidimensional tori, such as harmonic lattice vibration, remain stable against the introduction of small nonlinear perturbations. In other words, the motion of the perturbed system is restricted to the invariant tori close to the invariant tori of the unperturbed system, provided that the frequencies of the unperturbed motion are incommensurate. This theorem was first proved for canonical normal system with nondegenerate unperturbed frequencies, i.e.

$$\det\left|\frac{\partial^2 H_0}{\partial y_i \partial y_k}\right| \neq 0, \tag{2}$$

but later the theorem is extended to degenerate cases by Arnold[27] and especially by Nisida[28] by reducing them to nondegenerate cases by means of the Birkhoff transformation. The invariant tori in these theories are not uniform integrals and do not conflict with Poincaré-Fermi theorem. These invariant tori will be broken under the larger nonlinear perturbation, and the system is expected to become ergodic, although no analytical theory is presented yet. The computer studies of these problems are given in §§5 and 6, which form the main parts of the present article.

A trajectory of a system is described as a geodesics on a space of a

certain metric. The geodesic flow on a manifold with negative curvature is shown ergodic by Anosov.[29] This kind of system is called a C-system. In C-systems two orbits with close initial data are exponentially divergent. Recently Sinai[30] proved that a system composed of more than two hard spheres contained in a parallelepipedic box with rigid walls is ergodic and further it is a K-system. For the definition of K-system some mathematical preliminaries are required and thus we do not enter into it here.[27] We further notice that in real thermodynamical systems the long time average $\overline{f}$ defined by

$$\overline{f}=\lim_{T\to\infty}\frac{1}{T}\int_{t-T/2}^{t+T/2} f\,dt \tag{3}$$

can be replaced by a short time average

$$\widehat{f}=\frac{1}{\tau}\int_{t-\tau/2}^{t+\tau/2} f\,dt \tag{4}$$

provided that $\tau>\tau_0$, where τ_0 is the characteristic relaxation time of the system. In other words, we say that the system is thermodynamical if the relation

$$\widehat{f}=\overline{f}=f^* \tag{5}$$

holds. For the establishment of thermodynamical state, it is conjectured that

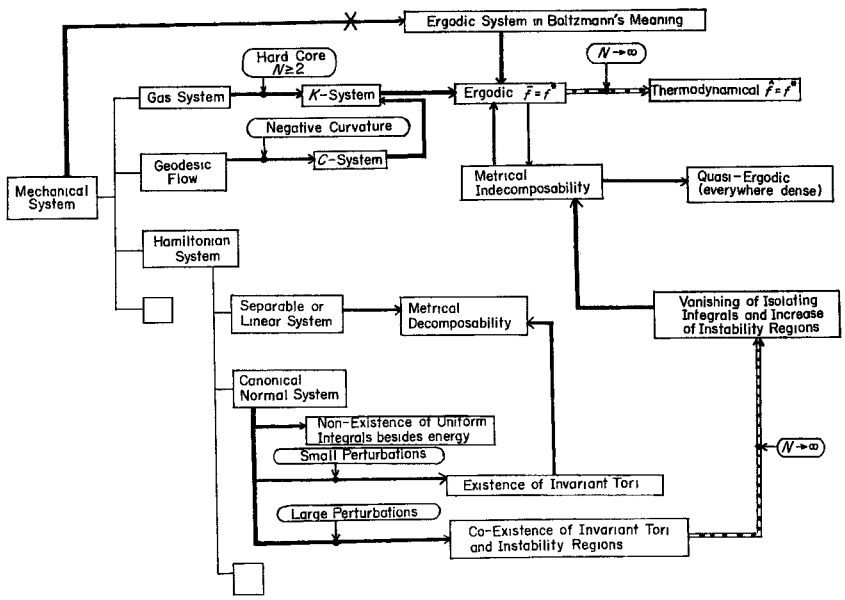

Fig. 1. Diagram showing the relation among various ergodic theories. $\boxed{A}\xrightarrow{C}\boxed{B}$ means that B follows from A by the introduction of a property C. The dotted lines indicate conjectures.

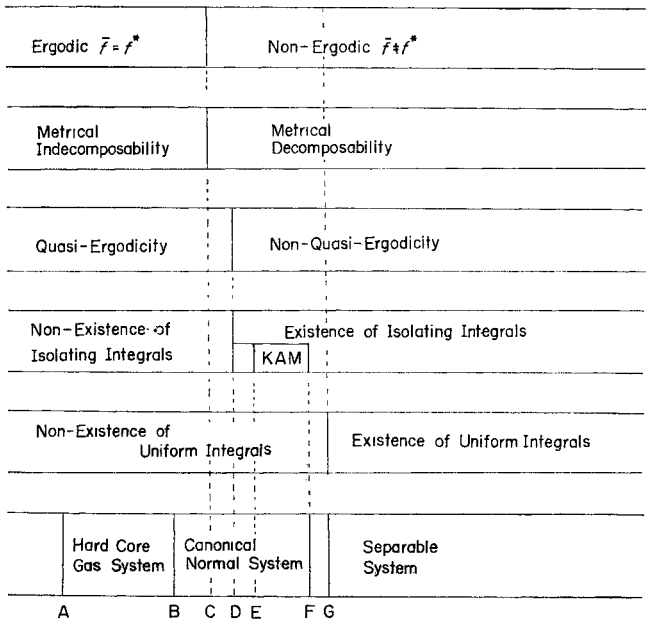

Fig. 2. Classification of mechanical systems.

the thermodynamical limit ($n\to\infty$, $V\to\infty$, $n/V=$const) will be necessary. Thus Sinai's proof that the gas system for $n>2$ is ergodic will be extended to the statement that the gas system for $n\to\infty$ is thermodynamical. Figures 1 and 2 are the summary of the present section. In Fig. 1 we show the interrelation among the results of various ergodic theories for dynamical systems. Figure 2 is the relations of the domains where the classifications of dynamical systems hold. The vertical lines indicate the boundaries of the classifications and their mutual positions. It is conjectured that for $n\to\infty$, the solid vertical lines at C.D.E.F move to the right up to the vertical line at G and thus KAM region vanishes. In this way, almost all the physical system will become thermodynamical, as expected.

