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Nonlinear Coupled Oscillators: Modal Equation Approach*

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A one-dimensional system of equimass particles coupled by identical nonlinear springs is studied. The equations of motion are expressed in terms of the normal coordinates of the corresponding linear system. Selection rules are developed for interactions among the modes, and the number of interaction terms in the modal equations is reduced by considering the case of a single dominant mode. The equations are considerably simplified by judicious approximation, and their validity checked by direct numerical computation. In terms of the resulting coupled Mathieu equations it is possible to investigate stability questions and to explain recent results of computational experiments. The bearing on ergodicity and time-correlation is discussed.

1. INTRODUCTION

Among the early problems run on the MANIAC I at Los Alamos almost 20 years ago was one suggested by Enrico Fermi. The computational capacity of this early computer was estimated to be sufficient for performing numerical experiments on the one-dimensional crystal studied by Peierls [1] in his classic paper. The plan was to numerically integrate the equation of motion of a linear array of 10–100 equimass particles connected by nonlinear springs. The end particles would be immersed in reservoirs (in some unspecified way), and the average energy of each particle would then be used to determine the thermal conductivity of the system as a function of the form and magnitude of the spring nonlinearity.

There seemed to be no particular reason for passing to the limit of a continuous system and then rediscretizing for numerical integration since the system to be modeled was already discrete and the effect of "Umklapp" terms [1] could not be

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excluded. It was expected that the number of particles would be varied, and this effect was also studied.

The program was set up (in machine language, of course) and tested by running the case in which the end particles were fixed in position and the springs were linear. A system of 64 particles was started in the lowest mode and integrated using the simple Euler's method over about 20 periods to check the accuracy of the numerical scheme with a satisfactory result. At this point it was decided to run the same problem with a quadratic term in the force law for the springs still keeping the ends fixed so that the approach to equipartition of energy could be observed. The unexpected results of these calculations, which show no tendency toward ergodicity, are contained in the report [2] referred to as FPU in the literature.

Since that paper there have been many studies of the FPU cases as well as the continuum model which have led to a fairly satisfactory understanding of certain of the original results. An interesting unpublished calculation was made by Tuck [3] quite early, one which brings home the nonergodic nature of the FPU case. In the original work, weak nonlinearities led to a quasirecurrence of the initial conditions to the extent that some 99 % of the total energy returned to the first mode, the one initially excited. Due to the inherent calculational error in the simple integration scheme being used, it was not possible to distinguish between the error and a real failure to attain the initial conditions more exactly so the computation was terminated. In a more accurate computation Tuck extended the run to find a somewhat lower peak for the energy in the first mode at roughly double the quasi-recurrence time. Further computation led to additional equally spaced diminishing peaks but then the peaks began to increase and finally achieved a value much closer to the initial state than had the first recurrence. This "superperiod" appears to belong to a smaller resonance denominator in the perturbation expansion than the one associated with the first recurrence.

There have been some recent calculations [4–6] of the original problem with reservoirs to study the lattice thermal conductivity, but the major activity [7–15] has centered on the ergodic problem. An important development was the discovery [16–19] that there is a "region of stochasticity" where the FPU system exhibits a behavior quite different from the original results and more like an ergodic system. This has been verified and the boundary of the region has been further studied [20–23].

When periodic or quasiperiodic motion of a dynamical system is the object of of study, it is most natural and useful to describe the system in terms of the normal modes of the linear system. In the case of nearest neighbor interaction, however, the description is simple in terms of the position variables but this simplicity does not carry over to the normal modes, most of which interact with each other. In this paper we carry out the transformation to normal modes and make successive simplifications to reduce the number of participating modes.

First, it is assumed that one mode is dominant so that its approximate behavior can be described independently of the changes in the remaining small amplitude modes. The observation that the modes which initially participate in the development of the system are those lying near the dominant mode allows a reduction in the number of equations that need to be considered. This simplification is tested empirically and shown to be a reasonable approximation. In terms of the simpler system, conclusions are drawn, one of the more important being the relation between the size of the nonlinear term and the onset of the instability of the dynamical equations which is a necessary condition for ergodicity.

2. Modal Equations of Motion

The system to be studied consists of $N + 1$ particles labelled 0, 1, 2,..., N from the left and all having the same mass. They are connected together into a one-dimensional system by identical springs and for the present purposes the end particles labelled 0 and N are fixed in position for all time. Dimensional units are chosen so that the particle masses and the linear coefficient (Hooke's law constant) for the springs are both unity. The system coordinates are the displacements of the particles from their equilibrium positions denoted by x_j for the particle labelled j and the corresponding velocities $\dot{x}_j$, positive displacements being measured to the right. For the present system,

$$\dot{x}_0(t) = x_0(t) = \dot{x}_N(t) = x_N(t) = 0. \tag{1}$$

The force exerted on particle j by particle $j - 1$ because of the spring connection is given by

$$F_j = x_{j-1} - x_j + \lambda(x_{j-1} - x_j)^2 + \mu(x_{j-1} - x_j)^3,$$

where λ and μ are constants and the equations of motion

$$\begin{aligned}\ddot{x}_j = {} & x_{j+1} - 2x_j + x_{j-1} + \lambda[(x_{j+1} - x_j)^2 - (x_j - x_{j-1})^2] \\ & + \mu[(x_{j+1} - x_j)^3 - (x_j - x_{j-1})^3] \qquad (j = 1, 2,..., N - 1)\end{aligned} \tag{2}$$

follow from the Hamiltonian

$$H = \sum_{j=1}^{N} [\dot{x}_j^2/2 + (x_j - x_{j-1})^2/2 + \lambda(x_j - x_{j-1})^3/3 + \mu(x_j - x_{j-1})^4/4]. \tag{3}$$

Due to the possible change in sign of the cubic part of the Hamiltonian, systems with nonlinearities arising from such terms can exhibit a "breaking of the chain"

and other anomolous behavior at large energies. Earlier studies included such systems but this paper will be confined to the case $\lambda = 0$.

