# ENERGY SHARING AND EQUILIBRIUM FOR NONLINEAR SYSTEMS

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A Thesis submitted for the degree of Doctor of Philosophy
in the University of Adelaide
Department of Mathematics
December, 1963.

CONTENTS

## SUMMARY

A study is made of a one-dimensional system of identical particles in which the forces between neighbours are nonlinear. Identical springs connect adjacent particles, which each have an effective dianeter d. The end two particles, held fixed at a distance L apart, behave like rigid walls. A collision occurs between any two adjacent particles when they come into contact with their centres a distance d apart; otherwise the force of interaction between the two particles is linear. Symmetric motion, which is defined relative to the centre of the system, is shown to be destroyed in these nonlinear systems, while antisymmetry is conserved. An efficient method for carrying out the numerical computations on the model is developed, and the question of the numerical error is discussed.

If the system were linear, the energy $E_i$ in the i-th normal mode would be a constant of the motion. However, in the nonlinear system $E_i$ is constant only between collisions, having a finite jump discontinuity at each collision. Expressions for the coupling and energy sharing between the modes at a collision are derived exactly. It is shown that energy is shared amongst all the modes, irrespective of whether or not the system is set in motion in one particular mode. However, the rate of energy sharing is found to be dependent on the initial conditions. Partitioning of the total energy amongst the degrees of freedom is demonstrated by numerical computation of the time average $\langle E_i \rangle$ of the energy in each mode.

An equation of state, and an expression for the energy of the system as a function of thermodynamic variables, may be simply derived via statistical mechanics by the use of an isobaric grand partition function. Since the energy is always known, expected values for the temperature and pressure of any system may be computed. These provide a check for the numerical values of those variables arising from the computations. The estimates for the pressure and the temperature are derived from the forces acting on the end particles, which are held fixed, and from the total kinetic energy, respectively. Fluctuations in these estimates are computed in order to demonstrate that the system tends towards a state of equilibrium. The behaviour of the velocity autocorrelation function is also discussed.

The evidence provided by this investigation strongly suggests that these nonlinear systems are ergodic. It is concluded that this model should be useful in providing numerical verification of other results in statistical mechanics. Some suggestions for further investigation are offered.

This thesis contains no material which has been accepted for the award of any other degree or diploma in any University. To the best of my knowledge and belief the thesis contains no material previously published or written by another person, except where due reference is made in the text of the thesis.

R.S. Northcote

## ACKNOWLEDGEMENTS

It is a pleasure to thank my supervisor, Professor R.B. Potts, for suggesting this nonlinear model as a topic for research. I should also like to thank him for the encouragement, helpful advice, and criticism he has given throughout the duration of this work. Without his guidance and enthusiastic interest this thesis would not have been written.

I should also like to thank Dr. C.A. Hurst and Mr. J.G. Sanderson, with whom I have had several helpful discussions. Miss. Mary Chapman drew the figures, and Miss Alison Shierlaw typed the manuscript; to them I offer my sincere thanks for their excellent work. I also wish to thank the staff of the Computing Centre for their help in preparing, and checking, the data in the tables. Some of the computations were carried out on a 7090 through the generosity of IBM while Professor Potts was a visitor at the IBM Research Center, Yorktown Heights, New York, U.S.A.

I gratefully acknowledge the support of the Australian Government for an award under the British Commonwealth Scholarship and Fellowship Plan.

# CHAPTER 1

# INTRODUCTION

## 1.1 Fermi, Pasta, and Ulan's Computations

Considerable interest has been shown in the surprising results obtained by Fermi, Pasta, and Ulam [1] who carried out numerical computations on a one-dimensional nonlinear system and found, rather unexpectedly, very little tendency towards equipartition of energy amongst the linear normal modes. They considered an assembly of point particles coupled by forces which were linear except for small nonlinear terms. The interaction potential between two adjacent particles a distance r apart was assumed to be of the form

$$\phi(r) = \tfrac{1}{2}\gamma(r-a)^2 + \phi_1(r), \qquad ---(1.1)$$

where a and $\gamma$ are constants, and $\phi_1(r)$ is a perturbation term which gives rise to small nonlinear forces. In the cases studied these forces were quadratic, cubic, or broken linear.

If there are N + 2 particles*, and $x_i$ is the displacement of the i-th particle from its equilibrium position, then the equations of motion for the quadratic case are given by

$$\ddot{x}_i - (x_{i+1} - 2x_i + x_{i-1}) = \lambda[(x_{i+1} - x_i)^2 - (x_i - x_{i-1})^2]$$
$$(i = 1,..,N), \qquad ---(1.2)$$

* Some authors choose N + 2 particles while others choose N + 1, leading to confusion in the literature. In this thesis we choose N + 2 particles with the end two held fixed, in which case there are N degrees of freedom.

together with the boundary conditions $x_o \equiv x_{N+1} \equiv 0$. $\lambda$ is a constant which was chosen so that the nonlinear term was always small compared with the linear term.

The results of one of the computations carried out by FPU for the system of equations (2) are illustrated in Fig. 0. When the system was started from rest with all the energy in the first linear mode, for example, energy was shared amongst only the first few modes in an almost periodic manner. After some time the system returned very close to the initial configuration, with nearly all the energy in the first mode. The qualitative features of these results were typical of the three different types of systems studied. No explanation was given by FPU for the apparent lack of ergodicity in these nonlinear systems. It was conjectured that quasi-states may exist in certain systems which are approximately nonlinear. However, many physicists (and others) have been puzzled by the failure of these systems to show the approach to equilibrium which is normally expected of such nonlinear systems.

## 1.2 An Explanation by Ford

An explanation of the observations made by FPU has been provided by Ford [2], who investigated the general form of the Kryloff and Bogoliuboff series solution to the Eqs. (2). For the linear system defined by (2) with $\lambda = 0$, the normal mode frequencies $\omega_i$ are given by

$$\omega_i = 2 \sin[\tfrac{1}{2} i\pi/(N+1)] \quad (i = 1,..,N). \qquad ---(1.3)$$

Ford showed that appreciable energy sharing can occur in the nonlinear systems only if there is internal resonance amongst the frequencies $\omega_i$, i.e. only if there is a dependence relation of the form

$$\sum_{i=1}^{N} n_i \omega_i = 0 \qquad ---(1.4)$$

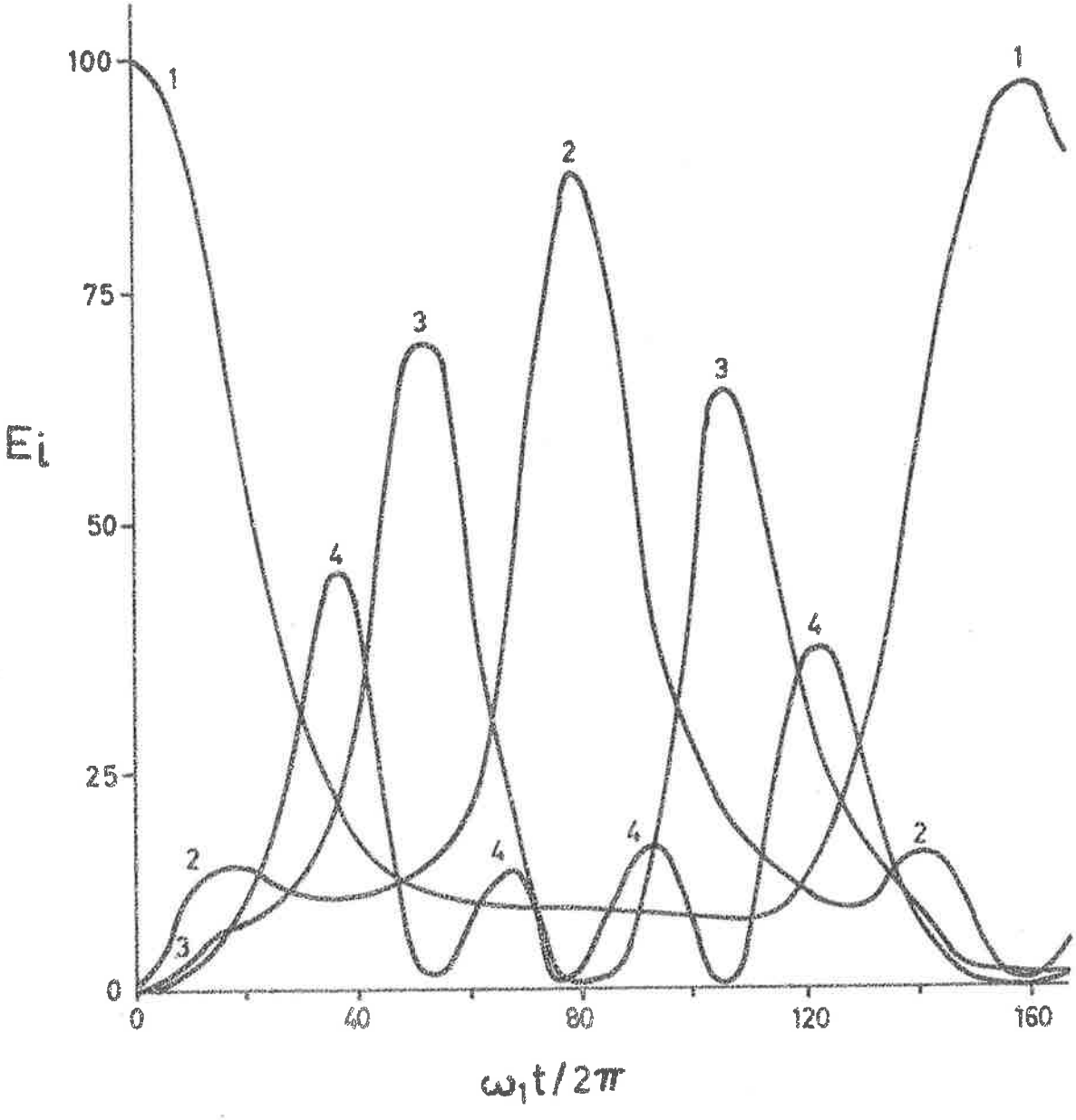


FIGURE 0. The energy $E_i$, as a percentage of the total energy E, for the first four linear modes computed by Fermi, Pasta, and Ulam. $N = 31$, $\lambda = \cdot 25$, $E_i = \delta_{i1} E$ at $t = 0$, $E_5 < \cdot 20E$, $E_k < \cdot 07E$ for $k > 5$.

for some nonzero collection of integers $\{n_i\}$. When N + 1 is a prime or a power of two the $\omega_i$ given by (3) are linearly independent on the integers. Thus Ford concluded that the systems studied by FPU could not exhibit appreciable energy sharing, as the only cases considered were for N + 1 equal to a power of two. This argument is only valid in the case of very weak coupling in which $\lambda \approx 0$. The actual values of $\lambda$ used by FPU were as large as 1, in which case Ford suggested that the condition (4) should be replaced by an approximate condition. This condition for energy sharing, which was derived by Ford and Waters [3] in a more recent paper, is

$$\sum_{i=1}^{N} n_i \omega_i \lesssim \lambda. \qquad \text{---(1.5)}$$

When N is sufficiently large, $\omega_1 \simeq \omega_2/2 \simeq \omega_3/3 \ldots$, where the approximation becomes poorer as one reads to the right. This further explains the results obtained by FPU. As $\lambda$ is increased from zero one would expect appreciable energy sharing amongst higher and higher modes.

The Eqs. (2) may be transformed into the form

$$\ddot{q}_i + \omega_i^2 q_i = \lambda \sum_{j,k=1}^{N} A_{jk} q_j q_k \quad (i = 1,..,N), \qquad \text{---(1.6)}$$

where the $A_{jk}$ are determinable constants. The $q_i$ are the normal coordinates in the linear system, and are obtained from the coordinates $x_i$ by a simple linear transformation. Wigner-Brillouin perturbation theory was used by Ford and Waters to provide a solution (to order $\lambda^2$) for the particular case when N = 2. The condition (5) resulted from generalization of the necessary conditions for energy sharing in this simple system. Exact solutions to (6) were obtained for systems of N = 2,3,5, and 15 particles. The object was to show that, although there is little energy sharing when the frequencies $\omega_i$ are given by

(3) (when N + 1 is a prime or a power of 2), resonance occurs if the frequencies are chosen such that $\omega_i = 2i/N$. Although this was certainly demonstrated, it should have been pointed out that the criterion (5) is not a sufficient condition for resonance. This is shown by the results for the case N = 5. The $\omega_i$ given by (3) then satisfy $\omega_1 + \omega_3 - \omega_5 = 0$, yet there was no resonance evident in the corresponding computations.

## 1.3 Ergodicity and Equilibrium

Ford and Waters suggested that if ergodicity is necessary for an approach to equilibrium, then the weakly nonlinear systems of the type investigated by FPU should be abandoned. However they were reluctant to believe that these systems do not exhibit an approach to equilibrium, and therefore offered the alternative suggestion that ergodicity may not be a necessary prerequisite for equilibrium. There is evidence that many physically interesting systems are not ergodic. A consequence of the conjecture is that an analytic solution of the approach to equilibrium should be more readily obtainable.

In support of this, Ford and Waters showed many similarities between their nonlinear resonant systems and linear systems. They used the perturbation theory to show the existence of stable normal modes in the nonlinear resonant systems, and also found an analytic constant of the motion different from the total energy. Although these systems were nonergodic, equipartition of energy amongst the linear modes (in the time average) was apparent in some of the resonant systems. The partial success of the perturbation schemes in providing an analysis of these systems led them to believe that the problems of irreversible systems are on the verge of solution.

Jackson [4] gave a more comprehensive account of the question of ergodicity by a discussion of the existence of constants of the motion. He concluded that only limited information about ergodicity can be obtained from a study of constructing constants of a particular form, and that the satisfaction

of (4) would be unlikely to play any role in the "coarse-grained" ergodicity of systems with any finite $\lambda$.

In his paper Jackson also developed a different perturbation theory which was later [5] applied to the systems of the type studied by FPU, and Ford and Waters. The analysis was then compared with results obtained from computer solutions of the equations of motion. While agreeing that Ford's observation is true in the case of weak coupling, Jackson showed that "the non-ergodic behaviour of these systems does not result simply from the incommensurability of the uncoupled frequencies $\{\omega_i\}$, but also from the particular form of mode interaction and the initial conditions used in all the calculations, both of which affect the coupled frequency spectrum $\{\Omega_i\}$..... A theoretical examination of the dependence of the coupled frequencies $\{\Omega_i\}$ on the initial conditions shows that the ergodic behaviour will, in general, be strongly dependent on the initial conditions."

To illustrate these remarks, Jackson compared the recurrence time $\tau_\lambda$ (defined as the time required for the near-recurrence of the initial conditions) determined from the theoretical and computer solutions. It was found that there was wide disagreement between the theoretical and computed values for $\tau_\lambda$ for the FPU results when low order theory was used. The conclusion was that the FPU cases are not in the limit of weak coupling and a higher order analysis is necessary. Jackson's higher order analysis, which was only valid for $\lambda \lesssim \cdot 85$, showed very good agreement with the computer solutions for values of $\lambda$ up to $\cdot 75$, and for $N = 3$ and 8. The energy curves obtained by FPU for $N = 31$ and $\lambda = \frac{1}{4}$ were also predicted much more accurately than by Ford's analysis. Although there was an increase in the amount of energy exchanged between the modes as $\lambda$ was increased, the recurrence times $\tau_\lambda$ decreased. This feature would not preclude the possibility of an ergodic behaviour except that in these systems energy is transmitted to the higher modes only via the intermediary ones, independently of the form of the nonlinearity. To remove this property,

Jackson introduced imperfections into the system by having different coupling constants $\lambda_i$ between pairs of particles. Although there was considerably more energy sharing in these new systems, a periodic behaviour was still apparent so they could not be described as ergodic.

## 1.4 A Different Nonlinear Model

It is not intended to pursue further the investigations on the nonlinear systems of the type introduced by FPU. However, as a contribution to the study of the behaviour of nonlinear systems, this thesis [6] embodies an investigation into the energy sharing and equilibrium properties of a different model. A one-dimensional assembly of particles is considered in which nonlinearity is introduced by assuming that collisions occur between adjacent particles which each have an effective diameter d. The advantages of the model are that the computations are facilitated because the system behaves linearly between collisions, nonlinear effects can be made small or large merely by altering the mean energy per degree of freedom of the system, and the model has physical realism.

Considerable effort has been devoted to the development of an efficient and accurate method for the numerical computations, and to the conservation of computer storage space to avoid the use of magnetic tapes, or other backing storage. Before becoming involved in the mathematical detail and discussion in the next few chapters it should be noted that the model is essentially very simple. The basic information to be determined is:

1. the motion of the system, determined from linear equations which are used to compute the particle position and velocity coordinates at each collision, and the times at which these occur;
2. the energies in the linear modes, which are evaluated from the known positions and velocities after each collision;

3. the mean temperature, obtained from the average kinetic energy of the system;
4. the mean pressure, derived from the average forces acting on the fixed end particles.

Subsidiary computations are carried out at suitable intervals of time to obtain estimates for the fluctuations in the temperature and the pressure, and the velocity autocorrelation function.

# CHAPTER 2

# THE MODEL

## 2.1 Definition of the Model

By the one-dimensional model is meant a system of N + 2 particles, each of mass M and effective diameter d, constrained to move on a straight line. The end particles, held fixed at a distance L apart, behave like rigid walls. There are therefore N degrees of freedom in the model. If the particles are equally spaced, the distance between an adjacent pair is $\ell$, where

$$(N+1)\ell = L. \qquad ---(2.1)$$

It is supposed that adjacent particles are connected to each other by identical springs of spring constant $\gamma$ and natural length a - d.

The force of interaction between two adjacent particles, with centres a distance r apart, is

$$f = -\gamma(r-a), \qquad ---(2.2)$$

a linear function of r. Nonlinearity is introduced into the system by supposing that adjacent particles suffer elastic collisions when they meet, their centres then being a distance d apart. The system is thus a conservative one, with a potential energy of interaction given by

$$\phi(r) = \infty \qquad r \leqslant d,$$

and

$$\phi(r) = \phi_0 + \tfrac{1}{2}\gamma(r-a)^2 \qquad r > d. \qquad ---(2.3)$$

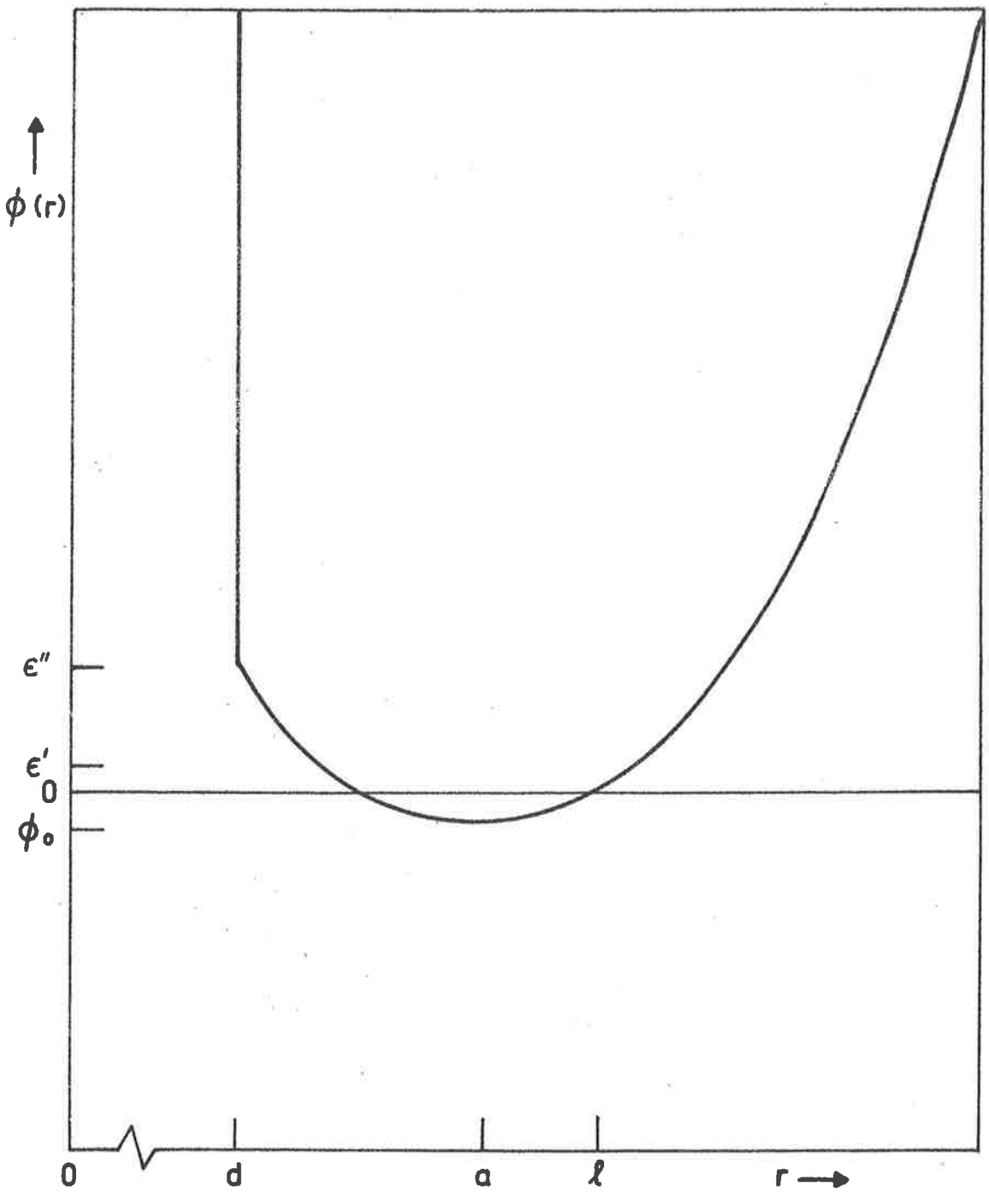


FIGURE 1. The potential $\phi(r) = \phi_0 + \frac{1}{2}\gamma(r-a)^2$, where $\phi_0 = -\frac{1}{2}\gamma(\ell-a)^2$ if $\phi(\ell)=0$, between particles of diameter d with centers r apart. The spring has constant $\gamma$, natural length a-d. The systems studied have a mean energy/particle given by $\epsilon'$ or $\epsilon''$.

A graph of this function is sketched in Fig. 1. If the potential energy is taken to be zero when the particles are equally spaced, then $\phi(\ell) = 0$, and

$$\phi_0 = -\tfrac{1}{2}\gamma(\ell-a)^2. \qquad ---(2.3a)$$

If the displacement of the i-th particle from its equilibrium position is $x_i$ at time t, then the equations of motion of the system, between collisions, are*

$$M\ddot{x}_i - \gamma(x_{i+1} - 2x_i + x_{i-1}) = 0, \qquad ---(2.4)$$

together with the boundary conditions $x_0 \equiv x_{N+1} \equiv 0$ for all t.

A collision occurs between particles j - 1 and j when any of the equalities

$$x_j - x_{j-1} + \ell - d = 0 \quad (j = 1,2,..,N+1) \qquad ---(2.5)$$

is satisfied, where we have made use of the boundary conditions. The equality signs in (5)** are replaced by inequality signs between collisions, i.e. between collisions

$$x_j - x_{j-1} + \ell - d > 0 \quad (j = 1,2,..,N+1). \qquad ---(2.6)$$

When a collision occurs, the positions of the particles are unaltered, but there is a discontinuity in at least one of the velocities. For a collision between particles j - 1 and j at time t, the velocities of the colliding particles immediately after the collision are determined according to the scheme:

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* It will be assumed that the range of the suffices i and j is (1,2,..,N), except where another range is specified, or the context indicates a different interpretation.

** Reference to equations in the same chapter will not include the chapter number associated with the number of the equation.

| collision index j | velocity changes |
|---|---|
| 1 | $\dot{x}_1(t_+) = -\dot{x}_1(t_-)$ |
| 2,...,N | $\dot{x}_{j-1}(t_+) = \dot{x}_j(t_-)$, $\dot{x}_j(t_+) = \dot{x}_{j-1}(t_-)$ |
| N+1 | $\dot{x}_N(t_+) = -\dot{x}_N(t_-)$. ---(2.7) |

The collision indices j = 1 and j = N+1 correspond to collisions on the left and right walls, respectively. All other collisions are internal. The equations (4) together with the conditions (6) and (7) completely define the motion of the assembly of particles.

## 2.2 The Mathematical Solution

Equation (4) may be rewritten, in matrix notation, in the form

$$\ddot{\underset{\sim}{x}} + \underset{\sim}{R}\,\underset{\sim}{x} = \underset{\sim}{0}, \qquad \text{---(2.8)}$$

where $\underset{\sim}{x}$ is the position vector at any instant, and $\underset{\sim}{R}$ is the positive definite matrix given, respectively, by

$$\underset{\sim}{x} = \begin{bmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ x_N \end{bmatrix}, \text{ and } \underset{\sim}{R} = \frac{\gamma}{M}\begin{bmatrix} 2 & -1 & 0 & 0 & \cdot\cdot & 0 & 0 \\ -1 & 2 & -1 & 0 & & & \\ 0 & -1 & 2 & -1 & & & \\ \cdot & \cdot & \cdot & \cdot & & & \\ 0 & & & & -1 & 2 & -1 \\ 0 & 0 & & \cdot\cdot & 0 & -1 & 2 \end{bmatrix}. \qquad \text{---(2.9)}$$

The vector $\underset{\sim}{x}$ is of order N; $\underset{\sim}{R}$ is of order N × N.

The solution of (8) may be written down immediately in the form

$$\underset{\sim}{x}(t) = \cos[\underset{\sim}{R}^{\frac{1}{2}}(t-t_0)]\underset{\sim}{x}(t_0) + \underset{\sim}{R}^{-\frac{1}{2}}\sin[\underset{\sim}{R}^{\frac{1}{2}}(t-t_0)]\dot{\underset{\sim}{x}}(t_0),$$

from which it follows that

$$\dot{\underset{\sim}{x}}(t) = -\underset{\sim}{R}^{\frac{1}{2}}\sin[\underset{\sim}{R}^{\frac{1}{2}}(t-t_0)]\underset{\sim}{x}(t_0) + \cos[\underset{\sim}{R}^{\frac{1}{2}}(t-t_0)]\dot{\underset{\sim}{x}}(t_0).$$

These last two equations may be written together in the form

$$\begin{bmatrix} \underset{\sim}{x}(t) \\ \dot{\underset{\sim}{x}}(t) \end{bmatrix} = \underset{\sim}{A}(t-t_o) \begin{bmatrix} \underset{\sim}{x}(t_o) \\ \dot{\underset{\sim}{x}}(t_o) \end{bmatrix}, \qquad ---(2.10)$$

where

$$\underset{\sim}{A}(t) = \begin{bmatrix} \underset{\sim}{A}_1(t) & \underset{\sim}{A}_2(t) \\ \underset{\sim}{A}_3(t) & \underset{\sim}{A}_1(t) \end{bmatrix}, \qquad ---(2.11)$$

and

$$\underset{\sim}{A}_2(t) = \underset{\sim}{R}^{-\frac{1}{2}} \sin(\underset{\sim}{R}^{\frac{1}{2}}t), \qquad ---(2.12a)$$

$$\underset{\sim}{A}_1(t) = \dot{\underset{\sim}{A}}_2(t), \qquad ---(2.12b)$$

$$\underset{\sim}{A}_3(t) = -\underset{\sim}{R}\,\underset{\sim}{A}_2(t). \qquad ---(2.12c)$$

The transformation (10) is the exact solution of the system, provided that no collisions have occurred in the time interval $(t_o,t)$, i.e. the system is linear throughout the interval. If a collision occurs between particles $j-1$ and $j$ at time $\tau$, the changes in the velocities given by (7) may be represented in matrix notation by

$$\dot{\underset{\sim}{x}}(\tau+) = \underset{\sim}{T}(\tau)\,\dot{\underset{\sim}{x}}(\tau-). \qquad ---(2.13)$$

$\underset{\sim}{T}(\tau)$ is obtained from the unit matrix $\underset{\sim}{I}$, of order $N \times N$, by reversing the sign of the unit element in the first or last row if $j = 1$ or $N+1$, respectively, and by interchanging rows $j-1$ and $j$ if $1 < j < N+1$. Thus, when there are collisions, the position and velocity vectors at any time $t$ are

$$\begin{bmatrix} \underset{\sim}{x}(t) \\ \dot{\underset{\sim}{x}}(t) \end{bmatrix} = \underset{\sim}{A}(t-t_n) \begin{bmatrix} \underset{\sim}{x} & \underset{\sim}{0} \\ \underset{\sim}{0} & \underset{\sim}{T}(t_n) \end{bmatrix} \underset{\sim}{A}(t_n-t_{n-1}) \cdots \begin{bmatrix} \underset{\sim}{I} & \underset{\sim}{0} \\ \underset{\sim}{0} & \underset{\sim}{T}(t_1) \end{bmatrix} \underset{\sim}{A}(t_1-t_o) \begin{bmatrix} \underset{\sim}{x}(t_o) \\ \dot{\underset{\sim}{x}}(t_o) \end{bmatrix}$$

$$= \underset{\sim}{B}(t-t_o) \begin{bmatrix} \underset{\sim}{x}(t_o) \\ \dot{\underset{\sim}{x}}(t_o) \end{bmatrix}, \qquad ---(2.14)$$

say, where the collisions have occurred at times $t_i\,(i = 1,..,n)$.

The transformation (14) is the basis for computations on the nonlinear system. From it the values of the $\underset{\sim}{x}$ coordinates and their derivatives at any time t may be obtained from their values at time $t_o$, provided that the collisions can be determined.

## 2.3 Symmetry and Antisymmetry

Let $\underset{\sim}{K}$ be the orthogonal matrix which is obtained by reversing the order of the rows in the unit matrix $\underset{\sim}{I}$ of order $N \times N$, i.e.

$$\underset{\sim}{K} = \begin{bmatrix} 0 & 0 & .. & 0 & 1 \\ . & . & & 1 & 0 \\ 0 & 1 & & . & . \\ 1 & 0 & .. & 0 & 0 \end{bmatrix}, \qquad ---(2.15)$$

and let $\underset{\sim}{Q}$ be the partitioned matrix of order $2N \times 2N$

$$\underset{\sim}{Q} = \begin{bmatrix} \underset{\sim}{K} & \underset{\sim}{0} \\ \underset{\sim}{0} & \underset{\sim}{K} \end{bmatrix}. \qquad ---(2.16)$$

The matrix $\underset{\sim}{K}$ commutes with a matrix $\underset{\sim}{C}$ of the same order if and only if $\underset{\sim}{C}$ is centrosymmetric, i.e. has elements which satisfy

$$C_{i,j} = C_{N+1-i,\ N+1-j}. \qquad ---(2.17)$$

The proof of this theorem is trivial since, if $\delta_{i,j}$ is the Kronecker delta function, $K_{i,j} = \delta_{N+1,i+j}$.

As $\underset{\sim}{R}$ is a centrosymmetric matrix, the partitioned blocks of $\underset{\sim}{A}(t)$, which are given by (12), are also centrosymmetric and each commutes with $\underset{\sim}{K}$. Hence $\underset{\sim}{Q}$ commutes with $\underset{\sim}{A}(t)$, for all t. It follows from group representation theory that the matrices $\underset{\sim}{A}(t)$ are reducible, the reduction being effected by the same similarity transformation which reduces $\underset{\sim}{Q}$ to diagonal form.

Symmetric and antisymmetric position and velocity coordinates may be defined by the orthogonal transformation

$$\begin{bmatrix} \underset{\sim}{y}_S(t) \\ \underset{\sim}{y}_{AS}(t) \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} \underset{\sim}{I} & \underset{\sim}{K} & \underset{\sim}{0} & \underset{\sim}{0} \\ \underset{\sim}{0} & \underset{\sim}{0} & \underset{\sim}{I} & \underset{\sim}{K} \\ -\underset{\sim}{K} & \underset{\sim}{I} & \underset{\sim}{0} & \underset{\sim}{0} \\ \underset{\sim}{0} & \underset{\sim}{0} & -\underset{\sim}{K} & \underset{\sim}{I} \end{bmatrix} \begin{bmatrix} \underset{\sim}{x}(t) \\ \dot{\underset{\sim}{x}}(t) \end{bmatrix} = \underset{\sim}{H} \begin{bmatrix} \underset{\sim}{x} \\ \dot{\underset{\sim}{x}} \end{bmatrix}, \qquad ---(2.18)$$

where $\underset{\sim}{y}_S$ represents the symmetric position and velocity coordinates, and $\underset{\sim}{y}_{AS}$ the antisymmetric coordinates. For convenience we choose N to be even, in which case $\underset{\sim}{y}_S$ and $\underset{\sim}{y}_{AS}$ are each N-dimensional vectors, and the partitioned blocks of $\underset{\sim}{P}$ are each of order $\frac{1}{2}N \times \frac{1}{2}N$. $\underset{\sim}{P}$ is the required matrix which reduces $\underset{\sim}{Q}$ to diagonal form, i.e.

$$\underset{\sim}{P}\ \underset{\sim}{Q}\ \underset{\sim}{P}' = \begin{bmatrix} \underset{\sim}{I} & \underset{\sim}{0} \\ \underset{\sim}{0} & -\underset{\sim}{I} \end{bmatrix}. \qquad ---(2.19)$$

Thus, in the new coordinate system defined by (18), the transformation (10) becomes

$$\begin{bmatrix} \underset{\sim}{y}_S(t) \\ \underset{\sim}{y}_{AS}(t) \end{bmatrix} = \underset{\sim}{P}\ \underset{\sim}{A}(t-t_o)\underset{\sim}{P}' \begin{bmatrix} \underset{\sim}{y}_S(t_o) \\ \underset{\sim}{y}_{AS}(t_o) \end{bmatrix}, \qquad ---(2.20)$$

where $\underset{\sim}{P}\ \underset{\sim}{A}(t)\underset{\sim}{P}'$ may be represented in the form

$$\underset{\sim}{P}\ \underset{\sim}{A}(t)\underset{\sim}{P}' = \begin{bmatrix} \underset{\sim}{A}_{11}(t) & \underset{\sim}{0} \\ \underset{\sim}{0} & \underset{\sim}{A}_{22}(t) \end{bmatrix}. \qquad ---(2.21)$$

Equations (20) and (21) demonstrate the well known property that symmetry and antisymmetry are conserved in the linear system. The reduction of $\underset{\sim}{A}(t)$ by $\underset{\sim}{P}$ is more complete than indicated, but it is more useful here to leave it in the form given in (21).

We now investigate what happens in the nonlinear system. The matrices $\underset{\sim}{T}(t_i)$ in (14) do not, in general, commute with $\underset{\sim}{K}$, so that $\underset{\sim}{B}(t)$ and $\underset{\sim}{Q}$ do not commute. If $\underset{\sim}{P}\ \underset{\sim}{B}\ \underset{\sim}{P}'$ is partitioned in the form

$$\underset{\sim}{P}\ \underset{\sim}{B}\ \underset{\sim}{P}' = \begin{bmatrix} \underset{\sim}{B}_{11} & \underset{\sim}{B}_{12} \\ \underset{\sim}{B}_{21} & \underset{\sim}{B}_{22} \end{bmatrix},$$

the noncommutativity of $\underset{\sim}{B}$ and $\underset{\sim}{Q}$ implies

$$\begin{bmatrix} \underset{\sim}{B}_{11} & -\underset{\sim}{B}_{12} \\ \underset{\sim}{B}_{21} & -\underset{\sim}{B}_{22} \end{bmatrix} \neq \begin{bmatrix} \underset{\sim}{B}_{11} & \underset{\sim}{B}_{12} \\ -\underset{\sim}{B}_{21} & -\underset{\sim}{B}_{22} \end{bmatrix}.$$

It may therefore be deduced that the matrices $\underset{\sim}{B}(t)$ are irreducible in general, i.e. symmetry and antisymmetry are not conserved together. Furthermore, as energy is conserved in the nonlinear system, conservation of symmetry together with non-conservation of antisymmetry (or vice versa) is also impossible.