§5. Existence of isolating integrals and instability regions

As mentioned in §4, there exists no uniform integral other than energy in canonical normal systems. This kind of integral is assumed uniform with respect to a parameter μ, provided that μ is small. However, it is possible that there exist integrals at some fixed value of μ. These integrals are sometimes called isolating, third or adelphic integrals. The KAM invariant tori are isolating integrals. Search for such integrals has been carried out for a long time, especially by astronomers. Recently, with the motion of stars in the galaxy in mind, computer studies have been made for the motion of a

particle in various potential fields with axial symmetry. Among others,[31] Hénon and Heiles[32] considered the motion in a plane containing the symmetry axis of the potential fields. They discussed the system with Hamiltonian given by

$$H=\frac{1}{2}(\dot{x}^2+\dot{y}^2)+U(x,y), \tag{6}$$
$$U(x,y)=\frac{1}{2}\left(x^2+y^2+2x^2y-\frac{2}{3}y^3\right).$$

By virtue of the energy integral, if we put $x=0$, we have an orbit in the $(y,\dot{y},\dot{x})$ space. Hénon-Heiles represented the results of computation by plotting in the $(y,\dot{y})$ plane the consecutive points crossing the $x=0$ plane with positive $\dot{x}>0$. When the total energy is small, the consecutive points in the $(y,\dot{y})$ plane lie exactly on a curve, called level curve. These curves form a one-parameter family which covers completely the available area, and also show the existence of the stable points and the separatrix (Fig. 3). On increasing the energy, however, the available area is divided into two; one is

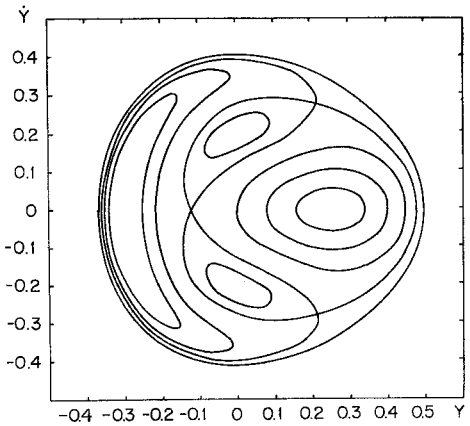

Fig. 3. Hénon-Heiles' level curves. Total energy $E=0.0833$.

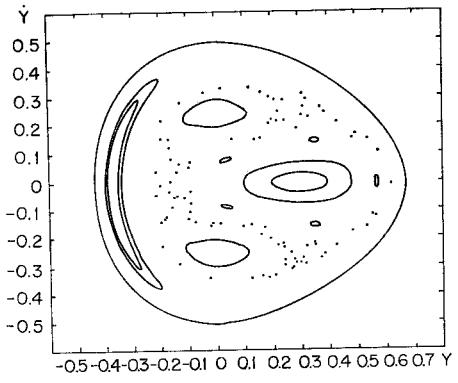

Fig. 4. Hénon-Heiles' level curves. Total energy $E=0.12500$. The dots in the unstable region belong to a single orbit.

filled by level curves and the other is rather random and is devoid of level curves. This random region lies around the separatrix mentioned above (Fig. 4). The existence of level curves means the existence of isolating integrals, which can be identified as the invariant tori found by Kolmogorov. The instability region near the separatrix is also found in the magnetic surface in a plasma studied by Mel'nikov[33] and others.[34] Same kind of study is carried out by Walker and Ford[35] in a system with isolated or double resonances. All these studies show the existence of isolating integrals as well as the instability region arising from the amplitude instability. This is regarded to be

consistent with KAM theory. Furthermore according to Ford and Lunsford,[36] in the anharmonic oscillators with resonant nonlinear terms, for example, in a system with Hamiltonian

$$H=J_1+2J_2+3J_3+\gamma[\alpha J_1 J_2^{1/2}\cos 2(\varphi_1-\varphi_2) +\beta(J_1J_2J_3)^{1/2}\cos(\varphi_1+\varphi_2-\varphi_3)] \tag{7}$$

expressed in terms of action-angle variables, irreversibility occurs even in limit of $\gamma\to 0$. They showed this by calculating the instability region and the separation of two trajectories initially started with a small distance.

Recently Aizawa[37] discussed a nonlinear spring with the Hamiltonian

$$H=\frac{1}{2}\sum_{i=1}^{N}\dot{x}_i^2+\frac{1}{4}\sum_{i=1}^{N}(x_i-x_{i+1})^4. \tag{8}$$

He found the nonlinear normal modes and studied on computer their stability for the cases of $N=3$ and 4 by the method of Hénon and Heiles. In the unstable region where the isolating integral is missing, the system has a property of C-system just like the Ford-Lunsford[36] model discussed above. It is also surmised that for $N\to\infty$ the unstable region covers all the energy surface, and thus the system results in the thermodynamical state.