Introduce normal modes through

$$x_j = i \sum_{k=-N}^{N} (a_k/\omega_k) \exp(-i\pi_j k/N), \tag{4}$$

where $\omega_k = 2 \sin(\pi k/2N)$. We chose these slightly nonstandard variables in order to keep the nonlinear term as simple as possible. For x_j to be real, i.e., $x_j = x_j^*$, we require $a_k^* = a_{-k}$ and the boundary condition (1) will be satisfied if $a_k = a_{-k}$. Substituting into the quartic term of the Hamiltonian, we find

$$\begin{aligned}\sum_{j=1}^{N} (x_j - x_{j-1})^4 &= \sum \frac{a_k a_{k'} a_{k''} a_{k'''}}{\omega_k \omega_{k'} \omega_{k''} \omega_{k'''}} \exp[-i\pi_j(k + k' + k'' + k''')/N] \\ &\quad \times [1 - \exp(i\pi k/N)][1 - \exp(i\pi k'/N)] \\ &\quad \times [1 - \exp(i\pi k''/N)][1 - \exp(i\pi k'''/N)] \\ &= \sum a_k a_{k'} a_{k''} a_{k'''} \exp[-i\pi(j - \tfrac{1}{2})(k + k' + k'' + k''')/N], \end{aligned} \tag{5}$$

where the sums extend over j and all k's. The relation $a_k = a_{-k}$ is used to eliminate the imaginary part of the exponential, and the j-sum becomes

$$\sum_{j=1}^{N} \cos[(j - \tfrac{1}{2})(k + k' + k'' + k''')\, \pi/N] = N \cdot D(k + k' + k'' + k'''), \tag{6}$$

where $D(0) = 1$, $D(\pm 2N) = -1$ and $D(\cdot) = 0$ otherwise.

Finally,

$$\sum_{j=1}^{N} (x_j - x_{j-1})^4 = N \sum a_k a_{k'} a_{k''} a_{k'''} D(k + k' + k'' + k'''), \tag{7}$$

where the right side sum is over all k's.

The complete Hamiltonian becomes

$$H = (N/2) \sum [(\dot{a}_k/\omega_k)^2 + a_k^2] + (\mu N/4) \sum a_k a_{k'} a_{k''} a_{k'''} D(k + k' + k'' + k'''), \tag{8}$$

with the equation of motion for normal mode k,

$$\ddot{a}_k = -\omega_k^2 a_k - \mu \omega_k^2 \sum_{k'k''k'''} a_{k'} a_{k''} a_{k'''} D(k + k' + k'' + k''') \tag{9}$$

or, in terms of the canonically conjugate $p_k = \partial H/\partial \dot{a}_k = (N/\omega_k^2)\, \dot{a}_k$,

$$H = \frac{1}{2} \sum \left[\frac{\omega_k^2}{N} p_k^2 + N a_k^2\right] + (\mu N/4) \sum a_k a_{k'} a_{k''} a_{k'''} D(k + k' + k'' + k'''). \tag{10}$$

3. Numerology

Single Mode Initial Excitation

In the case of a nonlinear term in the Hamiltonian, quartic in the coordinates, the D-function in (9) requires that for mode k to be excited by modes k', k'', k''', not necessarily distinct, the following congruence must be satisfied:

$$k \equiv (k' + k'' + k''')(\text{mod } 2N), \tag{11}$$

where use has been made of the fact that k and $-k$ are the same mode since a_k and a_{-k} satisfy the same equation.

An excited mode $k_0 (| k_0 | < N)$ can excite other modes given by

$$k \equiv (2j + 1)\, k_0 (\text{mod } 2N), \tag{12}$$

for *any* integer j. If a mode k is excited then $k \pm 2k_0$ can be excited by (11). Since k_0 is excited initially (12) follows by induction. Relation (12) is also sufficient because from (11) odd multiples of k_0 can only excite another odd multiple of k_0.

Writing (12) as an equality, it is evident that both sides can be divided by $d = (k_0, N)$, the greatest common divisor, thus, replacing (12) by its *irreducible form*

$$k/d \equiv (2j + 1)(k_0/d)[\text{mod } 2(N/d)], \tag{13}$$

where k_0/d and N/d are now relatively prime. It is assumed from now on that (12) is in irreducible form so that $(k_0, N) = 1$. This assumption is convenient since systems with the same irreducible form are dynamically similar.

From $(k_0, N) = 1$ it follows that $(k_0, 2N) = 1, 2$ according to whether k_0 is odd or even. For odd k_0,

$$(k_0, 2N) = 1 = sk_0 + 2tN, \tag{14}$$

for some integers s and t from the Euclidean algorithm. It is clear s must be odd, and the second equality is just (12) with $k = 1$, from which it follows that *all* odd modes are excited from k_0. If k_0 is even, hence, N odd, $(k_0, 2N) = 2 = sk_0 + 2tN$. There is always a solution with odd s for if s were even, then

$$2 = sk_0 + 2tN = (s + N)\, k_0 + (2t - k_0)\, N = s'k_0 + 2t'N \tag{15}$$

leads to an odd s'. Thus, we have (12) with $k = 2$. Let $k_0 = 2$, then from (12) all modes twice an odd integer are excited. Moreover, for each such, another solution of the congruence is $k = 2(2j + 1 - N) \equiv 2(N - 2j - 1)(\text{mod } 2N)$, which is twice a distinct even integer since N is odd. Thus *all* even modes are included.

It follows immediately from the preceding that if $k_0 = 1$ and $N = 2, 3$ then no other mode is excited. Similarly, if $k_0 = 2$ and $N = 3$ no further excitation occurs. These results may be combined and generalized to *reducible* k_0, N by the following corollary.

COROLLARY. *If* $k_0 = 2N/3$, $2N/4$, *or* $2N/6$ *no further excitation occurs and* k_0 *is a stable mode.*

Multiple Initial Excitation

If more than one mode is present initially, interactions take place which result in richer spectra. This is particularly true when initial modes have opposite parity, but even with modes of the same parity, the stability described previously may be lost.

It suffices to consider only two of the initially excited modes—of opposite parity if possible. As before, assume the system is in irreducible form, i.e., if k_{0i} and k_{0j} are the two initial modes in a system of $N + 1$ particles, then the greatest common divisor $d = (k_{0i}, k_{0j}, N) = 1$.

The main result is: *If* k_{0i} *and* k_{0j} *are of opposite parity, all modes* k *are excited; if not, then all modes of that parity are excited.*

Consider first the case of opposite parity. Let $k_{0i} = u$ (ungerade) be the odd, and $k_{0j} = g$ (gerade) the even mode. From the congruence (11), excited states are given by

$$k \equiv (au + bg) (\text{mod } 2N), \tag{16}$$

where a, b are integers such that $a + b$ is odd. The latter follows immediately by induction.

For this case

$$(u, g, 2N) = 1 = ru + sg + 2tN, \tag{17}$$

where $r + s$ is odd or can be made so by:

$$ru + sg = ru + gu + sg - ug = (r + g)\, u + (s - u)\, g = r'u + s'g, \tag{18}$$

where r' has the same parity as r but s' has opposite parity from s, so $r' + s'$ is odd [24]. Thus, (17) has the form of (16) with $k = 1$. It is clear how (11) can be used with $k = 1$ and an even mode to generate all modes.