There is one exception to these observations. When the nonlinear system is completely antisymmetric initially, collisions always occur in conjugate pairs. Indeed if particles $j - 1$ and $j$ collide at time $t_i$, then so also do particles $N + 1 - j$ and $N + 2 - j$. For this pair of collisions at $t_i$, $\underset{\sim}{T}(t_i)$ is centrosymmetric. The matrix $\underset{\sim}{B}(t)$ for any $t$ then commutes with $\underset{\sim}{Q}$, so that $\underset{\sim}{B}$ is reducible. Antisymmetry is therefore conserved in this special case. This conservation of antisymmetry is unstable because a small admixture of symmetric motions will gradually force collisions to occur other than in conjugate pairs.

When the system is initially symmetric, it is simple to show that the symmetry is destroyed immediately a collision occurs. If we write

$$\underset{\sim}{z} = \begin{bmatrix} \underset{\sim}{I} & \underset{\sim}{K} \\ -\underset{\sim}{K} & \underset{\sim}{I} \end{bmatrix} \underset{\sim}{x},$$

where $\underset{\sim}{I}$ and $\underset{\sim}{K}$ are each of order $\frac{1}{2}N \times \frac{1}{2}N$ ($N$ even), then the system is symmetric if and only if

$$z_i \equiv 0 \equiv \dot{z}_i. \qquad (i = \tfrac{1}{2}N+1,..,N) \qquad ---(2.22)$$

When a collision occurs between particles $j - 1$ and $j$ at time $t$ (assume $j > \frac{1}{2}N$), then the velocities of the colliding particles are interchanged, and we have

$$\dot{z}_{j-1}(t-) = \dot{x}_{j-1}(t-) - \dot{x}_{N+2-j}(t-) = 0,$$

$$\dot{z}_{j}(t-) = \dot{x}_{j}(t-) - \dot{x}_{N+1-j}(t-) = 0,$$

$$\dot{z}_{j-1}(t+) = \dot{x}_{j}(t-) - \dot{x}_{N+2-j}(t-),$$

$$\dot{z}_{j}(t+) = \dot{x}_{j-1}(t-) - \dot{x}_{N+1-j}(t-),$$

and

$$\dot{z}_{j-1}(t+) = -\dot{z}_{j}(t+) \neq 0.$$

Symmetry has obviously been destroyed. It is even simpler to show that symmetry is also destroyed when $j = 1$ or $N + 1$, and the cases for $1 < j \leq \frac{1}{2}N$ are analagous to the above.

To sum up, symmetry and antisymmetry are each conserved in the linear system (no collisions). In the nonlinear system neither symmetry nor antisymmetry is conserved, except in the special case when the system is completely antisymmetric. We shall usually avoid this special case when choosing the initial conditions for numerical computations on the model, although we shall investigate some cases in which the initial conditions are only slightly perturbed from complete antisymmetry in order to observe the instability of the antisymmetric motion.

# CHAPTER 3

# THE NUMERICAL METHOD OF COMPUTATION

## 3.1 The General Method

Suppose that a collision has occurred at time $t_n$, and that $\underset{\sim}{x}(t_n)$ and $\dot{\underset{\sim}{x}}(t_n+)$ are the position and velocity vectors immediately after the collision. After a subsequent time interval h, the position and velocity vectors can be found from

$$\begin{bmatrix} \underset{\sim}{x}(t_n+h) \\ \dot{\underset{\sim}{x}}(t_n+h) \end{bmatrix} = \underset{\sim}{A}(h) \begin{bmatrix} \underset{\sim}{x}(t_n) \\ \dot{\underset{\sim}{x}}(t_n) \end{bmatrix}. \qquad ---(3.1)$$

This iteration is then repeated, the m + 1-st iteration being given by

$$\begin{bmatrix} \underset{\sim}{x}[t_n+(m+1)h] \\ \dot{\underset{\sim}{x}}[t_n+(m+1)h] \end{bmatrix} = \underset{\sim}{A}(h) \begin{bmatrix} \underset{\sim}{x}(t_n+mh) \\ \dot{\underset{\sim}{x}}(t_n+mh) \end{bmatrix}. \qquad ---(3.2)$$

After each iteration the inequalities (2.6) are tested. If no inequality is violated further iterations are performed until one of the inequalities, say the j-th, is not satisfied. This indicates that a collision between particles j - 1 and j has occurred in the previous time interval h. This procedure establishes the time $t_{n+1}$ of the next collision to within h; in fact, if the first inequality to be unsatisfied is found after the m + 1-st iteration, a first estimate of $t_{n+1}$ is taken as

$$t_{n+1}' = t_n + mh.$$

The corresponding estimates of the position and velocity vectors immediately before this collision are

$$\underset{\sim}{x}(t_{n+1}') = \underset{\sim}{x}(t_n+mh),$$

and

$$\dot{\underset{\sim}{x}}(t_{n+1}') = \dot{\underset{\sim}{x}}(t_n+mh).$$

To enable a more accurate estimate of $t_{n+1}$ to be made, K matrices $\underset{\sim}{A}(h_i)$ $(i = 1,2,..,K)$ are evaluated, where $h_1$ is some convenient starting interval, and $h_{i+1} = p^{-1}h_i$, p being an integer greater than one. If $m_i + 1$ iterations have been computed with $\underset{\sim}{A}(h_i)$, then an estimate of $t_{n+1}$ is

$$t_{n+1}' = t_n + \sum_{i=1}^{K} m_i h_i, \qquad ---(3.3)$$

and

$$0 < t_{n+1} - t_{n+1}' < h_K. \qquad ---(3.4)$$

A final estimate of $t_{n+1}$ is obtained by making use of the known values of the position and velocity vectors at time $t_{n+1}'$. If $h_K$ is sufficiently small, an extrapolation to $O[(\delta t)^3]$ by Newton's method will establish $t_{n+1}$ to the accuracy of the computer. The final estimate of the collision time is then

$$t_{n+1} = t_{n+1}' + \Delta t, \qquad ---(3.5)$$

where $\Delta t$ is the small time correction established by the extrapolation. The values of the position and velocity vectors at time $t_{n+1}$ are computed by extrapolation from the values at time $t_{n+1}'$.

Having determined the time $t_{n+1}$ and the values of the position and velocity vectors immediately before the collision, the velocities of the colliding particles are altered according to the scheme (2.7) to determine the velocity vector $\dot{\underset{\sim}{x}}(t_{n+1}+)$ immediately after the collision. The whole process is then

repeated to determine the time of the next collision, and so on.

The elements of the matrices $\underset{\sim}{A}(h_i)$ $(i = 1,2,..,K)$ are determined from Eqs. (2.11) and (2.12). For the numerical evaluation of these matrices using economized polynomial approximations for $\sin(\underset{\sim}{R}^{\frac{1}{2}}t)$ and $\cos(\underset{\sim}{R}^{\frac{1}{2}}t)$, it is necessary to determine an expression for the elements of $\underset{\sim}{R}^r$, for positive integers r.

## 3.2 An Expression for the Elements of $\underset{\sim}{R}^r$.

Consider the matrix

$$\underset{\sim}{R}_1 = -(M/y)\underset{\sim}{R}, \qquad ---(3.6)$$

where $\underset{\sim}{R}$ is given by Eq. (2.9). $\underset{\sim}{R}_1$ is a band matrix, of order $N \times N$, with nonzero elements on the principal diagonal and the two adjacent diagonals. The nonzero elements in any row are given by the three coefficients in the binomial expansion of $(1-x)^2$, with the exception that there are only two elements in each of the first and last rows. In general, the nonzero elements in any row of $\underset{\sim}{R}_1{}^r$ are given by the $2r + 1$ coefficients in the binomial expansion of $(1-x)^{2r}$. This condition is valid for all elements for which the row and column suffices i and j, respectively, satisfy the inequalities

$$r < i + j < 2(N+1) - r. \qquad ---(3.7)$$

The first r and the last r rows have fewer than $2r + 1$ elements. Furthermore, the elements for which i and j do not satisfy (7), i.e.

$$i + j \leq r, \text{ or } i + j \geq 2(N+1) - r, \qquad ---(3.8)$$

are not the appropriate binomial coefficients, but a combination of two or three of these coefficients. This property is due to "end effects" in the matrix multiplication.

We now make the hypothesis that the elements of $\underset{\sim}{R}_1{}^r$, for $r > 0$, are given by the expression

$$\left[\underset{\sim}{R_1}^{r}\right]_{ij} = \sum_{s=0}^{2r}(-)^s\left[\binom{2r}{s} - \binom{2r}{r-m} - \binom{2r}{r-m'}\right]\delta_{i+r,j+s}, \quad ---(3.9)$$

where $\delta_{i,j}$ is the Kronecker delta function,

$$m = i + j, \quad ---(3.10)$$

and

$$m' = 2(N+1) - m. \quad ---(3.11)$$

It is also assumed that

$$\binom{2r}{k} = 0 \quad \text{for } k < 0. \quad ---(3.12)$$

It follows that when i and j satisfy one of the inequalities in (8) there is a correction to be made to the appropriate binomial coefficient, and that when both inequalities hold, which can only occur when $N < r$, there are two corrections.

The proof of (9) is by induction. The hypothesis is obviously true for $r = 1$, for any valid N. Assume the result holds for the general case in which $r = n$. Then for $r = n + 1$

$$\left[\underset{\sim}{R_1}^{n+1}\right]_{ij} = \sum_{k=1}^{N}\left[\underset{\sim}{R_1}^{n}\right]_{ik}\left[\underset{\sim}{R_1}\right]_{kj}$$

$$= \sum_{k=1}^{N}\left\{\sum_{s=0}^{2n}(-)^s\left[\binom{2n}{s} - \binom{2n}{n-i-k} - \binom{2n}{n+i+k-2N-2}\right]\delta_{i+n,k+s}\right\}$$

$$\times \left(\delta_{k,j+1} - 2\delta_{k,j} + \delta_{k,j-1}\right). \quad ---(3.13)$$

The properties

$$\sum_k \delta_{i,k}\,\delta_{k,j} = \delta_{i,j}, \quad ---(3.14)$$

and

$$\delta_{i,k-m} = \delta_{i+m,k} \quad ---(3.15)$$

follow immediately from the definition of the Kronecker delta function. It may also be shown that

$$\binom{2n+2}{s} = \binom{2n}{s} + 2\binom{2n}{s-1} + \binom{2n}{s-2}. \qquad ---(3.16)$$

The last relation is valid for all integers s if the condition (12) is imposed. Using (14), (15), (12), and (16) in succession, the result

$$\sum_{k=1}^{N}\left\{\sum_{s=0}^{2n}(-)^s\binom{2n}{s}\delta_{i+n,k+s}\right\}(\delta_{k,j+1}-2\delta_{k,j}+\delta_{k,j-1})$$

$$= \sum_{s=0}^{2n+2}(-)^s\binom{2n+2}{s}\delta_{i+n+1,j+s}$$

may be derived. A similar analysis of the remaining contributions in (13) yields the required result (9), with r replaced by n + 1. The initial hypothesis is then proved by induction. Note that the proof is independent of N.

The required expression for the elements of $\underset{\sim}{R}^r$ is now obtained directly from (6) and (9) in the form

$$\left[\underset{\sim}{R}^r\right]_{ij} = (\gamma/M)^r \sum_{s=0}^{2r}(-)^{r+s}\left[\binom{2r}{s}-\binom{2r}{r-m}-\binom{2r}{r-m'}\right]\delta_{i+r,j+s}, \qquad ---(3.17)$$

where m and m′ are given by (10) and (11), respectively, and the condition (12) is imposed.

## 3.3 The Evaluation of $\underset{\sim}{A}(t)$

If approximations to the functions cos θ and sin θ can be represented by the economized polynomials

$$\cos\theta \approx \sum_{r=0}^{n} c_{2r}\,\theta^{2r} \qquad |\theta| \leq \tfrac{1}{2}\pi, \qquad ---(3.18)$$

and

$$\sin\theta \approx \sum_{r=0}^{n} c_{2r+1}\,\theta^{2r+1} \qquad |\theta| \leq \tfrac{1}{2}\pi, \qquad ---(3.19)$$

of degree 2n and 2n + 1, respectively, then

$$\cos(\underset{\sim}{R}^{\frac{1}{2}}t) \simeq \sum_{r=0}^{n} c_{2r}\, \underset{\sim}{R}^{r}\, t^{2r},$$

and

$$\underset{\sim}{R}^{-\frac{1}{2}} \sin(\underset{\sim}{R}^{\frac{1}{2}}t) \simeq \sum_{r=0}^{n} c_{2r+1}\, \underset{\sim}{R}^{r}\, t^{2r+1}.$$

The range of validity of these last two approximations is

$$|t| \leq \tfrac{1}{4}\pi(\gamma/M)^{-\frac{1}{2}}, \qquad \text{---(3.20)}$$

$$= \tfrac{1}{4}\pi \text{ units}$$

if we choose $(\gamma/M)^{-\frac{1}{2}}$ as the unit of time. For t in this range, the partitioned blocks of $\underset{\sim}{A}(t)$ in Eqs. (2.12) are given, to order n, by

$$\underset{\sim}{A}_1(t) = \sum_{r=0}^{n} c_{2r}\, \underset{\sim}{R}^{r}\, t^{2r}, \qquad \text{---(3.21a)}$$

$$\underset{\sim}{A}_2(t) = \sum_{r=0}^{n} c_{2r+1}\, \underset{\sim}{R}^{r}\, t^{2r+1}, \qquad \text{---(3.21b)}$$

and

$$\underset{\sim}{A}_3(t) = -\underset{\sim}{R}\,\underset{\sim}{A}_2(t). \qquad \text{---(3.21c)}$$

The elements of $\underset{\sim}{A}(t)$ are evaluated from (17) and (21) using the coefficients in (18) and (19). However the structure of $\underset{\sim}{A}(t)$ makes possible a considerable reduction in the number of elements requiring evaluation. It is evident that the elements in the i-th row of $\underset{\sim}{A}_1(t)$, for example, are symmetric about the i-th element in that row, i.e.

$$\left[\underset{\sim}{A}_1(t)\right]_{i,i+k} = \left[\underset{\sim}{A}_1(t)\right]_{i,i-k},$$

providing the column subscripts are valid. In general, if N is sufficiently large, i may be chosen so that both $m > n$ and $m' > n$ are satisfied for every element in the i-th row. Since

$1 \leqslant j \leqslant N$ and, in (21), $0 \leqslant r \leqslant n$, this amounts to satisfying the condition

$$n \leqslant i \leqslant N + 1 - n.$$

With i in this range, the second and third terms in (17) are each zero for all r (r = 1,2,..,n). The elements in the i-th row of $\underset{\sim}{A}_1(t)$ are then

$$\left[\underset{\sim}{A}_1(t)\right]_{i,i+k} = (-)^k \sum_{r=0}^{n} \binom{2r}{r-k} c_{2r} z^{2r} \quad (k = 0,1,..,n), \qquad ---(3.22)$$

where

$$z = (\gamma/M)^{\frac{1}{2}} t. \qquad ---(3.23)$$

The variable z is then a measure of the time in terms of the unit $(\gamma/M)^{-\frac{1}{2}}$.

When $i < n$ there are elements $[\underset{\sim}{A}_1(t)]_{ij}$ for which $m \leqslant n$. For such elements a correction must be subtracted from the appropriate value derived from (22). The corrections, which are obtained from (17) and (21a), are

$$C_m = (-)^m \sum_{r=0}^{n} \binom{2r}{r-m} c_{2r} z^{2r},$$

where m is defined by (10). This term is just the element $[\underset{\sim}{A}_1(t)]_{i,i+m}$ given by (22). Consideration of the cases for which $m' < n$ when $i > N + 1 - n$ shows that the correction terms are then $C_{m'}$.

In order to compute each of the $N^2$ elements of $\underset{\sim}{A}_1(t)$ to the n-th order it is apparent that only the n + 1 quantities

$$B_{1k} = (-)^k \sum_{r=0}^{n} \binom{2r}{r-k} c_{2r} z^{2r} \quad (k = 0,1,..,n) \qquad ---(3.24)$$

need be evaluated. The $c_{2r}$ are the coefficients in the n-th order approximation to cos θ given by (18), and z is defined by (23). Since $B_{1k}$ is zero for $k > n$, every element of $\underset{\sim}{A}_1(t)$ may

now be expressed in the form

$$[\underset{\sim}{A}_1(t)]_{ij} = B_{1k} - B_{1m} - B_{1m'}, \qquad ---(3.25)$$

where

$$k = |i-j|, \qquad ---(3.26)$$

m and m′ are given by (10) and (11), respectively, and t is restricted to the range given by (20).

The elements of the other blocks of $\underset{\sim}{A}(t)$ may be evaluated from expressions which are analogous to (24) and (25), and which are derived in the same way. Indeed, the elements of $\underset{\sim}{A}_2(t)$ and $\underset{\sim}{A}_3(t)$ are found to the n-th order from

$$B_{2k} = (-)^k (y/M)^{-\frac{1}{2}} \sum_{r=0}^{n} \binom{2r}{r-k} c_{2r+1} z^{2r+1} \quad (k = 0,1,..,n), \qquad ---(3.27)$$

and

$$B_{3k} = (-)^{k+1} (y/M)^{\frac{1}{2}} \sum_{r=0}^{n} \binom{2r+2}{r+1-k} c_{2r+1} z^{2r+1} \quad (k = 0,1,..,n+1), \qquad ---(3.28)$$

respectively. Note that $B_{1k}$ and $B_{2k}$ are each the sum of terms from the k-th order up to the n-th order, and are therefore of the k-th order, while $B_{3k}$ is of the (k-1)-st order if $k > 0$. Hence the (i,j)-th elements of each of $\underset{\sim}{A}_1$ and $\underset{\sim}{A}_2$ are of the k-th order, and the corresponding elements of $\underset{\sim}{A}_3$ are of the (k-1)-st order ($k > 0$), where k is defined by (26).

## 3.4 The Extrapolation Procedure

At the time $t_{n+1}'$ given by (3), all the inequalities (2.6) are satisfied. However, if the particles j - 1 and j collide at time $t_{n+1}$, then at $t_{n+1}'$

$$x_j(t_{n+1}') - x_{j-1}(t_{n+1}') + \ell - d = \eta > 0, \qquad ---(3.29)$$

where $\eta \ll \ell - d$, and j is an integer in the range $1 \leq j \leq N+1$. Since the velocity coordinates are known at $t_{n+1}'$, a zeroth order estimate of $\Delta t$ in (5) is

$$\Delta t = - \eta/(\dot{x}_j - \dot{x}_{j-1}). \qquad ---(3.30)$$

To the next order, $\Delta t$ is the smallest positive root of the cubic polynomial

$$a_0 t^3 + a_1 t^2 + a_2 t + a_3 = 0, \qquad ---(3.31)$$

which is given by the collision condition at $t_{n+1}$, i.e.

$$x_j(t_{n+1}) - x_{j-1}(t_{n+1}) + \ell - d = 0. \qquad ---(3.32)$$

The coordinates $x_{j-1}$ and $x_j$ at $t_{n+1}$ are determined by the linear transformation

$$\begin{bmatrix} \underset{\sim}{x}(t_{n+1}) \\ \underset{\sim}{\dot{x}}(t_{n+1}) \end{bmatrix} = \underset{\sim}{A}(\delta t) \begin{bmatrix} \underset{\sim}{x}(t_{n+1}') \\ \underset{\sim}{\dot{x}}(t_{n+1}') \end{bmatrix}, \qquad ---(3.33)$$

where terms up to $O[(\delta t)^3]$ only are retained in $\underset{\sim}{A}(\delta t)$. The required elements of $\underset{\sim}{A}(\delta t)$ are found from expressions of the form (25) using the first order elements obtained from (24), (27), and (28). These elements are

$$B_{11} = c_0 + 2c_2(y/M)t^2, \qquad B_{12} = - c_2(y/M)t^2,$$
$$B_{21} = c_1 t + 2c_3(y/M)t^3, \qquad B_{22} = - c_3(y/M)t^3,$$
$$B_{31} = -2(y/M)t[c_1 + 3c_3(y/M)t^2], \qquad B_{32} = (y/M)t[c_1 + 4c_3(y/M)t^2],$$
and
$$B_{33} = -c_3(y/M)^2 t^3. \qquad ---(3.34)$$

The coefficients $a_i$ in (31) are now found, from (32), (33), and (34), to be given by

$$a_0 = c_3(y/M) \begin{cases} [2\dot{x}_1 - \dot{x}_2] & j = 1 \\ [3(\dot{x}_j - \dot{x}_{j-1}) + \dot{x}_{j-2} - \dot{x}_{j+1}] & 1 < j < N+1 \\ [-2\dot{x}_N + \dot{x}_{N-1}] & j = N+1, \end{cases} \qquad ---(3.35a)$$

$$a_1 = c_2(y/M) \begin{cases} [2x_1 - x_2] & j = 1 \\ [3(x_j - x_{j-1}) + x_{j-2} - x_{j+1}] & 1 < j < N+1 \\ [-2x_N + x_{N-1}] & j = N+1, \end{cases} \qquad ---(3.35b)$$

$$a_2 = c_1(\dot{x}_j - \dot{x}_{j-1}) \qquad \text{all } j, \qquad ---(3.35c)$$

$$a_3 = c_0(x_j - x_{j-1}) + \mathcal{C} - d \qquad \text{all } j, \qquad ---(3.35d)$$

where the position and velocity coordinates are those at time $t_{n+1}'$, and $c_0 = c_1 = 1$, $c_2 = -\frac{1}{2}$, and $c_3 = -\frac{1}{6}$, to this order.

With the estimate of $\Delta t$ given by (30) as a first approximation, Newton's method may be applied to the polynomial (31) to obtain an accurate estimate of $\Delta t$. The position and velocity vectors at $t_{n+1}$ can then be determined by extrapolation from the known vectors at $t_{n+1}'$, using the transformation $\underset{\sim}{A}(\Delta t)$ in (33). The elements of $\underset{\sim}{A}(\Delta t)$ are determined, up to $O[(\Delta t)^3]$, from the quantities evaluated in (34).

## 3.5 Quantitative Evaluation of the Theory

The numerical computations were carried out on IBM 1620 and IBM 7090 computers using single-length floating point arithmetic (for most of the calculation), i.e. eight significant decimal figures (8 fig.). The elements of the iteration matrices $\underset{\sim}{A}(h_i)$ $(i = 1,2,..,K)$ are therefore computed correct to 8 fig., or to ten decimal places (10D) for the higher order elements. The second condition arises because the positions (or velocities) of any two particles are not necessarily of the same order of magnitude, but the probability of these magnitudes differing by more than $10^2$ is negligible. In particular, the small numerical error involved in computing the elements of $\underset{\sim}{A}(t)$ to 10D only is more than compensated by the increase in the speed of the computation over the cases in which higher order terms are considered.

The coefficients $c_{2r}$ and $c_{2r+1}$ used to evaluate the elements of $\underset{\sim}{A}(t)$ are derived in Appendix 1. To achieve the desired accuracy in $\underset{\sim}{A}(t)$ these coefficients are obtained from the first seven terms of the Chebyshev series expansions for $\cos\theta$ and $\sin\theta$, and are computed to 12D. The values so obtained are listed in Table A1 in the appendix. It immediately follows that the elements of $\underset{\sim}{A}(t)$, for $|t| \leq \frac{1}{4}\pi$ units, need be

computed to only the 6-th order at the most.

The initial time interval $h_1$ for the iteration procedure should be made as large as possible to increase the speed of the computation, yet should be small enough to avoid missing any collisions. In general this second condition is more restrictive than the range of validity (20) for the numerical approximations to $\underset{\sim}{A}(h_1)$. It was found, experimentally, that suitable starting intervals are approximately $h_1 = \cdot 4$ units for $N < 10$, and $h_1 = \cdot 2$ units for $10 < N < 40$. The computation is most efficient if succeeding iteration intervals are bisected when a collision is indicated. For the final extrapolation, which includes terms to $O[(\delta t)^3]$, the range of validity is

$$6c_4 (\gamma/M)^2 t^4/c_0 < 10^{-10}$$

$$\text{i.e.} \qquad |t| < 2\sqrt{5} \times 10^{-3} \text{ units.} \qquad \text{---(3.36)}$$

The iteration procedure may therefore be used for any time interval in the range $t_1 < |t| \leq t_2$, where $t_1 = 2\sqrt{5} \times 10^{-3}$ units and $t_2 = \frac{1}{4}\pi$ units. Since $t_2/t_1 < 2^8$, at most only 9 matrices are required for the computations. As every element of $\underset{\sim}{A}(h_i)$ can be computed to the n-th order from the $3n + 4$ quantities given by (24), (27), and (28), where we have since shown that $n = 6$, the total computer storage required for the iteration matrices is less than 200 words. This is despite the fact that there are over 4000 elements in each matrix when $N = 32$.

The analysis in this and the preceding chapter emphasises one of the main advantages of the model; that the computation may be reduced to a very simple form. Numerical computations have been carried out on systems for which N was 3,4,7,8,15,16, 31, and 32. These values of N were chosen because of Ford's suggestion that the nonlinear systems studied by FPU could not show appreciable energy sharing when $N + 1$ is a prime or a power of two. Realistic values were assigned to the parameters M, $\gamma$, $\ell$, a, and d of the model, the values so assigned being given in Table I. The unit of time is therefore

$$(\gamma/M)^{-\frac{1}{2}} \simeq \cdot 2739 \times 10^{-12} \text{ sec.} \qquad \text{---(3.37)}$$

TABLE I. The numerical values assigned to the parameters in the computation. The particles each have mass M, effective diameter d, and a mean separation of $\ell$ - d. Adjacent particles are connected by springs which have spring constant y and natural length a - d.

| Parameter | Numerical Value |
|---|---|
| M | $3{\cdot}0 \times 10^{-23}$ gm |
| y | 400 dyne/cm |
| $\ell$ | $4{\cdot}000 \times 10^{-8}$ cm |
| a | $3{\cdot}995 \times 10^{-8}$ cm |
| d | $3{\cdot}400 \times 10^{-8}$ cm |

The quantities which are used to evaluate the typical iteration matrix $\underset{\sim}{A}(t)$, $t = 10^{-13}$ sec ($\simeq$ ·36 units), are given in Table II. In this instance there are only sixteen terms which are non-zero to 10D. For smaller t, even fewer terms are needed to determine $\underset{\sim}{A}(t)$. To compute the elements for the iteration matrices correct to 8 fig. or 10D, we used the luxury (if it can be called that) of double precision floating point arithmetic in the computations on the 7090 (using FORTRAN II), and rounded the results so obtained to 8 fig. These values were then held in the fixed store for use in the computation of the collisions, where only single precision arithmetic was used for the iterations.

Measured in terms of the average time taken to compute a collision, the speed of the computation is approximately proportional to N. For N = 31, the 7090 calculated 100 collisions per particle, and carried out all the additional computations required, in about 70 minutes. Ample means for checking the accuracy of the computer programme are available since the total energy of any system is constant, the motion is reversible, and antisymmetry is conserved if the initial configuration is antisymmetric. A listing of the FORTRAN II programme for the computations on an IBM 7090 is given in Appendix 3. The numerical methods analysed in this chapter, and in Appendix 1, are

TABLE II. The quantities $B_{1k}$, $B_{2k}$, and $B_{3k}$, determined from (24), (27), and (28), respectively, which are used to evaluate the elements of the matrix $\underset{\sim}{A}(t)$, where $t = 10^{-13}$ sec. Only the terms up to $\underset{\sim}{O}(10^{-10})$ are included in the table, and each value is given to, at most, 8 decimal figures.

| k | $B_{1k}$ | $B_{2k} \times 10^{13}$ | $B_{3k} \times 10^{-13}$ |
|---|---|---|---|
| 0 | + ·87104 581 | + ·95643 508 | - ·24927 959 |
| 1 | ·06375 2649 | ·02163 6636 | + ·12177 429 |
| 2 | ·00072 12057 | ·00014 53505 | ·00284 61863 |
| 3 | ·00000 32300 | ·00000 04634 | ·00001 92566 |
| 4 | ·00000 00077 | ·00000 00009 | ·00000 00616 |
| 5 | | | ·00000 00001 |

programmed in SUBROUTINE COLLN and SUBROUTINE MATRIX of the programme. SUBROUTINE COLLN has been modified slightly to increase the speed of the computation, as the most frequently used starting interval for the iterations is $h_1 \simeq$ ·18 units, and only 15 terms, at most, are required for each $\underset{\sim}{A}(h_i)$.

## 3.6 Error Analysis

An error $\epsilon$ is expected in each of the position and velocity coordinates found from an iteration of the form (1). Each position coordinate, for example, can be reduced to the sum of $2n + 2$ products of two terms when the elements of $\underset{\sim}{A}(h)$ are computed to the n-th order. The computations are carried out to a fixed number of decimal figures (8 fig.), and there is a truncation associated with each sum or product of two floating point numbers. However, if the summation is so arranged that the smaller (high order) contributions are added before the larger contributions, the total error in determining each coordinate is limited to the final truncation to 8 figures. The mean error in the absolute value of each position and velocity is, therefore, $\epsilon = -\frac{1}{2}$ in the eighth figure, for each iteration.

Error is also introduced whenever the extrapolation procedure is used in the final determination of a collision. To minimize this it is necessary to compute the time increment $\Delta t$ given by (30) and the elements given by (34) using double precision arithmetic, otherwise the error in the extrapolation procedure would be much greater than that in any one iteration. When the elements in (34) have been evaluated, $\underset{\sim}{x}(t_{n+1})$ and $\dot{\underset{\sim}{x}}(t_{n+1})$ are computed to single precision by extrapolation from $\underset{\sim}{x}(t_{n+1}')$ and $\dot{\underset{\sim}{x}}(t_{n+1}')$. The expected error in computing the extrapolation is then of the same magnitude as the error in an ordinary iteration. Because information on each system is required at exact intervals of time (usually $h_1$), there are normally two extrapolations for every collision; one in the computation of the collision, and another to get back in step with the equal time intervals.

For repeated iterations and extrapolations there is a linear build-up in the total error. An actual estimate of this error is difficult to obtain as all the values of $X = |x_j|$, say, are distributed about a mean $\bar{X}$. If $p_k$ is the probability that X lies in the range

$$10^{a+k} \leq X < 10^{a+k+1},$$

where k is any integer, and a is a constant integer, then the expected error in X after I iterations is

$$\epsilon(I) = -\tfrac{1}{2} I \, 10^{a-7} \, \Sigma_k \, p_k \, 10^k.$$

The error therefore depends on the probability distribution function for X. To illustrate this consider the following possibilities:

(a) $\bar{X} = 10^a$, $p_{-1} = \cdot 4$, $p_0 = \cdot 5$, all other $p_k$ negligible, then

$$\epsilon(I) = - \cdot 27 \times 10^{a-7} \, I = - \cdot 27 \times 10^{-7} \, I\bar{X};$$

(b) $\bar{X} = 5 \times 10^a$, $p_{-1} = \cdot 2$, $p_0 = \cdot 8$,

$$\epsilon(I) = - \cdot 41 \times 10^{a-7} \, I \simeq - \cdot 08 \times 10^{-7} \, I\bar{X};$$

(c) $\bar{X} = \cdot 9 \times 10^{a}$, $p_{-1} = \cdot 1$, $p_0 = \cdot 7$, $p_1 = \cdot 2$,

$$\epsilon(I) = - 1 \cdot 36 \times 10^{a-7} I \simeq - \cdot 15 \times 10^{-7} I\bar{X}.$$

In these rough examples the error in the eighth figure ($10^{a-7}$) of X increases as $\bar{X}$ increases, yet the relative error $\epsilon(I)/\bar{X}$ is by no means constant. In estimating the error in any positive quantity X we shall assume that X always lies in some range

$$10^{a} \leq X < 10^{a+1},$$

where a is some integer, and predict that the error estimate so obtained is within a factor of 10 of the actual error.

With the above assumptions, the mean error in the absolute value X of each position and velocity coordinate after I iterations and C collisions is

$$\epsilon_X(I,C) = - \cdot 5 \times 10^{a-7}(I+2C). \qquad ---(3.38)$$

Since $(X+\epsilon)^2 \simeq X(X+2\epsilon)$, the predicted error in the total energy E of the system is proportional to $2\epsilon_X \times 2N$, i.e.

$$\epsilon_E(I,C) = - 2 \times 10^{b-7} (I+2C)N, \qquad ---(3.39)$$

where $10^{b} \leq E < 10^{b+1}$, b being an integer.

For constant E (apart from the error), $\epsilon_E$ is directly proportional to I + 2C, the total number of iterations and extrapolations. The errors in the energy of several systems of N = 31 particles on which computations were carried out are given in Table III. The discrepancies between the predicted and computed values are well within the tolerance suggested above. The given figures are a striking illustration of the fact that the errors are a function of E, as well as of I and C.

The error is, of course, dependent on the accuracy of the floating point arithmetic routines (or instructions) used on the computer on which the computations are carried out. Most of the computations were done on an IBM 7090 computer, with FORTRAN II

TABLE III. The computed and predicted errors in the mean energy per degree of freedom E/N for different systems of N = 31 particles, after I iterations and C collisions had been computed. The values given are the errors in the eighth significant figure of the numerical values for E/N.

| $(E/N) \times 10^{14}$ | I | C | Computed Error | Predicted Error |
|---|---|---|---|---|
| •4 | 27000 | 3000 | - 35700 | - 66000 |
| •4 | 24000 | 3000 | - 36100 | - 60000 |
| •7 | 15000 | 3000 | - 44200 | - 42000 |
| •7 | 15000 | 3000 | - 44800 | - 42000 |

as the source programme language. Thus eight significant figures are retained with truncation after each arithmetic operation. On a different computer (or if the programme had been written in a different language) more figures might be retained, possibly with rounding instead of truncation. In such cases the error would be much smaller, and could sometimes be positive instead of being always negative. Since each system studied has physical meaning, we may regard the small loss in energy as a gradual loss of heat from the system, which could otherwise be said to be isolated in a heat bath at a constant temperature. Before concluding this section it is interesting to discuss what effects the numerical error has on the dynamical properties of such systems.

To check the reversibility of the motion the velocities of a system of N = 31 particles were reversed after 500 collisions had occurred. The path of the system in phase space was retraced closely for over 200 collisions before an "incorrect" collision was noted. Over 400 collisions and 2000 iterations were computed before the motion strayed significantly from the expected path. It should be pointed out that, although the mean expected error in each position and velocity coordinate after this number of iterations and collisions is only about -1400 units in the eighth decimal place, the "spread" in the error is very large.

In another case a system of N = 16 particles was set in motion with all the energy in the 16-th mode initially, i.e. the system was completely antisymmetric. As the error increased so too did the times between two collisions which should have occurred simultaneously in a conjugate pair. However 150 collisions occurred before the total energy in the symmetric modes exceeded ·001% of the total energy of the system during the longer time interval between any two pairs of conjugate collisions. Thereafter there was an increase in the rate at which the antisymmetry was destroyed. After 170 collisions the energy in the symmetric modes was not less than 1·5% of the total energy, while after 230 collisions the system was no longer dominantly antisymmetric. Although the numerical error can be expected to play a direct part in the loss of antisymmetry, it indirectly leads to a rapid increase in the symmetric modes, due to the instability of the conservation of antisymmetry in the presence of symmetric perturbations. Results of numerical computations which verify the properties of antisymmetric systems are given in Tables IX - XI in the next chapter.

Finally, the linear model (no collisions) was run for a system of N = 32 particles. Over 6000 iterations were computed, a period corresponding to 1600 collisions in the equivalent non-linear system, yet the configuration of the system remained in the first mode with an error of less than ·001%.