§6. Experiments on one- and two-dimensional vibrations

a. Models for computer experiments

In this section we consider the systems of one-dimensional lattice of $(N+2)$ identical particles as well as of two-dimensional square lattice of $(N+2)\times(N+2)$ particles, both with fixed-boundary conditions, interacting through quadratic harmonic potentials and quartic anharmonic potentials, i.e.

$$V(r)=\frac{1}{2}r^2+\frac{1}{4}\lambda r^4 \tag{9}$$

between nearest neighbors. As will be explained later, we have to make computer experiments with larger amplitudes in order to get thermal equilibrium. Larger amplitude might, however, cause the collapse of the lattice in case of cubic potential. The Hamiltonians of the systems considered here are assumed to be given for one- and two-dimensional cases respectively by

$$H_1=\frac{1}{2}\sum_{i=1}^{N}p_i^2+\sum_{i=0}^{N}V(x_{i+1}-x_i), \tag{10}$$

$$x_0=x_{N+1}=0,$$

and

$$H_2=\frac{1}{2}\sum_{i,j=1}^{N}p_{ij}^2+\sum_{i,j=0}^{N}V(x_{i+1,j}-x_{ij})+\sum_{i,j=0}^{N}\gamma V(x_{i,j+1}-x_{ij}), \tag{11}$$

$$x_{0,l}=x_{N+1,l}=x_{m,0}=x_{m,N+1}=0$$

$$l, m=0, \cdots, N+1,$$

where p_i's or p_{ij}'s are momenta of particles and the second and third terms in H_2 represent the central-force potentials and noncentral-force potentials between nearest neighbors respectively. The anharmonic coupling constant λ can be varied at our disposal. This enables us to see the effect of the anharmonicity upon the behaviors of our systems, which is impossible on using the δ-function type strong anharmonicity. Initially one of the normal modes is excited and the motion of all the particles are calculated using a set of differential-difference equations by means of the Runge-Kutta-Gill method. The energy of each normal mode and other necessary quantities are calculated. The normal modes of anharmonic lattices are defined, as mentioned in §3, as those of the corresponding harmonic lattice. Thus the energies of the harmonic parts of the total Hamiltonians H_1 and H_2 are given respectively by the normal coordinates Q_k's and Q_{ij}'s

$$\varepsilon_k=\frac{1}{2}(\dot{Q}_k^2+\omega_k^2Q_k^2), \tag{12}$$

$$\omega_k=2\sin\left(\frac{k\pi}{2(N+1)}\right), \tag{13}$$

$$\varepsilon_{ij}=\frac{1}{2}(\dot{Q}_{ij}^2+\omega_{ij}^2Q_{ij}^2), \tag{14}$$

$$\omega_{ij}=2\left(\sin^2\frac{i\pi}{2(N+1)}+\gamma\sin^2\frac{j\pi}{2(N+1)}\right)^{1/2}. \tag{15}$$

A useful check of consistency of numerical calculation is provided by the conservation of total energy defined by the sum of kinetic, harmonic and anharmonic potential energies. The conservation of energy was confirmed within the error less than 0.01% in all the calculations, on using the time increment of less than 1/50 of the period, $2\pi/\omega$, of the highest frequency mode.

Our computer experiments were done firstly in two-dimensional case[38] and thereafter in one-dimensional case,[39),*] with almost similar results for both ones. The advantage of the two-dimensional model over the one-dimensional one is that in the two-dimensional case one can choose elastic constant γ so as to make the distribution of normal frequencies convenient for our purpose,

*) The detailed reports of experiments described in this section are also given in these references.

by making some of the frequencies nearly equal to one another even in a system of small number of particles, although the two-dimensional system is accompanied with the inconvenience of providing larger boundary effect. For example, the frequencies and the periods of the normal modes in the case of $N=3$ (9 movable particles) and $\gamma=0.9$ are given in Table I, which shows that (1, 3), (3, 1) and (2, 2) modes have almost equal frequencies. As a consequence the resonance condition, proposed by Ford[12] and Jackson[13] will be satisfied, and the exchange of energy among normal modes will take place easily. Furthermore the periods of the normal modes lie in small range between 2.47 and 5.96, and this will give rise to the exchange of the energy among all normal modes in rather short computation time. In one-dimensional lattices, the distribution of normal frequencies depends only on the number of particles and the resonance condition mentioned above is supposed to be realized more easily in a system of much more particles. This circumstances, however, will be improved by introducing impurities with different masses and/or spring constants, as treated by Jackson, or by exciting a normal mode with larger energy. The latter attempt was achieved by Ooyama et al.,[39] and the result will also be described below.

Table I. Normal frequencies and periods in the case of $N=3$, $\gamma=0.9$.

Mode number	ω_{ij}	$2\pi/\omega_{ij}$
1, 1	1.06	5.96
1, 2	1.54	4.07
1, 3	1.91	3.29
2, 1	1.59	3.95
2, 2	1.95	3.22
2, 3	2.25	2.79
3, 1	1.99	3.17
3, 2	2.28	2.75
3, 3	2.55	2.47

b. Energy sharing among normal modes

Some characteristic behaviors of energy sharing among normal modes can be found in the square lattice of $N=3$ when we excite the (2, 2) mode with the anharmonic coupling constant $\lambda=0.5$ under the initial conditions

$$\begin{aligned} Q_{ij} &= \begin{cases} 2.0 & \text{for } (i,j)=(2,2) \\ 0 & \text{otherwise} \end{cases} \\ \dot{Q}_{ij} &= 0 \qquad \text{for all } (i,j). \end{aligned} \tag{16}$$