For two odd modes

$$(u_1, u_2, 2N) = 1 = ru_1 + su_2 + 2tN, \tag{19}$$

where $r + s$ must be odd to satisfy this equation so we are assured of a solution of

$$1 = (au_1 + bu_2)(\text{mod } 2N), \tag{20}$$

for $a + b$ odd corresponding to (16). With $k = 1$ and no even modes, all odd modes and only odd modes can be reached with (11).

Finally, with two even modes,

$$(g_1, g_2, 2N) = 2 = rg_1 + sg_2 + 2tN, \tag{21}$$

where N must be odd and s can be made to have opposite parity from r by using (15), so that the solution,

$$2 = (ag_1 + bg_2)(\text{mod } 2N), \tag{22}$$

can be used with (11) to generate all even modes.

EXAMPLE a. Let $k_0 = 4$, $N = 18$. Since $(4, 18) = 2$, $2 \to k_0$, $9 \to N$; since k_0 is even, all even modes less than N are excited, namely: 2, 4, 6, 8.

EXAMPLE b. Let $k_0 = 4$, $N = 17$. Irreducible. All even modes to $k = 16$ are excited.

EXAMPLE c. Let $k_0 = 3$, $N = 21$. Thus $(3, 21) = 3$, $1 \to k_0$, $7 \to N$; all odd modes 1, 3, 5 excited.

EXAMPLE d. Let $k_0 = 5$, $N = 22$. Irreducible. All odd modes 1, 3,..., 21 excited.

EXAMPLE e. Let $k_0 = 5$, $N = 15$. Since $k_0 = (2N/6)$, this is a stable mode, no others are excited.

EXAMPLE f. Let $k_{01} = 4$, $k_{02} = 6$, $N = 22$. Since $(4, 6, 22) = 2$, $2 \to k_{01}$, $3 \to k_{02}$, $11 \to N$; all states of irreducible form are excited; all even states of reducible form excited.

4. COMPUTATIONAL SCHEME

The numerical work was performed on the MANIAC II at the Los Alamos Scientific Laboratory. Its characteristics are implied by its multiplication time and memory access of 6μ's and 3μ's, respectively. More important is the convenience and directness afforded by the MADCAP programming language [25]. Single precision is represented by 43 binary bits ($\sim$13 decimal digits). Full precision in the

initial conditions was achieved by first using double precision arithmetic and then rounding to standard word length.

Some preliminary numerical experiments were made to determine a satisfactory integration scheme. Several Runge–Kutta methods were examined; using the total energy of the system as a criterion, it was found that an approach due to Butcher [26], specifically his formula 3, was sufficiently accurate with integration steps of $\Delta t = 0.01$ that the truncation error was of the same order of magnitude as the rounding error. Even for long runs of several thousand time units and for relatively large nonlinear terms, the energy check rarely exceeded one part in 10^5, and was usually much better. Moreover, if the initial conditions, i.e., the initially excited modes, were of one parity, that parity was retained throughout the calculation; thus, checks on the error-free operation of the computer were available. In addition, there was a more quantitative control over the introduction of small amounts of initial modes of opposite parity—so-called seeding.

In general, the one-dimensional displacement coordinate x_j (from equilibrium) and the associated velocity $\dot{x}_j$ were taken as dependent variables. At regular time intervals, Fourier analyses of these coordinate and velocity profiles were made so as to determine modal amplitudes a_k and $\dot{a}_k$. From these, the uncoupled linear modal energies were obtained.

It was of interest to examine the behavior with time of the nonlinear modal energies including the coupling terms. The energy terms associated with each mode were those that corresponded to terms occurring in the modal equations of motion. The number of such terms increases rapidly with N; however, it was straightforward to compute such modal energies for $N \leqslant 8$.

5. Integration of Modal Equations

The FPU and later studies seem to show that for small nonvanishing values of the nonlinear coefficient the systems are periodic to the accuracy of the calculations. This is especially clear in some of the recent work [18, 22], where it is shown by means of extrapolation of the relation between the lifetime of an initially excited single mode and the nonlinear parameter. The situation is that we have a system where, at $\mu = 0$, there are normal modes with an infinite lifetime. By continuity, it is expected that by taking μ sufficiently small any arbitrarily given lifetime can be exceeded, but the unexpected result is that this can be achieved for a $\mu > M > 0$, for some M.

Although the normal modes occupy a special position, being the infinite lifetime states for $\mu = 0$, it is likely that there are similar states for other values of μ. Configurations which are stable for nonzero values of μ have been found and are called "solitons" [27, 28]. It is possible that there are disjoint ranges of μ over

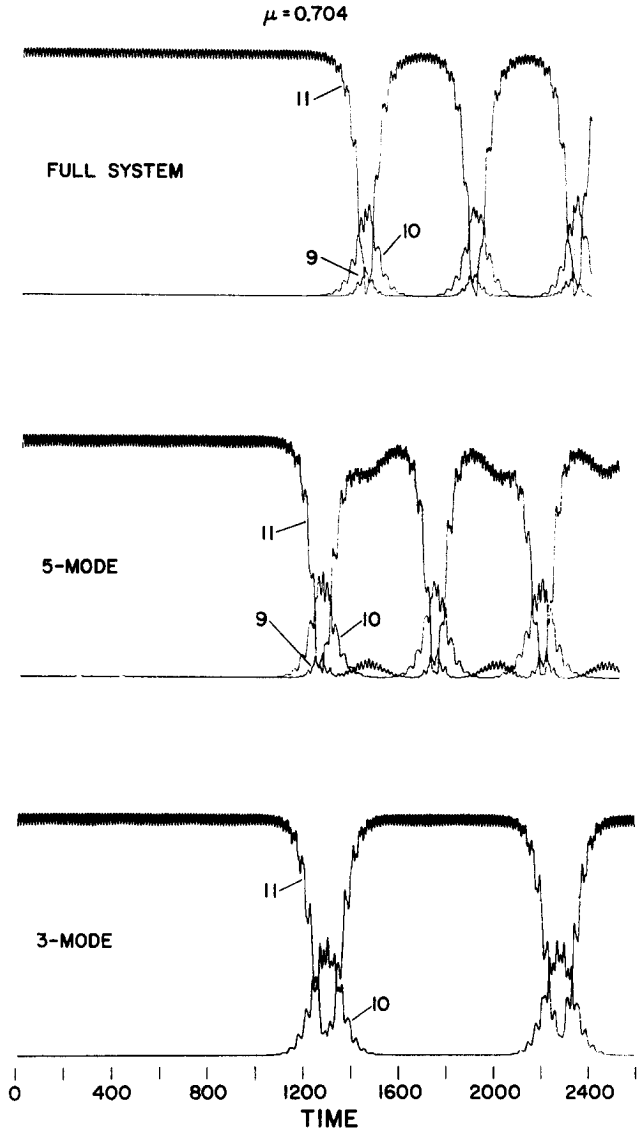

FIG. 1. Plot of three modal energies for the system and two approximations. The full system was integrated using the original coordinates, whereas the 5- and 3-mode systems were integrated directly in terms of the modal amplitudes. The value of σ (cf., Eq. (27)) for these systems was 0.042.