From the analysis and discussion in this chapter we can conclude that the numerical computations are efficient, and economical on computer storage requirements. Furthermore, the numerical error is no greater than that expected.

# CHAPTER 4

# ENERGY SHARING

## 4.1 The Linear Normal Modes

The eigenvalues and the corresponding eigenvectors of the matrix $\underset{\sim}{R}$ defined by Eq. (2.9) are well known. The elements of the orthogonal symmetric matrix $\underset{\sim}{S}$ which transforms $\underset{\sim}{R}$ into diagonal form are given by

$$S_{ij} = \left(\frac{2}{N+1}\right)^{\frac{1}{2}} \sin\left(\frac{ij\pi}{N+1}\right). \qquad ---(4.1)$$

In the linear system normal coordinates are determined by the transformation

$$\underset{\sim}{q} = \underset{\sim}{S}\ \underset{\sim}{x}, \qquad ---(4.2)$$

and the normal modes vibrate with frequencies $\omega_i/2\pi$, where

$$\omega_i = 2\left(\frac{\gamma}{M}\right)^{\frac{1}{2}} \sin\left(\frac{\frac{1}{2}i\pi}{N+1}\right). \qquad ---(4.3)$$

Note that $\omega_i$ is a monatonically increasing function of i, and $0 < \omega_i < 2(\gamma/M)^{\frac{1}{2}}$.

## 4.2 Equations for the Coupling and Energy Sharing

The potential energy of interaction between two adjacent particles is given by Eq. (2.3). Since there are N + 1 distinct pairs of adjacent particles, the total potential energy of the system is

$$\text{P.E.} = (N+1)\phi_0 + \tfrac{1}{2}\gamma \sum_{j=1}^{N+1} (x_j - x_{j-1} + \ell - a)^2$$

$$= \tfrac{1}{2}\gamma \Big[ \sum_{j=1}^{N+1} (x_j - x_{j-1})^2 \Big] + (N+1)[\phi_0 + \tfrac{1}{2}\gamma(\ell - a)^2]$$

$$= \tfrac{1}{2} M \underset{\sim}{x}' \underset{\sim}{R} \underset{\sim}{x},$$

if we choose $\phi_0$ as in Eq. (2.3a). The total energy of the system is therefore

$$E = \tfrac{1}{2} M (\underset{\sim}{x}' \underset{\sim}{R} \underset{\sim}{x} + \dot{\underset{\sim}{x}}' \dot{\underset{\sim}{x}}) \qquad ---(4.4)$$

or, in terms of the normal coordinates of the linear system,

$$E = \tfrac{1}{2} M \sum_{i=1}^{N} (\omega_i^2 q_i^2 + \dot{q}_i^2). \qquad ---(4.5)$$

If the system were linear

$$E_i = \tfrac{1}{2} M (\omega_i^2 q_i^2 + \dot{q}_i^2), \qquad ---(4.6)$$

the energy associated with the i-th normal mode, would also be a constant of the motion. However in the nonlinear system $E_i$ is constant only between collisions, having a finite jump discontinuity at the time of each collision. For a collision at time t the changes in these energies are

$$\Delta E_i(t) = \tfrac{1}{2} M [\dot{q}_i(t+)^2 - \dot{q}_i(t-)^2]$$

$$= \tfrac{1}{2} M \, \Delta\dot{q}_i(t) [2\dot{q}_i(t-) + \Delta\dot{q}_i(t)], \qquad ---(4.7)$$

where

$$\Delta\dot{q}_i(t) = \dot{q}_i(t+) - \dot{q}_i(t-). \qquad ---(4.8)$$

To express $\Delta\dot{q}_i(t)$ in terms of the velocities of the colliding particles, (2) and the conditions (2.7) may be used to show that, when the two particles j - 1 and j collide*,

---

* In this chapter the range of permissible values for the suffix j is always (1,2,..,N+1), unless otherwise specified.

$$\Delta\dot{q}_i(t) = \begin{cases} 2S_{i1}\,\dot{x}_1(t+) & j = 1 \\ [S_{ij} - S_{i,j-1}][\dot{x}_j(t+) - \dot{x}_{j-1}(t+)] & 1 < j < N+1 \\ 2S_{iN}\,\dot{x}_N(t+) & j = N+1 \end{cases}$$

If the elements $S_{ij}$ are evaluated from (1), simple trigonometrical manipulation reduces each of these expressions to the form

$$\Delta\dot{q}_i(t) = [8/(N+1)]^{\frac{1}{2}} \sin[\tfrac{1}{2}i\pi/(N+1)]\cos[\tfrac{1}{2}i(2j-1)\pi/(N+1)]\,|\Delta\dot{x}_j(t)|, \qquad ---(4.9)$$

where $|\Delta\dot{x}_j(t)|$, which is proportional to the magnitude of the impulse at each collision, is given by

$$|\Delta\dot{x}_j(t)| = \begin{cases} 2\dot{x}_1(t+) & j = 1 \\ \dot{x}_j(t+) - \dot{x}_{j-1}(t+) & 1 < j < N+1 \\ -2\dot{x}_N(t+) & j = N+1. \end{cases} \qquad ---(4.10)$$

Equation (9) may be written more conveniently as

$$\Delta\dot{q}_i(t) = [y(N+1)/2M]^{-\frac{1}{2}}\,\omega_i\,C_{ij}\,|\Delta\dot{x}_j|, \qquad ---(4.11)$$

where $\omega_i$ is given by (3), and

$$C_{ij} = \cos[\tfrac{1}{2}i(2j-1)\pi/(N+1)]. \qquad ---(4.12)$$

The matrix $\underset{\sim}{C}$ is of order $N \times (N+1)$. Equation (11) shows that there is 'coupling' between the modes whenever a collision occurs, while (7) gives the corresponding changes in the energies $E_i$.

## 4.3 The Coupling between the Modes

The increment $\Delta\dot{q}_i(t)$ for a collision j at time t is the product of three factors; the magnitude of the impulse at the collision, the coupling term $C_{ij}$, and a modulating term which is directly proportional to the frequency $\omega_i$. The impulsive force is determined by the velocities of the colliding particles, and therefore increases, on the average, as the total energy of the system increases.

The absolute value of the coupling term is a maximum ($|C_{ij}| = 1$) when

$$i(2j-1) = 2m(N+1), \qquad ---(4.13)$$

for some integer m. Of all the cases for which the condition (13) is approximately satisfied, there are two which will be of particular interest in the discussion to follow. When collisions occur between particles which are close to the left wall ($j \simeq 1$), or the right wall ($j \simeq N+1$), $|C_{ij}| \simeq 1$ for the first few modes ($i \simeq 1$), provided $N >> 1$ (i.e. $N^{-1} < \cdot 1$ say). The coupling term is also large in magnitude for the modes $i = 2k$ and $i = N-2(k-1)$, ($k \simeq 1$), when collisions occur near the centre of the system ($j \simeq [\frac{1}{2}(N+1)]$). As the integer approximations become worse the numerical value of $|C_{ij}|$ decreases. Although $|C_{ij}|$ can be large for the low modes, in general the increment $\Delta\dot{q}_i$ will be larger in magnitude for the high modes because of the modulating term, which is proportional to $\omega_i$.

The sign of $\Delta\dot{q}_i$, which is determined by $C_{ij}$, is positive if

$$4m - 1 < i(2j-1)/(N+1) < 4m + 1 \qquad ---(4.14)$$

for some integer m, and negative otherwise.

## 4.4 The Energy Sharing

The energy sharing arises from the discontinuities in the kinetic energy associated with each mode when collisions occur. It is seen from (7) that the increments $\Delta E_i$ in the energy of the i-th mode are dependent on the normal velocity coordinates $\dot{q}_i(t-)$ immediately before a collision, and on their increments $\Delta\dot{q}_i(t)$. Because the latter are proportional to the frequency $\omega_i$, it follows that the rate of energy sharing for the high modes should be much greater than that for the low modes, if N is large.

Since $C_{ij}\,\Delta\dot{q}_i > 0$ for all i and j, the energy increment $\Delta E_i(t)$ is positive if

$$C_{ij}\ \dot{q}_i(t-) > 0. \qquad ---(4.15)$$

When

$$C_{ij}\ \dot{q}_i(t-) < 0, \qquad ---(4.16)$$

$\Delta E_i(t)$ is positive or negative according as

$$|\Delta\dot{q}_i(t)| \gtrless 2|\dot{q}_i(t-)|. \qquad ---(4.17)$$

The potential energies of each mode are continuous functions of time throughout the motion. However, as the system behaves linearly during the time interval between collisions, there is energy sharing between the potential and kinetic energies of each mode. This form of energy sharing is periodic with period $T_i = 2\pi/\omega_i$ for the i-th mode, and is therefore much more rapid for high modes than for low modes. It follows then that the kinetic energies of the modes, and hence the discontinuities in these at each collision, are dependent on the frequencies $\omega_i$. This dependence is negligible unless the time between any two collisions is of the order of $(\gamma/M)^{-\frac{1}{2}}$.

## 4.5 A Dominant Mode

Suppose that at some time during the motion the k-th mode becomes dominant, in the sense that the energy $E_k$ is a large fraction of the total energy E of the system. If the first mode is dominant, with $\dot{q}_1 > 0$ and $|\dot{q}_1| >> |\dot{q}_i|$ $(i \neq 1)$, then the next collision will most probably occur near the right wall. When $j > \frac{1}{2}(N+1)$, $C_{1j} < 0$, and in this case $C_{1j}\ \dot{q}_1 < 0$. Similar considerations when the k-th mode is dominant will show that the collisions j most likely to occur subsequently are those for which $C_{kj}\ \dot{q}_k < 0$. From (16) and (17) it is seen that this condition will usually lead to a decrease in $E_k$.

The above argument does not preclude the possibility that during the motion some mode may become dominant. Indeed, if the model is to exhibit ergodicity, this is to be expected. Such a condition could occur, for example, when the potential energy $\frac{1}{2}M\omega_k^2 q_k^2$ of the k-th mode is much larger than the corresponding

kinetic energy. At subsequent collisions there would be an increase in the kinetic energy, and in the total energy $E_k$ of the mode, if either $|\Delta\dot{q}_k(t)| > 2|\dot{q}_k(t-)|$, or $C_{kj}\,\dot{q}_k(t-) > 0$. However if $E_k$ is a large fraction of E after any collision there is a greater probability that at the next collision $\Delta E_k$ will be negative, rather than positive.

## 4.6 The Numerical Computations

The above analysis does not yield an exact expression for the amount of energy sharing to be expected over any time interval. However it does indicate qualitatively that energy is shared between all modes, that the rate of energy sharing is greater for the higher modes, and that the probability of any mode becoming, or remaining, dominant is small. For quantitative results we turn to the computer solutions of the motion for different numbers of particles.

For any given N, the initial configuration of the system may be taken to be

$$E_i = \delta_{ik} E,$$

say. This corresponds to the k-th normal mode in the linear system. Since collisions must occur if the model is to be nonlinear, there is a lower bound on the total energy E of any nonlinear system. In the numerical computations we always chose $k = 1$ or $k = N$. To avoid the special case of the conservation of antisymmetry discussed earlier, the initial configuration was usually perturbed slightly from these ideal conditions, but the perturbation was such that the total energy in all the modes other than the k-th was not more than ·002E. Both weakly coupled and strongly coupled systems have been investigated, the strength of the coupling being dependent on the total energy of the system. As the energy is increased, so too is the collision rate, and the average magnitude of the impulse at each collision. The initial behaviour of any system is strongly dependent on the starting configuration, the number of particles, and the mean energy per particle.

For the values of the parameters used in the computations (see Table I, p29), the potential energy of interaction between two particles about to collide is $\phi(d+) = \cdot 708 \times 10^{-14}$ ergs, and $\phi_0 = -\cdot 5 \times 10^{-16}$ ergs. If we denote the mean energy per particle* by

$$\epsilon = E/N, \qquad \text{---(4.18)}$$

Then the energies of the systems studied were given by $\epsilon' = \cdot 4 \times 10^{-14}$ ergs, and $\epsilon'' = \cdot 7 \times 10^{-14}$ ergs. These energy levels are illustrated in Fig. 1 (p.10). It is evident that systems with energies $N\epsilon'$ will be weakly nonlinear, while those with energies $N\epsilon''$ will be much more strongly nonlinear. This conclusion is supported in the next chapter where a plot of the theoretical energy-pressure curve $P = P(\epsilon)$ in Fig. 6 also shows that systems in which $\epsilon = \epsilon'$ are weakly nonlinear. We now discuss the computed results for systems in which the initial configuration is slightly perturbed from the k-th mode; the three cases considered are $k = 1$, $k = N$ ($N$ odd), and $k = N$ ($N$ even).

## 4.6.1 Case k = 1

When a system is started in the first mode there is a gradual loss of energy from that mode with an increase in the energies of all the other modes. The energy loss from the first mode is explained by the fact that most of the collisions occur initially in the neighbourhood of one of the walls (the right wall if $\dot{q}_1(0) > 0$) and, as was noted above, the condition $C_{1j}\,\dot{q}_{1j} < 0$ is usually satisfied. It was also shown that for such collisions $|C_{1j}| \simeq 1$, if $N >> 1$. The loss of energy is then a maximum, even though the actual loss is small due to the modulating term. The second and third modes increase more rapidly than the others, initially. This is because $C_{2j} > 0$ if

---

* Note that there are N+2 particles in the system. However, since the end two have zero kinetic energy we exclude them from consideration, and refer to $\epsilon$ loosely as the mean energy per particle, although it is really the mean energy per degree of freedom.

$j < N/4$ or $3N/4 < j$, and there is an almost continuous stepwise increase in $E_2$ as $C_{2j}\,\dot{q}_2 > 0$ at almost every collision. Although the coupling at each collision is often stronger for the third mode, $E_2$ increases more rapidly than $E_3$ as $C_{3j}\,\dot{q}_3$ is often negative, leading to some decreases in $E_3$. As the increments $E_i$ for the higher modes are negative almost as often as they are positive, there is no appreciable increase in the energies $E_i$ initially. Eventually, while the first mode is still dominant, the sign of $\dot{q}_1$ is reversed. While the magnitude of $\dot{q}_1$ is small, the first inequality in (17) is satisfied for some collisions, and there are small positive increments in $E_1$. There is then a period without collisions during which the entire system of particles 'swings' in the opposite direction to the original motion. Collisions then occur predominantly in the neighbourhood of the other wall, leading to further losses of energy from the first mode. After some time the configuration of the system bears little resemblance to the initial state, and the modes begin to exchange energy freely in a more random manner. Frequently one mode is found to have much more energy than any of the others. There is, however, no evidence of the periodic behaviour found in the systems studied by FPU and others. The only significant difference in the energy sharing properties of weakly and strongly coupled systems started in the first mode appeared to be the rate at which energy was shared amongst all the modes.

In Fig. 2 $E_1$ and $E_2$ have been plotted as a percentage of the total energy E for the system $N = 15$, which was started in the first mode with $\epsilon = \epsilon''$. The curve is a histogram because of the constancy of the energies between collisions. $E_1$ decreased initially until, after about 20 collisions, $|\dot{q}_1|$ was small. The increments $\Delta E_1$ were then negligible, and for several collisions $E_1$ remained almost constant. The explanation for this behaviour is that $T_1 = 2\pi/\omega_1$ is long compared with the average time between collisions, so that $\dot{q}_1$ does not alter appreciably from one collision to the next. The whole system of particles then swung in the opposite direction until the 37-th

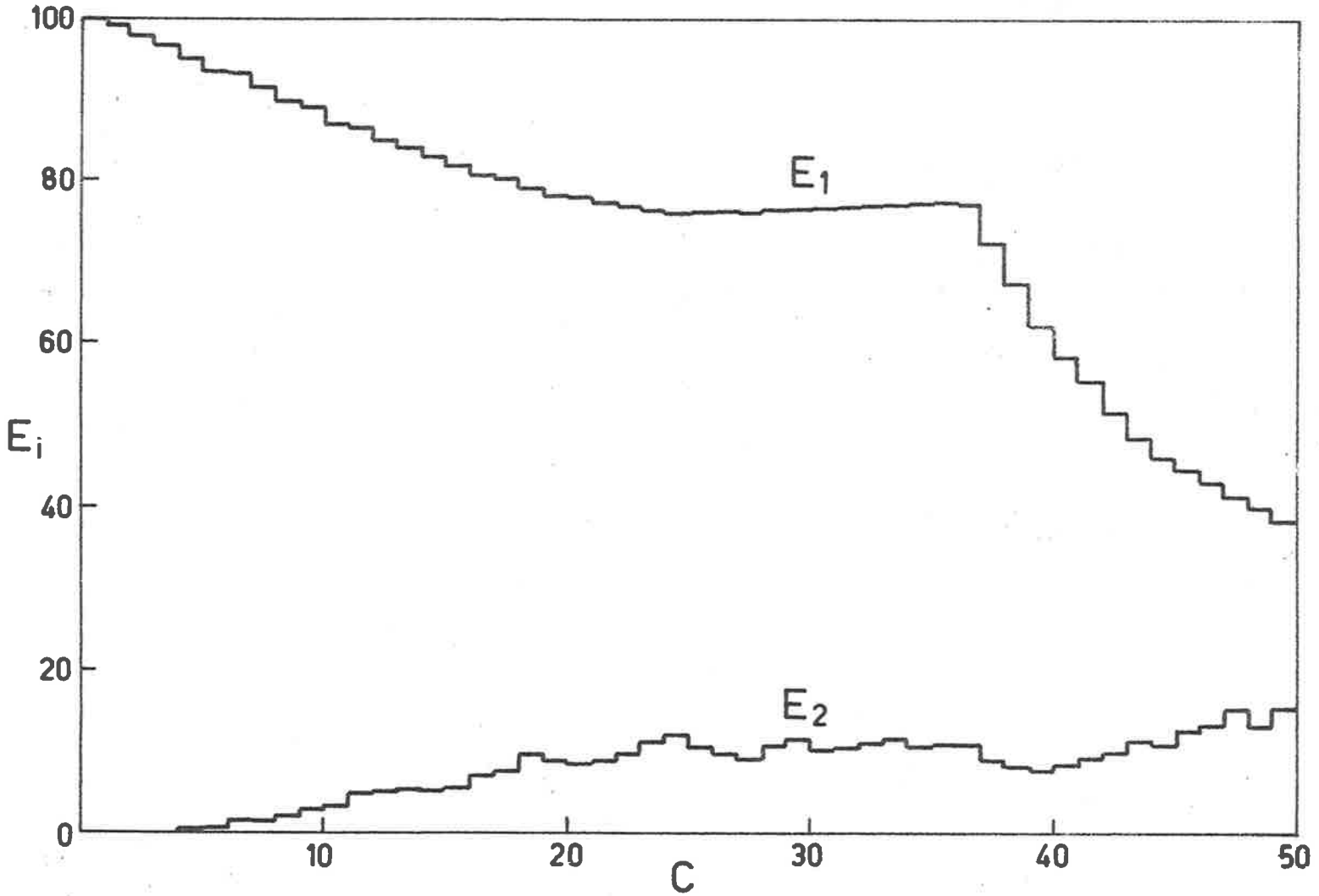


FIGURE 2. The energy in the first two modes after C collisions for N=15 particles, mean energy/particle $\epsilon=\epsilon''$, and $E_i=\delta_{ik}E$ at t=0, with k=1.

collision occurred on the left wall. $E_1$ then decreased more rapidly again. The predominance of collisions in the neighbourhood of first the right wall, and then the left wall, is clearly shown in Table IV. As the energy became distributed amongst all the modes, the fluctuations in the numbers of collisions between each pair of adjacent particles in any given period decreased.

TABLE IV. The numbers of collisions between particles j - 1 and j in intervals of C collisions in the system N = 15, $\epsilon = \epsilon''$, and $E_1 \simeq E$ at t = 0.

| C | j = 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 - 20 | | | | | | | | | | | 1 | 2 | 2 | 6 | 4 | 5 |
| 21 - 36 | | | | | | | | | 1 | 2 | 2 | 1 | 3 | 4 | 2 | 1 |
| 37 - 50 | | 4 | 3 | 2 | 2 | 2 | 1 | | | | | | | | | |

The partition of the total energy amongst all the modes at intervals up to 1500 collisions is shown in Table V. Once the first mode has ceased to be dominant it is apparent that energy is freely exchanged between all the modes. This is further illustrated by computation of the time averages $\langle E_i \rangle$ of the energies, given by

$$\langle E_i \rangle = \tau^{-1} \int_0^{\tau} E_i(t)dt. \qquad ---(4.19)$$

Numerical values for these averages are given in Table VI. The approach to equipartition of the energy amongst the modes, in the time average, is strongly evident.

In a similar system with the same starting configuration except that $\epsilon = \epsilon'$, the decay of energy from the first mode is much slower. The collision rate in this system was not much more than 25% of the rate in the more strongly nonlinear system. Tables for the energies $E_i$ and their time averages $\langle E_i \rangle$ at intervals up to 750 collisions are given in Appendix 2. The approach to equipartition is still evident, even though the system is only weakly nonlinear.

TABLE V. The energies $E_i$, as percentages of E, after C collisions and time z units for the case N = 15, $\epsilon = \epsilon''$, and k = 1. $[z = (\gamma/M)^{+\frac{1}{2}}t]$

| C | z | i=1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | ·0 | 100·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 |
| 5 | ·6 | 95·2 | ·4 | ·6 | ·4 | ·2 | ·0 | ·0 | ·0 | ·0 | ·1 | ·4 | ·8 | 1·0 | ·7 | ·2 |
| 10 | ·8 | 88·8 | 2·1 | 1·8 | ·4 | ·1 | ·6 | ·4 | ·0 | ·6 | 1·8 | 2·0 | 1·1 | ·3 | ·0 | ·0 |
| 15 | 1·2 | 82·9 | 4·9 | 2·4 | ·3 | ·5 | ·1 | ·7 | 3·1 | 3·2 | ·8 | ·0 | ·5 | ·4 | ·1 | ·0 |
| 30 | 2·9 | 76·4 | 11·3 | 2·0 | 2·3 | ·6 | 1·5 | ·9 | ·1 | ·7 | 1·9 | ·8 | ·2 | ·9 | ·3 | ·3 |
| 45 | 13·2 | 46·4 | 10·9 | 1·1 | 1·6 | 5·3 | 4·7 | 3·5 | 2·4 | ·6 | ·7 | 1·4 | ·7 | 1·8 | 13·4 | 5·6 |
| 60 | 15·7 | 32·5 | 12·0 | ·9 | 1·0 | ·7 | 4·2 | 6·1 | 2·8 | ·4 | ·1 | 11·0 | 14·8 | 2·6 | 5·6 | 5·2 |
| 75 | 21·0 | 33·3 | 9·2 | 3·5 | 4·0 | ·1 | 2·2 | 1·9 | 3·6 | 2·8 | 8·1 | 3·7 | 8·7 | 1·9 | 4·6 | 12·5 |
| 90 | 28·4 | 17·2 | 5·8 | 6·6 | 1·8 | 5·5 | 3·5 | 2·6 | 2·3 | 6·0 | 13·4 | 14·1 | 9·9 | 9·4 | ·4 | 1·6 |
| 105 | 32·7 | 21·2 | 15·4 | ·5 | 3·8 | 1·6 | 1·5 | 14·5 | 1·6 | 2·1 | 1·1 | 4·0 | 2·1 | 2·2 | 19·4 | 9·2 |
| 120 | 39·2 | 9·9 | 13·8 | 1·2 | 3·1 | 8·1 | 8·6 | 10·5 | 9·0 | ·6 | 3·7 | 8·0 | ·1 | 12·9 | 7·8 | 3·0 |
| 135 | 47·2 | 11·9 | 6·0 | 5·0 | 4·0 | 5·7 | 1·6 | 2·6 | 4·3 | 3·7 | 2·5 | 10·0 | 8·9 | ·4 | 19·1 | 14·3 |
| 150 | 57·6 | 12·0 | 3·7 | 2·5 | 1·0 | 5·5 | 12·7 | 14·5 | 8·5 | 4·1 | 4·5 | 2·1 | 12·5 | 4·8 | 2·9 | 8·6 |
| 300 | 123·4 | 6·2 | 1·0 | 28·5 | 15·1 | ·3 | 7·2 | 3·8 | 1·8 | 3·2 | 23·1 | ·4 | ·1 | 2·3 | 6·5 | ·6 |
| 450 | 196·3 | 7·3 | 11·4 | 7·6 | 40·6 | 4·2 | ·7 | 4·0 | 6·6 | 1·0 | 2·0 | 4·1 | 1·9 | 4·9 | ·1 | 3·6 |
| 600 | 262·5 | 4·3 | 1·7 | 24·4 | 2·2 | 23·4 | 20·1 | 3·2 | 2·6 | ·5 | 4·5 | ·8 | 2·4 | ·5 | 6·1 | 3·3 |
| 750 | 326·2 | 6·3 | 10·5 | 5·6 | 4·5 | ·5 | ·7 | 8·7 | 1·5 | 5·7 | 29·3 | 7·2 | 2·9 | 6·1 | 6·4 | 4·1 |
| 900 | 395·8 | 5·7 | 6·0 | 1·3 | 5·3 | 3·1 | 9·3 | 16·8 | 11·3 | 4·6 | 4·3 | 4·7 | 2·7 | 2·1 | 13·2 | 9·6 |
| 1050 | 470·0 | ·9 | 3·5 | 9·2 | 3·3 | 6·8 | 3·3 | 7·8 | 6·1 | 5·9 | 7·4 | 1·0 | ·5 | 7·4 | 32·2 | 4·8 |
| 1200 | 528·9 | 11·2 | 12·9 | 1·1 | 21·2 | 10·3 | 10·4 | 3·0 | ·3 | 4·9 | ·6 | ·7 | 11·6 | 1·9 | 4·9 | 5·0 |
| 1350 | 593·9 | 7·1 | 1·5 | ·1 | 1·2 | ·5 | 1·1 | 9·8 | 5·2 | 26·8 | 9·0 | 13·3 | 10·0 | 2·9 | 7·3 | 4·2 |
| 1500 | 668·3 | 11·5 | 5·8 | 3·4 | 6·1 | 8·1 | 2·4 | 1·5 | ·8 | 5·9 | 34·3 | 11·6 | 1·6 | 1·1 | 1·4 | 4·5 |

TABLE VI. The percentage time averages $\langle E_i \rangle$ after C collisions and time z for N = 15, $\epsilon = \epsilon''$, and k = 1.

| C | z | i = 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | ·0 | 100·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 |
| 5 | ·6 | 99·0 | ·1 | ·1 | ·1 | ·2 | ·1 | ·1 | ·1 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 |
| 10 | ·8 | 96·8 | ·5 | ·6 | ·5 | ·3 | ·2 | ·1 | ·2 | ·2 | ·2 | ·1 | ·1 | ·1 | ·1 | ·1 |
| 15 | 1·2 | 93·1 | 1·7 | 1·5 | ·7 | ·3 | ·3 | ·4 | ·6 | ·5 | ·3 | ·2 | ·1 | ·2 | ·2 | ·1 |
| 30 | 2·9 | 83·9 | 6·5 | 2·1 | 1·0 | ·8 | ·9 | ·8 | ·8 | ·6 | ·5 | ·3 | ·3 | ·4 | ·4 | ·5 |
| 45 | 13·2 | 76·1 | 9·6 | 2·4 | 1·3 | 1·2 | 1·0 | 2·2 | 1·3 | 1·0 | ·5 | ·9 | ·3 | ·7 | ·6 | ·7 |
| 60 | 15·7 | 69·7 | 10·2 | 2·2 | 1·3 | 1·3 | 1·3 | 3·4 | 1·4 | 1·2 | ·6 | 1·6 | 1·0 | 1·0 | 1·8 | 2·0 |
| 75 | 21·0 | 60·6 | 9·7 | 2·2 | 1·7 | 1·1 | 1·3 | 3·4 | 2·8 | 2·7 | 1·4 | 1·6 | 2·8 | 1·4 | 2·4 | 4·7 |
| 90 | 28·4 | 52·4 | 9·2 | 3·0 | 1·9 | 1·4 | 1·6 | 2·8 | 3·1 | 3·0 | 3·3 | 2·4 | 4·4 | 2·3 | 2·6 | 6·6 |
| 105 | 32·7 | 47·9 | 9·8 | 3·1 | 2·5 | 1·5 | 2·3 | 3·7 | 3·0 | 3·3 | 3·2 | 2·6 | 4·7 | 2·9 | 3·5 | 6·1 |
| 120 | 39·2 | 43·4 | 11·2 | 2·8 | 2·6 | 1·7 | 2·5 | 4·3 | 3·2 | 3·4 | 3·1 | 2·8 | 4·6 | 3·0 | 3·8 | 7·5 |
| 135 | 47·2 | 37·9 | 10·8 | 3·1 | 2·8 | 2·2 | 2·7 | 4·1 | 4·9 | 3·3 | 3·6 | 3·3 | 5·9 | 3·0 | 4·7 | 7·8 |
| 150 | 57·6 | 33·4 | 10·3 | 2·8 | 2·6 | 4·0 | 3·2 | 4·6 | 4·5 | 3·0 | 4·6 | 3·0 | 6·5 | 3·1 | 4·7 | 9·8 |
| 300 | 123·4 | 19·6 | 7·8 | 5·9 | 4·5 | 5·5 | 6·2 | 6·6 | 5·5 | 4·1 | 5·6 | 5·3 | 5·7 | 4·5 | 4·6 | 8·6 |
| 450 | 196·3 | 13·5 | 8·7 | 7·4 | 6·1 | 5·6 | 6·2 | 7·4 | 5·4 | 5·2 | 6·9 | 5·2 | 5·9 | 5·2 | 4·1 | 7·1 |
| 600 | 262·5 | 11·3 | 9·2 | 8·8 | 6·7 | 5·6 | 6·1 | 6·6 | 6·0 | 5·3 | 6·5 | 5·4 | 5·8 | 5·2 | 4·9 | 6·7 |
| 750 | 326·2 | 9·9 | 9·1 | 9·2 | 6·7 | 5·7 | 6·2 | 6·8 | 6·0 | 5·7 | 7·1 | 5·4 | 5·8 | 5·4 | 4·8 | 6·3 |
| 900 | 395·8 | 8·7 | 9·5 | 8·6 | 6·9 | 5·7 | 6·1 | 6·7 | 5·9 | 6·1 | 6·8 | 5·9 | 5·6 | 6·1 | 4·8 | 6·7 |
| 1050 | 470·0 | 7·9 | 9·1 | 8·2 | 6·4 | 6·3 | 6·0 | 6·5 | 5·9 | 6·1 | 6·8 | 5·9 | 5·6 | 6·5 | 5·3 | 7·3 |
| 1200 | 528·9 | 7·5 | 8·5 | 8·2 | 6·5 | 6·6 | 6·2 | 6·3 | 5·9 | 6·0 | 6·6 | 6·1 | 5·8 | 6·7 | 5·4 | 7·7 |
| 1350 | 593·9 | 7·3 | 7·9 | 8·1 | 6·8 | 7·0 | 6·2 | 6·3 | 5·8 | 6·4 | 6·4 | 5·9 | 5·9 | 6·7 | 5·7 | 7·5 |
| 1500 | 663·3 | 7·2 | 7·5 | 7·8 | 6·6 | 6·6 | 6·3 | 6·5 | 6·3 | 6·5 | 6·6 | 6·4 | 6·1 | 6·7 | 5·6 | 7·3 |

4.6.2 Case k = N, N odd

In systems for which the initial configuration is $E_N = E$, there is a very rapid loss of energy from the N-th mode. Most of the collisions occur near the centre of the system initially, and the first few have indices j which are even if $\dot{q}_N > 0$. This explains the loss of energy from the N-th mode, since the condition $C_{Nj}\,\dot{q}_N < 0$ is satisfied when such collisions occur. The energy loss is large because at each collision $|C_{Nj}| \simeq 1$, and the modulating term is a maximum. Furthermore, the increments $|\Delta\dot{q}_N|$ are so large that $\dot{q}_N$ quickly becomes negative. Any further collisions for which j is even will lead to small increases in $E_N$. However when $\dot{q}_N < 0$, collisions for which j is odd soon begin to occur, leading to further decreases in $E_N$. After a short time $E_N$ is almost negligible. The energies $E_{N-2}$, $E_{N-4}$,.. increase rapidly initially. It has been shown that $|C_{ij}| \simeq 1$ for i = N-2, N-4,.., and i = 2,4,.. when collisions occur in the neighbourhood of $j = [\frac{1}{2}(N+1)]$. When the modulating term is taken into account it is obvious that rapid increases in $E_{N-2}$, $E_{N-4}$,... are to be expected. An interesting feature is that $E_2$ increases slowly but fairly steadily. Indeed, for large N, it is not long before $\langle E_2 \rangle$ becomes greater than $\langle E_N \rangle$. The coupling term $C_{2j}$ is negative for a large number of collisions initially. While $\dot{q}_2$ remains negative the increment $\Delta E_2$ at each collision, although small, is always positive, leading to a slow but steady increase in $E_2$.

In Fig. 3 we have plotted $E_{13}$ and $E_{15}$ for the first 50 collisions in a system which was started very close to the N-th mode, with N = 15 and $\epsilon = \epsilon''$. The rapid exchange of energy between these two modes is clearly shown. Values for the energies $E_i$ and the time averages $\langle E_i \rangle$ for all modes are given in Tables VII and VIII, respectively. The approach of the time averages to equipartition is again evident. Comparison with Fig. 2 and Tables V and VI shows that this approach is more rapid for the system started in the N-th mode, because of the more rapid exchange of energy initially.

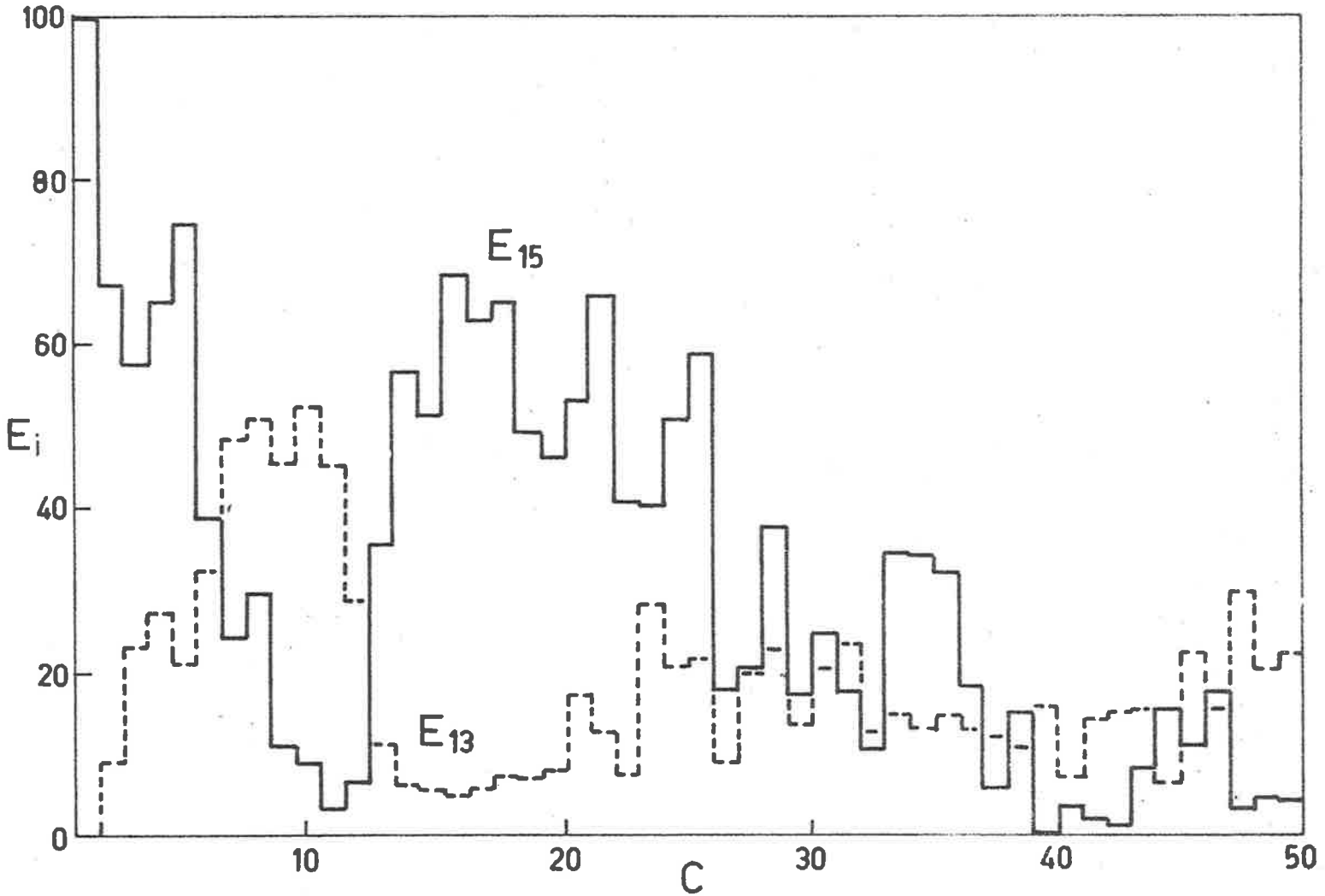


FIGURE 3. The energy in the 13th and 15th modes after C collisions for the case N=15, $\epsilon=\epsilon''$, k=15.