In all the experiments described here we take the initial conditions of zero initial velocities ($\dot{Q}=0$). Thus we do not repeat to write explicitly this condition in what follows. We find, as shown in Fig. 5, that at the initial stage, the energy of the (2, 2) mode is not transfered to the other modes appreciably and the motion itself seems periodic and stable, but, after an elapse of a certain amount of time, which we call the induction period, abrupt energy transfer to (1, 3) and (3, 1) modes takes place. The existence of the induction period implies that, during this period, the energies of the normal modes

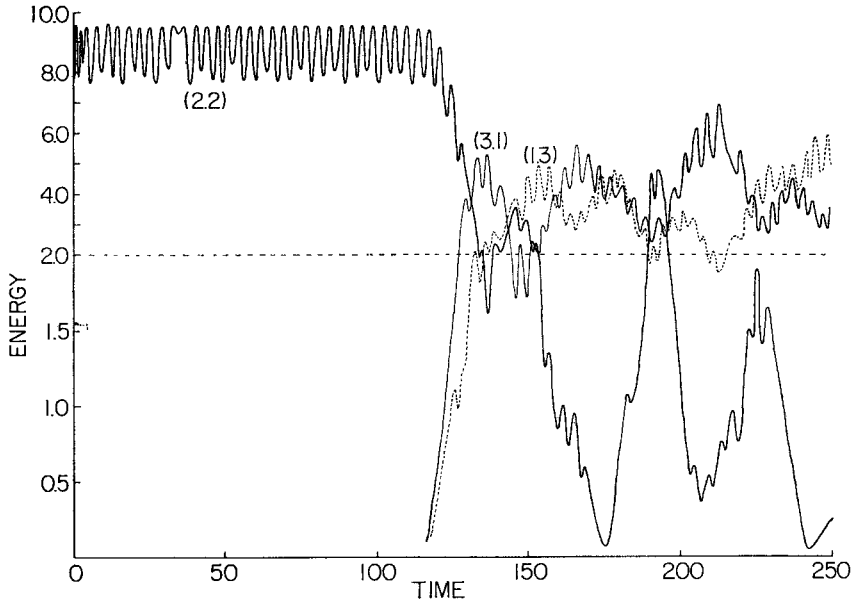

Fig. 5. Energy sharing among normal modes in a two-dimensional square lattice with $N=3$, $\gamma=0.9$ and $\lambda=0.5$. The (2, 2) mode only is excited.

other than the excited one (2, 2) increase slowly up to certain critical values. Thus if, besides exciting the (2, 2) mode initially, we excite all the other modes with very small amount of energies (for example about the order of 10^{-3} of the energy of the main excited mode), we expect that the induction period is reduced greatly and the thermal equilibrium is attained in a shorter time. Thus on exciting the (2, 2) mode by the initial conditions

$$Q_{ij}=\begin{cases}2.0 & \text{for } (i,j)=(2,2)\\ 0.1 & \text{otherwise,}\end{cases} \tag{17}$$

the induction period is found to become 1/4 of the case of Fig. 5 and almost all modes are excited at the final stage of computation.

The energy sharing among normal modes in two-dimensional lattice described above is achieved by the presence of resonance condition. However the resonance condition need not be satisfied strictly as pointed out by Jackson, provided that anharmonicity is large. Thus in a system without strict resonance condition or even in a one-dimensional system one can expect the same kind of energy sharing. This is really the case, and we find the induction periods also in one-dimensional anharmonic lattices.

Here we note that, because of the symmetry properties of the initial condition and the potential energy of quadratic and quartic types the even modes can never be excited, when an odd mode is initially excited. This

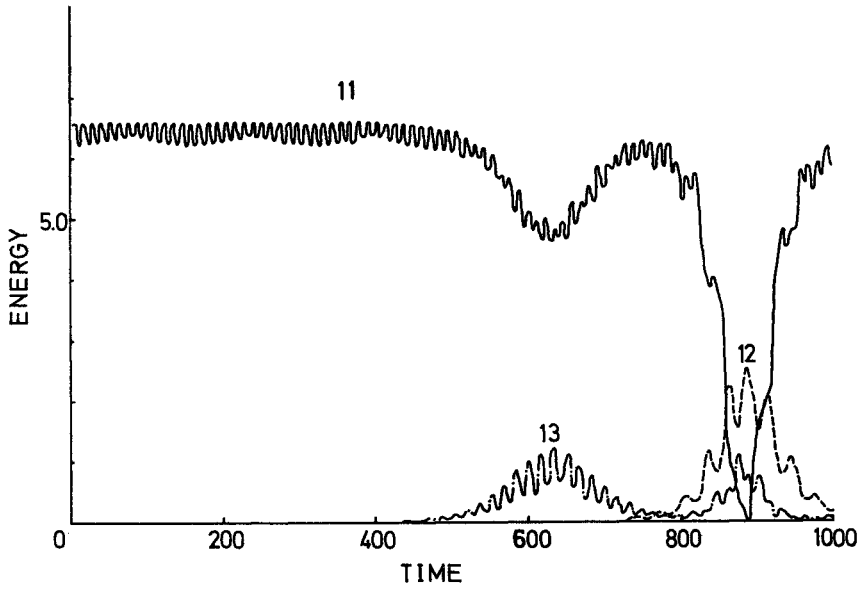

Fig. 6. Energy sharing among normal modes in a one-dimensional lattice with $\lambda=0.1$. The 11th mode is excited. The 9th mode becomes excited, but is omitted here. Single precision. In this connection an erratum should be made. In Fig. 7 in the previous paper[39] $\lambda=0.1$ should read $\lambda=0.088$.