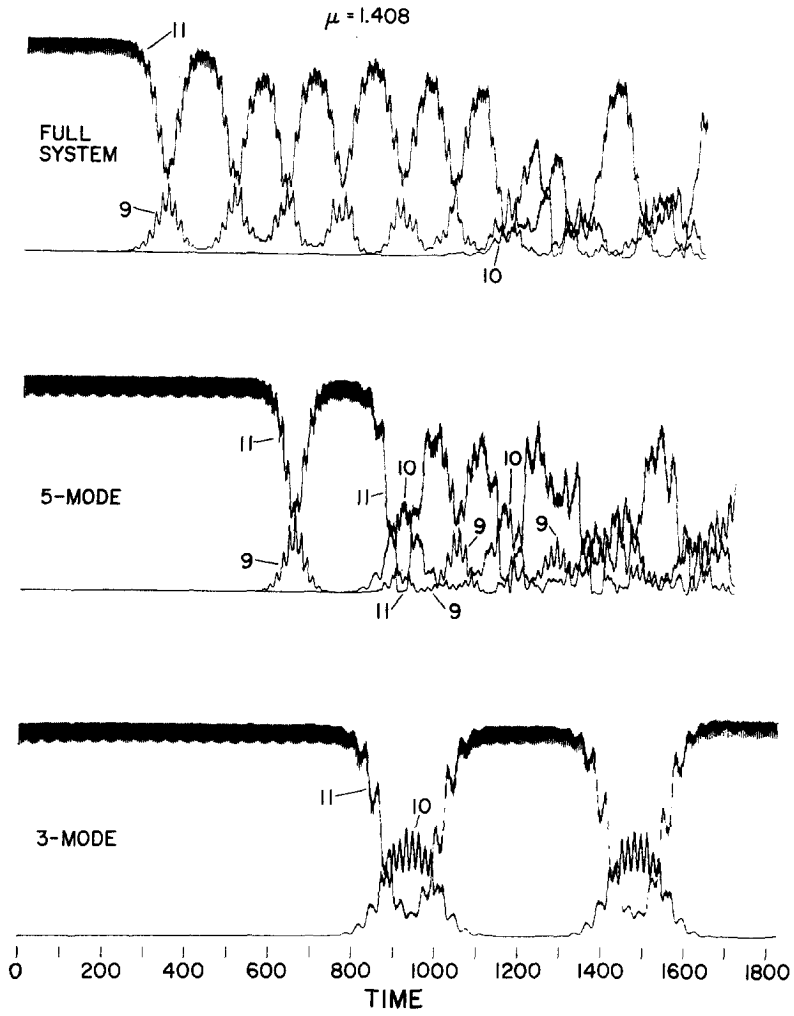

FIG. 2. A similar plot to Fig. 1 with a value of $\sigma = 0.085$.

which the lifetimes of these states are infinite or at least very long. The normal modes are the simplest, however, and in view of this discussion may not be so special as they first appear.

It would be useful, therefore, to study the system in terms of the a_k variables. Unfortunately, the number of terms in the normal mode equations is of order N^3 and the equations become unmanageable for reasonably sized N. The usual procedure for integrating the full system is to carry out the dynamic calculation in coordinate space and then transform to the a_k variables when needed for output.

Of particular interest is the system [22] in which most of the energy was initially in mode 11 with $N = 16$. It was observed that for small μ, the bulk of the energy was retained in the 11th mode for a long time before energy sharing commenced. The present paper is concerned mainly with that system, specifically the early phases.

The final degradation of mode 11 occurs because some of the modes which were initially small grow to a size comparable to mode 11. It is found that the modes that are the main participants in this action are the neighboring modes 9, 10, 12, and 13. By restricting our attention to five modes, the number of nonlinear terms in the modal equations is reduced to 49. For the system involving modes 10, 11, and 12 the number of terms is 10. It, therefore, becomes possible to integrate the modal equations directly and the results for 5-mode and 3-mode systems are shown for two values of μ in Figs. 1 and 2 together with the integration of the full equations carried out in coordinate space. The 3-mode system is, for example,

$$\ddot{a}_k + \omega_k^2(a_k + 3\mu f_k) = 0 \qquad (k = 10, 11, 12), \tag{23}$$

where

$$\begin{aligned} f_{10} &= a_{11}^2(2a_{10} + a_{12}) + a_{10}(2a_{12}^2 + a_{10}^2), \\ f_{11} &= a_{11}^3 + 2a_{11}(a_{10}^2 + a_{10}a_{12} + a_{12}^2), \\ f_{12} &= a_{11}^2(2a_{12} + a_{10}) + a_{12}(2a_{10}^2 + a_{12}^2). \end{aligned} \tag{24}$$

Figure 1 describes a system in which mode 11 is stable until modes 10 and 12 appear; at this point mode 11 decays and a copious interchange of energy among the modes occurs, a process referred to as "induction." The detailed correspondence of the full system with the 3-mode and 5-mode systems is seen to be quite acceptable, at least to induction time.

The system in Fig. 2 exhibits some new features. There are some interchanges between mode 11 and modes 9 and 13. This is precisely the behavior found in the FPU cases and a quasiperiodicity might be expected. Again, however, the even modes adjoining 11 grow and cause induction at the last part of the run. Although the detailed correspondence is not so good at this larger value of σ, the induction by mode 10 is qualitatively correct. Mode 9 appears earlier in the full system as compared to the 5-mode system owing to the presence of mode 1 which couples to 9 according to (11). The important occurrence is the first appearance of the even modes adjoining mode 11.