TABLE VII. The percentage energies $E_i$; N = 15, $\epsilon = \epsilon''$, k = 15.

| C | z | i = 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | 100 |
| 5 | 1·0 | ·0 | 1·9 | ·0 | ·7 | ·0 | ·3 | ·0 | ·3 | ·7 | ·1 | ·4 | ·1 | 21·0 | ·1 | 74·6 |
| 10 | 3·4 | ·0 | 9·9 | ·1 | 6·2 | ·3 | ·6 | 1·3 | ·4 | 5·9 | ·1 | 12·3 | ·5 | 52·5 | ·8 | 9·1 |
| 15 | 8·7 | ·0 | 10·6 | ·1 | ·8 | ·1 | 2·8 | ·1 | 1·9 | 4·9 | ·1 | 19·8 | ·6 | 5·9 | 1·2 | 51·0 |
| 30 | 13·7 | ·1 | 7·1 | 1·4 | 2·7 | 1·6 | 1·2 | 1·8 | 8·2 | ·5 | 20·1 | 16·8 | 7·5 | 13·3 | ·3 | 17·3 |
| 45 | 27·4 | ·5 | 9·7 | 3·3 | 6·0 | 8·1 | 7·8 | ·0 | 4·4 | 3·5 | 23·0 | 5·1 | ·1 | 6·7 | 6·0 | 15·8 |
| 60 | 35·2 | 3·8 | 7·2 | 1·5 | ·4 | ·3 | 2·7 | ·1 | 2·8 | 10·2 | 11·9 | 16·4 | 5·3 | 31·4 | 2·7 | 3·2 |
| 75 | 43·2 | 4·3 | 9·5 | 6·3 | 11·7 | 7·1 | 9·9 | 5·3 | 6·2 | 9·7 | 2·0 | ·2 | 8·2 | 6·8 | 6·5 | 6·3 |
| 90 | 50·6 | ·3 | 16·3 | 22·6 | 6·8 | 11·5 | ·4 | 3·1 | ·5 | 11·8 | 3·4 | ·5 | 1·2 | ·4 | 17·5 | 3·7 |
| 105 | 58·1 | ·6 | 4·7 | 14·4 | 9·6 | 3·7 | 8·0 | 3·2 | 1·8 | 1·7 | ·6 | 14·7 | 13·3 | 10·3 | 2·3 | 11·2 |
| 120 | 64·2 | 3·8 | ·4 | 15·6 | ·7 | 13·0 | 5·8 | 10·6 | 8·9 | ·6 | 3·4 | 1·4 | 9·2 | 11·7 | 12·2 | 2·6 |
| 135 | 70·1 | 3·9 | ·1 | 3·3 | 1·0 | 14·6 | 2·4 | 1·1 | 6·4 | 16·3 | 7·2 | 1·5 | 12·4 | 1·6 | 19·7 | 8·5 |
| 150 | 77·2 | 2·4 | 5·0 | 3·9 | 3·9 | 19·0 | 7·6 | 5·7 | 4·1 | 1·0 | 13·5 | 10·5 | 5·8 | 2·2 | 13·6 | 1·8 |
| 300 | 151·7 | 1·4 | 1·2 | ·1 | 9·0 | ·8 | 11·9 | 4·7 | 25·1 | 2·8 | 5·6 | 4·3 | 2·8 | 2·5 | 17·3 | 10·7 |
| 450 | 228·4 | ·4 | 24·8 | 7·8 | 4·0 | 5·4 | 2·9 | 14·5 | 5·4 | 11·6 | 6·3 | 1·9 | 3·5 | 7·0 | 1·3 | 3·0 |
| 600 | 296·2 | 5·1 | 15·3 | 3·8 | 3·0 | 6·8 | 2·8 | 17·0 | 4·5 | 6·0 | ·5 | 6·3 | 4·7 | 17·5 | 2·9 | 3·8 |
| 750 | 353·3 | 8·5 | 6·9 | 3·7 | 4·7 | 1·2 | 2·5 | 4·1 | 13·9 | 4·1 | 3·9 | 9·7 | 1·9 | 14·4 | 2·7 | 17·8 |
| 900 | 415·7 | 21·9 | 2·4 | 2·7 | 1·8 | 5·8 | 8·7 | 2·4 | 5·8 | 10·3 | 11·0 | ·7 | 9·7 | 3·0 | 11·3 | 2·5 |
| 1050 | 499·6 | 6·9 | ·1 | 8·5 | 1·5 | 8·5 | 4·2 | 17·8 | 9·4 | 20·9 | ·5 | 1·0 | ·6 | 8·8 | 2·2 | 9·2 |
| 1200 | 553·8 | ·8 | 7·3 | 5·2 | 15·0 | 15·2 | 7·9 | 5·9 | 4·4 | 12·8 | 4·6 | 2·0 | 1·2 | ·3 | 2·1 | 15·4 |
| 1350 | 611·9 | 24·7 | ·2 | 2·2 | 4·5 | 1·0 | 2·2 | 1·3 | 21·5 | 10·6 | 9·6 | ·2 | 1·1 | ·6 | 12·8 | 7·5 |
| 1500 | 677·6 | 7·9 | 22·5 | 3·8 | 3·7 | 10·8 | 10·5 | 2·1 | ·1 | ·3 | 2·1 | 10·8 | 2·5 | ·2 | 3·0 | 19·7 |

TABLE VIII. The percentage time averages $\langle E_i \rangle$; N=15, $\epsilon=\epsilon''$, k=15.

| C | z | i=1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | 100 |
| 5 | 1·0 | ·0 | 1·5 | ·0 | ·8 | ·1 | ·3 | ·2 | ·4 | ·7 | ·2 | 1·0 | ·3 | 18·8 | ·3 | 75·4 |
| 10 | 3·4 | ·0 | 6·1 | ·1 | 3·8 | ·2 | ·4 | ·8 | ·6 | 3·5 | ·3 | 7·0 | ·5 | 40·8 | ·7 | 35·5 |
| 15 | 8·7 | ·0 | 9·3 | ·1 | 3·0 | ·4 | 1·4 | 1·8 | 1·3 | 7·1 | ·7 | 14·5 | ·7 | 30·1 | ·7 | 28·8 |
| 30 | 13·7 | ·0 | 7·5 | ·1 | 2·8 | ·4 | 1·2 | 2·0 | 1·6 | 5·4 | 1·4 | 12·6 | ·8 | 23·5 | 1·6 | 39·1 |
| 45 | 27·4 | ·1 | 11·0 | ·6 | 3·2 | 1·7 | 2·7 | 3·3 | 2·9 | 7·0 | 3·8 | 10·7 | 2·5 | 18·9 | 4·6 | 26·9 |
| 60 | 35·2 | ·5 | 9·8 | 1·4 | 2·7 | 1·4 | 2·4 | 3·7 | 3·6 | 7·3 | 6·1 | 11·1 | 3·7 | 18·6 | 4·7 | 22·8 |
| 75 | 43·2 | 1·1 | 9·2 | 2·0 | 2·9 | 2·1 | 2·8 | 4·7 | 4·0 | 7·6 | 6·7 | 11·4 | 3·9 | 16·3 | 5·1 | 20·3 |
| 90 | 50·6 | 1·2 | 10·0 | 3·6 | 4·3 | 3·1 | 2·9 | 5·3 | 3·8 | 7·5 | 6·1 | 10·2 | 4·3 | 14·4 | 5·1 | 18·1 |
| 105 | 58·1 | 1·1 | 10·3 | 7·0 | 4·5 | 2·8 | 3·7 | 5·1 | 3·7 | 7·4 | 6·1 | 9·6 | 4·4 | 13·0 | 5·1 | 16·1 |
| 120 | 64·2 | 1·2 | 9·6 | 7·8 | 4·6 | 2·9 | 3·6 | 5·4 | 3·8 | 7·4 | 5·9 | 9·3 | 5·1 | 12·8 | 5·8 | 14·9 |
| 135 | 70·1 | 1·4 | 8·9 | 8·0 | 4·3 | 3·8 | 3·6 | 5·5 | 4·1 | 7·3 | 5·7 | 8·6 | 5·4 | 12·3 | 6·7 | 14·4 |
| 150 | 77·2 | 1·5 | 8·2 | 7·5 | 4·1 | 4·7 | 3·7 | 5·5 | 4·4 | 7·6 | 5·8 | 8·8 | 5·8 | 11·4 | 7·1 | 13·9 |
| 300 | 151·7 | 2·8 | 7·2 | 6·5 | 3·9 | 5·9 | 6·4 | 6·2 | 5·4 | 6·9 | 6·7 | 7·4 | 5·6 | 8·8 | 9·0 | 11·4 |
| 450 | 228·4 | 2·9 | 6·0 | 5·7 | 5·3 | 6·6 | 5·9 | 6·4 | 5·4 | 7·3 | 6·5 | 7·4 | 7·2 | 9·1 | 8·5 | 9·8 |
| 600 | 296·2 | 4·5 | 7·5 | 5·4 | 5·4 | 7·8 | 6·2 | 6·3 | 5·6 | 6·8 | 6·2 | 7·2 | 6·8 | 8·1 | 7·6 | 8·6 |
| 750 | 353·3 | 5·8 | 7·8 | 5·4 | 5·4 | 7·5 | 6·1 | 5·9 | 5·5 | 6·8 | 6·3 | 6·7 | 6·7 | 8·1 | 7·6 | 8·5 |
| 900 | 415·7 | 7·0 | 7·4 | 5·2 | 6·0 | 7·0 | 6·6 | 6·0 | 5·6 | 7·0 | 6·1 | 6·9 | 6·3 | 7·9 | 7·2 | 7·9 |
| 1050 | 488·6 | 8·0 | 7·0 | 5·1 | 6·0 | 7·2 | 6·8 | 6·0 | 5·6 | 6·5 | 6·2 | 6·7 | 6·0 | 7·9 | 7·2 | 7·8 |
| 1200 | 553·8 | 7·9 | 6·8 | 5·2 | 6·0 | 7·0 | 6·8 | 6·4 | 5·9 | 6·5 | 6·1 | 6·5 | 6·2 | 7·8 | 7·3 | 7·5 |
| 1350 | 611·9 | 8·2 | 6·7 | 5·1 | 6·2 | 6·9 | 6·9 | 6·6 | 5·8 | 6·5 | 6·1 | 6·3 | 6·0 | 7·9 | 7·2 | 7·5 |
| 1500 | 677·6 | 8·2 | 7·0 | 5·3 | 6·0 | 6·7 | 6·8 | 6·5 | 5·8 | 6·6 | 6·2 | 6·4 | 6·0 | 7·7 | 7·0 | 7·7 |

4.6.3 Case k = N, N even

It has already been shown theoretically (§2.3) that antisymmetric motion is conserved in a system which is completely antisymmetric. However, in the presence of small symmetric perturbations, the conservation of antisymmetry is expected to be unstable. To demonstrate this property computations were carried out on systems of particles in which the initial configuration was within ·001% of $E_N = E$, with N even. In Table IX values are given for the energies $E_i$ and time averages $\langle E_i \rangle$ for all modes in a system of N = 16 particles which was completely antisymmetric initially. The antisymmetry is obviously conserved for some time; although there is energy in the odd modes after some collisions, there is no contribution to the corresponding time averages $\langle E_i \rangle$ as the energies in these modes are zero after the next collision, which occurs immediately. The build-up in the numerical error, however, gradually introduces symmetric perturbations. As discussed in §3.6, collisions no longer occur exactly in conjugate pairs, and the time averages $\langle E_i \rangle$ for the symmetric modes begin to increase.

One might argue that this is entirely due to the numerical error, rather than to the instability of the conservation of antisymmetry in the presence of the perturbations. To disprove this hypothesis computations were carried out on a similar system which was slightly perturbed (< ·001%) from the previous initial configuration. After only 30 collisions and 240 iterations the energies in the symmetric modes were as high as ·01E at a time when they should have been zero. This increase in the energies of the symmetric modes cannot be accounted for by the numerical error alone. Values for the energies $E_i$ and time averages $\langle E_i \rangle$ for this system are given in Tables X and XI. It is obvious that the small initial symmetric perturbation leads to a rapid sharing of energy amongst all the modes.

Apart from the antisymmetry considerations, the cases k = N (N even) are very similar to the cases k = N (N odd) which were discussed above. Energy is shared predominantly by the modes N, N-2, N-4,.., and to a lesser extent by the modes

TABLE IX. Percentage energies $E_i$ and time averages $\langle E_i \rangle$ for the antisymmetric system $N = 16$, $\epsilon = \epsilon''$, $E_{16} \equiv E$ at $t = 0$.

(a) Mode Energies

| C | z | i=1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | 100 |
| 30 | 23·8 | ·0 | 10·8 | ·0 | ·6 | ·0 | 5·1 | ·0 | 21·9 | ·0 | 8·8 | ·0 | 1·2 | ·0 | 26·1 | ·0 | 25·5 |
| 60 | 41·8 | ·0 | ·7 | ·0 | 8·6 | ·0 | 23·9 | ·0 | 10·0 | ·0 | 1·7 | ·0 | 10·7 | ·0 | 3·2 | ·0 | 41·1 |
| 90 | 56·2 | ·1 | 14·0 | ·5 | 21·0 | 1·1 | ·7 | 1·6 | 3·6 | 1·7 | 15·6 | 1·4 | 14·8 | ·8 | 3·7 | ·2 | 19·2 |
| 95 | 56·8 | ·0 | 20·1 | ·0 | 19·1 | ·0 | 4·2 | ·0 | 2·3 | ·0 | 12·1 | ·0 | 18·9 | ·0 | 3·1 | ·0 | 23·3 |
| 120 | 66·1 | ·1 | 23·3 | ·3 | 1·1 | ·1 | 10·6 | ·5 | 10·8 | 3·4 | 8·6 | 6·9 | 15·6 | 6·7 | 8·5 | 2·6 | 1·2 |
| 125 | 67·6 | ·0 | 19·3 | ·0 | 14·1 | ·0 | 3·6 | ·0 | 1·1 | ·0 | 26·1 | ·0 | 3·3 | ·0 | 32·0 | ·0 | ·5 |
| 150 | 78·0 | ·0 | 15·9 | ·0 | 23·0 | ·0 | 6·8 | ·0 | 25·9 | ·0 | 18·0 | ·0 | 8·7 | ·0 | ·5 | ·0 | 1·2 |
| 180 | 90·5 | ·0 | ·0 | ·0 | 7·6 | ·0 | 12·5 | ·0 | 19·0 | ·1 | 24·9 | ·1 | 12·5 | ·0 | 12·9 | ·1 | 10·3 |
| 210 | 103·4 | ·1 | 16·3 | ·0 | 1·5 | ·4 | 26·4 | 1·0 | 6·7 | 2·0 | 7·1 | ·8 | 9·1 | ·6 | 3·5 | 1·4 | 23·2 |
| 240 | 120·1 | ·1 | 12·5 | 2·7 | 25·3 | ·2 | 6·3 | 8·9 | 19·3 | 2·4 | 1·4 | 7·1 | 4·6 | ·8 | ·1 | ·8 | 7·5 |

(b) Energy time averages

| | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | 100 |
| 30 | 23·8 | ·0 | 9·0 | ·0 | 4·8 | ·0 | 3·8 | ·0 | 5·9 | ·0 | 7·3 | ·0 | 11·5 | ·0 | 28·8 | ·0 | 28·7 |
| 60 | 41·8 | ·0 | 6·9 | ·0 | 4·9 | ·0 | 9·6 | ·0 | 6·4 | ·0 | 9·9 | ·0 | 11·6 | ·0 | 24·5 | ·0 | 26·3 |
| 90 | 56·2 | ·0 | 6·5 | ·0 | 6·3 | ·0 | 11·9 | ·0 | 7·0 | ·0 | 10·9 | ·0 | 12·0 | ·0 | 21·4 | ·0 | 23·8 |
| 120 | 66·1 | ·0 | 8·3 | ·0 | 7·4 | ·0 | 11·9 | ·0 | 7·2 | ·0 | 10·3 | ·0 | 11·7 | ·0 | 21·4 | ·0 | 21·8 |
| 150 | 78·0 | ·0 | 9·9 | ·0 | 9·5 | ·0 | 10·9 | ·0 | 9·1 | ·0 | 10·4 | ·0 | 11·9 | ·0 | 19·2 | ·0 | 19·2 |
| 180 | 90·5 | ·0 | 9·7 | ·0 | 8·7 | ·0 | 14·2 | ·0 | 9·3 | ·0 | 11·0 | ·0 | 11·7 | ·0 | 17·7 | ·0 | 17·7 |
| 210 | 103·4 | ·0 | 9·2 | ·0 | 9·4 | ·0 | 14·4 | ·1 | 9·5 | ·1 | 11·1 | ·1 | 11·4 | ·1 | 17·4 | ·2 | 16·9 |
| 240 | 120·1 | ·0 | 10·4 | ·1 | 9·7 | ·6 | 14·2 | ·7 | 9·6 | ·5 | 10·6 | ·5 | 10·5 | ·6 | 15·6 | 1·2 | 15·2 |

TABLE X. The percentage energies $E_i$ for the (perturbed) system: N=16, $\epsilon=\epsilon''$, k=16.

| C | z | i=1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | 100 |
| 2 | ·0 | ·0 | ·3 | ·2 | ·7 | 1·1 | ·5 | 3·1 | ·0 | 5·0 | ·4 | 5·3 | 2·7 | 3·6 | 6·2 | 1·2 | 69·7 |
| 3 | ·1 | ·0 | 1·1 | ·0 | 2·6 | ·0 | 2·0 | ·0 | ·1 | ·0 | 1·7 | ·0 | 10·7 | ·0 | 24·7 | ·0 | 57·0 |
| 4 | ·1 | ·0 | 1·5 | ·3 | 1·4 | ·1 | ·2 | ·6 | ·0 | 2·0 | ·1 | ·1 | 2·8 | 2·2 | 23·0 | 3·1 | 62·7 |
| 5 | ·9 | ·0 | 1·9 | ·0 | ·6 | ·0 | ·4 | ·0 | ·1 | ·0 | 1·1 | ·0 | ·4 | ·0 | 21·4 | ·0 | 74·1 |
| 6 | 1·0 | ·0 | 3·6 | ·0 | 2·9 | ·0 | 1·0 | ·0 | 3·0 | ·0 | 8·8 | ·0 | 10·0 | ·0 | 32·1 | ·0 | 38·6 |
| 7 | 1·0 | ·0 | 4·8 | ·3 | 3·1 | 1·0 | ·1 | ·5 | ·0 | ·1 | 3·3 | 2·5 | 6·9 | 4·7 | 42·0 | 2·4 | 28·3 |
| 8 | 2·0 | ·0 | 6·2 | ·0 | 3·4 | ·0 | ·3 | ·0 | 1·8 | ·0 | 2·7 | ·0 | 4·4 | ·0 | 53·8 | ·0 | 27·5 |
| 15 | 10·7 | ·0 | 4·5 | ·0 | 9·3 | ·0 | 1·9 | ·0 | ·1 | ·0 | ·1 | ·0 | 1·0 | ·0 | 19·8 | ·0 | 63·2 |
| 30 | 22·5 | ·0 | 14·3 | ·0 | 3·0 | ·1 | 2·2 | ·4 | 6·8 | ·7 | 1·6 | 1·0 | 8·0 | ·8 | 40·6 | ·3 | 20·0 |
| 60 | 38·2 | ·5 | 5·4 | 1·9 | 16·2 | ·8 | 16·4 | ·1 | 1·7 | 1·4 | 24·3 | ·4 | 2·7 | 2·8 | 14·9 | 10·3 | ·3 |
| 90 | 53·2 | 1·6 | ·5 | 3·7 | 3·8 | 6·5 | 1·1 | 10·5 | 9·3 | 1·0 | 27·5 | 4·1 | 5·5 | 8·3 | 3·6 | 12·8 | ·1 |
| 120 | 63·9 | ·9 | ·6 | 1·6 | 12·9 | 12·6 | 3·8 | ·4 | ·8 | 1·9 | 2·6 | 1·0 | 13·6 | 4·2 | 10·8 | 4·6 | 27·7 |
| 160 | 81·3 | 2·6 | ·3 | 4·2 | 4·2 | 8·5 | 5·7 | 5·7 | 8·7 | 13·3 | 5·1 | 7·5 | 5·3 | 3·9 | 4·4 | 14·1 | 6·6 |
| 320 | 144·7 | ·2 | ·7 | 11·2 | 2·6 | 6·8 | 3·5 | 1·5 | 18·9 | 10·9 | 20·3 | 1·8 | 4·1 | 1·8 | 2·2 | 12·3 | 1·1 |
| 480 | 216·3 | 2·4 | 12·3 | 3·3 | ·6 | 12·3 | 18·6 | 6·2 | 1·6 | 8·5 | 1·7 | 2·2 | 8·7 | 12·3 | 6·6 | 1·7 | 1·1 |
| 640 | 280·5 | ·2 | ·6 | 2·3 | 10·2 | 9·2 | 9·2 | 6·1 | 24·7 | ·9 | 3·7 | 4·9 | 3·5 | 5·5 | ·7 | 1·5 | 16·7 |
| 800 | 345·7 | 3·5 | 4·7 | ·2 | ·7 | 6·4 | 4·8 | 2·3 | 5·9 | 3·0 | 10·1 | 10·1 | ·6 | 4·8 | 7·6 | 20·0 | 15·2 |
| 960 | 407·9 | 1·7 | 1·9 | 1·1 | 3·6 | 12·6 | 1·9 | 2·3 | 16·9 | 3·7 | 15·3 | 14·0 | 12·9 | 4·6 | 4·0 | 3·1 | ·3 |
| 1120 | 473·6 | 15·1 | 3·5 | ·4 | 3·5 | 7·0 | ·8 | 24·2 | 11·8 | 2·4 | 1·2 | 1·0 | 4·8 | 3·1 | 3·4 | 14·3 | 3·5 |
| 1280 | 543·5 | 15·6 | 2·6 | 5·1 | 3·1 | 1·5 | 3·9 | ·9 | 10·2 | 9·1 | 1·2 | 19·9 | 2·5 | 3·9 | 6·4 | 4·1 | 10·0 |
| 1440 | 611·2 | ·6 | 2·7 | 6·7 | ·9 | 6·8 | 17·1 | 8·6 | 5·1 | 2·5 | 30·2 | ·5 | ·7 | 7·4 | ·4 | ·9 | 8·9 |
| 1600 | 684·1 | 1·1 | 5·3 | 4·1 | 1·3 | 2·0 | 5·2 | 5·6 | 23·7 | 3·2 | 16·1 | 3·4 | 1·2 | 2·6 | 9·5 | 12·1 | 3·6 |

TABLE XI. The percentage time averages $\langle E_i \rangle$; N = 16, $\epsilon = \epsilon''$, k = 16.

| C | z | i=1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | ·0 | 100 |
| 5 | ·9 | ·0 | 1·8 | ·0 | ·8 | ·0 | ·6 | ·0 | ·1 | ·0 | 1·1 | ·0 | 1·5 | ·0 | 21·2 | ·0 | 72·8 |
| 10 | 3·1 | ·0 | 6·1 | ·0 | 3·8 | ·0 | ·7 | ·0 | 1·3 | ·0 | 3·9 | ·0 | 7·3 | ·0 | 43·6 | ·0 | 33·4 |
| 15 | 10·7 | ·0 | 8·7 | ·0 | 4·4 | ·0 | 2·3 | ·0 | 4·4 | ·0 | 8·1 | ·0 | 12·9 | ·0 | 26·9 | ·0 | 32·3 |
| 30 | 22·5 | ·0 | 8·9 | ·0 | 4·9 | ·0 | 3·7 | ·0 | 5·1 | ·1 | 7·2 | ·1 | 11·9 | ·1 | 28·8 | ·0 | 29·1 |
| 45 | 28·9 | ·0 | 7·8 | ·2 | 4·8 | ·3 | 4·7 | ·7 | 4·9 | ·5 | 7·1 | ·8 | 11·1 | 1·0 | 27·2 | ·6 | 28·4 |
| 60 | 38·2 | ·1 | 7·6 | ·3 | 5·6 | ·5 | 5·6 | ·9 | 4·2 | 1·2 | 9·4 | 1·5 | 8·8 | 2·0 | 27·7 | 1·6 | 23·1 |
| 75 | 45·9 | ·2 | 6·5 | ·6 | 5·4 | ·7 | 6·1 | 1·2 | 3·9 | 2·4 | 10·6 | 1·6 | 9·1 | 2·9 | 24·9 | 3·1 | 20·8 |
| 90 | 53·2 | ·3 | 5·6 | ·8 | 5·0 | 1·5 | 5·6 | 1·6 | 4·4 | 3·1 | 11·2 | 3·4 | 9·0 | 3·4 | 22·2 | 3·5 | 19·3 |
| 105 | 57·5 | ·4 | 5·3 | 1·0 | 5·3 | 2·0 | 5·6 | 1·8 | 4·6 | 3·1 | 10·9 | 3·7 | 9·1 | 3·5 | 20·6 | 4·4 | 18·5 |
| 120 | 63·9 | ·5 | 4·8 | 1·3 | 6·0 | 3·4 | 6·0 | 1·7 | 4·9 | 3·4 | 10·2 | 3·9 | 10·3 | 3·3 | 18·9 | 4·3 | 17·1 |
| 140 | 72·0 | ·6 | 4·3 | 1·5 | 6·9 | 3·6 | 5·6 | 1·8 | 5·2 | 3·8 | 9·4 | 4·6 | 10·2 | 3·8 | 17·7 | 4·4 | 16·6 |
| 160 | 81·3 | ·7 | 3·9 | 1·6 | 6·8 | 3·9 | 5·6 | 1·9 | 5·3 | 4·8 | 9·7 | 4·8 | 10·1 | 3·7 | 16·8 | 4·9 | 15·8 |
| 320 | 144·7 | 2·0 | 6·0 | 4·8 | 6·7 | 5·2 | 5·8 | 4·1 | 5·7 | 5·7 | 8·0 | 4·8 | 7·7 | 5·2 | 12·0 | 5·5 | 10·7 |
| 480 | 216·3 | 2·7 | 6·0 | 4·5 | 5·9 | 4·8 | 5·9 | 5·0 | 6·7 | 5·8 | 7·8 | 5·9 | 7·3 | 5·6 | 10·6 | 6·3 | 9·1 |
| 640 | 280·5 | 2·6 | 5·2 | 5·0 | 6·7 | 4·8 | 6·2 | 5·6 | 6·4 | 6·1 | 7·4 | 6·0 | 7·0 | 5·5 | 9·5 | 6·7 | 9·3 |
| 800 | 345·7 | 3·2 | 5·3 | 4·9 | 6·3 | 4·9 | 5·9 | 5·7 | 6·3 | 6·4 | 7·8 | 5·9 | 6·7 | 5·8 | 9·0 | 6·6 | 9·2 |
| 960 | 407·9 | 3·5 | 5·4 | 5·5 | 6·0 | 5·4 | 6·0 | 6·0 | 6·1 | 6·2 | 7·8 | 5·8 | 6·5 | 5·8 | 8·8 | 6·5 | 8·7 |
| 1120 | 473·6 | 3·7 | 5·7 | 5·8 | 5·7 | 5·3 | 5·9 | 6·5 | 6·4 | 6·3 | 7·8 | 5·6 | 6·5 | 5·9 | 8·5 | 6·4 | 8·2 |
| 1280 | 543·5 | 4·5 | 5·2 | 5·5 | 5·4 | 5·2 | 6·1 | 6·6 | 6·3 | 6·1 | 7·6 | 5·6 | 6·5 | 5·8 | 8·2 | 6·6 | 8·5 |
| 1440 | 611·2 | 4·5 | 5·2 | 6·3 | 5·4 | 5·2 | 6·4 | 6·6 | 6·3 | 6·1 | 7·4 | 5·9 | 6·2 | 5·9 | 8·0 | 6·6 | 8·0 |
| 1600 | 684·1 | 4·2 | 5·0 | 6·4 | 5·1 | 5·5 | 6·6 | 6·4 | 6·6 | 6·1 | 7·3 | 5·9 | 6·2 | 6·1 | 8·0 | 6·6 | 8·0 |

2,4,.., initially. These, of course, are the antisymmetric modes. Gradually, however, energy becomes freely distributed amongst all the modes.

The general behaviour of every system studied was very similar, once the initial conditions had ceased to be dominant. In particular, a slight variation in the number of particles from N = 31 to N = 32, say, did not yield essentially different results, provided we exclude the special antisymmetric system from consideration. That is, the nonlinear systems studied here do not show less energy sharing when N + 1 is a prime or a power of two, which was a reason given by Ford for the lack of energy sharing in the systems studied by FPU. In our systems if all the energy was initially in one normal mode, it became freely distributed amongst all the modes, provided there was sufficient energy for at least one collision to occur. Data from some of the other computations carried out are given in Appendix 2. The evidence suggested in the theory and supported by the numerical computations strongly suggests that these systems are ergodic.

# CHAPTER 5

# THE STATISTICAL MECHANICS OF THE MODEL

## 5.1 The Isobaric Grand Partition Function

In statistical mechanics the grand partition function of an assembly of N particles confined to a volume V is defined by

$$Z_g(T,\mu,V) = \Sigma_{(N)}\ Z(T,N,V)\exp(N\mu/kT), \qquad ---(5.1)$$

where $Z(T,N,V)$ is the ordinary partition function. T is the absolute temperature of the assembly, $\mu$ is the chemical potential, and k is Boltzmann's constant. The partition functions are related to thermodynamic variables via the equations

$$F = -kT\ \ell n\ Z(T,N,V), \qquad ---(5.2)$$

and

$$PV = kT\ \ell n\ Z_g(T,\mu,V), \qquad ---(5.3)$$

where P is the pressure, and F the Helmholtz free energy. If E is the total energy of the assembly and S the entropy, then

$$F = E - TS = \mu N - PV. \qquad ---(5.4)$$

The equations above suggest that an isobaric grand partition function [7] be defined by

$$Z_i(T,N,P) = \Sigma_{(V)}\ Z(T,N,V)\exp(-PV/kT). \qquad ---(5.5)$$

The corresponding thermodynamic potential $\mu N$, the Gibb's free energy, will be given as a function of T, N, and P by

$$\mu N = - kT\ \ell n\ Z_i(T,N,P).$$

From (4), and the first and second laws of thermodynamics,

$$d(\mu N) = - SdT + VdP + \mu dN,$$

so that

$$\frac{\partial}{\partial P}(\mu N) = V, \qquad ---(5.6a)$$

and

$$\frac{\partial}{\partial T}(\mu N) = - S. \qquad ---(5.6b)$$

Equations (4) and (6) together yield

$$E = \mu N - T \frac{\partial}{\partial T}(\mu N) - P \frac{\partial}{\partial P}(\mu N),$$

i.e.

$$E = kT\left[ T \frac{\partial}{\partial T}(\ell n\ Z_i) + P \frac{\partial}{\partial P}(\ell n\ Z_i) \right]. \qquad ---(5.7)$$

This equation expresses the total energy of the assembly as a function of the temperature and the pressure if the number of particles in the assembly is fixed. Also, if the volume V is given, then P is derived implicitly from (6a), which may be written as

$$V = - kT \frac{\partial}{\partial P} \ell n\ Z_i(T,N,P). \qquad ---(5.8)$$

## 5.2 Evaluation of $Z_i(T,N,P)$

In statistical mechanics the partition function of a one dimensional assembly of particles with N degrees of freedom is shown to be

$$Z = \left(\frac{M\ k\ T}{2\pi\ \hbar^2}\right)^{\frac{1}{2}N} Z_C, \qquad ---(5.9)$$

where $\hbar$ is Planck's constant, and $Z_C$ is the configurational partition function of the assembly. In our model this is given by

$$Z_C = \int \cdots \int \exp\left[ - \sum_{j=1}^{N+1} \phi(y_j - y_{j-1})/kT \right] dy, \qquad ---(5.10)$$

integrated over $0 = y_0 < y_1 < \cdots < y_{N+1} = L$, where we have written $y_j = j\ell + x_j$. On replacing the variable V by the variable L of our assembly we obtain, from (5) and (9),

$$Z_i(T,N,P) = \left(\frac{M\ k\ T}{2\pi\ \hbar^2}\right)^{\frac{1}{2}N} \int_0^\infty \exp(-PL/kT) Z_C(T,N,L)\,dL$$

$$= \left(\frac{M\ k\ T}{2\pi\ \hbar^2}\right)^{\frac{1}{2}N} \bar{Z}_C(T,N,P/kT). \qquad ---(5.11)$$

where $\bar{Z}_C$ is the Laplace transform of $Z_C$.

If $\mathcal{L}$ is defined as the Laplace transform operator

$$\mathcal{L}[f(r)] = \int_0^\infty \exp(-Pr/kT)[f(r)]\,dr, \qquad ---(5.12)$$

repeated use of the convolution formula,

$$\mathcal{L}\left[\int_0^r f(r-\lambda)g(\lambda)\,d\lambda\right] = \mathcal{L}[f(r)].\mathcal{L}[g(r)],$$

gives

$$\bar{Z}_C(T,N,P/kT) = \left\{\mathcal{L}\left[\exp[-\phi(r)/kT]\right]\right\}^{N+1}. \qquad ---(5.13)$$

Since $\exp[-\phi(r)/kT] = 0$ for $r \leq d$,

$$\mathcal{L}\left[\exp[-\phi(r)/kT]\right] = \exp(-Pd/kT)\mathcal{L}\left[\exp[-\phi(r+d)/kT]\right],$$

which reduces to a standard Laplace transform when the functional form of $\phi$ given by Eq. (2.3) is introduced. Indeed,

$$\mathcal{L}\left[\exp[-\phi(r+d)/kT]\right] = \exp\left(-[\phi_0+\tfrac{1}{2}\gamma(a-d)^2]/kT\right) \times \mathcal{L}\left[\exp\left(-\tfrac{1}{2}\gamma[r^2-2r(a-d)]/kT\right)\right]$$

$$= \exp\left(-[\phi_0+\tfrac{1}{2}\gamma(a-d)^2]/kT\right) \mathcal{L}'[\exp(-r^2/4a^2)],$$

where

$$a = (kT/2\gamma)^{\frac{1}{2}},$$

and $\mathcal{L}'$ is the Laplace operator given by (12) when P/kT is replaced by

$$\beta = [P-\gamma(a-d)]/kT.$$

The remaining transform, which may be found in standard tables [8] of Laplace transforms, is

$$\mathcal{L}'[\exp(-r^2/4\alpha^2)] = 2\alpha \exp(\alpha^2\beta^2) \int_{\alpha\beta}^{\infty} \exp(-t^2)dt.$$

After a process of back substitution into the various equations, the isobaric grand partition function for the assembly of particles is finally evaluated to be

$$Z_i(T,N,P) = \left(\frac{M\ k\ T}{2\pi\ \hbar^2}\right)^{\frac{1}{2}N} \left[(kT/\gamma)^{\frac{1}{2}} F(y) \exp\left(-[Pd+\phi_0+\tfrac{1}{2}\gamma(a-d)^2]/kT\right)\right]^{-N+1}, \qquad ---(5.14)$$

where

$$y = [P-\gamma(a-d)](\gamma kT)^{-\frac{1}{2}}, \qquad ---(5.15)$$

and

$$F(y) = \exp(\tfrac{1}{2}y^2) \int_{y}^{\infty} \exp(-\tfrac{1}{2}s^2)ds \qquad ---(5.16)$$

is an error function which has been tabulated [9].