symmetry, however, is easily broken by the presence of errors introduced in the process of computation, and therefore the even modes can be excited. This is seen in Fig. 6. When one excite the 11th mode, the 13th and 9th modes are easily excited after the elapse of the induction period and then the 12th mode begins to be excited. Clearly this is due to the computation errors. By a more precise calculation using the double precision program (see Fig. 7), we found that the 12th mode begins to be excited at a later time than the experiment given in Fig. 6. The induction period does not change and the computation result remains unaltered by the more precise calculation up to the time when the energy begins to be transferred to the 12th mode in Fig. 6. On the other hand in real physical systems, we never have such an ideal system as is completely isolated from the surrounding medium. The interaction of surrounding medium has the effect of introducing the errors of energies of the normal modes, although the total energy of the system is kept almost constant. In our present computer experiments, the computation errors do change the normal mode energies appreciably but do not destroy the conservation of total energy. As is mentioned already, a check of computation errors is done by the conservation of the total energy. Of course the errors of the conservation of the total energy increases gradually as the time proceeds, but we could not find the abrupt increase of the errors even when the 12th mode becomes excited. The computation errors are generally to be avoided,

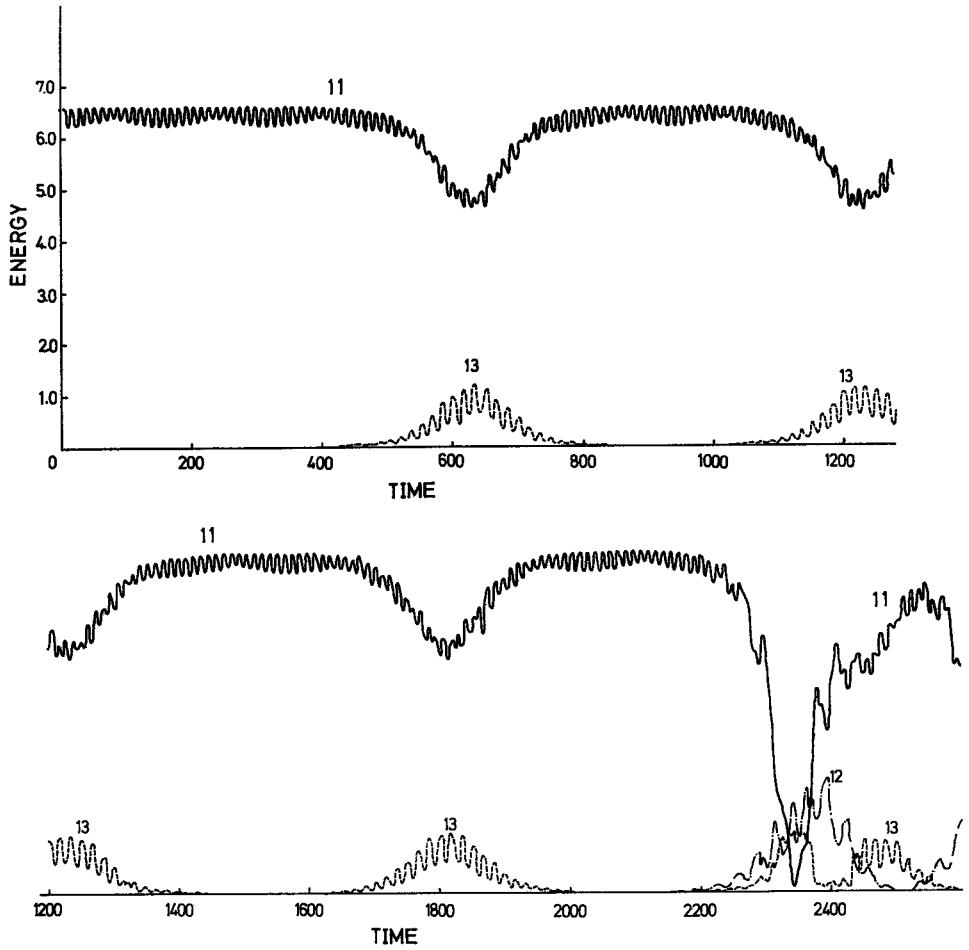

Fig. 7. Energy sharing among normal modes in a one-dimensional lattice with $\lambda=0.1$. Double precision. Compare Fig. 7 with Fig. 6.

but in our present purpose this effect turns out to be not always annoying but rather to be regarded positively as a necessary effect by interpreting it as the interaction of the surrounding medium in real systems. We adopt this view, but otherwise, our system is never ergodic.

Therefore after the elapse of the induction period we expect that all the modes are excited and the system reaches a thermal equilibrium. In anharmonic lattice vibration, however, the normal mode energies are not necessarily same to all the modes. It is better to see whether the velocities of the particles obey Maxwell distribution or not when the energy sharing among normal modes takes place. We found that the long time averages of the kinetic energies of individual particles tend to a constant value, and those of the products of the velocities of different particles have a tendency to vanish

after elapsing the induction period.[39] This also confirms the establishment of thermal equilibrium.