In all of these runs a small amount of energy ($\sim 10^{-17}$) was placed in the even modes initially, The even modes are prohibited from participating if they start with zero amplitude by the results of Section 3. It is found [18, 29] that the growth of the even modes is exponential for sufficiently large μ. A logarithmic plot of a typical

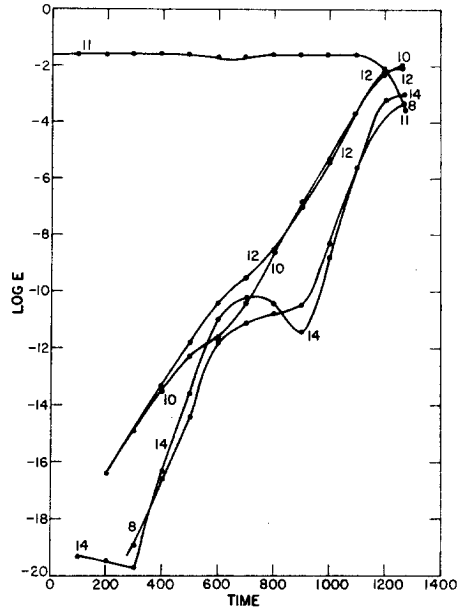

FIG. 3. Logarithm of the modal energy for $\sigma = 0.056$ with initial seeding in all modes. The dip in mode 11 and the erratic behavior around $t = 650$ is probably an FPU cycle before induction at $t = 1200$.

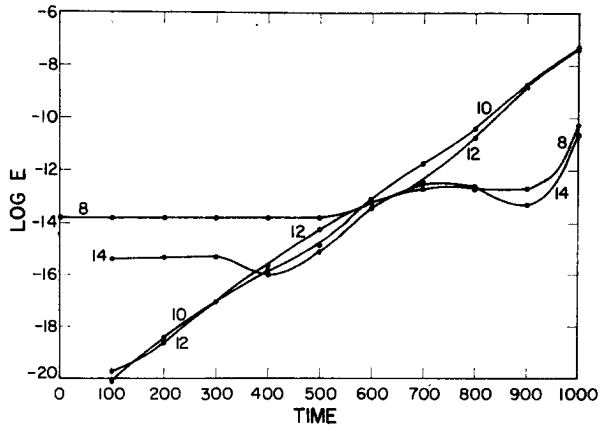

FIG. 4. Logarithm of the modal energy for $\sigma = 0.056$ with initial seeding of mode 8.

even mode growth is given in Figs. 3 and 4. It is interesting to note that even when the 8th mode only is "seeded" initially, modes 10 and 12 grow exponentially and cause the eventual decay of 11 as shown in Fig. 4.

6. Coupled Mathieu Equations

Equations (23) for three modes and the 5-mode equations describing the inter-

of the system, particularly the growth of the small amplitude modes which eventually cause the decay of the principal driving mode. In this section further simplifications of the reduced Eqs. (23) will be carried out. Although this will bring about a somewhat poorer quantitative agreement with the full integration scheme, the qualitative features of the system are preserved and the analytic tractability of the resulting equations will be of heuristic value in understanding the behavior of these systems.

It was possible to reduce the number of modes under consideration because the system was one in which a single mode was dominant, and, at least for the particular mode chosen, it was observed that only neighboring modes participated in the initial phases. Besides reducing the number of equations, the dominance of a single mode allows further approximations, namely the retention of only those nonlinear terms containing the principal mode as a cubic or quadratic in which case the system (23) becomes:

$$\begin{aligned} \ddot{a}_{10} &= -\omega_{10}^2 a_{10} - 3\mu\omega_{10}^2 a_{11}^2(2a_{10} + a_{12}), \\ \ddot{a}_{11} &= -\omega_{11}^2 a_{11} - 3\mu\omega_{11}^2 a_{11}^3, \\ \ddot{a}_{12} &= -\omega_{12}^2 a_{12} - 3\mu\omega_{12}^2 a_{11}^2(2a_{12} + a_{10}). \end{aligned} \tag{25}$$

The energy in the 11th mode is substantially constant until the other modes reach a significant size so the energy integral for that mode can be approximated by

$$N[(\dot{a}_{11}/\omega_{11})^2 + a_{11}^2 + \tfrac{3}{2}\mu a_{11}^4] = N(\alpha_{11}^2 + \tfrac{3}{2}\mu\alpha_{11}^4), \tag{26}$$

where $\alpha_{11} \equiv a_{11}(0)$ and the system is initially at rest. Now let

$$\begin{aligned} a_{11} &= \alpha_{11}\cos\phi, \\ \sigma &= \tfrac{3}{2}\mu\alpha_{11}^2, \\ m &= \sigma/(1 + 2\sigma), \\ \tau &= (1 + 2\sigma)^{1/2}\,\omega_{11}t, \end{aligned} \tag{27}$$

then (26) becomes

$$(d\phi/d\tau)^2 = 1 - m \sin^2 \phi, \tag{28}$$

describing an elliptic function of the first kind with period

$$T_\tau = (1 + 2\sigma)^{1/2}\, \omega_{11} T = 4 \int_0^{\pi/2} \frac{d\phi}{(1 - m \sin^2 \phi)^{1/2}} \equiv 2\pi J(m). \tag{29}$$

The corresponding angular frequency is given by

$$\Omega_{11} = 2\pi/T = (1 + 2\sigma)^{1/2}\, \omega_{11}/J(m). \tag{30}$$

Using $a_{11} = \alpha_{11} \cos \phi$ in the remaining two equations of (25) we find

$$\begin{aligned} \ddot{a}_{10} &= -\omega_{10}^2 a_{10} - 2\omega_{10}^2 \sigma(\cos^2 \phi)(2a_{10} + a_{12}), \\ \ddot{a}_{12} &= -\omega_{12}^2 a_{12} - 2\omega_{12}^2 \sigma(\cos^2 \phi)(2a_{12} + a_{10}). \end{aligned} \tag{31}$$

These equations were integrated with (28) until a_{10} and a_{12} became comparable with a_{11}. The growth of these modes is exponential and the logarithm of the rate measured in decades per thousand time units is plotted as a function of σ and marked "coupled system" in Fig. 5. Additional values for runs using the complete

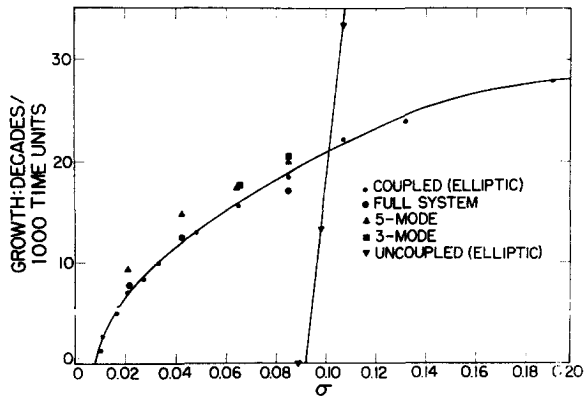

FIG. 5. Comparison of growth rates for different approximations to $N = 16$ coupled and uncoupled systems.

set of equations and the reduced set of the last section are also shown. The shape of this curve is to be compared with Fig. 10 of [22].