An equation of state for the model is now derived from (8) and (14) in the form

$$P + \gamma(\ell-a) = (\gamma kT)^{\frac{1}{2}} F(y)^{-1}. \qquad ---(5.17)$$

Koppell [10] has derived an equation similar to this. However the above evaluation of the function $\overline{Z}_C$ is much simpler [11] than the complicated saddle point method which Koppell used to evaluate $Z_C$. The use of the grand partition function avoids the saddle point method and thereby greatly simplifies the mathematical analysis.

A similar criticism was made over ten years ago by Lewis and Wannier [12] of a paper by Berlin and Kac [13]. The latter derived the spherical properties of a ferromagnet by a lengthy saddle point evaluation of the partition function. Lewis and Wannier showed that "the mathematical manipulation can be

reduced to almost nothing" through the use of the grand partition function. They also felt that "this observation is of some consequence in a domain of research in which progress has been largely impeded by mathematical difficulties". Of course it has to be borne in mind that the different partition functions give the same mean values of the thermodynamic quantities, but would give different results for fluctuations, and other quantities in which second-order terms are important.

## 5.3 The Pressure and Energy Equations

Our equation of state (17) clearly shows that the difference between the pressure of the nonlinear system and the pressure due to the tension in the springs is given by a correction term, which is a function of the temperature, and the function $F(y)$ defined by (15) and (16). Nagamiya [14] has considered a model in which the mutual interaction energy between particles was taken to be

$$\phi(r) = \phi_0 + \tfrac{1}{2}\gamma(r-a)^2 \qquad -\infty < r < \infty.$$

Here no cut-off was assumed to exist at $r = d$. The model was therefore linear, and the equation of state derived was

$$P + \gamma(\ell - a) = 0. \qquad \text{---(5.18)}$$

This is just our equation of state (17) with the correction term replaced by zero. The correction term, then, represents the difference between the linear and the nonlinear cases. The result in the linear case is, of course, formulated in Hooke's Law.

For further comparison it is possible to recast (17) in the form

$$x = \gamma(\ell - d)(\gamma kT)^{-\frac{1}{2}} = -y + F(y)^{-1}. \qquad \text{---(5.19)}$$

One could assume that there is a minimum distance between molecular centres, say d, in Nagamiya's model. By adding an appropriate term in each side of (18) and effecting some minor rearrangement we have

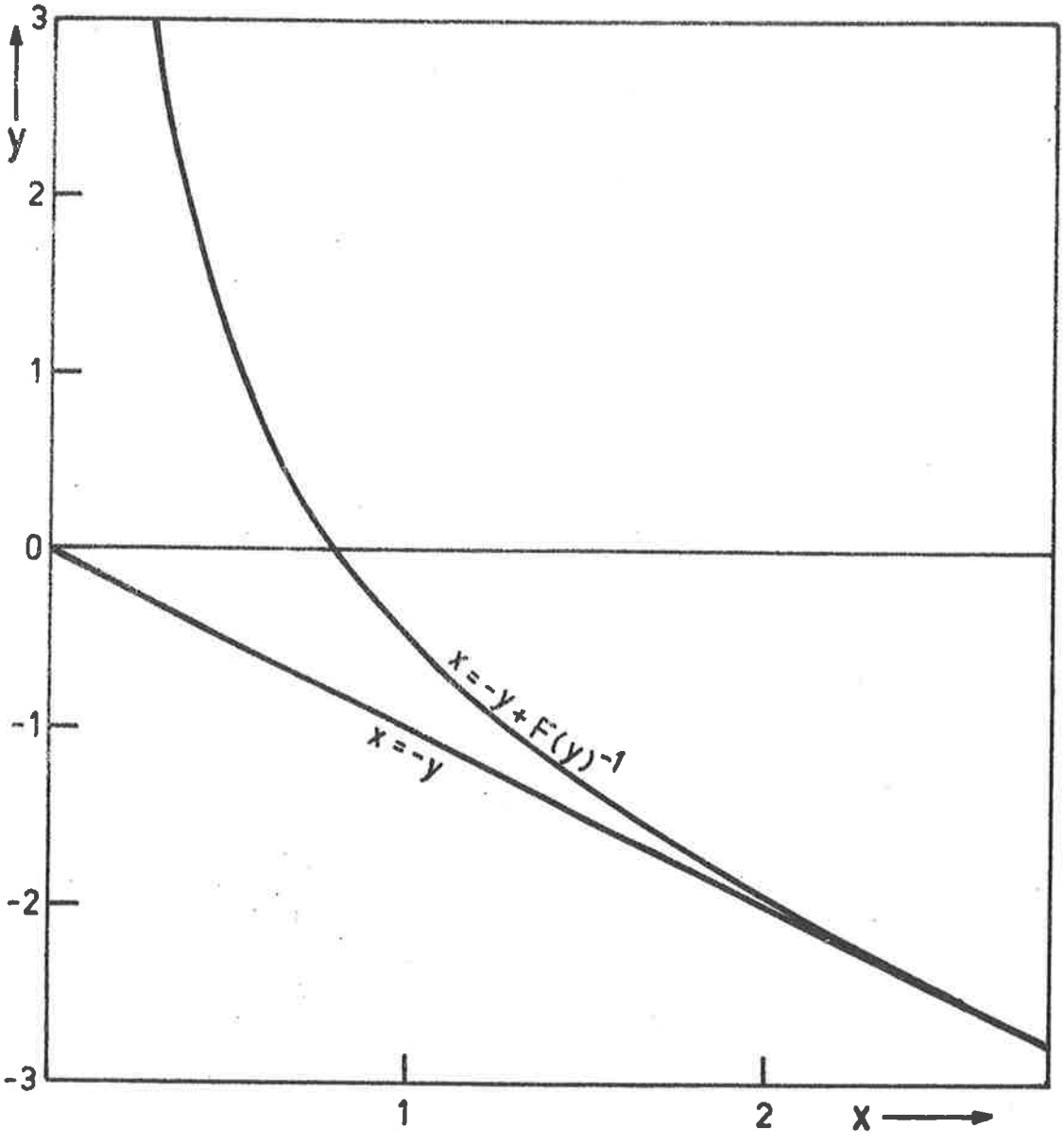


FIGURE 4. Curves for the equation of state, in dimensionless form, for both the linear and nonlinear systems. $x=y(\ell-d)(ykT)^{-\frac{1}{2}}$, and $y=[P-y(a-d)](ykT)^{-\frac{1}{2}}$.

$$x = \gamma(\ell-d)(\gamma kT)^{-\frac{1}{2}} = -y. \qquad ---(5.20)$$

Equations (18) and (19) are represented graphically in Fig. 4. Note that, for any given abscissa x, the difference between the y coordinates of the nonlinear and linear curves in the figure is

$$y - y_1 = x + y = F(y)^{-1}, \qquad ---(5.21)$$

where $y_1$ is the ordinate of the linear curve.

The total energy of the assembly may be obtained from (7) and (14) in the form

$$E = (N+\tfrac{1}{2})kT + \tfrac{1}{2}(N+1)\gamma^{-1}\left[P^2 - \gamma^2(\ell-a)^2 - (\gamma kT)^{\frac{1}{2}}F(y)^{-1}[P+\gamma(a-d)]\right], \qquad ---(5.22)$$

where we have used $\phi_0 = -\frac{1}{2}\gamma(\ell-a)^2$. On using (17) to eliminate F(y), the energy is found to be given by

$$E/(N+1) = kT - \tfrac{1}{2}(\ell-d)[P+\gamma(\ell-a)] - \tfrac{1}{2}(N+1)^{-1}kT.$$

When N is assumed to be infinite the mean energy per particle defined by Eq. (4.18) is

$$\epsilon = kT - \tfrac{1}{2}(\ell-d)[P+\gamma(\ell-a)]. \qquad ---(5.23)$$

In linear systems the pressure is given by (18), and $\epsilon = kT$, as expected.

For given values of the parameters $\gamma$, $\ell$, a, and d, (15), (17), and (23) is a set of three independent equations in the four variables $\epsilon$, P, T, and y. Any one of these variables may therefore be expressed as a function of any one of the others. Theoretical values for the expected temperature and pressure of any assembly may therefore be computed. Sketches of the curves $T = T(\epsilon)$ and $P = P(\epsilon)$, for the numerical values of the parameters given in Table I (p.29), have been drawn in Figs. 5 and 6, respectively. The pressure of a linear system with the given parameters is $P = -\cdot 2 \times 10^{-7}$ dyne. It is clear from Fig. 7 that the model becomes approximately linear when $\epsilon < \cdot 25 \times 10^{-14}$ ergs.

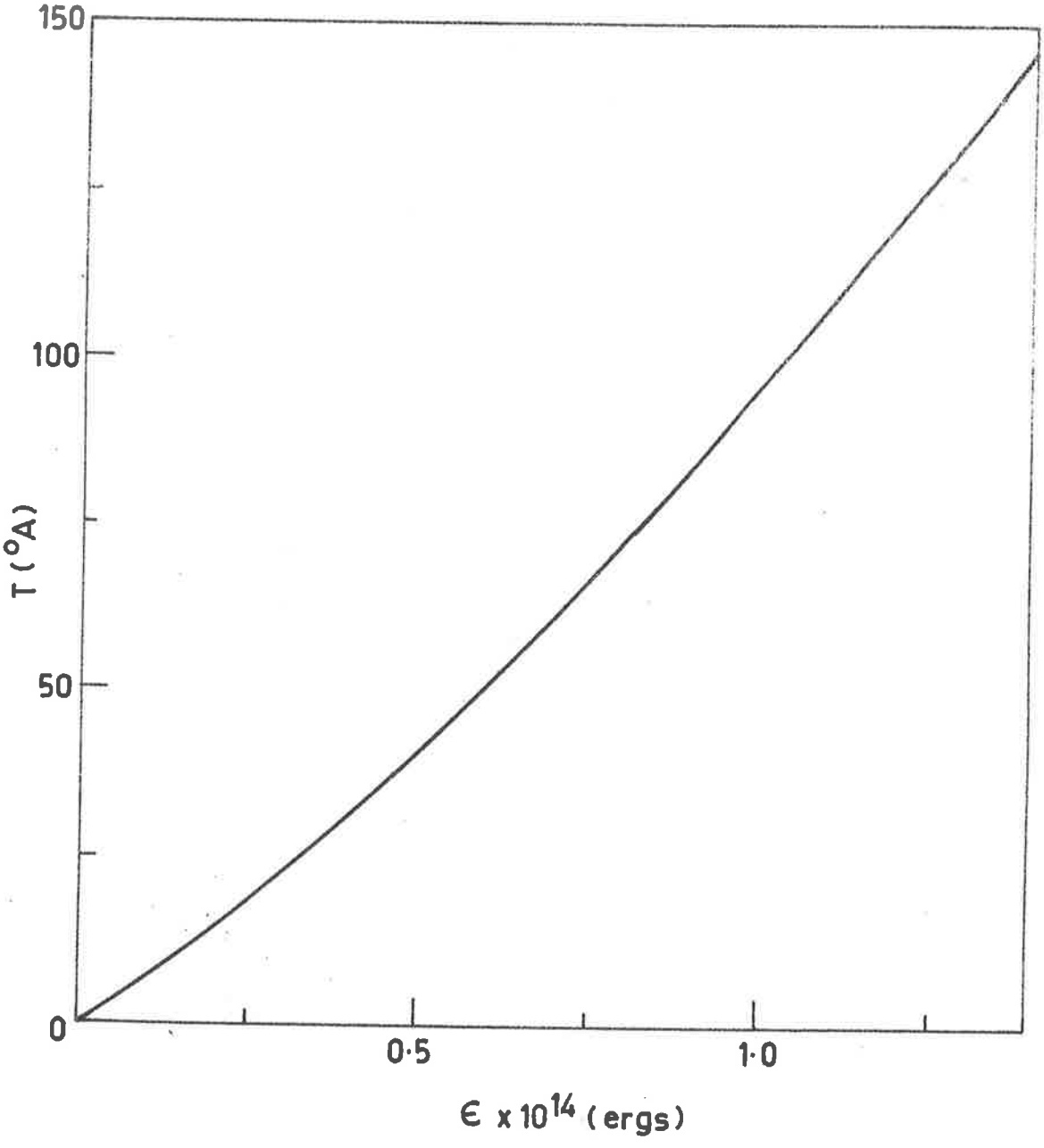


FIGURE 5. The thermodynamic temperature T as a funcion of the mean energy/particle ε, for the specific values of the parameters given in Table I.

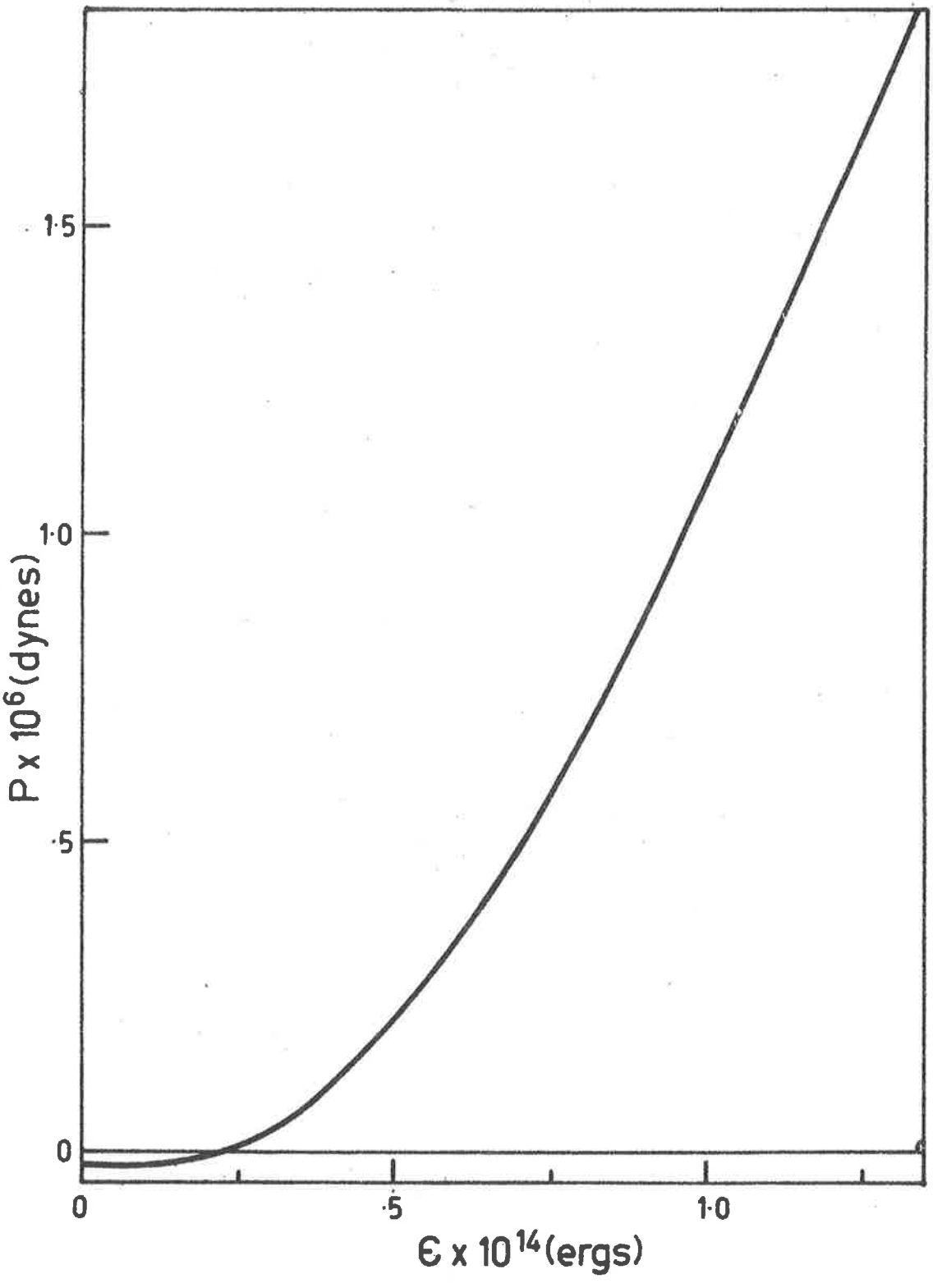


FIGURE 6. The thermodynamic pressure P as a function of $\epsilon$, for the values of the parameters given in Table I.

Because $\epsilon$ is then small compared with $\phi(d+) = \cdot 708 \times 10^{-14}$ ergs, the cut-off in the potential at r = d has little effect, i.e. few collisions, if any, occur. This is further evidenced by reference to Fig. 1 (p.10). Note also that the model appears to be weakly nonlinear when $\epsilon = \epsilon' = \cdot 4 \times 10^{-14}$ ergs, which is the mean energy per particle for some of the systems on which computations were carried out.

## 5.4 Fluctuations

Fluctuations in the temperature and the pressure are expected in an isolated assembly. The relative fluctuations in the temperature T are given by

$$\sigma_T^2 = \overline{(T - \bar{T})^2} / \bar{T}^2 , \qquad ---(5.24)$$

where $\bar{T}$ is the phase average of T. However, because we are using ideal walls for the calculation of the pressure, we cannot consider fluctuations in the actual pressure. This is because any estimate of the pressure requires a finite time for computation. We therefore consider fluctuations in the time average of the pressure [15] defined by

$$\sigma^2_{<P>} = \overline{(<P> - \overline{<P>})^2} / \overline{<P>}^2 . \qquad ---(5.25)$$

Computation of these fluctuations will yield further evidence on whether or not the mean temperature and pressure of any system approach equilibrium values.

The ergodic theorem states that the phase average (e.g. $\bar{T}$) is the same as the limiting value of the time average (e.g. <T>). As our systems appear to be ergodic (Chapt. 4), we make estimates of the fluctuations by computing time averages of T and <P>, rather than phase averages. It would also be convenient to derive expected values for the fluctuations from statistical mechanics. However, as has already been pointed out, we cannot obtain the correct values for the expected fluctuations in the microcanonical systems being studied from $Z_i$, which was evaluated by considering an isobaric grand canonical ensemble.

# CHAPTER 6.

# COMPUTATION OF THE THERMODYNAMIC VARIABLES

In the last chapter the statistical mechanics of the model was developed, i.e. expressions were found for the thermodynamic variables when N was assumed to be infinite. Mathematical expressions will now be found for the corresponding variables of the finite model.

## 6.1 The Mean Temperature

Since there are N degrees of freedom in the model, it follows from the equipartition principle that

$$\langle KE \rangle = \tfrac{1}{2} Nk \langle T \rangle,$$

where <KE> denotes the time average of the kinetic energy of the system. The time average of the temperature is therefore given by

$$\langle T \rangle = 2 \langle KE \rangle / (Nk). \qquad ---(6.1)$$

A measure of the instantaneous temperature is taken as $T = 2 \times KE/(Nk)$.

The time average of the kinetic energy over any time interval $(0,\tau)$ is

$$\langle KE \rangle = \tfrac{1}{2} M \tau^{-1} \int_0^\tau \dot{\underset{\sim}{x}}' \, \dot{\underset{\sim}{x}} \, dt. \qquad ---(6.2)$$

If there are no collisions in this interval (i.e. the system

behaves linearly) then, on integrating by parts and rearranging,

$$\tfrac{1}{2}M \int_0^\tau (\dot{\underset{\sim}{x}}' \dot{\underset{\sim}{x}} - \underset{\sim}{x}' \underset{\sim\sim}{R} \underset{\sim}{x})dt = \tfrac{1}{2}M[\underset{\sim}{x}' \dot{\underset{\sim}{x}}]_0^\tau,$$

where we have used Eq. (2.8) to evaluate $\underset{\sim}{x}' \ddot{\underset{\sim}{x}}$. But from Eq. (4.4), since the system is conservative,

$$\tfrac{1}{2}M \int_0^\tau (\dot{\underset{\sim}{x}}' \dot{\underset{\sim}{x}} + \underset{\sim}{x}' \underset{\sim\sim}{R} \underset{\sim}{x})dt = \tau E.$$

Addition of the last two equations yields the time average of the kinetic energy over the interval $(0,\tau)$, if no collisions occur:

$$\langle KE \rangle = \tfrac{1}{2}E + \tfrac{1}{4}M\, \tau^{-1} [\underset{\sim}{x}' \dot{\underset{\sim}{x}}]_0^\tau. \qquad ---(6.3)$$

As $\tau$ increases the second term tends to zero, giving the expected result for the linear system $\langle KE \rangle = \tfrac{1}{2}E$ in the limit as $\tau \to \infty$.

When there are collisions during the interval $(0,\tau)$, there is a correction term $C'$ in (3) so that

$$\langle KE \rangle = \tfrac{1}{2}E + \tfrac{1}{4}M\, \tau^{-1} [\underset{\sim}{x}' \dot{\underset{\sim}{x}}]_0^\tau + C', \qquad ---(6.4)$$

where

$$C' = -\tfrac{1}{4}M\, \tau^{-1} \Sigma_i [\underset{\sim}{x}' \dot{\underset{\sim}{x}}]_{t_i-}^{t_i+},$$

and $t_i$ $(i = 1,2,\ldots)$ are the times at which the collisions occur. If we define

$$D' = [\underset{\sim}{x}' \dot{\underset{\sim}{x}}]_{t-}^{t+},$$

then, for a collision between particles $j-1$ and $j$ at time $t$,

$$D' = x_{j-1}(t)[\dot{x}_{j-1}(t+) - \dot{x}_{j-1}(t-)] + x_j(t)[\dot{x}_j(t+) - \dot{x}_j(t-)].$$

On using Eqs. (2.5) and (2.7) this may be reduced to

$$D' = -(\ell - d)\, |\Delta \dot{x}_j(t)|,$$

where $|\Delta\dot{x}_j(t)|$ is given by Eq. (4.10). The correction term for the nonlinear case in which there are collisions is therefore

$$C' = \tfrac{1}{4}M\,\tau^{-1}(\ell-d)\Sigma_i|\Delta\dot{x}_j(t_i)|, \qquad ---(6.5)$$

where the summation is over all collisions between particles $j-1$ and $j$ at times $t_i$ during the time interval.

The time average $\langle T\rangle$, which we shall call the mean temperature, is computed from (1), (4), and (5), i.e.

$$\langle T\rangle = E/(Nk) + \tfrac{1}{2}M(Nk\tau)^{-1}\left\{[\underset{\sim}{x}'\dot{\underset{\sim}{x}}]_0^\tau + (\ell-d)\Sigma_i|\Delta\dot{x}_j(t_i)|\right\}. \qquad ---(6.6)$$

## 6.2 The Mean Pressure

Between collisions the forces exerted by the constraints holding particles 0 and $N+1$ fixed are

$$f_0 = -\gamma(x_1+\ell-a),$$

and

$$f_{N+1} = \gamma(-x_N+\ell-a),$$

respectively. Since the model is one-dimensional, these forces are the instantaneous pressures acting on the left and right walls, respectively, provided there are no collisions on the walls. Thus, in the linear system, the time average of the mean pressure acting on the two walls taken over an interval $(0,\tau)$ is

$$\langle P\rangle = -\gamma(\ell-a) - \tfrac{1}{2}\gamma\,\tau^{-1}\int_0^\tau (x_1-x_N)dt. \qquad ---(6.7)$$

From Eq. (2.8) it follows that

$$\gamma\int_0^\tau (x_1-x_N)dt = -\gamma(\underset{\sim}{\alpha}_1'-\underset{\sim}{\alpha}_N')[\dot{\underset{\sim}{x}}]_0^\tau, \qquad ---(6.8)$$

where $\underset{\sim}{\alpha}_1'$ and $\underset{\sim}{\alpha}_N'$ are the first and last rows, respectively, of the matrix $\underset{\sim}{R}^{-1}$. Since this integral is finite, in the limit as $\tau\to\infty$,

$$\langle P\rangle \to -\gamma(\ell-a), \qquad ---(6.9)$$

which is the result for the linear system predicted in Eq.(5.18).

When there are end collisions, however, there are additional contributions to the pressure due to impulses on the walls. A measure of the time average of the pressure over the interval $(0,\tau)$ in the nonlinear system is therefore given by

$$\langle P\rangle = -\gamma(\ell-a) - \tfrac{1}{2}\gamma\tau^{-1}\int_0^\tau (x_1-x_N)dt + C''. \quad ---(6.10)$$

For an end collision the impulse of the impact on the wall is $2M|\dot{x}_i|$, $i = 1$ or $N$. If $\Sigma'$ and $\Sigma''$ denote summation over all collisions on the left and right walls, respectively, then

$$C'' = M\tau^{-1}[\Sigma'|\dot{x}_1| + \Sigma''|\dot{x}_N|]. \quad ---(6.11)$$

The definite integral in (10) is evaluated by summing the partial integrals for the time intervals between each pair of collisions. Thus

$$-\gamma\int_0^\tau (x_1-x_N)dt = \gamma(\underset{\sim}{\alpha}_1'-\underset{\sim}{\alpha}_N')\left\{[\underset{\sim}{\dot{x}}]_0^\tau - \Sigma_i[\underset{\sim}{\dot{x}}]_{t_i-}^{t_i+}\right\}, \quad ---(6.12)$$

the summation being taken over all collisions at times $t_i$ $(i = 1,2,\ldots)$. To simplify this expression we introduce

$$D'' = (\gamma/M)(N+1)\ (\underset{\sim}{\alpha}_1' - \underset{\sim}{\alpha}_N')[\underset{\sim}{\dot{x}}]_{t-}^{t+}.$$

Since

$$(\gamma/M)(N+1)\ \underset{\sim}{\alpha}_1' = (N,N-1,\ldots,1),$$

and

$$(\gamma/M)(N+1)\ \underset{\sim}{\alpha}_N' = (1,2,\ldots,N),$$

then, for a collision between particles $j-1$ and $j$ at time $t$,

$$D'' = [N+1-2(j-1)][\dot{x}_{j-1}(t+)-\dot{x}_{j-1}(t-)]+[N+1-2j][\dot{x}_j(t+)-\dot{x}_j(t-)],$$

the boundary conditions being assumed. By using the collision conditions (2.7) this may be reduced to

$$D'' = \begin{cases} 2(N-1) \quad |\dot{x}_1(t)| & j = 1 \\ -2|\dot{x}_j(t)-\dot{x}_{j-1}(t)| & 1 < j < N+1 \\ 2(N-1) \quad |\dot{x}_N(t)| & j = N+1. \end{cases}$$

Thus, if $\Sigma''$ denotes summation over all internal collisions,

$$-\gamma \int_0^\tau (x_1 - x_N)dt = \gamma(\underset{\sim}{\alpha}_1' - \underset{\sim}{\alpha}_N')[\dot{\underset{\sim}{x}}]_0^\tau$$

$$+2M[-(N-1)\Sigma'|\dot{x}_1| + \Sigma''|\dot{x}_j - \dot{x}_{j-1}| - (N-1)\Sigma'''|\dot{x}_N|]/(N+1).$$

On adding up all the contributions in (10) we obtain the estimate for the pressure in the form

$$\langle P\rangle = -\gamma(\ell - a) + \tfrac{1}{2}\gamma\tau^{-1}(\underset{\sim}{\alpha}_1' - \underset{\sim}{\alpha}_N')[\dot{\underset{\sim}{x}}]_0^\tau + M(N+1)^{-1}\tau^{-1}\Sigma_i|\Delta\dot{x}_j(t_i)|, \qquad ---(6.13)$$

where the summation is over all collisions between particles $j-1$ and $j$ at times $t_i$ $(i = 1,2,\ldots)$, and $|\Delta\dot{x}_j(t)|$ is determined from Eq. (4.10). Provided the time interval $(0,\tau)$ is large, we shall call this estimate the mean pressure of the system.

In the limit as $\tau \to \infty$,

$$\langle P\rangle \to -\gamma(\ell - a) + \beta, \qquad ---(6.14)$$

where

$$\beta = \lim_{\tau\to\infty} M(N+1)^{-1}\tau^{-1}\Sigma_i|\Delta\dot{x}_j(t_i)|. \qquad ---(6.15)$$

$\beta$, then, represents the difference between the pressures of the corresponding linear and nonlinear thermodynamic systems. From Eq. (5.17) we should expect that, for large N and large $\tau$, the numerical estimates for $\beta$ and T should satisfy the relation

$$\beta(\gamma kT)^{-\frac{1}{2}} = F(\gamma)^{-1}, \qquad ---(6.16)$$

where $\gamma$ and $F(\gamma)$ are defined by Eqs. (5.15) and (5.16), respectively. This last equation is just Eq. (5.21) written in a different form. Thus $\beta(\gamma kT)^{-\frac{1}{2}}$ should yield the vertical

distance of separation between the curves for the linear and nonlinear equations of state, drawn in Fig. 4 (p.61), at the x coordinate determined by T.

## 6.3 Results of the Computations

The numerical computations for different systems showed that the mean temperatures and pressures approach the values predicted theoretically. That a small number of particles gives a good approximation to the infinite assembly seems a characteristic of molecular dynamics. Even when we chose N as small as 7 or 8 the mean temperature approached to within 4% of the predicted temperature for the infinite assembly, while the error in the mean pressure was of the order of 30%. We will now discuss fully the largest systems on which computations were carried out, and only refer to the results for smaller systems for comparison.

In Fig. 7 we plot <T> for the two systems in which N = 31, $\epsilon = \epsilon'' = \cdot 7 \times 10^{-14}$ ergs, and the initial configurations were $E_1 = E$ and $E_N = E$, respectively. It is quite clear that <T> approaches near the thermodynamic value in each case. Figure 8 shows the behaviour of <T> in the two similar systems in which $\epsilon = \epsilon' = \cdot 4 \times 10^{-14}$ ergs. In a linear system in which all the energy is in the i-th normal mode, say, the curve of <T> as a function of the time t will oscillate periodically about the mean $E/(Nk)$ with a period $2\pi/\omega_i$. The oscillations about the mean will decrease to zero as $t \to \infty$. This explains the periodic oscillations in the curve labelled k = 1. In the weakly non-linear system the first mode remained dominant for a considerable time as there was little energy sharing with the other modes, and the oscillations in <T> are therefore to be expected. The period of these oscillations is approximately $2\pi/\omega_1 = 1 \cdot 753 \times 10^{-11}$ sec. However, as the energy becomes distributed amongst all the modes, <T> begins to approach near the thermodynamic value of $31 \cdot 7^{\circ}$A. The approach is slow because of the dominance of the first mode for such a long time. Because of this, the numerical estimate of $\sigma_T^2$ for this system should be

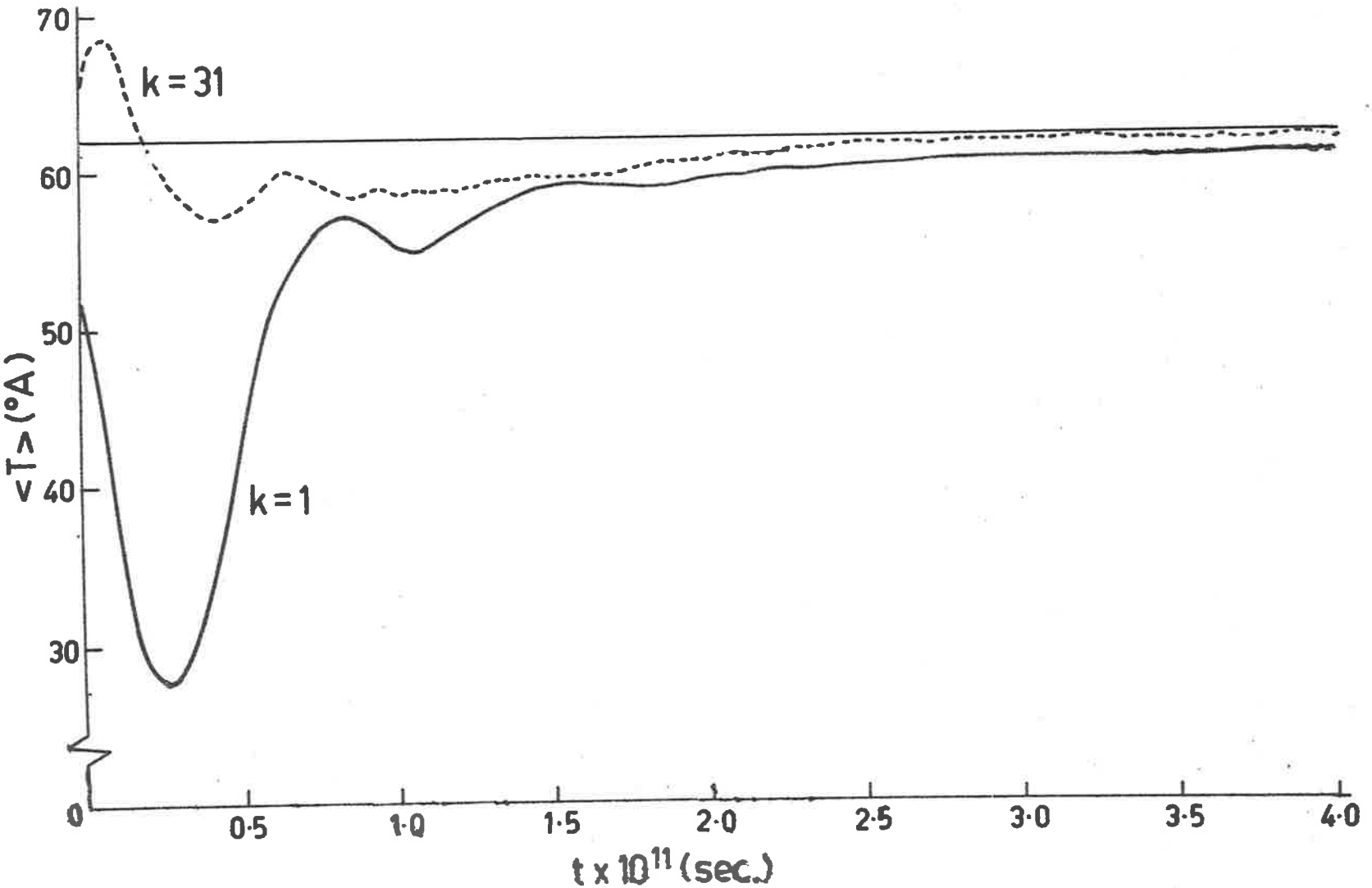


FIGURE 7. The mean temperature computed for the systems N=31, $\epsilon=\epsilon''$, and $E_i=\delta_{ik}E$ at t=0. The predicted thermodynamic temperature is $T'' = 62{\cdot}07^{\circ}A$.