c. Induction period

The induction period found in the computer experiments described above seems to be an essential feature for the establishment of a thermal equilibrium in the anharmonic lattice vibration. For quantitative purpose, we define the induction period T by the time required for the energy of the initially excited mode to be reduced to the one half of the initial value. When other conditions are same, the induction period becomes larger, the smaller the coupling constant λ is. Figure 8 shows the relation between $1/T$ and λ. It is thus surmised that there exists a critical value λ_{c_2} under which the induction period becomes infinite and the system is not ergodic. However one has to notice that this result is obtained by admitting the computation errors. On decreasing λ, the induction period becomes long and thus the 12th mode becomes excited before the induction period elapses. As one sees in Fig. 7 which is obtained by a more precise calculation with the double precision program, the 13th and 9th modes only are excited and the system is periodic although at $t=2300$, the 12th mode becomes excited due to the computation errors. In this case of small λ, the induction period varies according to the degree of precision in the calculation. We can say that there is another critical value λ_{c_1}, under which only the 9th and the 13th modes are excited and the system behaves

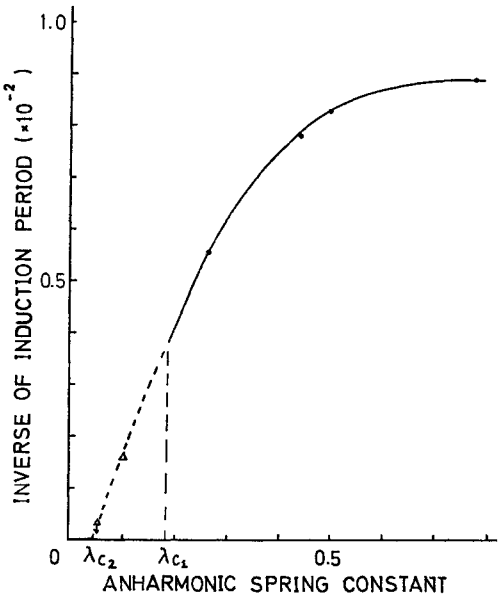

Fig. 8. Inverse of the induction period vs anharmonic coupling constant.

periodically until the 12th mode becomes excited. The inverse of the time necessary for these two modes to be excited lies on the extention of $1/T \sim \lambda$ relation. This is easily understood, because the induction period defined above is just the time necessary for the 13th mode to be excited.

d. Exponential lattice

As mentioned in §1, Toda[18] has found the "normal" modes*) and solitary waves (solitons) in an exponential lattice with the potential

$$V(r) = \frac{a}{b}(e^{-br} + br)$$
$$= \frac{a}{b} + \frac{ab}{2}r^2 - \frac{ab^2}{6}r^3 + \cdots, \tag{18}$$

where r is the deviation from the equilibrium distance of the neighboring particles and a and b are constants. The existence of stable "normal" modes or solitons seems contradictory to the ergodic properties of the anharmonic lattice. The stability problems of solitons are discussed by Ooyama et al.[20] Here we present the same kind of the experiments described above in the lattices of the potential (18). Figure 9 is the result of the calculation on the energy sharing among the modes when one excites the 11th mode ($N=15$, $a=0.471$, $b=2.127$, $ab=1$, $ab^2/2=1.06$), and shows that after the elapse of the induction period the system reaches a thermal equilibrium. On the other hand, Fig. 10 ($a=0.646$, $b=1.54$, $ab=1$, $ab^2/2=0.77$) shows rather periodic behavior. The anharmonicity in the potential is expressed by $ab^2/2$. This quantity is 0.77 for Fig. 10 but it is 1.06 for Fig. 9. For smaller $ab^2/2=0.5$ ($a=1$, $b=1$) we have striking periodic behavior as shown in Fig. 11, which corresponds to Fig. 7 in the quartic anharmonic potential.

In concluding this section, mention is to be made further. Chirikov et al.[40] made similar experiments on the system with the same Hamiltonian given by Eqs. (8) and (9), and found the same phenomena as ours. They considered as essential the time required for the energy sharing to take place among the modes including the eventh, and regarded it as a measure of instability. According to our present discussion, the computation errors are necessary for the complete energy sharing, but the measure of instability defined by Chirikov et al. is easy to change by different computer programs, and thus cannot be regarded as a characteristic quantity of the system. Recently Inoue[41] studied the system of two anharmonically coupled oscillators by the Mori[42] theory of

*) The meaning of "normal" mode used here is different from the normal mode without " " defined in the above section. The "normal" mode with " " is the motion of such a wave as its shape does not change with time.