If ϕ in (31) can be approximated as Ωt with constant driving frequency Ω, which is the case for small σ, then the system consists of two coupled Mathieu equations.

Letting $\tau = \Omega t$ be the independent variable, and using (30), we bring Eq. (31) to the form:

$$\begin{aligned} \ddot{a}_{10} + [J(m)(\omega_{10}/\omega_{11})]^2 [a_{10} + ma_{12} + m \cos 2\tau(2a_{10} + a_{12})] = 0, \\ \ddot{a}_{12} + [J(m)(\omega_{12}/\omega_{11})]^2 [a_{12} + ma_{10} + m \cos 2\tau(2a_{12} + a_{10})] = 0. \end{aligned} \tag{32}$$

If these equations are decoupled by removing a a_{12} from the first equation and a_{10} from the second, each takes on the canonical form of a Mathieu equation:

$$\ddot{y} + (a + 2q \cos 2\tau)\, y = 0, \tag{33}$$

where for the first, for example:

$$\begin{aligned} a &= [J(m)\ \omega_{10}/\omega_{11}]^2 \approx (1 + m/2)(\omega_{10}/\omega_{11})^2, \\ q &= ma. \end{aligned} \tag{34}$$

The growth of a mode will depend, in this case, on how close the quantity a is to unity, and on the magnitude of q. The growth rate can be found on the chart of the characteristic exponent shown in Fig. 6. To first order, the boundaries of the instability region are given by $a = 1 \pm q$ [30]:

$$\begin{aligned} [J(m)\ \omega/\omega_{11}]^2 \approx (1 + m/2)(\omega/\omega_{11})^2 = 1 \pm m(\omega/\omega_{11})^2, \\ m = 2[1 - (\omega_{11}/\omega_{12})^2],\ 2/3[\omega_{11}/\omega_{10})^2 - 1] = 0.19,\ 0.08, \end{aligned} \tag{35}$$

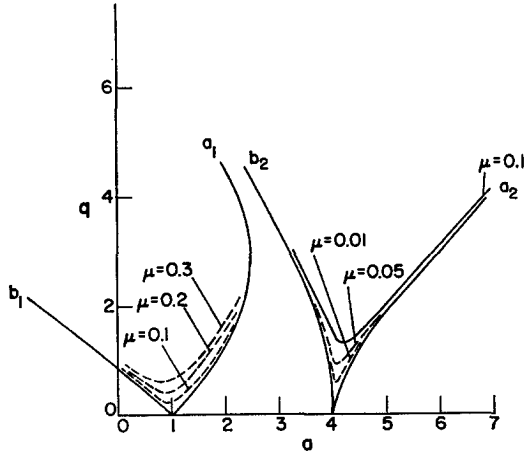

FIG. 6. Growth rate $\exp(\mu\tau)$ for unstable regions of Eq. (33).

so that exponential growth of mode 10 can be expected to begin at $m = 0.08$, hence, $\sigma = 0.095$. The uncoupled equations were integrated numerically and the results plotted in Fig. 5 showing good agreement with the calculated value.

The important point is that the behavior of the uncoupled cases is quite different from the coupled cases as brought out in Fig. 5. This can be understood in the following way. The natural frequencies of the mode 10 coupled with mode 12 system will vary between ω_{10} and ω_{12}, roughly, according to

$$\sin[(\omega_{10} + \omega_{12})/2] \cos[\omega_{10} - \omega_{12})/2]$$

slowly varying around the average $(\omega_{10} + \omega_{12})/2$, a frequency much closer to ω_{11} than was ω_{10} or ω_{12}. It can be expected, therefore, that instability will occur for a smaller value of σ and the growth rates will increase more slowly. In fact, a formula of the form (35) with $(\omega_{10} + \omega_{12})/2\omega_{11}$ substituted for ω/ω_{11} can be conjectured:

$$\sigma \approx A\left[\left(\frac{2\omega_{11}}{\omega_{10} + \omega_{12}}\right)^2 - 1\right] = A\left[\sec^2 \frac{\pi}{2N} - 1\right] \approx A\frac{\pi^2}{8N^2}, \qquad (36)$$

depending only on N and independent of the driving mode. Several computer runs with $N = 8$ and $N = 32$ were made for comparison with the $N = 16$ runs and are plotted in Fig. 7. Runs at $N = 32$ but without the approximation $\phi = \Omega t$ (i.e., the elliptic equation for mode 11 was integrated at each step) were made to show the agreement for small σ and are also shown. For $A = 2$ we find $\sigma_{cr} = 0.04$,

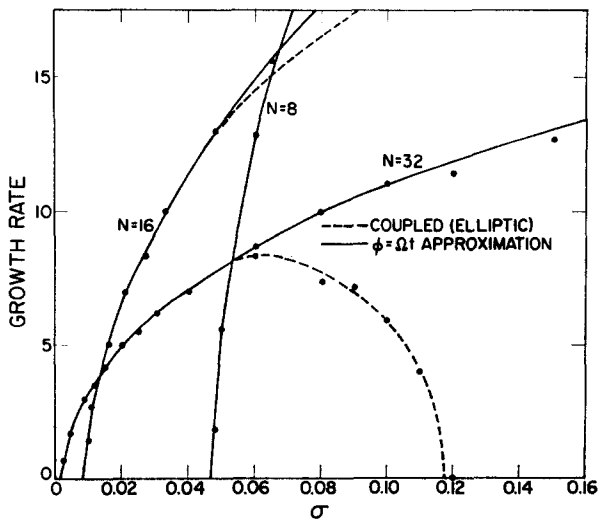

FIG. 7. Growth rate for different values of N and for $\phi = \Omega t$ approximation.

0.01, 0.0025 for $N = 8, 16, 32$, respectively, and in substantial agreement with the computed values. Some of the values used for Figs. 5 and 7 are given in Table I.

In the equation of motion (9), it is evident that a coefficient of the linear term could be given any value, except 0, by an appropriate change in the time scale. All

TABLE I

Comparison of Growth in Decades/Thousand Time Units for Full Equations, 5-Mode, 3-Mode, Coupled Mathieu with Elliptic Function Driver, and Coupled Mathieu with $\phi = \Omega t$.