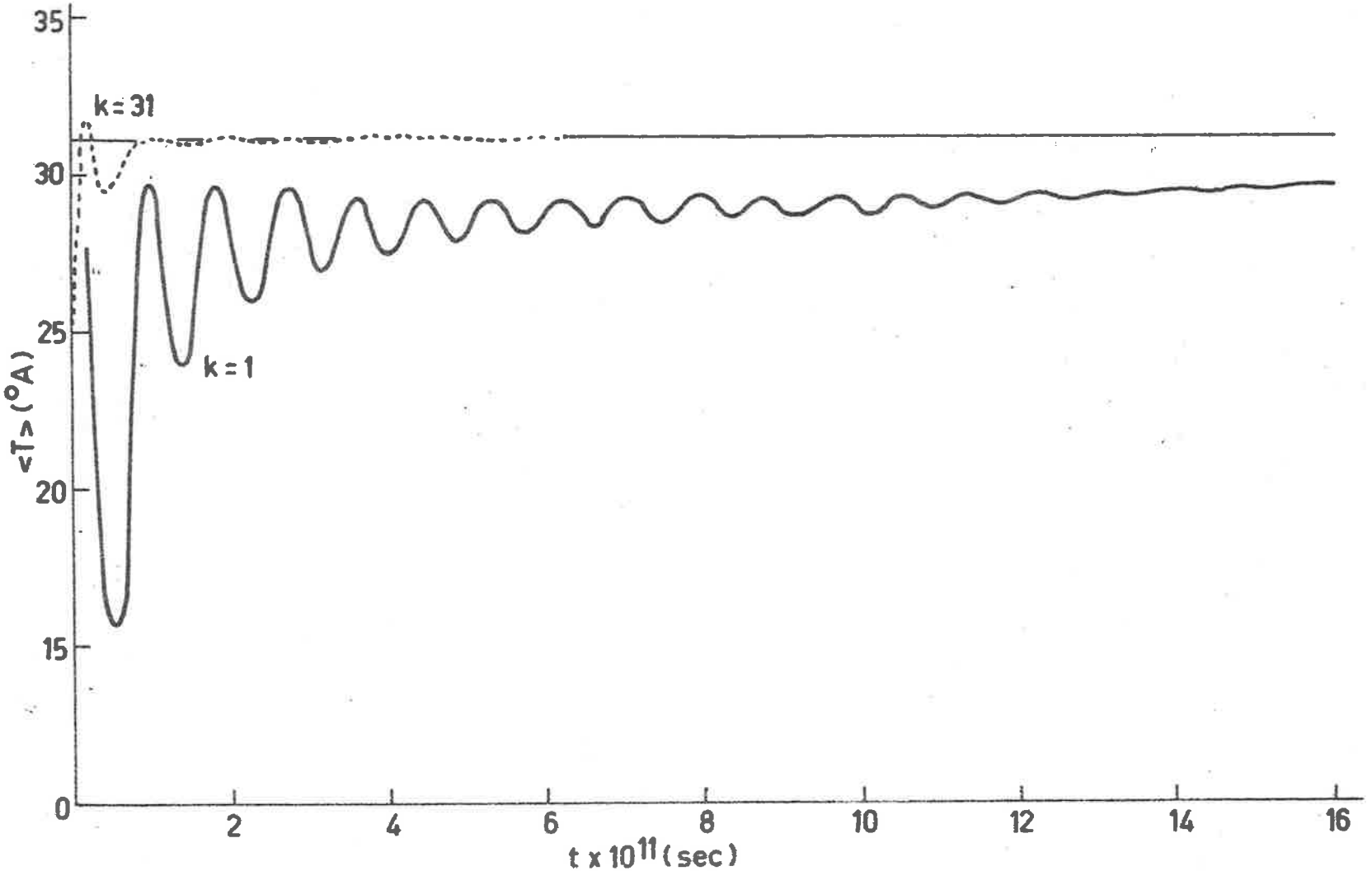


FIGURE 8. The mean temperature for the weakly nonlinear systems N=31; $\epsilon=\epsilon'$ $E_i=\delta_{ik}E$ at t=0. $T' = 31{\cdot}7^{\circ}A$. The distinctly linear behaviour of the system for k=1 is apparent.

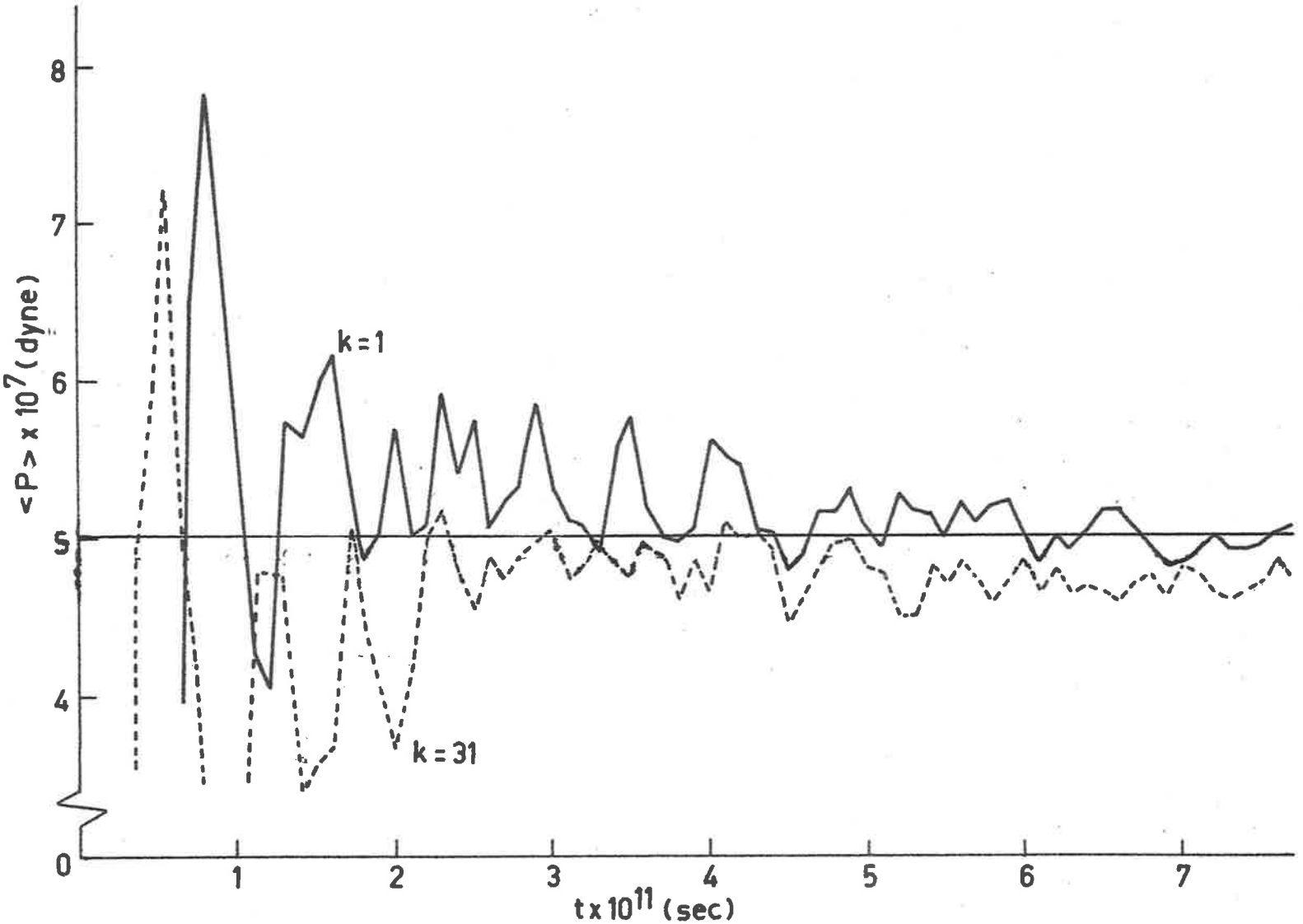


FIGURE 9. The mean pressure for the systems N=31, $\epsilon=\epsilon''$, $E_i=\delta_{ik}E$ at t=0. The predicted thermodynamic pressure is $P'' = \cdot 503 \times 10^{-6}$ dyne.

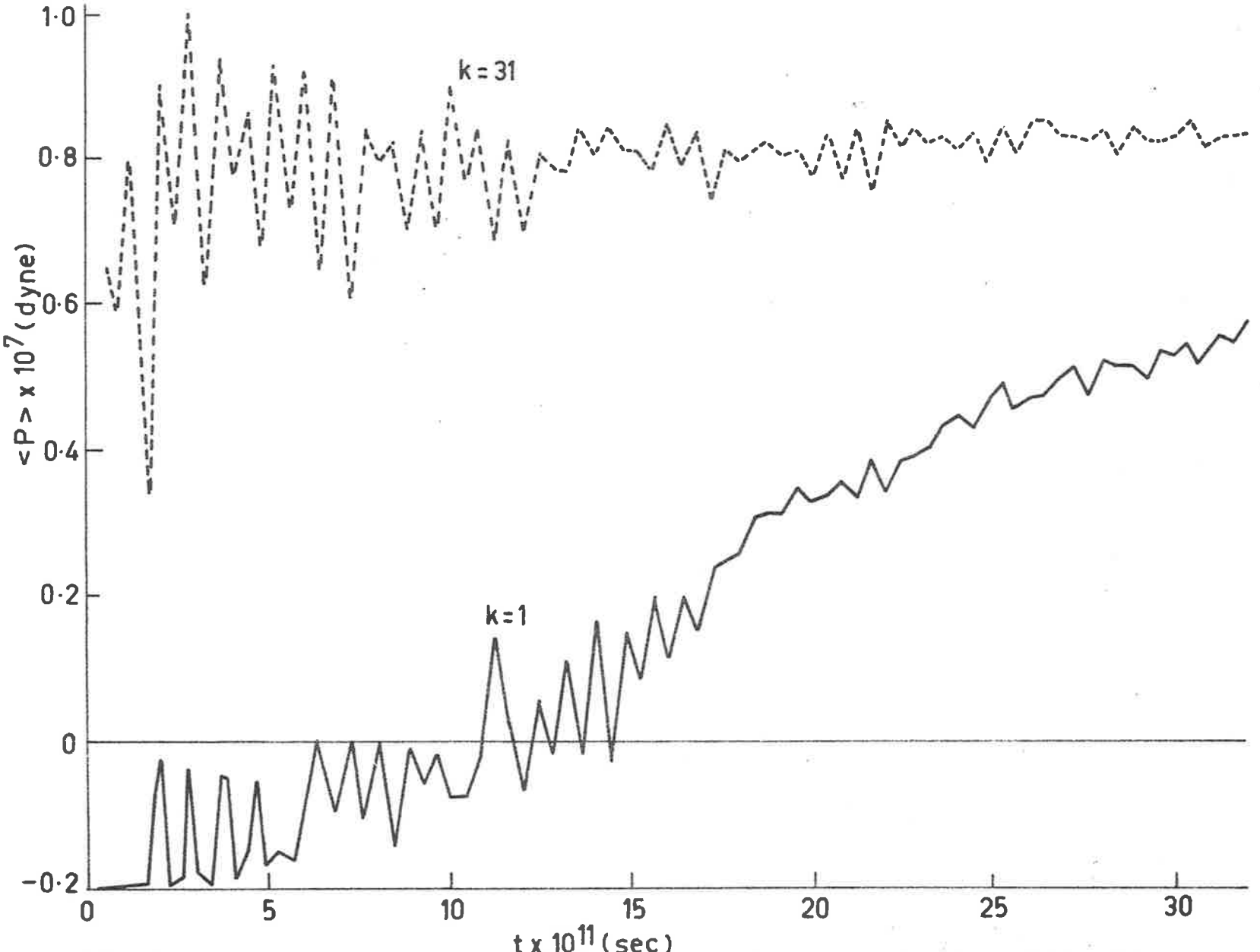


FIGURE 10. The mean pressure for N=31, $\epsilon=\epsilon'$, $E_i=\delta_{ik}E$ at t=0. $P' = \cdot 106\times10^{-6}$ dyne.

much larger than the corresponding estimates for the other systems.

Figures 9 and 10 show that the mean pressure <P> also approaches near the predicted thermodynamic values in each of the four systems discussed above. In the more strongly nonlinear systems (Fig. 9) <P> rapidly approaches the predicted value, and then fluctuates near this value with decreasing variations. The system corresponding to the curve k = 1 in Fig. 10 is obviously strongly linear initially, since the pressure given by Hooke's Law for the linear system is $P_1 = -\cdot 200 \times 10^{-7}$ dyne. This conclusion is supported by the remarks made above about this particular system. As in the case for the temperature <T>, the pressure <P> approaches the thermodynamic value as t increases, indicating a nonlinear behaviour.

Some actual values for <T> and <P>, together with the relative fluctuations $\sigma_T^2$ and $\sigma_{<P>}^2$ computed from Eqs. (5.24) and (5.25), respectively, are given in Table XII for systems of N = 15 and N = 31 particles. For N = 15 the values of <T> for the given systems differ from the predicted thermodynamic temperatures by about 2·5%. For similar initial time intervals the results for N = 31 show that, with one exception, the estimates for <T> are within about 1% of the thermodynamic values. However, for second time intervals corresponding to collisions 1500 - 3000 when N = 31, the error is about ·6% when $\epsilon = \epsilon'$, and remains near 1% when $\epsilon = \epsilon''$, with no exception. The smaller relative error when $\epsilon = \epsilon'$ is to be expected as the time intervals considered are considerably larger than those considered in the more strongly nonlinear systems in which $\epsilon = \epsilon''$. It is seen that the larger systems (N = 31) give results which are much closer to the thermodynamic temperatures (N = ∞). The computed values for $\sigma_T^2$ when N = 31 indicate that the temperatures of these systems approach equilibrium values. As expected, the corresponding relative fluctuations for N = 15 are larger. The computed values for the mean pressure, although not as accurate as those for the mean temperature, also show an approach near to

TABLE XII. Time averages of the temperature <T> and pressure <P>, together with the relative fluctuations $\sigma_T^2$ and $\sigma_{<P>}^2$, respectively, over intervals of C collisions and time t sec for systems of (a) N = 15 and (b) N = 31 particles; $E_k$ = E at t = 0, and $\epsilon$ = E/N. x and y give the values of the variables in the dimensionless equation of state Eq. (5.19).

| $\epsilon$ | k | C × $10^{-1}$ | t × $10^{10}$ | <T> | $\sigma_T^2$ | <P> × $10^6$ | $\sigma_{<P>}^2$ | x | y | x + y |
|---|---|---|---|---|---|---|---|---|---|---|
| (a) | | | | | | | | | | |
| $\epsilon'$ | 1 | 0-75 | 3·13 | 30·9 | ·048 | ·0647 | ·0626 | 1·837 | -1·772 | ·065 |
| $\epsilon'$ | 15 | 0-75 | 3·01 | 31·2 | ·048 | ·0779 | ·0143 | 1·827 | -1·753 | ·075 |
| $\epsilon''$ | 1 | 0-75 | ·89 | 60·7 | ·036 | ·4361 | ·0022 | 1·311 | -1·062 | ·249 |
| $\epsilon''$ | 15 | 0-75 | ·97 | 60·3 | ·035 | ·3922 | ·0032 | 1·315 | -1·089 | ·226 |
| (b) | | | | | | | | | | |
| $\epsilon'$ | 1 | 0-150 | 3·31 | 30·6 | ·078 | ·0605 | ·7578 | 1·846 | -1·784 | ·062 |
| | | 150-300 | 2·66 | 31·5 | ·018 | ·0875 | ·0048 | 1·820 | -1·738 | ·082 |
| $\epsilon'$ | 31 | 0-150 | 2·85 | 31·3 | ·023 | ·0813 | ·0080 | 1·825 | -1·748 | ·077 |
| | | 150-300 | 2·65 | 31·5 | ·022 | ·0988 | ·0008 | 1·820 | -1·730 | ·090 |
| $\epsilon''$ | 1 | 0-150 | ·77 | 61·4 | ·016 | ·5101 | ·0042 | 1·303 | -1·015 | ·288 |
| | | 150-300 | ·85 | 61·5 | ·015 | ·4476 | ·0004 | 1·302 | -1·049 | ·253 |
| $\epsilon''$ | 31 | 0-150 | ·85 | 61·6 | ·019 | ·4695 | ·0025 | 1·301 | -1·036 | ·265 |
| | | 150-300 | ·87 | 61·4 | ·017 | ·4494 | ·0003 | 1·303 | -1·048 | ·255 |

TABLE XIII. The theoretically predicted thermodynamic values for the temperature T and the pressure P. x and y are the coordinates of the appropriate points on the nonlinear curve in Fig. 4, which represents Eq. (5.19).

| $\epsilon$ | T | P × $10^6$ | x | y | x + y |
|---|---|---|---|---|---|
| $\epsilon' = ·4 \times 10^{-14}$ | 31·72 | ·1060 | 1·814 | - 1·718 | ·096 |
| $\epsilon'' = ·7 \times 10^{-14}$ | 62·07 | ·5031 | 1·296 | - 1·014 | ·282 |

the predicted pressures. Again, the results are, in general, closer to the thermodynamic values when N = 31 than when N = 15. Of course the fluctuations $\sigma_{<P>}^2$ should tend to zero if <P> approaches an equilibrium value. The given estimates for $\sigma_{<P>}^2$ when N = 31 therefore support the conclusion that the mean pressures do, in fact, approach equilibrium values. It should be pointed out that no contributions to $\sigma_T^2$ and $\sigma_{<P>}^2$ were computed for the first 5N collisions when $\epsilon = \epsilon'$, and for the first 10N collisions when $\epsilon = \epsilon''$. A point of interest is that the average rate of collisions per degree of freedom C/Nt is approximately the same for every system with the same energy per degree of freedom $\epsilon$. This rate increases rapidly as $\epsilon$ increases, being about three times greater for $\epsilon = \epsilon''$ than for $\epsilon = \epsilon'$.

The values obtained for the variables x and y determined from Eqs. (5.19) and (5.17) are also given in Tables XII and XIII. Almost every pair of coordinates x and y computed for the systems in which N = 31 gives a point which lies very close to the curve for the nonlinear equation of state in Fig. 5. Indeed the reason for not plotting these points is that they are so close to each other, and to the curve, as to be almost indistinguishable on such a small figure. As suggested by Eq. (5.21), the theoretical value for x + y for any given $\epsilon$ is the vertical distance between the linear and the nonlinear curves in Fig. 5, and is therefore a measure of the difference between the linear and nonlinear systems. Comparison of the values for x + y in the tables shows that the points (x,y) for N = 15 are not as close to the curve for the equation of state as are the corresponding points for N = 31. In other words, the systems in which N = 15 do not show the difference between the linear and nonlinear models as well as do the systems with N = 31. However we suggest that, if sufficient computations had been carried out with N = 31, say, for different mean energies $\epsilon$, the curve for the equation of state could have been obtained experimentally. In particular, we conclude that the numerical computations provide an adequate evaluation of the thermodynamic properties of the nonlinear model.

# CHAPTER 7

# THE AUTOCORRELATION FUNCTION

## 7.1 Introduction

The volume of the total phase space available to an isolated microcanonical system of total energy E is finite. From this it can be concluded that the path in phase space which represents the motion of the system must be closed, in which case the system must eventually return to its initial configuration, before repeating the previous motion. The length of time for such a repetition is known as the Poincaré recurrence time of the system. It is known that the existence of an equilibrium state with fluctuations need not be inconsistent with Poincaré cycles, and that small fluctuations from equilibrium should have small Poincaré cycles while large fluctuations should have very long Poincaré cycles. Mazur and Montroll [16] have exhibited several formulae which show that the Poincaré cycles which are most relevant in the analysis of typical experimental situations involve directly only a small number of variables. The formulae given usually involved certain correlation functions of the variables. Mazur and Montroll also showed that a dynamical function is ergodic when its phase correlation function tends to zero as $t \to \infty$. Thus the character of any system can be deduced from correlation functions of variables which are functions of the motion of the system. An example of such a function is the velocity autocorrelation function associated with the i-th particle in our system of N degrees of freedom. This is defined by

$$\rho_{N,i}(t') = \frac{\lim_{T\to\infty} < p_i(t)p_i(t+t') >}{\lim_{T\to\infty} < p_i(t)^2 >} \qquad ---(7.1)$$

where $p_i$ is the momentum of the i-th particle. Before discussing the numerical results obtained for this function for the

nonlinear systems studied, we evaluate $\rho_{N,i}(t')$ for the linear systems.

## 7.2 The Linear Case

The autocorrelation function defined above is readily evaluated for the linear system by transforming the integrands in (1) into the normal coordinates defined in Eq. (4.2), and their derivatives. The solution to the equations of motion of the linear system in terms of the normal coordinates is

$$q_i(t) = q_i(0)\cos\omega_i t + \omega_i^{-1}\dot{q}_i(0)\sin\omega_i t, \qquad ---(7.2)$$

where the $\omega_i$ are given by Eq. (4.3). By transforming into the normal coordinates and using (2) we obtain

$$\dot{x}_i(t)\dot{x}_i(t+t') = \sum_{j,k=1}^{N} S_{ij}S_{ik}\dot{q}_j(t)[-\omega_k q_k(t)\sin\omega_k t' + \dot{q}_k(t)\cos\omega_k t']. \qquad ---(7.3)$$

It is simple to show that

$$\lim_{T\to\infty} \langle \dot{q}_j(t)q_k(t) \rangle = 0,$$

and

$$\lim_{T\to\infty} \langle \dot{q}_j(t)\dot{q}_k(t) \rangle = \tfrac{1}{2}M^{-1}E_j\delta_{jk},$$

where $E_j$ is defined in Eq. (4.6). Hence

$$\lim_{T\to\infty} \langle \dot{x}_i(t)\dot{x}_i(t+t') \rangle = \tfrac{1}{2}\sum_{j=1}^{N} S_{ij}^{\,2}E_jM^{-1}\cos\omega_j t'. \qquad ---(7.4)$$

Since $p_i = M\dot{x}_i$, the autocorrelation function for the linear system is

$$\rho_{N,i}(t) = \frac{\sum_{j=1}^{N} S_{ij}^{\,2}E_j\cos\omega_j t}{\sum_{j=1}^{N} S_{ij}^{\,2}E_j}, \qquad ---(7.5)$$

a function which is obviously periodic in t. There are two special cases of interest when the autocorrelation function in (5) is reduced to a very simple form.

(a) When the energy of the linear system is equipartitioned amongst all the modes,

$$\rho_{N,i}(t) = \sum_{j=1}^{N} S_{ij}^{2} \cos \omega_j t$$

$$= (N+1)^{-1} \sum_{j=1}^{N} \Big(1-\cos[2ij\,\pi/(N+1)]\Big)\cos \omega_j t. \qquad ---(7.6)$$

(b) If the configuration of the system is $E_j = \delta_{jk}E$, so that all the energy is in the k-th mode, then

$$\rho_{N,i}(t) = \cos \omega_k t. \qquad ---(7.7)$$

## 7.3 An Estimate for the Nonlinear Case

Equations (5), (6), and (7) are offered as an interesting basis for comparison with the autocorrelation functions for the nonlinear systems that have been studied. Unfortunately, the autocorrelation function is not easily evaluated in the nonlinear case; indeed we are forced to resort to a numerical approximation to obtain estimates for the necessary time averages in (1). As the method of computing the motion for each system facilitated the obtaining of information at equal time intervals h, an estimate of the autocorrelation function defined in (1) was taken as

$$\rho_{N,i}(t) = \frac{\sum_{r=0}^{n} \dot{x}_i(rh)\dot{x}_i(t+rh)}{\sum_{r=0}^{n} \dot{x}_i(rh)^2}, \qquad (t = 0,h,2h,\ldots). \qquad ---(7.8)$$

The estimate for $t = mh$ has no meaning unless $m \ll n$, i.e. $m < \cdot 05n$ say. In Fig. 11 we have plotted the curve obtained

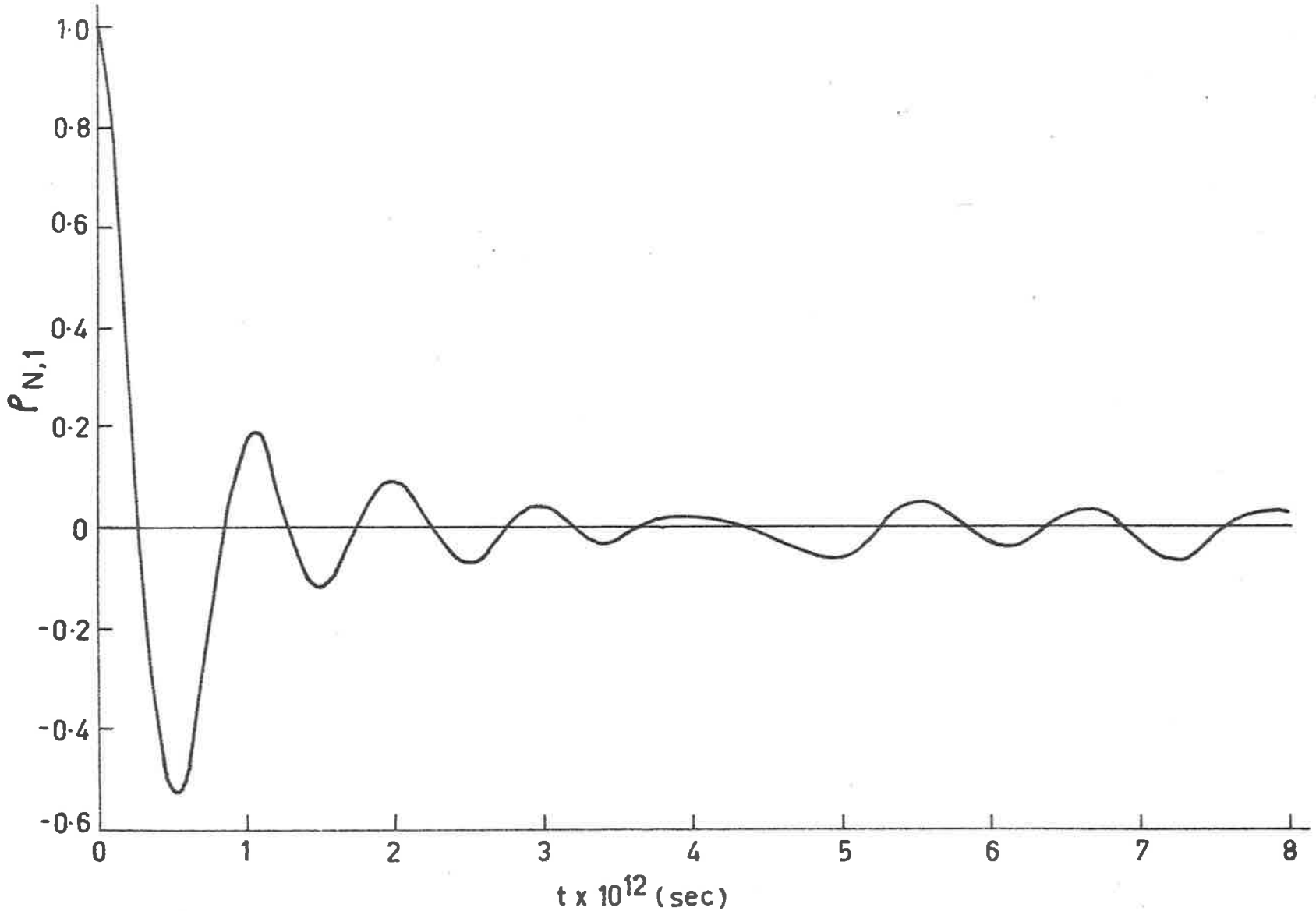


FIGURE 11. The velocity autocorrelation function $\rho_{N,1}$ for the system N=31, $\epsilon=\epsilon'$, k=1.

for $\rho_{N,1}(t)$ for the system N = 31, $\epsilon = \epsilon'$, and $E_1 = E$ at t = 0. This estimate of the autocorrelation function was obtained from a computation which ran for 12000 intervals with $h = \cdot 5 \times 10^{-13}$ sec, and the function is plotted for only 160 such intervals. Although this system appeared to be the most weakly nonlinear of all the systems studied, the curve plotted bears no comparison with the autocorrelation function for the linear system started in the first mode. In the latter system $\rho_{N,1}(t) = \cos \omega_1 t$, and the period of oscillations is $2\pi/\omega_1 \simeq 17 \cdot 5 \times 10^{-12}$ sec compared with an initial period of oscillation of about $10^{-12}$ sec in the nonlinear case. The curve plotted in Fig. 11 is typical of the corresponding curves for every system studied. In particular, $\rho_{N,1}(t)$ appeared to be independent of N, and of the rate of collisions in the systems. In every case the time between the first two maxima was about $10^{-12}$ sec, and thereafter the curve fluctuated with a maximum amplitude of about ·15.

The curves were only obtained for 200 intervals of t, i.e. up to $t = 20 \times 10^{-12}$ sec when $h = 10^{-13}$ sec., as computing $\rho_{N,1}(t)$ for more intervals of t would have required running the whole computation much further than was necessary to obtain satisfactory results for the other properties of these systems, which have been discussed earlier in this thesis. It is not possible to draw any conclusions from the curves obtained for the autocorrelation function, but it is significant that our nonlinear model enables a dynamical estimate of this function to be made. The curve drawn in Fig. 11 therefore provides an interesting comparison with the hypothetical curve drawn by Mazur and Montroll in Fig. 3 of their paper.

# CHAPTER 8

## CONCLUSIONS

It has been clearly shown that, in contrast to the systems studied by FPU, and others, our simple nonlinear systems show a behaviour which can reasonably be described as ergodic. This is evidenced in the first place by the equipartition of the energy of each system amongst all the linear modes, in the time average. The rate at which this energy sharing occurs is much more rapid for systems in which all the energy is initially in a high mode than for those in which only the first mode is excited at the start of the motion. However, energy is freely exchanged amongst all the modes once the effect of the initial conditions is no longer dominant.

Secondly, the rapid approach of the temperature and pressure estimates to equilibrium values, which are near those predicted theoretically for the thermodynamic system, is further evidence of the ergodic nature of these systems. The results of the numerical computations (e.g. in Table XII) show that the thermodynamic behaviour of each system of N particles is almost identical when long intervals of time, in which the systems no longer show dependence on the initial conditions, are considered.

It is remarkable that such small systems (e.g. N = 31) should yield numerical results which are in excellent agreement with the theoretical results derived via statistical mechanics for the thermodynamic system. The inherent simplicity of the nonlinear model enabled an efficient and relatively accurate numerical method to be developed to carry out calculations on

the model. For the small values of N used, the speed and economies of the computation enabled estimates of the pressure, temperature, and the autocorrelation function to be obtained quickly, without recourse to magnetic tapes for intermediate storage, whereas the computational time for N = 128, say, would have been prohibitive with the limited computing facilities at our disposal. It is suggested that a numerical verification of some of the other results of statistical mechanics could be obtained from this model. In particular, a calculation of the entropy function and its fluctuations for both a system and a subsystem could be attempted. This should lead to a numerical evaluation of the H-theorem.

It would be interesting to try to derive the macroscopic properties of the model by the generation of a stochastic process. The time intervals between two collisions could be chosen at random from a probability distribution. The trajectory of any system in phase space may then be followed by repeated application of the linear transformation (2.10) for the selected time intervals, together with a random choice of collision after each iteration. This method should yield systems which are statistically equivalent to the ones which have been discussed in this thesis.

# APPENDIX 1

## ECONOMIZED POLYNOMIAL APPROXIMATIONS TO Cos θ and Sin θ

The coefficients $c_{2r}$ and $c_{2r+1}$ in the economized polynomial approximations to cos θ and sin θ, respectively, given by Eqs. (3.18) and (3.19), may be derived from the Chebyshev series expansions for these functions.

The Chebyshev polynomial $T_r(x)$ of degree r in x is defined by

$$T_r(x) = \cos(r \arccos x). \qquad \text{---(A1.1)}$$

It is a well known property of these polynomials [17] that, in a given finite range, a function of a real variable is represented more accurately by a Chebyshev series approximation of prescribed degree than by a truncated Taylor series expansion of the same degree. Clenshaw [18] has compiled tables for the first ten coefficients of the infinite series

$$\cos \tfrac{1}{2}\pi x = {\sum_{r=0}^{\infty}}' a_{2r}\, T_{2r}(x) \qquad |x| \leq 1, \qquad \text{---(A1.2)}$$

and

$$\sin \tfrac{1}{2}\pi x = x{\sum_{r=0}^{\infty}}' a_{2r}\, T_{2r}(x) \qquad |x| \leq 1, \qquad \text{---(A1.3)}$$

where the prime denotes that the coefficient $a_0$ is halved in the summation. The Chebyshev polynomials may be derived from the recurrence relation

$$T_{r+1}(x) - 2x\, T_r(x) + T_{r-1}(x) = 0,$$

with $T_0(x) = 1$, and $T_1(x) = x$. Since $|T_r(x)| \leq 1$ for all x, the

absolute error due to truncation of either (2) or (3) after the n+1-st term, say, is given by

$$|\text{Error}| < \sum_{r=n+1}^{\infty} |a_{2r}|.$$

Hence the number of terms to be retained in the Chebyshev series in order to obtain any desired accuracy is readily ascertained.

If the infinite series (2) and (3) are each truncated after the n+1-st term, they may then be expressed in the form of Eqs. (3.18) and (3.19), respectively, after making the change of variable $\theta = \frac{1}{2}\pi x$. The elements of $\underset{\sim}{A}(t)$ given by Eqs. (2.11) and (3.21) are computed correct to eight significant figures, or to ten decimal places for the smaller elements, when only the first seven terms in each of (2) and (3) are retained. The coefficients $c_{2r}$ and $c_{2r+1}$ computed from the first seven coefficients $a_{2r}$ evaluated by Clenshaw for (2) and (3), respectively, are given to 12D in Table A1. These coefficients are used in the appropriate equations in §3.3 to evaluate the elements of $\underset{\sim}{A}(t)$ to within the prescribed error.

TABLE A1. The coefficients $c_{2r}$ and $c_{2r+1}$ in the economized polynomial approximations to cos θ and sin θ, respectively, given by Eqs. (3.18) and (3.19) in which n = 6. The coefficients are evaluated to 12D from the first seven terms in each of Eqs. (2) and (3).

| r | $c_{2r}$ | $c_{2r+1}$ |
|---|---|---|
| 0 | + ·999999 999999 | + 1·000000 000000 |
| 1 | − ·499999 999970 | − ·166666 666664 |
| 2 | + ·041666 666473 | + ·008333 333320 |
| 3 | − ·001388 888417 | − ·000198 412667 |
| 4 | + ·000024 801040 | + ·000002 755695 |
| 5 | − ·000000 275247 | − ·000000 025030 |
| 6 | + ·000000 001991 | + ·000000 000154 |

# APPENDIX 2

## TABLES OF VALUES FOR $E_i$ and $\langle E_i \rangle$

The tables which follow are supplementary to Tables V-XI which appear in Chapter 4 to illustrate the energy sharing properties of the nonlinear systems being investigated. Each table gives the energies $E_i$ in the linear normal modes as percentages of the total energy E, and/or the time averages $\langle E_i \rangle$ of these energies for some system. The $E_i$ given correspond to the partition of E just before the C-th collision at time z units $[z = (\gamma/M)^{\frac{1}{2}}t]$, and the $\langle E_i \rangle$ are the time averages for the interval 0 to z units.