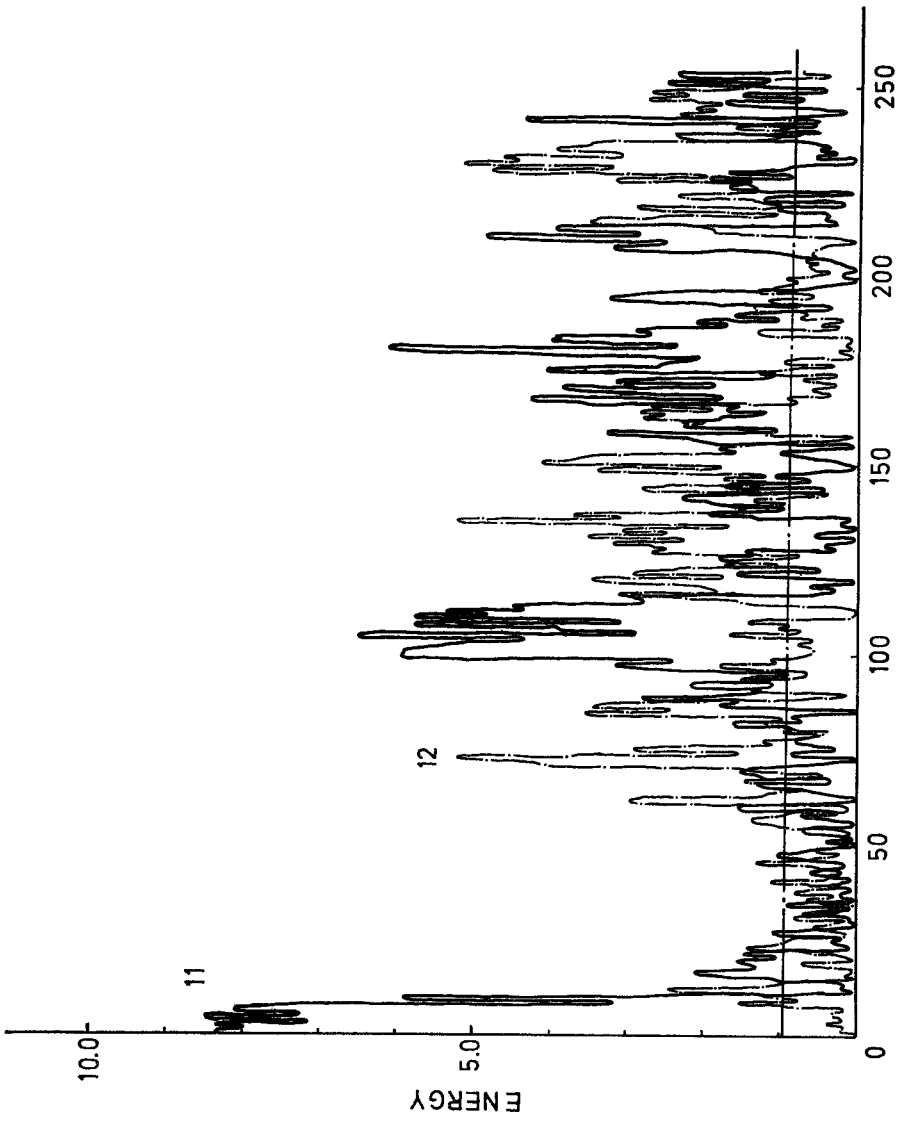

Fig. 9. Energy sharing in the exponential lattice. $N=15$, $a=0.471$, $b=2.127$, $ab^3/2=1.06$.

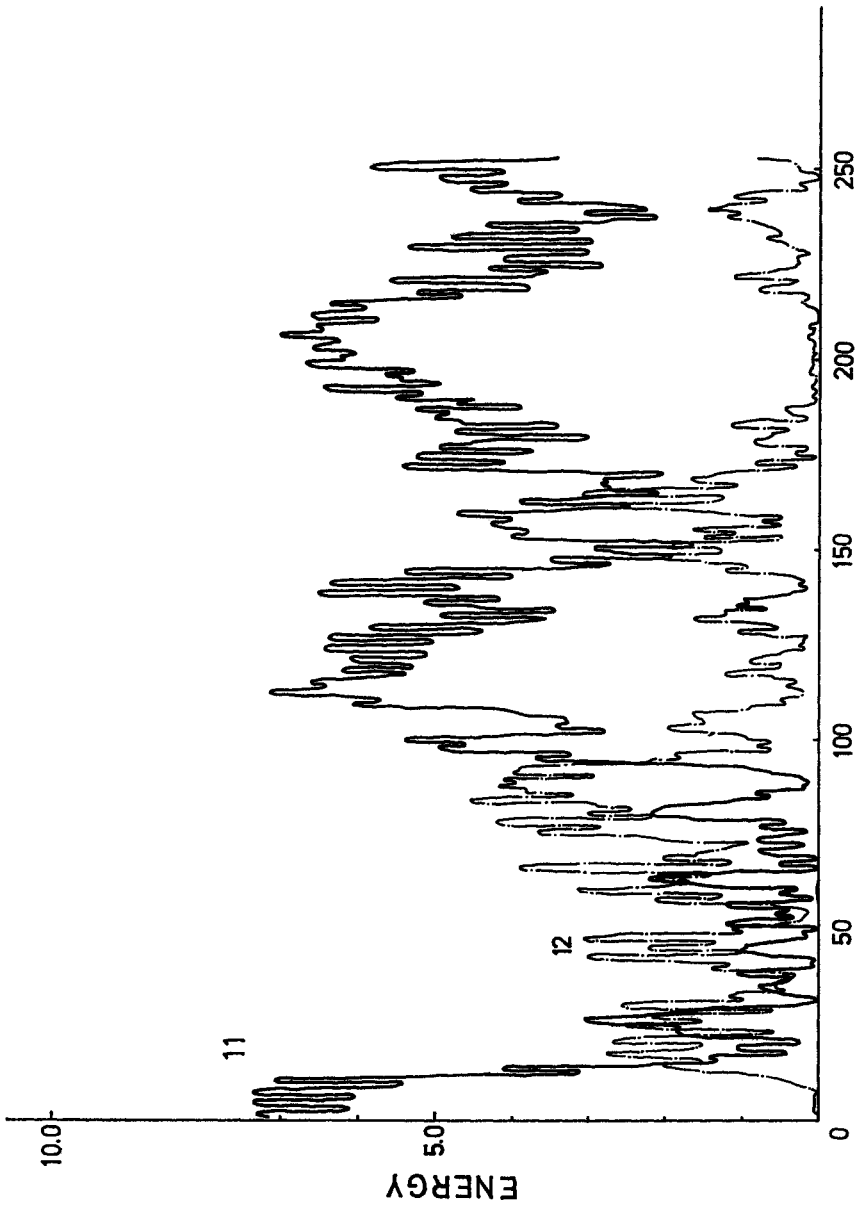

Fig. 10. Energy sharing in the exponential lattice. $N=15$, $a=0.646$. $b=1.54$, $ab^2/2=0.77$.