σ	Full equations	5-mode system	3-mode system	Coupled Mathieu system	Coupled Mathieu $\phi = \Omega t$
0.021	7.8	9.3	—	7.0	7.0
0.042	12.6	14.8	14.9	12.5	11.2
0.064	—	17.4	—	15.5	14.8
0.085	17.0	19.9	20.5	18.5	16.9

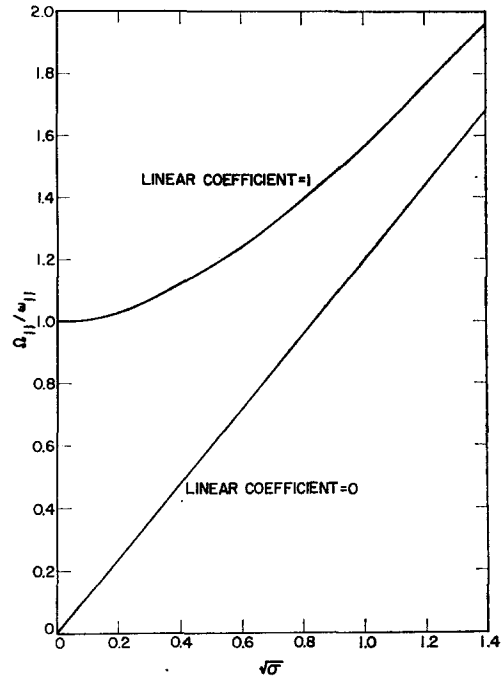

FIG. 8. Variation of the dominant frequency with σ with and without linear term.

cases will, thus, have been considered if the values 0 and 1 for the linear coefficient are investigated. Moreover, when the linear term is absent, changes in μ or in initial amplitudes are equivalent to a change in time scale so that, given N, only a single problem need be run for a given distribution of the initial excitation. The drawback of studies on problems with no linear term is that the plots of the linear modal energies contain a kinetic energy term only and the graphs tend to be more jagged because they fail to account for an appreciable amount of energy.

In the case of no linear term or if $\sigma \gg 1$, then $m \to \frac{1}{2}$ and $J(m) \to 1.18$; thus, asymptotically, $\Omega_{11} \approx 1.20(\sigma)^{1/2}\, \omega_{11}$, equality holding when the linear coefficient is 0. A plot of Ω/ω vs $(\sigma)^{1/2}$ for the cases of linear coefficients 0 and 1 is given in Fig. 8.

7. Growth of Small Modes—Stability

It is, of course, only under the unusual circumstances of stability given in Section 3 that a single mode will not excite others. In general, when a single mode is excited at one phase of the oscillation other modes will be seen if a snapshot is taken at a different phase. Moreover, one can expect modes not prohibited by the selection rules of Section 3 to begin to grow. The manner in which these other modes grow is crucial to any discussion of ergodicity.

The notions of irreversibility and ergodicity are connected with the behavior, over long times, of the difference between trajectories in phase space of two systems whose initial states differ only slightly. The exponential divergence of such trajectories, in time, signals the irreversible behavior of the system and also forms a basis for the expectation that the mapping of at least one small neighborhood will inhabit larger and larger regions of the phase space and even at an exponential rate. The time scale for ergodicity is as relevant as its existence since a system which resists ergodicity over times comparable with those appropriate to the observed physical phenomena cannot be assumed to be ergodic in deriving the description of those phenomena.

To study this behavior one could form the difference of the equations of motion describing two initially close systems. Alternatively, a small amount of energy could be put in modes otherwise forbidden by the selection rules. Thus, the energy in these "seeded" modes can be studied as a function of time and compared with the unperturbed situation in which the energy in those modes is strictly zero. This is the case studied here with the further simplifying assumption that only one mode is excited initially. In the event that more than one mode is initially excited a strong interchange of energy will cause changes in the frequencies of those modes since they are amplitude dependent and the consequent variation of Ω complicates the simple Mathieu analysis given in Section 6 so that the critical value of σ is thereby changed. No experiments were performed along these lines.

On the other hand, the goal of the present study is to show how a highly ordered system randomizes, in some sense, so that the choice of an initially ordered system with a single mode excited is quite natural.

The two systems are the set of Eq. (9) and the same set with a_k replaced by $a_k + \epsilon_k$. The differences of these equations are

$$\ddot{\epsilon}_k = -\omega_k^2 \epsilon_k - 3\,\mu\omega_k^2 \sum_{k'k''k'''} \epsilon_{k'} a_{k''} a_{k'''} D(k + k' + k'' + k'''), \tag{37}$$

where terms quadratic and cubic in ϵ_k have been dropped. If we restrict the a_k to a

effect of initial error in the specification of the system. The growth of $\epsilon_k(0)$ seed is the growth of initial error of this magnitude and the induction time is also the time when the system has "forgotten" the initial state. Any intrinsic uncertainty in the initial state will determine a "memory time" for the system and configurations further apart in time than this amount will be uncorrelated. An initial ball in phase space can be expected to grow exponentially in at least one dimension for values of σ above some critical value.

On the other hand it should be mathematically possible, subject to the restrictions imposed by the growth of roundoff error, to integrate the equations backward in time ($-\Delta t \rightarrow \Delta t$) to the initial state. *This is possible even from the so-called stochastic region.* How can this "undoing" of truncation error be understood?

Consider an unstable system after a period of exponential growth. The growth is associated with the largest positive eigenvalue of the dynamical transformation from one time to the next in the integration, at least in some average way. It follows that after a long time a state of the system has been reached in which the eigenvector belonging to that eigenvalue is dominant and other eigenvectors have been suppressed. If now all of the velocities are reversed in that state, the dynamical reversibility of the equation of motion guarantees that the new eigenvector will belong to an eigenvalue which is the negative of the previous one. The equations of motion are the same since our system is symmetric in the time.

If, at the time the integration is reversed, a perturbation due to machine roundoff occurs so that some of the eigenvector belonging to the largest positive eigenvalue for the reversed equation is introduced then that eigenvector will grow on the backward integration at the same rate as the observed growth on the forward integration. Exponential growth of a perturbation means a constant propagation velocity within the machine representation of numbers from the less significant to the more significant bits.

In Fig. 9 the growth of the unstable modes associated with $\sigma = 0.042$, $N = 16$, and driving mode 11 is plotted to $t = 1500$, well into the "stochastic" region which

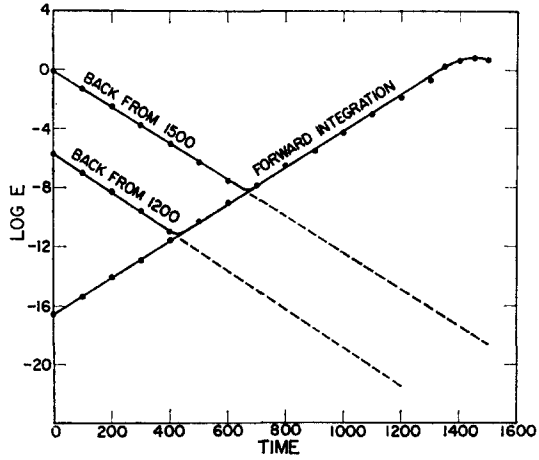

FIG. 9. Average of the logarithms of the energies in modes 10 and 12 plotted for a forward integration to $t = 1500$ and integrated backward from $t = 1200$ and $t = 1500$.