In the tables in this appendix z and i are represented by Z and I, respectively. For simplicity the system to which each table refers is labelled $n_1 - n_2 - n_3$, where $n_1 = N$; $n_2 = 1$ or 2 according as the energy of the system is given by $\epsilon = \epsilon'$ or $\epsilon''$, respectively; $n_3 = k$ if the initial configuration of the system was slightly perturbed from the k-th mode, i.e. $E_i \simeq \delta_{ik}E$ at $t = 0$, except for the antisymmetric system in Table A2.15 when the initial configuration was not perturbed from the k-th mode. When N = 31 or 32 the table is split into two sections, the first of which gives the $E_i$ and/or $\langle E_i \rangle$ for the modes 1-16, while the second part gives the required values for the remaining modes.

TABLE A2.1. PERCENTAGE MODE ENERGIES AND TIME AVERAGES FOR THE SYSTEM 7-2-1.

| A. MODE ENERGIES * | | | | | | | | | B. TIME AVERAGES | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| C | Z | I=1 | 2 | 3 | 4 | 5 | 6 | 7 | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
| 0 | .0 | 99.9 | .0 | .0 | .0 | .0 | .0 | .0 | 99.9 | .0 | .0 | .0 | .0 | .0 | .0 |
| 2 | 1.2 | 94.4 | .6 | 1.3 | 1.5 | 1.3 | .8 | .2 | 99.1 | .1 | .2 | .2 | .2 | .1 | .1 |
| 4 | 1.6 | 83.2 | 7.0 | 6.6 | 2.3 | .1 | .3 | .6 | 95.4 | 1.5 | 1.4 | .6 | .3 | .4 | .3 |
| 6 | 2.0 | 79.4 | 7.4 | 1.5 | 6.3 | 4.9 | .6 | .1 | 92.0 | 2.7 | 1.5 | 1.7 | 1.2 | .6 | .3 |
| 8 | 7.3 | 59.8 | 12.5 | 3.0 | 12.0 | 4.3 | 3.9 | 4.6 | 82.4 | 10.8 | 2.1 | 1.5 | 1.6 | .9 | .7 |
| 10 | 7.9 | 39.4 | 31.7 | 11.2 | 7.6 | 1.8 | 7.1 | 1.1 | 79.5 | 11.7 | 2.4 | 1.7 | 2.0 | 1.9 | .9 |
| 12 | 8.7 | 34.1 | 30.6 | 4.0 | 15.4 | 7.0 | 1.5 | 7.4 | 75.6 | 13.0 | 2.5 | 2.2 | 2.2 | 2.7 | 1.9 |
| 14 | 11.0 | 33.4 | 14.4 | 3.3 | 12.7 | 4.4 | 11.7 | 20.1 | 66.5 | 13.7 | 3.0 | 4.1 | 2.6 | 4.1 | 6.0 |
| 16 | 14.0 | 24.9 | 6.3 | 14.0 | 21.4 | 6.5 | 7.7 | 19.2 | 59.7 | 12.9 | 3.7 | 6.7 | 2.5 | 4.1 | 10.4 |
| 24 | 21.6 | 22.9 | 13.0 | 9.3 | 2.4 | 13.2 | 26.2 | 13.1 | 46.0 | 10.8 | 6.8 | 6.4 | 8.0 | 7.6 | 14.4 |
| 32 | 29.2 | 3.2 | 5.7 | 28.7 | 24.6 | 19.8 | 3.8 | 14.3 | 38.0 | 13.1 | 6.9 | 8.0 | 8.7 | 13.4 | 12.0 |
| 40 | 37.4 | 1.2 | 3.1 | 53.8 | 10.5 | 15.9 | 14.0 | 1.4 | 29.8 | 11.7 | 15.2 | 8.0 | 9.1 | 13.4 | 12.8 |
| 48 | 46.3 | 3.8 | 20.4 | 11.3 | 3.1 | .8 | 25.1 | 35.6 | 25.1 | 12.7 | 14.3 | 9.9 | 8.3 | 15.2 | 14.5 |
| 56 | 55.7 | 3.4 | 28.1 | 2.4 | 17.9 | 7.4 | 7.7 | 33.2 | 21.3 | 14.7 | 15.4 | 9.9 | 9.0 | 14.2 | 15.5 |
| 64 | 61.6 | 1.1 | 13.5 | .7 | 39.6 | 28.5 | 4.9 | 11.7 | 19.5 | 15.3 | 14.3 | 10.7 | 11.2 | 13.7 | 15.3 |
| 72 | 70.1 | 7.5 | 36.0 | 28.9 | 10.0 | .6 | 14.2 | 2.9 | 17.4 | 17.9 | 14.4 | 11.1 | 11.2 | 12.7 | 15.3 |
| 80 | 76.3 | 27.0 | .0 | 15.5 | 17.9 | 14.5 | 21.9 | 3.3 | 17.6 | 17.0 | 14.3 | 11.6 | 11.6 | 13.1 | 14.7 |
| 140 | 148.2 | 13.1 | 15.7 | 27.6 | 9.6 | 1.3 | 5.3 | 27.5 | 15.5 | 16.7 | 13.7 | 12.9 | 11.5 | 15.3 | 14.4 |
| 280 | 277.0 | 41.9 | 3.7 | 11.5 | 15.1 | 11.0 | 14.7 | 2.0 | 17.3 | 16.4 | 14.0 | 14.6 | 11.8 | 13.6 | 12.3 |
| 420 | 426.4 | 4.7 | 7.9 | 19.5 | .8 | 16.4 | 33.0 | 17.6 | 15.0 | 17.6 | 13.8 | 13.2 | 11.5 | 13.8 | 15.2 |
| 560 | 596.0 | 8.7 | 13.7 | 4.5 | 2.9 | 50.2 | 2.7 | 17.2 | 12.4 | 16.4 | 13.1 | 14.2 | 13.2 | 15.2 | 15.5 |
| 700 | 746.0 | 3.1 | 6.0 | 3.7 | 47.4 | 25.7 | 8.9 | 5.1 | 12.8 | 15.4 | 13.4 | 14.3 | 13.3 | 15.0 | 15.9 |

TABLE A2.2. PERCENTAGE MODE ENERGIES AND TIME AVERAGES FOR THE SYSTEM 7-2-7.

| A. MODE ENERGIES * | | | | | | | | | B. TIME AVERAGES | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| C | Z | I=1 | 2 | 3 | 4 | 5 | 6 | 7 | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
| 0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | 99.9 | .0 | .0 | .0 | .0 | .0 | .0 | 99.9 |
| 2 | .2 | .2 | 4.5 | 3.7 | 8.9 | 16.4 | 4.5 | 61.9 | .1 | 3.1 | 2.6 | 6.3 | 11.5 | 3.1 | 73.2 |
| 4 | 2.8 | .0 | 11.9 | 1.6 | 2.6 | 23.2 | 2.3 | 58.4 | .0 | 9.4 | 1.1 | 2.5 | 18.2 | 2.0 | 66.9 |
| 6 | 6.6 | .1 | 5.9 | 2.0 | 16.0 | 35.0 | 2.7 | 38.4 | .0 | 8.4 | 1.7 | 7.4 | 27.7 | 2.3 | 52.5 |
| 8 | 8.8 | .8 | 3.3 | 10.4 | 2.0 | 4.0 | 18.7 | 60.8 | .2 | 6.9 | 3.5 | 6.6 | 21.5 | 6.0 | 55.4 |
| 10 | 11.3 | 2.1 | 1.2 | 6.6 | 12.6 | 16.5 | 36.6 | 24.3 | .5 | 5.9 | 4.6 | 6.9 | 19.6 | 10.4 | 52.1 |
| 12 | 14.2 | 3.4 | 2.6 | 10.4 | 4.6 | 21.3 | 35.9 | 21.8 | 1.1 | 5.3 | 5.7 | 6.8 | 19.8 | 16.1 | 45.3 |
| 14 | 19.5 | 1.6 | .1 | 11.4 | 4.3 | 25.3 | 45.1 | 12.2 | 1.4 | 4.2 | 6.5 | 9.6 | 19.1 | 24.2 | 34.9 |
| 16 | 21.1 | 1.1 | 1.0 | 14.2 | 13.9 | 16.3 | 8.3 | 45.3 | 1.4 | 4.0 | 6.8 | 9.9 | 19.2 | 23.6 | 35.1 |
| 24 | 28.9 | 1.3 | 4.8 | 44.9 | 10.8 | 9.3 | 19.7 | 9.3 | 1.3 | 4.3 | 9.6 | 10.2 | 23.7 | 18.4 | 32.4 |
| 32 | 39.5 | .4 | 10.5 | 28.1 | 35.8 | 4.1 | 3.8 | 17.2 | 1.1 | 4.6 | 17.5 | 12.0 | 23.1 | 15.1 | 26.6 |
| 40 | 44.4 | 4.4 | 24.9 | 13.6 | 26.2 | 19.4 | 4.3 | 7.2 | 1.4 | 6.3 | 17.1 | 14.5 | 21.6 | 13.9 | 25.1 |
| 48 | 53.3 | 32.3 | 18.7 | 3.6 | 5.5 | 9.5 | 26.1 | 4.3 | 5.1 | 9.5 | 14.9 | 13.5 | 19.4 | 15.2 | 22.4 |
| 56 | 65.4 | 22.1 | 6.3 | 21.6 | 7.6 | 29.8 | 10.4 | 2.1 | 10.6 | 9.7 | 12.9 | 12.0 | 18.8 | 15.6 | 20.4 |
| 64 | 71.0 | 19.7 | 4.6 | 8.4 | 17.0 | 9.2 | 37.7 | 3.4 | 12.0 | 9.2 | 13.2 | 12.4 | 18.2 | 15.3 | 19.7 |
| 72 | 77.2 | 9.8 | 23.5 | 8.9 | 9.1 | 9.8 | 27.6 | 11.4 | 12.5 | 10.5 | 12.3 | 12.0 | 19.0 | 14.7 | 19.0 |
| 80 | 88.0 | 5.4 | 20.5 | 15.0 | 9.6 | 6.5 | 24.7 | 18.3 | 12.4 | 11.5 | 12.4 | 11.7 | 18.7 | 15.0 | 18.4 |
| 140 | 157.9 | 2.2 | 33.7 | 15.6 | 20.7 | 2.8 | 13.1 | 11.9 | 17.0 | 14.0 | 11.2 | 13.5 | 14.0 | 14.4 | 15.9 |
| 280 | 283.2 | 2.0 | 28.7 | 4.4 | 10.3 | .6 | 48.8 | 5.1 | 20.8 | 15.0 | 11.0 | 12.9 | 11.8 | 13.8 | 14.7 |
| 420 | 440.8 | 36.3 | 17.5 | 3.3 | 10.6 | 15.6 | 6.7 | 10.1 | 16.9 | 14.0 | 12.5 | 14.8 | 13.2 | 14.4 | 14.1 |
| 560 | 581.0 | 58.6 | 3.0 | 1.5 | 5.9 | 4.9 | 16.0 | 10.1 | 17.9 | 15.3 | 12.3 | 13.5 | 13.1 | 14.3 | 13.6 |
| 700 | 733.9 | 1.2 | 31.4 | 1.7 | 1.3 | 12.0 | 43.6 | 8.8 | 17.0 | 15.0 | 12.7 | 13.3 | 13.7 | 14.7 | 13.6 |

TABLE A2.3. PERCENTAGE MODE ENERGIES AND TIME AVERAGES FOR THE SYSTEM 8-2-1.

| A. MODE ENERGIES | | | | | | | | | | B. TIME AVERAGES | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| C | Z | I=1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
| 0 | .0 | 100 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | 100 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| 8 | 1.3 | 78.9 | 9.5 | 3.2 | .2 | 3.0 | 2.4 | .3 | 2.4 | 84.7 | 6.6 | 3.2 | 1.2 | 1.8 | 1.2 | .7 | .5 |
| 16 | 8.7 | 35.2 | 17.8 | 4.1 | 5.4 | 2.3 | .1 | 6.3 | 28.9 | 72.4 | 11.9 | 3.8 | 2.5 | 1.4 | 1.4 | 3.0 | 3.7 |
| 24 | 14.2 | 29.9 | 5.7 | 10.1 | 15.1 | 9.4 | 8.9 | 11.1 | 9.6 | 58.8 | 9.6 | 8.1 | 3.5 | 4.8 | 3.1 | 3.3 | 8.8 |
| 32 | 23.3 | 3.8 | 16.9 | 19.6 | 8.8 | 14.9 | 1.4 | 21.1 | 13.5 | 42.3 | 8.9 | 7.6 | 9.5 | 10.1 | 7.6 | 4.4 | 9.7 |
| 40 | 29.3 | 11.9 | 2.6 | 30.8 | 17.2 | 4.4 | 2.9 | 9.0 | 21.3 | 35.3 | 9.0 | 11.8 | 10.1 | 9.3 | 7.4 | 6.3 | 10.8 |
| 48 | 36.0 | 26.5 | 9.8 | 1.2 | 3.6 | 9.0 | 5.5 | 33.4 | 11.1 | 32.1 | 8.5 | 10.7 | 9.2 | 9.3 | 8.0 | 12.2 | 10.0 |
| 56 | 42.2 | 22.2 | 4.2 | 14.0 | 31.3 | 7.9 | 7.9 | 2.4 | 10.1 | 31.2 | 8.0 | 10.2 | 10.1 | 9.5 | 8.2 | 13.2 | 9.6 |
| 64 | 45.9 | 13.9 | 11.5 | 4.1 | 8.3 | 9.2 | 15.6 | 24.7 | 12.8 | 29.5 | 7.8 | 10.0 | 9.9 | 10.2 | 9.0 | 13.3 | 10.2 |
| 72 | 51.3 | 3.2 | 12.2 | 3.1 | 2.3 | 24.9 | 21.5 | 22.9 | 9.9 | 27.1 | 8.4 | 9.6 | 11.1 | 10.0 | 10.1 | 13.0 | 10.7 |
| 80 | 58.4 | .7 | 7.0 | 14.2 | 16.4 | 18.3 | 26.9 | 15.1 | 1.4 | 24.0 | 9.2 | 9.9 | 10.9 | 10.9 | 10.9 | 13.0 | 11.2 |
| 120 | 108.1 | 9.3 | 12.0 | 11.3 | 3.3 | 3.1 | 41.1 | 12.9 | 7.1 | 17.5 | 9.0 | 10.1 | 10.0 | 10.2 | 10.9 | 18.2 | 14.2 |
| 160 | 139.8 | 3.8 | 8.5 | 7.5 | 21.0 | 17.2 | 35.0 | 5.0 | 2.0 | 15.3 | 8.8 | 9.2 | 10.3 | 12.0 | 12.5 | 17.5 | 14.3 |
| 200 | 178.1 | 6.7 | 1.2 | 13.2 | 15.3 | .9 | 6.5 | 17.6 | 38.5 | 13.7 | 9.0 | 10.5 | 10.2 | 11.6 | 12.8 | 17.1 | 15.2 |
| 240 | 209.2 | 1.4 | 29.5 | 12.3 | 26.7 | 3.3 | 1.2 | 3.7 | 22.0 | 12.4 | 10.9 | 10.7 | 10.3 | 11.3 | 12.2 | 16.6 | 15.7 |
| 320 | 282.7 | 7.7 | 6.9 | 5.5 | 27.9 | .7 | 1.5 | 4.5 | 45.4 | 11.7 | 9.7 | 12.5 | 13.0 | 11.6 | 12.1 | 14.8 | 14.7 |
| 400 | 353.1 | 29.1 | 23.7 | 8.4 | 2.7 | 1.8 | 11.0 | 10.9 | 12.5 | 10.7 | 13.0 | 11.6 | 13.0 | 11.6 | 11.5 | 14.8 | 13.8 |
| 480 | 425.2 | .5 | 7.8 | 11.7 | 16.3 | 16.1 | 7.9 | 18.7 | 21.1 | 11.6 | 12.4 | 12.3 | 12.4 | 11.2 | 12.1 | 14.6 | 13.3 |
| 560 | 507.1 | 11.3 | 5.7 | 25.2 | 16.0 | 14.6 | 7.2 | 8.6 | 11.4 | 11.8 | 13.0 | 12.1 | 12.2 | 10.9 | 11.8 | 15.1 | 13.1 |
| 640 | 583.9 | 22.8 | 3.3 | 1.9 | 5.1 | .6 | 44.7 | 4.0 | 17.7 | 11.9 | 13.5 | 11.7 | 12.1 | 11.1 | 12.0 | 14.9 | 12.8 |
| 720 | 643.4 | 15.1 | 7.9 | 8.8 | 26.0 | 19.1 | 7.2 | 1.9 | 14.0 | 12.7 | 13.0 | 11.5 | 12.3 | 11.3 | 12.1 | 14.2 | 13.0 |
| 800 | 714.2 | 2.0 | 23.4 | 17.6 | 20.7 | 5.1 | 27.6 | 1.2 | 2.5 | 12.2 | 14.0 | 11.7 | 12.3 | 11.1 | 11.8 | 13.6 | 13.3 |

TABLE A2.4. MODE ENERGIES AS PERCENTAGES OF E FOR THE SYSTEM 15-1-1.

| C | Z | I=1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | .0 | 100.0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| 5 | 19.4 | 99.7 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| 10 | 49.4 | 98.2 | .3 | .5 | .5 | .3 | .1 | .1 | .0 | .0 | .0 | .0 | .0 | .1 | .0 | .0 |
| 15 | 64.7 | 93.6 | 1.4 | 1.5 | .7 | .3 | .1 | .2 | .5 | .2 | .2 | .5 | .4 | .3 | .0 | .2 |
| 20 | 80.0 | 89.3 | 2.5 | 2.2 | 1.2 | .5 | .1 | .9 | .2 | .4 | .1 | .7 | .8 | .4 | .2 | .7 |
| 25 | 94.8 | 87.0 | 3.3 | 1.9 | 1.5 | 1.3 | .1 | .0 | .9 | .2 | .7 | .4 | 1.1 | .7 | .2 | .5 |
| 30 | 98.8 | 82.4 | 4.0 | 1.1 | 2.6 | 1.6 | .2 | 1.0 | 1.2 | 3.4 | .0 | .2 | .6 | .4 | 1.1 | .3 |
| 35 | 112.1 | 77.2 | 5.8 | .7 | 3.4 | 1.7 | .1 | 2.2 | 2.7 | .2 | .4 | 1.5 | .5 | 1.0 | 2.6 | .0 |
| 40 | 116.1 | 73.5 | 4.6 | .5 | 3.5 | .9 | .7 | .9 | .7 | 3.2 | 3.9 | .3 | 1.0 | 1.0 | 3.4 | 1.9 |
| 45 | 129.4 | 68.9 | 6.9 | .4 | 3.0 | 1.1 | 1.4 | 1.6 | 2.9 | 4.5 | 1.5 | 1.0 | .7 | 1.1 | .5 | 4.7 |
| 60 | 157.1 | 58.1 | 10.8 | 1.0 | 1.3 | 1.2 | 4.4 | 6.6 | 1.7 | .7 | 3.0 | 1.9 | 1.0 | 5.0 | .8 | 2.6 |
| 75 | 186.5 | 33.3 | 15.5 | 11.2 | 5.7 | .6 | 3.3 | 6.1 | .4 | 8.5 | 3.4 | 1.6 | .0 | 4.4 | 1.7 | 4.3 |
| 90 | 208.1 | 15.5 | 5.3 | 15.5 | .6 | 8.7 | 6.0 | 7.6 | 7.7 | 2.2 | 4.4 | 11.1 | 1.3 | 3.9 | 1.3 | 8.8 |
| 105 | 225.0 | 9.6 | 1.9 | 6.8 | 1.8 | 18.1 | 5.4 | .9 | 14.9 | 5.2 | 5.7 | 1.6 | 9.6 | 5.9 | 9.2 | 3.2 |
| 120 | 249.7 | 5.4 | 2.4 | 5.0 | .6 | .1 | 14.8 | 5.2 | 13.6 | 12.2 | .1 | 2.4 | 18.0 | 3.0 | 3.7 | 13.7 |
| 135 | 266.8 | 4.8 | 15.6 | 2.5 | 13.6 | .5 | 4.1 | 8.9 | 8.0 | 4.1 | .2 | 13.9 | 17.2 | 3.2 | .7 | 2.7 |
| 150 | 280.8 | 3.6 | 24.0 | 1.2 | 3.3 | 5.2 | .7 | 4.9 | 4.0 | 2.2 | 9.7 | 2.3 | 6.5 | 10.5 | 18.8 | 3.1 |
| 300 | 462.9 | 10.8 | 14.2 | 3.7 | .0 | 2.7 | .5 | 1.5 | 7.3 | 7.9 | 8.1 | 19.1 | 1.8 | 4.1 | 7.8 | 10.4 |
| 450 | 691.2 | 8.1 | 20.8 | 8.2 | 12.5 | 2.2 | 14.3 | 1.5 | 5.5 | 7.1 | .1 | 5.3 | 4.0 | 5.1 | .3 | 4.9 |
| 600 | 938.9 | 4.2 | 9.1 | 16.0 | 12.8 | 9.4 | 3.2 | .9 | 2.8 | 5.1 | 2.9 | 14.5 | .7 | 11.2 | 2.4 | 4.9 |
| 750 | 1141.9 | .6 | 23.7 | 4.2 | 9.5 | .1 | 5.0 | 17.0 | 4.9 | 4.9 | 1.7 | 8.8 | 10.0 | 6.4 | .6 | 2.7 |

TABLE A2.5. PERCENTAGE MODE ENERGY TIME AVERAGES FOR THE SYSTEM 15-1-1.

| C | Z | I=1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | .0 | 100.0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| 5 | 19.4 | 99.9 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| 10 | 49.4 | 99.3 | .1 | .2 | .2 | .1 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| 15 | 64.7 | 98.4 | .3 | .4 | .3 | .2 | .1 | .0 | .0 | .0 | .1 | .0 | .0 | .1 | .0 | .0 |
| 20 | 80.0 | 97.0 | .6 | .7 | .5 | .3 | .1 | .1 | .0 | .0 | .2 | .1 | .1 | .1 | .1 | .1 |
| 25 | 94.8 | 95.5 | 1.0 | .9 | .6 | .4 | .1 | .1 | .1 | .1 | .3 | .2 | .2 | .2 | .1 | .2 |
| 30 | 98.8 | 95.0 | 1.2 | 1.0 | .7 | .4 | .1 | .1 | .2 | .1 | .3 | .2 | .2 | .2 | .1 | .2 |
| 35 | 112.1 | 93.4 | 1.6 | .9 | .9 | .7 | .3 | .1 | .2 | .3 | .3 | .3 | .3 | .2 | .2 | .2 |
| 40 | 116.1 | 92.8 | 1.7 | .9 | 1.0 | .7 | .3 | .2 | .2 | .4 | .4 | .3 | .3 | .3 | .3 | .3 |
| 45 | 129.4 | 90.7 | 2.0 | .9 | 1.3 | .7 | .3 | .3 | .3 | .7 | .7 | .3 | .4 | .3 | .6 | .5 |
| 60 | 157.1 | 86.0 | 3.7 | .8 | 1.4 | .7 | .6 | .6 | .7 | .8 | 1.1 | .5 | .8 | .9 | .6 | .8 |
| 75 | 186.5 | 79.6 | 5.3 | 1.6 | 1.9 | .9 | 1.0 | 1.0 | .9 | 1.6 | 1.2 | .5 | 1.1 | 1.3 | .8 | 1.2 |
| 90 | 208.1 | 73.8 | 6.3 | 2.9 | 2.4 | 1.0 | 1.1 | 1.2 | 1.2 | 1.9 | 1.4 | 1.0 | 1.4 | 1.4 | 1.3 | 1.7 |
| 105 | 225.0 | 69.3 | 6.0 | 3.4 | 2.3 | 1.7 | 1.3 | 1.7 | 1.9 | 2.0 | 1.9 | 1.4 | 2.1 | 1.6 | 1.4 | 1.9 |
| 120 | 249.7 | 63.2 | 5.6 | 3.9 | 2.3 | 2.2 | 2.8 | 2.3 | 2.5 | 2.9 | 2.1 | 1.8 | 2.7 | 1.9 | 1.6 | 2.2 |
| 135 | 266.8 | 59.5 | 5.6 | 3.9 | 2.6 | 2.3 | 3.1 | 2.6 | 2.9 | 3.7 | 2.3 | 2.3 | 3.2 | 2.0 | 1.6 | 2.5 |
| 150 | 280.8 | 56.8 | 6.3 | 3.8 | 2.8 | 2.4 | 3.2 | 2.7 | 3.0 | 3.8 | 2.3 | 2.7 | 3.6 | 2.3 | 1.8 | 2.6 |
| 300 | 462.9 | 36.6 | 9.4 | 4.6 | 3.9 | 3.6 | 4.0 | 3.5 | 4.4 | 4.6 | 3.8 | 5.0 | 4.3 | 4.0 | 3.8 | 4.4 |
| 450 | 691.2 | 27.4 | 9.6 | 5.2 | 4.6 | 4.8 | 4.6 | 3.7 | 5.5 | 4.8 | 5.2 | 5.3 | 5.0 | 5.0 | 4.4 | 4.9 |
| 600 | 938.9 | 21.8 | 8.6 | 5.9 | 4.5 | 5.3 | 4.8 | 3.9 | 6.2 | 5.5 | 6.3 | 5.8 | 4.9 | 5.4 | 5.8 | 5.2 |
| 750 | 1141.9 | 18.3 | 9.2 | 7.4 | 4.7 | 5.4 | 4.8 | 4.4 | 5.9 | 6.6 | 6.0 | 5.9 | 5.0 | 5.4 | 5.9 | 5.3 |

TABLE A2.6. MODE ENERGIES AS PERCENTAGES OF E FOR THE SYSTEM 15-1-15.

| C | Z | I=1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | 100 |
| 5 | 11.4 | .0 | 2.4 | .1 | 1.2 | .3 | 1.3 | 1.2 | 1.9 | 2.5 | 2.5 | 16.2 | 6.2 | 60.8 | 3.4 | .0 |
| 10 | 24.4 | .0 | 1.2 | .0 | .4 | .1 | .5 | .4 | .6 | 1.9 | .7 | 5.9 | 3.0 | 13.0 | .3 | 72.0 |
| 15 | 39.2 | .0 | .7 | .1 | .5 | .2 | .7 | .5 | .8 | 1.1 | 2.7 | 10.2 | 3.5 | 5.0 | 3.8 | 70.2 |
| 20 | 47.9 | .0 | .3 | .6 | .3 | 1.9 | 2.9 | .3 | 1.4 | 10.7 | 1.8 | 10.2 | 18.5 | 6.8 | 5.1 | 39.1 |
| 25 | 60.3 | .0 | 1.6 | .0 | .5 | .2 | 1.4 | 2.3 | 3.1 | 2.7 | 4.0 | 43.2 | 1.4 | .4 | 11.1 | 28.0 |
| 30 | 72.4 | .3 | 2.2 | 1.1 | .5 | 1.0 | .7 | .4 | .5 | 7.1 | 5.7 | 5.0 | 18.0 | 6.5 | 30.5 | 20.3 |
| 35 | 82.6 | .0 | 2.9 | 1.4 | 1.9 | 5.3 | 1.8 | 14.2 | .4 | 5.3 | 3.9 | 1.6 | 9.0 | 32.5 | 4.3 | 15.3 |
| 40 | 86.9 | .0 | 4.2 | .7 | .9 | 3.2 | .9 | 11.1 | 7.1 | 10.3 | 7.1 | 6.4 | 4.3 | 26.7 | 5.8 | 11.5 |
| 45 | 96.2 | .3 | 3.9 | 1.4 | 2.4 | 4.1 | .9 | 7.5 | 1.1 | 4.2 | 3.5 | 7.2 | 12.3 | 11.6 | 22.6 | 16.9 |
| 60 | 126.3 | .7 | 7.8 | 4.6 | 1.5 | 4.6 | .2 | 2.3 | 6.4 | 5.2 | 1.2 | 4.6 | 10.1 | 6.3 | 31.5 | 12.8 |
| 75 | 153.4 | .1 | 12.0 | 4.0 | .8 | 4.6 | 4.2 | 2.7 | 1.8 | 17.6 | 3.0 | .2 | 17.0 | 18.4 | .7 | 12.8 |
| 90 | 184.9 | .0 | 17.6 | 2.2 | 5.3 | 4.7 | 6.0 | 6.8 | 3.5 | 10.6 | 23.6 | 7.0 | .3 | 5.8 | 1.0 | 5.8 |
| 105 | 207.7 | 1.0 | 11.5 | .5 | 14.8 | 23.1 | 5.2 | 4.2 | 21.3 | 3.6 | .2 | 1.3 | 2.4 | 9.3 | .7 | .9 |
| 120 | 230.8 | 1.6 | 9.9 | 1.0 | 11.3 | 5.0 | 14.7 | 7.2 | .9 | .2 | 16.8 | 4.2 | 7.6 | .6 | 3.3 | 15.5 |
| 135 | 251.2 | 3.2 | 10.2 | 8.1 | 7.1 | 1.5 | 8.0 | 1.6 | 3.0 | 12.2 | 4.7 | 7.2 | 7.3 | 14.1 | 9.9 | 1.9 |
| 150 | 269.1 | 6.2 | 8.1 | 1.1 | 5.9 | 7.2 | .0 | 7.1 | 10.6 | 8.6 | 14.4 | 5.3 | 4.3 | 7.6 | 2.4 | 11.3 |
| 300 | 477.9 | 6.2 | 7.5 | 4.0 | .6 | 14.3 | 8.4 | 6.5 | 5.0 | .5 | 18.7 | 4.6 | 1.6 | 12.8 | 2.5 | 6.9 |
| 450 | 682.3 | 1.3 | 38.7 | .3 | 16.0 | 2.2 | 3.2 | .9 | 3.1 | 4.6 | 1.3 | 20.8 | 1.8 | 1.0 | 1.0 | 3.6 |
| 600 | 888.3 | 13.1 | 1.8 | .2 | 11.5 | 3.3 | 3.0 | .7 | 10.3 | 21.4 | 11.8 | 3.6 | 5.1 | .4 | 9.3 | 4.5 |
| 750 | 1099.4 | 13.2 | 2.4 | 17.4 | 1.9 | 24.5 | 1.1 | 3.5 | 1.6 | 4.7 | 2.4 | 5.4 | 3.4 | 8.2 | 6.3 | 4.2 |

TABLE A2.7. PERCENTAGE MODE ENERGY TIME AVERAGES FOR THE SYSTEM 15-1-15.

| C | Z | I=1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | 100 |
| 5 | 11.4 | .0 | 1.0 | .1 | .8 | .2 | .9 | .7 | 1.3 | 2.2 | 2.0 | 9.5 | 2.9 | 26.0 | 1.4 | 51.0 |
| 10 | 24.4 | .0 | 1.0 | .1 | .5 | .2 | .7 | .5 | .9 | 1.8 | 1.4 | 6.5 | 2.3 | 24.6 | 1.7 | 57.8 |
| 15 | 39.2 | .0 | 1.0 | .1 | .7 | .2 | .8 | .6 | 1.1 | 2.0 | 1.6 | 7.1 | 2.5 | 31.1 | 2.3 | 49.0 |
| 20 | 47.9 | .0 | 1.0 | .1 | .5 | .2 | .8 | .6 | 1.2 | 2.3 | 1.5 | 6.7 | 2.8 | 25.7 | 2.2 | 54.5 |
| 25 | 60.3 | .0 | 1.3 | .1 | .5 | .4 | 1.0 | .6 | 1.3 | 3.4 | 1.4 | 10.5 | 2.9 | 22.0 | 3.3 | 51.3 |
| 30 | 72.4 | .0 | 1.4 | .2 | .6 | .5 | 1.0 | .7 | 1.2 | 3.4 | 2.6 | 11.8 | 3.7 | 21.7 | 6.3 | 44.9 |
| 35 | 85.6 | .1 | 1.5 | .3 | .7 | 1.2 | 1.0 | 1.4 | 1.3 | 3.6 | 4.0 | 10.6 | 4.4 | 21.2 | 7.6 | 41.2 |
| 40 | 86.9 | .1 | 1.6 | .3 | .8 | 1.3 | 1.0 | 1.8 | 1.5 | 3.9 | 4.2 | 10.3 | 4.4 | 21.6 | 7.6 | 39.7 |
| 45 | 96.2 | .1 | 1.8 | .4 | 1.0 | 1.5 | 1.1 | 2.5 | 1.5 | 3.9 | 4.7 | 10.0 | 4.8 | 21.5 | 8.0 | 37.3 |
| 60 | 126.3 | .2 | 3.4 | 1.1 | 1.9 | 2.6 | 1.4 | 2.9 | 2.4 | 4.0 | 4.5 | 8.9 | 5.0 | 19.5 | 10.2 | 32.1 |
| 75 | 153.4 | .2 | 4.8 | 1.7 | 2.0 | 2.6 | 2.4 | 3.5 | 2.4 | 5.0 | 4.4 | 8.1 | 6.5 | 17.1 | 10.9 | 28.4 |
| 90 | 184.9 | .2 | 6.6 | 2.0 | 1.9 | 2.6 | 2.6 | 3.7 | 3.9 | 6.0 | 5.4 | 7.5 | 6.0 | 15.8 | 9.5 | 26.2 |
| 105 | 207.7 | .2 | 7.6 | 2.2 | 3.0 | 2.9 | 2.8 | 3.9 | 4.5 | 5.7 | 6.2 | 7.1 | 5.6 | 14.8 | 8.8 | 24.7 |
| 120 | 230.8 | .3 | 7.8 | 2.3 | 4.0 | 3.5 | 3.3 | 3.9 | 5.5 | 5.6 | 6.2 | 6.7 | 5.7 | 13.8 | 8.3 | 23.1 |
| 135 | 251.2 | .5 | 7.9 | 2.5 | 4.4 | 3.6 | 3.5 | 3.9 | 5.8 | 5.9 | 6.1 | 6.7 | 6.1 | 13.3 | 8.4 | 21.5 |
| 150 | 269.1 | .7 | 7.9 | 2.6 | 4.4 | 4.1 | 3.5 | 4.1 | 5.8 | 6.5 | 6.2 | 6.7 | 6.1 | 12.9 | 8.4 | 20.3 |
| 300 | 477.9 | 3.1 | 6.7 | 4.0 | 6.8 | 5.0 | 5.8 | 4.6 | 5.6 | 7.0 | 7.0 | 6.3 | 5.8 | 9.9 | 8.4 | 14.0 |
| 450 | 682.3 | 3.3 | 7.7 | 5.5 | 7.4 | 4.8 | 5.6 | 5.6 | 5.7 | 6.7 | 6.5 | 7.1 | 5.8 | 8.8 | 7.6 | 11.8 |
| 600 | 888.3 | 5.2 | 8.8 | 5.2 | 7.2 | 5.3 | 5.4 | 5.6 | 6.1 | 6.4 | 6.3 | 7.0 | 5.8 | 7.9 | 7.2 | 10.6 |
| 750 | 1099.4 | 6.4 | 7.7 | 5.3 | 7.6 | 6.2 | 5.4 | 5.7 | 6.3 | 6.4 | 6.1 | 6.7 | 5.5 | 7.7 | 7.0 | 9.9 |

TABLE A2.8. MODE ENERGIES AS PERCENTAGES OF E FOR THE SYSTEM 16-1-1.