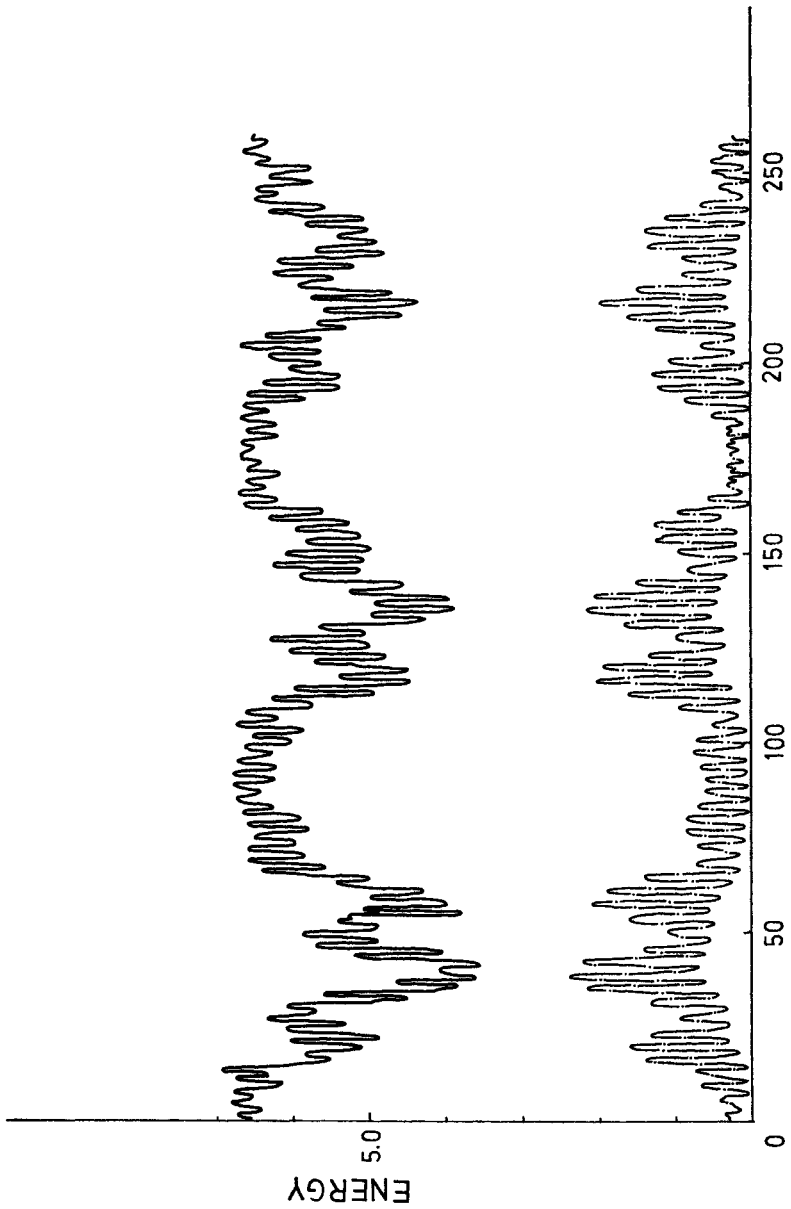

Fig. 11. Energy sharing in the exponential lattice. $N=15$, $a=1$, $b=1$, $ab^2/2=0.5$.

Brownian motion, and evaluated the frequency shift and the damping constant of the normal mode. Although the damping constant is shown to be anomalous at the resonance condition, it is rather periodic with positive and negative values alternately. It is expected that in the limit of large number of oscillators, the damping constant calculated in this manner really exhibits "damping".

§7. Discussion and quasi stochasticity

The recurrence phenomena and the non-ergodic properties of the anharmonic lattice vibrations found by Fermi et al.[10] and Saitô et al.[11] described in §3 can be explained by the result of Kolmogorov and others,[27] since as far as the anharmonic coupling constant λ is small, there exists invariant tori. We have also shown in §6 that there exists a critical value λ_c of the coupling constant λ so that depending on λ larger or smaller than λ_c, the system is ergodic or not. For $\lambda > \lambda_c$ the behavior of the system under the given initial condition is similar to those of the unstable region found by Hénon and Heiles[32] or by Ford and others.[35),36] These region, however, is not stochastic region in its strict meaning, because the behavior is completely deterministic as a solution of a set of differential equations. In spite of this, it is also to be noted that the use of the word "stochastic" in these region is not without reason. As shown in §§5 and 6, the behaviors of the systems in the unstable regions are irregular, oscillatory and aperiodic. Thus it would be better to say that the system is quasi-stochastic. It is difficult to define the degree of quasi-stochasticity, but whatever definition one may adopt, it is conjectured that the larger the system, the degree of quasi-stochasticity becomes larger.

In our experiments on anharmonic lattice vibrations, the computation errors which come in inevitably are found to play an essential role. We take into account positively the effect of the computation errors, since the initial conditions we adopted cannot give rise to the excitation of the even modes under mathematical rigor. Other initial conditions or other systems, such as having cubic potentials, do not require the computation errors. Chirikov[40] assigned the time required for the excitation of an even mode as a measure of the relaxation time to reach the equilibrium state.

In this paper we have presented the computer experiments made mainly in our laboratory, but still important problems remain unsolved. The studies for the case of cubic potentials, the effect of the impurities,*) and the dependence of the induction periods on the mode number or the number of particles etc. are now in progress, and other studies related to ergodicity as well are going on.

*) This was suggested by Professor Ford.

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