TABLE II

Modal Energies on Backward Integration

Mode	Initial energy	$t = 1200$	$t = 1500$	Return from 1200	Return from 1500
1	3.1×10^{-19}	6.4×10^{-5}	5.1×10^{-5}	1.7×10^{-17}	4.5×10^{-7}
2	1.2×10^{-18}	1.6×10^{-6}	2.5×10^{-5}	4.2×10^{-11}	1.5×10^{-5}
3	2.7×10^{-18}	7.5×10^{-9}	3.5×10^{-5}	1.3×10^{-17}	4.2×10^{-6}
4	4.7×10^{-18}	5.2×10^{-12}	1.9×10^{-4}	9.2×10^{-18}	1.3×10^{-7}
5	7.1×10^{-18}	1.5×10^{-14}	8.9×10^{-4}	5.1×10^{-18}	1.4×10^{-8}
6	9.9×10^{-18}	2.6×10^{-14}	3.7×10^{-3}	9.8×10^{-18}	5.5×10^{-8}
7	1.3×10^{-17}	2.8×10^{-11}	1.1×10^{-3}	1.4×10^{-17}	4.2×10^{-6}
8	1.6×10^{-17}	6.4×10^{-9}	4.1×10^{-2}	1.4×10^{-14}	3.0×10^{-4}
9	1.9×10^{-17}	8.4×10^{-6}	3.8×10^{-1}	1.4×10^{-13}	6.7×10^{-3}
10	2.2×10^{-17}	1.1×10^{-2}	4.2	1.9×10^{-6}	6.2×10^{-1}
11	20.57	21.05	11.4	20.57	19.04
12	2.7×10^{-17}	1.6×10^{-2}	4.6	1.6×10^{-6}	9.3×10^{-1}
13	2.9×10^{-17}	1.8×10^{-5}	5.6×10^{-1}	8.0×10^{-14}	1.7×10^{-3}
14	3.1×10^{-17}	8.7×10^{-9}	9.9×10^{-2}	1.3×10^{-14}	7.5×10^{-4}
15	3.2×10^{-17}	2.1×10^{-11}	1.0×10^{-2}	3.2×10^{-17}	1.3×10^{-5}

occurred at $t = 1350$. The system was integrated backward in time from $t = 1500$ and $t = 1200$ with the results shown in the figure and in Table II. Each of the curves for the return integration can be extrapolated to the time at which its integration was reversed and the ordinate will be the magnitude of the initial roundoff error. Extrapolation is necessary because the initially small values for the return leg are lost in the large dominant forward leg. The slope of the return graph is just the negative of the forward slope, belonging as it does, to the negative eigenvalue.

It is necessary that convergent systems be associated with each divergent system. From another view it arises from the conservation of density in phase since for each representative point that leaves a ball in phase space one must enter. The presence of a dissipative term does not change the mathematical reversibility if the positive dissipation is replaced by negative dissipation as necessary, although it may be physically unrealistic. That is, the system with $-t \to t$ is the reversed system and this involves a reversal of the sign of the dissipative term, in general.

In fact, for our initial conditions of zero velocity the past and future are symmetric so a divergent sytem must have been convergent in the past, at least with respect to the divergent mode under consideration.

8. Concluding Remarks

One result of the analysis is that the Mathieu term which is proportional to the square of the driving mode amplitude eventually dominates a forcing term proportional to the cube of driving mode amplitude even though the forcing term is much larger. A driving mode 11 gives a forcing term which should drive mode 1, and, indeed, mode 1 did grow in our system but a Mathieu term still dominated in the end.

If nonlinear terms proportional to a_{11}^2 and a_{11}^3 are retained, the equation of motion for mode 1 takes on the form (neglecting a_0)

$$\ddot{a}_1 + \omega_1^2 a_1(1 + 6\mu a_{11}^2) = \mu\omega_1^2 a_{11}^3 . \tag{38}$$

The computer results show that the forcing term on the right side of (38) determines the early behavior of the system, but eventually Mathieu terms in the total system become dominant. This forcing kind of resonance is the one which gives rise to the FPU behavior and has been used in the Wigner–Brillouin perturbation scheme [7] to describe that phenomenon. A study of stochasticity based on resonance with forcing terms is given in [19], but the effect of the Mathieu resonance would have to be included in a complete theory.

Forcing terms cause excitations whose amplitudes depend on how close the forcing frequency is to a natural frequency. At exact resonance the excitation is

a secular one which grows linearly in time as compared to the exponential growth of the Mathieu term. These considerations differ from the usual concerns in systems of this kind in that attention is focussed on the secular terms and on the instability growth instead of periodic and quasiperiodic components of the system. This circumstance arises, of course, from the goal of describing the ergodic behavior of the system and the unpredictability over long times rather than short-term predictable behavior.

Attention has been confined to the quartic nonlinear term of the Hamiltonian. The behavior with the cubic term included might be quite different and should be studied, together with higher order nonlinear terms. The Mathieu analysis is valid for the cubic nonlinearity, but the resonance is no longer subharmonic and is at $a = 4$ in (33) which is a narrower resonance. In addition, the cubic nonlinearity relates a driving mode k to a forcing term at mode $2k$, while the D-function connects k to mode $k/2$ through subharmonic Mathieu resonance.

The connection between the dimensionless Hamiltonian (3) and a typical physical lattice is discussed in [4, Appendix A]. A system of particles of mass 30 amu with an equilibrium separation of 3×10^{-8} cm and a sound velocity of 3×10^{5} cm/sec corresponds with dimensionless units of

time: 10^{-13} sec;

energy $= kT$: 4.5×10^{-12} erg;

temperature: 3.25×10^{4} K.

In [4], $N = 100$, $T = 300$, and the overall σ was about 0.1 for the quartic term. If it is assumed the principal mode had about 10% of the energy, its σ would be 0.01 and at that value nonlinear effects gave rise to a finite conductivity in the computer experiment. For $N = 100$, $\sigma = 0.01$ is well into the Mathieu region for the quartic. One must be careful, of course, to distinguish between heuristic experiments such as the present one designed to give information on the principles involved and true models of a physical system. The heuristic models generally involve far less computation but results must be examined with care and should be used to guide the theory and suggest further computation.
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