| C | Z | I=1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | .0 | 100.0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| 5 | 20.1 | 99.7 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| 10 | 37.3 | 97.9 | .3 | .5 | .5 | .3 | .1 | .1 | .0 | .0 | .0 | .0 | .0 | .0 | .1 | .0 | .0 |
| 15 | 53.4 | 95.5 | .9 | 1.1 | .9 | .5 | .3 | .1 | .1 | .0 | .0 | .1 | .0 | .0 | .2 | .2 | .1 |
| 20 | 69.5 | 93.1 | 1.3 | 1.2 | .8 | .5 | .1 | .1 | .1 | .0 | .2 | .9 | .8 | .3 | .1 | .3 | .3 |
| 25 | 87.5 | 91.4 | 1.8 | 1.1 | .8 | .6 | .0 | .6 | .9 | .1 | .4 | .3 | .4 | .3 | .2 | .1 | 1.0 |
| 30 | 103.0 | 90.6 | 2.0 | .4 | 1.2 | 1.5 | .1 | .3 | .4 | .7 | .3 | .0 | .2 | .2 | 1.0 | .2 | .8 |
| 35 | 120.0 | 89.9 | 2.4 | .1 | 1.5 | 1.5 | .1 | .1 | .1 | .0 | .4 | .6 | .1 | .2 | 2.1 | .6 | .1 |
| 40 | 136.4 | 86.8 | 4.0 | .2 | 1.0 | .1 | .8 | .6 | .1 | .1 | .0 | 1.0 | .6 | 1.8 | .5 | 2.1 | .2 |
| 60 | 167.6 | 66.2 | 8.8 | 1.5 | 3.2 | 2.5 | .6 | 1.6 | 1.0 | .3 | 1.4 | 1.8 | .8 | 6.4 | 1.5 | 2.2 | .3 |
| 80 | 198.2 | 49.9 | 14.1 | 2.4 | .3 | 2.3 | .7 | 2.9 | .8 | .1 | 9.4 | 1.5 | 1.4 | 7.2 | 1.5 | 3.7 | 1.7 |
| 120 | 254.4 | 17.2 | 7.6 | 3.2 | 2.6 | 2.3 | 10.0 | .9 | 6.9 | 14.8 | 5.4 | 7.3 | 1.3 | .7 | .1 | 13.8 | 5.9 |
| 160 | 300.0 | 3.4 | 4.4 | 1.1 | 4.8 | 7.5 | 12.5 | 5.7 | 10.9 | 14.5 | 13.0 | 15.7 | 1.3 | .9 | .6 | 1.8 | 1.9 |
| 200 | 353.3 | 7.1 | 3.1 | 3.1 | 5.5 | 8.9 | 2.6 | 4.0 | 3.8 | 7.2 | 9.8 | .2 | 24.1 | 9.3 | 3.6 | 1.3 | 6.6 |
| 240 | 413.7 | 8.9 | 8.7 | 10.5 | 8.2 | 5.5 | .2 | 2.8 | 7.1 | 31.6 | .6 | 8.0 | 3.7 | 1.0 | .2 | 2.8 | .1 |
| 320 | 507.7 | 3.6 | 1.4 | .5 | .2 | 12.5 | 13.5 | 14.8 | .4 | .5 | 11.1 | 7.0 | 1.0 | 12.7 | 4.6 | 12.6 | 3.4 |
| 400 | 641.5 | 4.4 | 8.4 | 3.4 | 9.1 | 1.7 | 5.5 | 3.5 | 1.4 | 6.2 | 1.8 | .6 | 7.9 | 21.3 | 1.5 | 3.1 | 20.4 |
| 480 | 755.5 | 3.9 | 14.5 | 1.0 | 5.7 | 3.1 | .0 | 1.8 | 5.1 | 5.4 | 7.8 | 3.2 | 4.7 | 3.4 | 13.2 | 19.9 | 7.3 |
| 560 | 864.3 | .9 | 2.3 | 2.7 | 1.0 | 9.9 | 1.5 | 4.0 | 14.5 | 5.5 | 22.2 | 3.4 | 8.9 | .1 | 8.9 | 8.7 | 5.4 |
| 640 | 961.5 | 4.5 | 16.6 | 1.1 | 3.6 | .1 | 15.4 | 6.4 | 1.8 | 9.4 | 13.3 | 3.3 | 4.9 | 8.9 | 2.6 | 5.2 | 2.8 |
| 720 | 1078.6 | 3.2 | 7.3 | 3.3 | 3.0 | 15.1 | 1.7 | .1 | 7.2 | 7.1 | 4.2 | 12.1 | 14.7 | 1.7 | 18.2 | .1 | 1.0 |
| 800 | 1188.5 | .9 | 11.1 | .5 | 5.3 | 9.6 | 5.6 | 19.8 | 18.1 | 1.1 | 11.0 | 8.6 | 2.3 | 2.4 | 1.5 | .2 | 1.9 |

TABLE A2.9. PERCENTAGE MODE ENERGY TIME AVERAGES FOR THE SYSTEM 16-1-1.

| C | Z | I=1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | .0 | 100.0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| 5 | 20.1 | 99.9 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| 10 | 37.3 | 99.6 | .0 | .1 | .1 | .1 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| 15 | 53.4 | 99.0 | .1 | .2 | .2 | .1 | .1 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| 20 | 69.5 | 98.1 | .3 | .4 | .3 | .2 | .1 | .0 | .0 | .0 | .1 | .1 | .1 | .1 | .1 | .1 | .1 |
| 25 | 87.5 | 96.9 | .6 | .5 | .4 | .3 | .1 | .1 | .1 | .1 | .1 | .2 | .1 | .1 | .1 | .1 | .3 |
| 30 | 103.0 | 96.0 | .8 | .5 | .5 | .4 | .1 | .1 | .2 | .1 | .2 | .2 | .2 | .1 | .2 | .1 | .3 |
| 35 | 120.0 | 95.1 | 1.0 | .4 | .6 | .6 | .1 | .1 | .2 | .1 | .2 | .3 | .2 | .2 | .4 | .2 | .3 |
| 40 | 136.4 | 94.4 | 1.3 | .4 | .6 | .6 | .1 | .2 | .2 | .2 | .2 | .3 | .2 | .2 | .6 | .3 | .3 |
| 60 | 167.6 | 91.1 | 2.6 | .5 | 1.1 | .6 | .2 | .2 | .3 | .3 | .3 | .3 | .3 | .4 | .8 | .5 | .4 |
| 80 | 198.2 | 85.6 | 3.6 | .8 | 1.0 | 1.2 | .3 | .6 | .4 | .8 | 1.0 | .6 | .6 | 1.1 | .9 | .8 | .7 |
| 120 | 254.4 | 73.6 | 4.2 | 1.3 | 1.2 | 2.5 | 1.2 | .9 | 1.1 | 2.5 | 2.1 | 1.1 | 1.5 | 1.8 | 1.4 | 1.4 | 2.0 |
| 160 | 300.0 | 64.7 | 4.9 | 2.1 | 1.9 | 3.0 | 2.3 | 1.7 | 1.7 | 3.4 | 3.3 | 1.8 | 1.8 | 1.8 | 1.6 | 1.9 | 2.1 |
| 200 | 353.3 | 55.7 | 4.6 | 1.9 | 2.5 | 4.3 | 2.5 | 2.0 | 2.0 | 4.1 | 3.6 | 2.5 | 3.2 | 2.3 | 2.3 | 2.6 | 3.7 |
| 240 | 413.7 | 48.5 | 4.7 | 2.2 | 3.4 | 4.6 | 3.2 | 2.7 | 2.4 | 4.5 | 4.1 | 3.0 | 4.2 | 3.0 | 2.9 | 2.8 | 3.8 |
| 320 | 507.7 | 41.2 | 5.1 | 3.1 | 4.5 | 4.6 | 3.3 | 3.4 | 2.6 | 4.4 | 4.6 | 3.2 | 4.1 | 3.9 | 4.0 | 3.8 | 4.3 |
| 400 | 641.5 | 34.0 | 5.1 | 3.2 | 4.4 | 4.2 | 4.5 | 3.2 | 2.8 | 4.4 | 4.7 | 4.2 | 4.8 | 4.2 | 5.2 | 6.1 | 5.2 |
| 480 | 755.5 | 30.0 | 5.0 | 3.5 | 4.5 | 4.2 | 4.9 | 4.1 | 3.8 | 4.2 | 4.6 | 4.1 | 4.9 | 4.7 | 5.9 | 6.3 | 5.4 |
| 560 | 864.3 | 26.5 | 5.1 | 3.5 | 4.3 | 4.6 | 4.6 | 4.2 | 4.0 | 4.6 | 5.1 | 4.9 | 5.2 | 5.2 | 6.2 | 6.3 | 5.6 |
| 640 | 961.5 | 24.2 | 5.5 | 4.2 | 4.6 | 4.9 | 4.9 | 4.3 | 4.3 | 4.6 | 5.3 | 4.9 | 5.2 | 5.1 | 6.1 | 6.2 | 5.5 |
| 720 | 1078.6 | 21.8 | 6.4 | 4.2 | 4.7 | 4.8 | 5.4 | 4.4 | 4.3 | 4.7 | 5.2 | 5.5 | 5.6 | 5.1 | 6.1 | 6.0 | 5.7 |
| 800 | 1188.5 | 20.1 | 6.2 | 4.3 | 5.7 | 5.4 | 5.3 | 4.4 | 4.5 | 4.9 | 5.3 | 5.4 | 5.7 | 5.0 | 5.9 | 6.0 | 5.9 |

TABLE A2.10. ENERGIES (A), AND TIME AVERAGES (B), FOR THE SYSTEM 31-1-1.

| C | Z | I=1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A. 0 | .0 | 100 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| 30 | 39.6 | 98.7 | .1 | .2 | .2 | .1 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| 60 | 101.9 | 96.8 | .5 | .4 | .2 | .0 | .1 | .1 | .0 | .0 | .0 | .0 | .0 | .0 | .1 | .1 | .0 |
| 90 | 163.5 | 93.7 | 1.4 | 1.0 | .3 | .1 | .1 | .0 | .1 | .1 | .2 | .1 | .2 | .3 | .7 | .2 | .0 |
| 120 | 197.1 | 87.1 | 2.8 | 1.1 | .3 | .5 | .5 | .2 | .1 | .3 | .1 | .2 | .0 | .1 | .2 | .1 | .2 |
| 150 | 231.0 | 83.3 | 3.5 | .8 | .6 | .4 | .5 | .1 | .3 | .1 | .3 | .3 | 1.0 | .3 | .1 | .0 | .3 |
| 310 | 446.0 | 48.0 | 13.0 | 2.9 | 2.1 | 1.9 | .6 | .6 | .1 | .0 | 2.1 | .1 | .1 | 1.2 | 3.4 | .3 | .5 |
| 620 | 651.2 | 4.6 | .1 | 1.9 | 1.9 | 14.5 | 2.1 | 2.8 | 10.1 | .6 | .2 | 10.3 | .7 | 2.6 | 5.8 | 1.0 | 2.3 |
| 930 | 850.0 | 2.1 | 3.1 | 2.2 | 3.4 | 9.5 | 2.6 | 3.0 | .4 | 1.6 | 7.1 | .9 | 1.2 | .2 | .6 | 1.0 | 1.1 |
| 1240 | 1043.4 | .3 | .5 | 2.7 | .6 | .7 | 5.0 | 1.2 | 1.6 | 12.8 | 6.2 | 2.8 | .3 | 1.4 | 6.3 | 6.7 | 1.9 |
| 1550 | 1232.1 | 1.3 | 8.9 | .6 | .4 | .9 | 1.6 | .9 | 1.1 | 1.8 | 12.0 | 1.1 | 2.5 | 1.4 | .9 | 4.1 | 1.8 |
| 1860 | 1442.2 | 8.0 | 3.1 | 1.4 | 4.8 | 2.9 | 1.3 | 4.7 | 2.6 | 4.4 | 2.4 | 1.3 | .0 | 1.9 | 2.6 | 2.1 | .9 |
| 2170 | 1666.5 | 6.7 | .5 | 3.7 | 5.2 | 1.4 | .9 | 2.0 | .3 | 2.2 | 9.2 | 5.4 | .2 | 3.7 | 1.6 | 1.9 | 1.6 |
| 2480 | 1836.9 | 4.9 | 2.3 | .8 | 9.1 | 1.5 | .2 | 1.9 | 3.4 | 1.0 | 1.3 | .1 | 1.7 | 1.7 | 7.3 | 1.8 | .3 |
| 2790 | 2045.3 | 1.7 | 4.5 | 2.1 | 4.2 | 2.0 | 7.6 | 2.1 | 3.0 | 6.1 | 3.0 | 2.8 | .3 | 3.2 | 5.3 | 1.1 | 1.2 |
| 3100 | 2252.7 | .5 | 2.8 | 3.8 | .5 | 2.1 | 2.3 | 1.3 | 6.8 | 3.3 | 6.2 | 4.5 | 1.9 | 4.5 | .3 | .9 | 10.7 |
| B. 0 | .0 | 100 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| 770 | 750.3 | 56.8 | 5.7 | 2.4 | 1.3 | 2.3 | .9 | 1.3 | .8 | 1.3 | 1.1 | 1.1 | 1.0 | 1.6 | 1.1 | 1.1 | 1.3 |
| 1550 | 1232.1 | 35.1 | 4.4 | 2.8 | 1.9 | 2.6 | 1.6 | 1.8 | 2.3 | 1.8 | 1.9 | 2.0 | 1.7 | 2.3 | 2.3 | 2.0 | 2.1 |
| 2320 | 1754.0 | 25.9 | 3.8 | 2.9 | 2.4 | 2.4 | 2.1 | 2.1 | 2.4 | 2.2 | 2.3 | 2.3 | 2.1 | 2.6 | 2.7 | 2.3 | 2.8 |
| 3100 | 2252.7 | 20.9 | 3.6 | 3.2 | 2.4 | 2.5 | 2.4 | 2.2 | 2.4 | 2.4 | 2.4 | 2.3 | 2.2 | 2.8 | 2.9 | 2.7 | 2.9 |

TABLE A2.10(CONT). ENERGIES (A), AND AVERAGES (B), FOR THE SYSTEM 31-1-1

| | C | Z | I=17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A. | 0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| | 30 | 39.6 | .0 | .0 | .0 | .0 | .1 | .0 | .1 | .1 | .0 | .0 | .0 | .0 | .1 | .0 | .0 |
| | 60 | 101.9 | .2 | .0 | .2 | .0 | .0 | .0 | .0 | .0 | .6 | .0 | .0 | .0 | .2 | .2 | .1 |
| | 90 | 163.5 | .2 | .0 | .0 | .1 | .2 | .0 | .0 | .3 | .0 | .1 | .0 | .0 | .1 | .4 | .2 |
| | 120 | 197.1 | .3 | .3 | .2 | .9 | .5 | .7 | .4 | .4 | .1 | .2 | .3 | .7 | .7 | .4 | .2 |
| | 150 | 231.0 | .1 | .2 | 1.4 | 1.1 | .1 | .6 | .6 | .5 | .2 | .4 | 1.1 | .3 | .6 | .4 | .4 |
| | 310 | 446.0 | 1.6 | .8 | .3 | 2.2 | 5.0 | .8 | 1.4 | .4 | 2.7 | .3 | .4 | 1.2 | 1.1 | 4.0 | .8 |
| | 620 | 651.2 | .5 | 2.0 | 5.8 | .5 | 5.8 | 3.8 | .8 | 8.3 | 1.6 | 2.3 | .3 | .1 | 3.9 | .7 | 2.0 |
| | 930 | 850.0 | 4.1 | 11.1 | .6 | 3.3 | 4.0 | .3 | 7.1 | .1 | 12.6 | 2.1 | 3.8 | .3 | .4 | .0 | 10.3 |
| | 1240 | 1043.4 | 8.8 | 2.9 | 12.3 | .7 | 3.7 | 1.3 | .5 | 1.3 | 1.4 | 3.8 | 2.8 | 3.2 | 3.8 | .9 | 1.5 |
| | 1550 | 1232.1 | 7.6 | 1.5 | 2.2 | .1 | 4.4 | 1.7 | 1.9 | 2.3 | .0 | 13.4 | 3.4 | 4.3 | 9.1 | .2 | 6.6 |
| | 1860 | 1442.2 | 7.7 | 4.4 | 3.3 | 2.8 | .4 | 6.2 | 5.8 | 5.7 | .8 | .2 | 3.9 | .4 | 4.9 | 4.4 | 4.6 |
| | 2170 | 1666.5 | 8.3 | 3.3 | .6 | .8 | 5.1 | 2.7 | 1.4 | 3.0 | .1 | 9.3 | 1.5 | 2.5 | .8 | 5.4 | 8.5 |
| | 2480 | 1836.9 | .8 | 11.3 | 1.0 | 2.2 | .5 | 10.8 | 4.6 | 2.7 | .6 | 1.6 | 16.0 | 2.2 | 1.0 | .7 | 4.8 |
| | 2790 | 2045.3 | 3.0 | 6.3 | 2.1 | .6 | 1.4 | 1.2 | 2.3 | 14.1 | 1.8 | .5 | 3.4 | 3.0 | 3.3 | 4.8 | 2.1 |
| | 3100 | 2252.7 | 5.3 | .6 | 1.7 | 11.4 | 4.2 | 1.3 | 4.7 | .4 | 4.7 | 1.1 | 7.8 | 1.3 | 2.3 | .6 | .3 |
| B. | 0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| | 770 | 750.3 | 1.3 | 1.5 | 1.5 | 1.1 | 1.5 | 1.3 | 1.4 | 1.1 | 1.0 | 1.5 | 1.2 | 1.1 | 1.2 | 1.3 | 1.0 |
| | 1550 | 1232.1 | 2.3 | 2.4 | 2.1 | 1.9 | 2.0 | 2.1 | 2.1 | 1.9 | 1.9 | 2.3 | 2.2 | 1.9 | 1.8 | 2.1 | 2.3 |
| | 2320 | 1754.0 | 2.5 | 2.7 | 2.3 | 2.4 | 2.4 | 2.3 | 2.7 | 2.4 | 2.3 | 2.5 | 2.4 | 2.3 | 2.1 | 2.8 | 2.7 |
| | 3100 | 2252.7 | 2.8 | 2.8 | 2.6 | 2.6 | 2.4 | 2.7 | 2.8 | 2.6 | 2.5 | 2.7 | 2.7 | 2.5 | 2.5 | 2.8 | 2.8 |

TABLE A2.11. ENERGIES (A), AND TIME AVERAGES (B), FOR THE SYSTEM 31-1-31.

| | C | Z | I=1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A. | 0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| | 30 | 26.8 | .0 | .2 | .6 | .3 | .2 | .4 | .2 | .0 | .9 | .2 | .9 | 1.2 | .8 | .2 | 1.6 | .2 |
| | 60 | 51.2 | .0 | .2 | 1.8 | .3 | .9 | 1.7 | .8 | .3 | 1.0 | .9 | .1 | 1.3 | .8 | 2.0 | 3.5 | 1.2 |
| | 90 | 74.7 | .0 | 1.2 | 4.1 | .0 | 1.4 | 2.3 | 1.8 | 2.9 | 1.5 | .5 | .6 | 1.4 | .3 | 1.5 | 6.5 | 11.3 |
| | 120 | 97.0 | .0 | 2.1 | 5.9 | .6 | 3.0 | .5 | .6 | 2.7 | 3.0 | .4 | 2.3 | 2.8 | 5.2 | 6.4 | 3.1 | 3.7 |
| | 150 | 118.7 | .0 | .5 | 2.6 | 2.1 | 1.5 | 11.4 | 3.0 | 4.7 | 3.0 | .5 | .8 | 4.8 | 6.5 | .4 | 1.9 | 3.2 |
| | 310 | 228.7 | .6 | 5.8 | .1 | 1.2 | .3 | 2.8 | 1.5 | 9.2 | 1.3 | 1.2 | 1.4 | 5.1 | .2 | .4 | 13.2 | 7.8 |
| | 620 | 450.4 | 2.8 | .6 | 3.6 | 2.9 | .9 | 3.1 | 1.8 | 1.9 | 2.7 | 2.3 | 5.8 | 2.6 | .3 | 5.0 | 2.7 | 18.4 |
| | 930 | 652.2 | .1 | 3.7 | 6.8 | 9.0 | .9 | 10.5 | 2.9 | 6.8 | 2.5 | .3 | 4.9 | 1.2 | 1.5 | .5 | 8.4 | 2.6 |
| | 1240 | 860.9 | .4 | 1.3 | 9.1 | .3 | .0 | 3.3 | 2.0 | 7.9 | .1 | 1.5 | 1.0 | 1.4 | 8.9 | .4 | 1.9 | 4.5 |
| | 1550 | 1067.7 | 3.1 | 2.1 | 3.4 | 6.1 | 3.7 | .2 | .5 | 6.6 | 10.7 | .2 | 1.3 | 1.6 | 7.9 | 2.9 | 2.1 | 1.8 |
| | 1860 | 1278.4 | 2.4 | 5.2 | 1.0 | 13.0 | 5.1 | 1.9 | 7.0 | 1.9 | .1 | 2.1 | 1.3 | 1.4 | .6 | 1.9 | 3.8 | 3.6 |
| | 2170 | 1454.1 | 3.1 | 2.6 | 9.2 | 9.6 | .6 | 1.3 | .1 | 3.3 | 4.6 | .8 | 3.2 | 10.8 | 5.4 | 4.3 | .3 | 5.3 |
| | 2480 | 1681.5 | 3.7 | 6.2 | .7 | 3.1 | 3.1 | 2.0 | .7 | 6.0 | 1.2 | 1.3 | 2.3 | 6.2 | .7 | .5 | 8.2 | 1.8 |
| | 2790 | 1870.6 | 7.9 | 8.1 | 7.8 | .5 | .3 | 3.3 | 3.1 | 4.7 | .6 | 4.3 | 6.3 | 2.2 | 4.0 | 5.1 | .5 | 3.5 |
| | 3100 | 2060.8 | .9 | 1.2 | 5.8 | 2.6 | 1.5 | 3.2 | 3.0 | .8 | 3.6 | 4.7 | 4.4 | 4.6 | 15.1 | .0 | .6 | 1.8 |
| B. | 0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| | 775 | 553.1 | 4.6 | .6 | 9.8 | 1.5 | .5 | 11.6 | 4.6 | 10.5 | .4 | 4.3 | 6.0 | 4.1 | 1.3 | 1.7 | 2.4 | .6 |
| | 1550 | 1067.7 | 1.4 | 3.6 | 3.9 | 3.3 | 2.3 | 3.8 | 3.7 | 3.1 | 3.1 | 3.3 | 3.0 | 3.5 | 3.0 | 3.0 | 3.2 | 3.7 |
| | 2325 | 1557.8 | 2.1 | 3.0 | 4.4 | 3.5 | 2.8 | 3.5 | 3.2 | 3.3 | 3.1 | 3.3 | 3.1 | 3.3 | 3.1 | 3.0 | 3.4 | 3.4 |
| | 3100 | 2060.8 | 3.0 | 3.4 | 3.7 | 3.1 | 2.7 | 3.5 | 3.4 | 3.5 | 3.1 | 3.5 | 3.2 | 3.1 | 3.0 | 3.1 | 3.2 | 3.3 |

TABLE A2.11(CONT). ENERGIES (A), AND AVERAGES (B), FOR THE SYSTEM 31-1-31.

| | C | Z | I=17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A. | 0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | 100 |
| | 30 | 26.8 | .7 | 1.0 | 5.5 | .4 | 7.0 | 1.9 | 3.9 | 1.2 | 14.9 | .0 | 23.8 | .1 | 20.5 | .7 | 10.4 |
| | 60 | 51.2 | 1.2 | 1.6 | .0 | 7.3 | 1.6 | 6.1 | .5 | 2.2 | .9 | 1.4 | 36.9 | .7 | 3.1 | 2.3 | 17.3 |
| | 90 | 74.7 | 5.4 | 2.9 | 1.5 | 7.0 | 2.3 | 4.4 | 4.7 | 7.8 | 6.9 | 11.2 | 1.0 | 2.7 | 2.6 | 1.6 | .7 |
| | 120 | 97.0 | 1.9 | 1.9 | 2.3 | 2.7 | 1.2 | 20.2 | 7.1 | 2.5 | 3.1 | 1.2 | 4.0 | 6.4 | .4 | 1.7 | 1.0 |
| | 150 | 118.7 | 1.7 | 2.0 | .2 | 5.9 | 2.0 | 5.4 | .5 | 2.3 | 9.7 | 4.2 | 2.8 | 5.1 | 2.7 | 7.4 | 1.5 |
| | 310 | 228.7 | 3.3 | .2 | 2.5 | 2.6 | 4.3 | .7 | 2.7 | 3.4 | 5.5 | 1.0 | 11.2 | 1.6 | 2.2 | .4 | 6.3 |
| | 620 | 450.4 | .1 | 1.9 | .5 | 2.7 | 10.4 | 4.7 | 3.1 | 1.3 | 2.8 | 3.7 | 2.5 | 4.6 | 1.2 | 1.8 | 1.5 |
| | 930 | 652.2 | .8 | 1.5 | 6.9 | 3.1 | .1 | 9.4 | 3.2 | .2 | 2.2 | .7 | 2.0 | .3 | 3.4 | 2.5 | 1.1 |
| | 1240 | 860.9 | 5.5 | .9 | .2 | .9 | 2.8 | 3.1 | 15.1 | 6.2 | 2.8 | 8.8 | 2.1 | 3.5 | 3.1 | .6 | .3 |
| | 1550 | 1067.7 | 4.1 | 1.6 | 2.7 | 3.6 | 1.3 | .1 | 3.0 | 5.1 | 2.1 | .4 | 6.7 | 3.5 | 8.3 | 2.5 | .5 |
| | 1860 | 1278.4 | .3 | 5.1 | 4.6 | 3.7 | 2.1 | 2.6 | 6.4 | 3.0 | .2 | .2 | 3.1 | 1.7 | 6.3 | .8 | 7.6 |
| | 2170 | 1454.1 | 1.2 | 1.1 | 2.3 | 5.1 | 5.0 | .4 | 1.5 | .3 | 3.8 | 3.2 | 5.4 | .1 | 4.0 | .9 | 1.2 |
| | 2480 | 1681.5 | 13.8 | .7 | 4.9 | 2.8 | 1.4 | 3.3 | 5.0 | 7.1 | 3.3 | 1.8 | 1.7 | .7 | 2.7 | .5 | 2.9 |
| | 2790 | 1870.6 | 3.8 | .6 | 3.3 | .5 | 6.4 | 1.5 | .5 | .3 | 3.2 | .4 | 5.2 | 8.5 | 1.6 | .2 | 1.8 |
| | 3100 | 2060.8 | 1.4 | 1.0 | 4.6 | 2.4 | 2.3 | 3.8 | 5.8 | 3.3 | 9.2 | 2.5 | 3.2 | 1.0 | 1.9 | 1.8 | 2.0 |
| B. | 0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | 100 |
| | 775 | 553.1 | 2.5 | 5.7 | .9 | .4 | 2.1 | .8 | 6.1 | .6 | 3.8 | 1.4 | .0 | 2.8 | 2.8 | 4.0 | 1.4 |
| | 1550 | 1067.7 | 3.1 | 3.2 | 2.3 | 3.2 | 2.6 | 3.4 | 3.0 | 3.1 | 3.1 | 3.0 | 4.2 | 2.8 | 4.0 | 3.5 | 4.6 |
| | 2325 | 1557.8 | 3.0 | 3.2 | 2.6 | 3.5 | 2.8 | 3.4 | 3.0 | 3.1 | 3.1 | 2.9 | 3.9 | 2.7 | 3.6 | 3.4 | 4.4 |
| | 3100 | 2060.8 | 3.1 | 3.2 | 2.7 | 3.3 | 3.0 | 3.4 | 3.0 | 3.1 | 3.1 | 3.0 | 3.6 | 2.9 | 3.5 | 3.3 | 3.9 |

TABLE A2.12. ENERGIES (A), AND TIME AVERAGES (B), FOR THE SYSTEM 31-2-1.

| | C | Z | I=1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A. | 0 | .0 | 100 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| | 30 | 1.7 | 91.8 | 1.2 | 1.6 | 1.2 | .5 | .1 | .0 | .0 | .0 | .1 | .3 | .4 | .2 | .0 | .1 | .2 |
| | 60 | 2.4 | 83.0 | 5.4 | 4.1 | 1.1 | .1 | .3 | .3 | .1 | .0 | .0 | .1 | .0 | .0 | .0 | .0 | .2 |
| | 90 | 3.5 | 77.0 | 9.0 | 2.5 | .9 | 1.6 | .3 | .6 | .6 | .1 | .5 | .2 | .1 | .4 | .3 | .3 | .9 |
| | 120 | 4.9 | 74.7 | 10.7 | 1.9 | 1.0 | .5 | 1.1 | .3 | .1 | .0 | .3 | .5 | .3 | .4 | .1 | .3 | .9 |
| | 155 | 7.6 | 75.5 | 11.0 | 2.2 | 1.1 | 1.0 | .2 | .7 | .1 | .5 | .1 | .3 | .1 | .3 | .6 | .1 | .6 |
| | 310 | 40.0 | 31.2 | 7.8 | 8.7 | 3.1 | 2.0 | 2.2 | .4 | 1.6 | .4 | 1.5 | .3 | .2 | 1.0 | .5 | .3 | .4 |
| | 620 | 100.0 | 5.6 | .1 | 9.7 | .3 | 3.6 | .4 | .3 | 3.7 | 8.4 | 1.4 | 1.6 | 2.3 | .3 | 14.3 | 1.8 | 1.6 |
| | 930 | 165.5 | 6.2 | 4.6 | 1.3 | 1.6 | 1.2 | 2.1 | 1.5 | 4.3 | 4.6 | 2.5 | 6.9 | 6.7 | 6.4 | 3.7 | 11.8 | .9 |
| | 1240 | 224.7 | 2.3 | 3.1 | 2.6 | 1.3 | 2.0 | 3.6 | .5 | 2.9 | 13.6 | 5.3 | 4.1 | 1.5 | 3.7 | 2.9 | 10.0 | 1.2 |
| | 1550 | 291.4 | .9 | 2.2 | 1.3 | 2.2 | 1.2 | 7.9 | 5.2 | 1.6 | .8 | 6.7 | .5 | 1.6 | 3.0 | 1.3 | .6 | .4 |
| | 1860 | 354.3 | .1 | 8.1 | 3.7 | .6 | 3.4 | 7.1 | 1.2 | 13.4 | 3.7 | 2.8 | 1.1 | 1.9 | .9 | 5.2 | 3.1 | .1 |
| | 2170 | 414.0 | 1.1 | 6.9 | 2.9 | 3.9 | .0 | .7 | 15.6 | .2 | 2.5 | 1.6 | 1.5 | 11.4 | 3.2 | .5 | 1.3 | 1.9 |
| | 2480 | 480.5 | .2 | .4 | 3.9 | .5 | .2 | 2.6 | 5.8 | .9 | 8.1 | 2.3 | 7.1 | .2 | 1.7 | 2.5 | 8.3 | 2.2 |
| | 2790 | 548.1 | .5 | 4.2 | 1.9 | 3.6 | 1.4 | 1.3 | 6.9 | .9 | 6.5 | 4.3 | 4.6 | .2 | .5 | 1.0 | 4.1 | 4.5 |
| | 3100 | 613.6 | 1.3 | 4.1 | 1.2 | .5 | 1.8 | 3.5 | .7 | 4.0 | 3.9 | .7 | 5.8 | 1.1 | 12.0 | 2.4 | 1.2 | 5.7 |
| B. | 0 | .0 | 100 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| | 775 | 131.1 | 26.2 | 5.0 | 4.2 | 3.0 | 1.8 | 1.6 | 1.7 | 2.1 | 2.2 | 2.6 | 1.9 | 2.0 | 1.9 | 3.1 | 2.2 | 3.2 |
| | 1550 | 291.4 | 13.2 | 3.9 | 6.2 | 2.4 | 2.3 | 2.4 | 2.3 | 2.2 | 2.8 | 2.8 | 2.9 | 2.0 | 2.6 | 3.5 | 2.7 | 3.1 |
| | 2325 | 448.2 | 9.0 | 4.5 | 4.7 | 2.2 | 2.7 | 2.5 | 2.6 | 2.3 | 2.9 | 3.1 | 3.0 | 2.7 | 3.0 | 3.7 | 3.0 | 3.4 |
| | 3100 | 613.6 | 6.9 | 4.1 | 4.1 | 2.3 | 2.4 | 2.4 | 2.6 | 2.3 | 2.9 | 3.0 | 3.1 | 2.5 | 3.1 | 3.8 | 3.0 | 3.7 |

TABLE A2.12(CONT). ENERGIES (A), AND AVERAGES (B), FOR THE SYSTEM 31-2-1.

| | C | Z | I=17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A. | 0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| | 30 | 1.7 | .3 | .1 | .0 | .1 | .4 | .6 | .4 | .2 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| | 60 | 2.4 | .4 | .3 | .0 | .0 | .0 | .4 | 1.2 | 1.4 | .5 | .0 | .2 | .1 | .1 | .4 | .3 |
| | 90 | 3.5 | 1.8 | 1.3 | .1 | .2 | .4 | .0 | .1 | .1 | .0 | .0 | .0 | .0 | .0 | .4 | .3 |
| | 120 | 4.9 | .3 | .3 | .0 | .0 | .1 | .7 | .2 | .2 | .2 | 1.7 | 1.1 | .1 | 1.2 | .3 | .3 |
| | 155 | 7.6 | .5 | .9 | .5 | .1 | .5 | .7 | .0 | .2 | .2 | .0 | .4 | .0 | .4 | .4 | .9 |
| | 310 | 40.0 | .6 | .0 | 1.6 | .2 | .1 | .3 | 4.0 | 8.4 | 4.8 | .3 | 1.7 | 1.4 | 2.5 | 3.3 | 9.4 |
| | 620 | 100.0 | 1.8 | 10.1 | 3.7 | 1.1 | .1 | .0 | 1.3 | 3.3 | 1.0 | 3.5 | 4.8 | 2.6 | 3.7 | 7.6 | .3 |
| | 930 | 165.5 | 1.2 | 1.7 | 4.1 | 2.6 | 4.0 | 4.0 | 2.6 | 1.3 | 1.7 | 1.9 | 1.9 | 5.4 | .2 | .0 | .8 |
| | 1240 | 224.7 | 2.9 | 1.4 | .3 | .6 | .3 | 4.3 | .7 | 3.2 | 9.2 | .9 | 9.5 | 1.2 | .5 | 2.2 | 2.2 |
| | 1550 | 291.4 | 12.7 | 1.5 | .5 | 12.4 | 4.4 | 3.1 | 1.2 | 3.1 | 8.8 | .2 | .5 | 7.3 | 2.1 | 3.3 | 1.6 |
| | 1860 | 354.3 | 3.8 | .5 | 2.6 | 3.0 | 1.3 | 4.5 | 4.2 | .8 | 5.2 | 1.8 | 1.5 | 1.8 | 3.9 | 5.0 | 3.6 |
| | 2170 | 414.0 | 1.8 | 2.2 | 10.1 | 1.4 | 2.3 | 5.6 | 2.4 | 6.0 | .3 | 2.3 | .4 | 1.1 | 3.0 | 4.9 | 1.5 |
| | 2480 | 480.5 | 1.8 | 5.0 | 11.1 | 6.4 | .3 | 13.8 | 1.2 | .7 | 2.1 | .4 | 2.9 | 1.3 | 3.1 | 2.5 | .6 |
| | 2790 | 548.1 | 8.2 | 1.6 | .0 | .3 | 2.3 | 13.7 | .0 | 2.6 | 3.6 | 4.0 | 2.3 | 5.6 | 1.3 | 7.0 | .8 |
| | 3100 | 613.6 | 1.5 | 1.3 | .5 | 6.0 | 4.9 | .3 | 5.4 | 1.0 | 7.9 | 3.0 | 9.2 | .6 | 4.2 | .8 | 3.6 |
| B. | 0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| | 775 | 131.1 | 1.9 | 2.0 | 1.8 | 2.4 | 2.0 | 2.0 | 2.4 | 2.7 | 3.0 | 2.6 | 1.9 | 3.2 | 2.5 | 2.4 | 2.5 |
| | 1550 | 291.4 | 2.7 | 2.9 | 2.3 | 3.1 | 2.6 | 3.0 | 2.8 | 3.0 | 3.3 | 2.9 | 2.7 | 3.4 | 2.6 | 2.4 | 2.9 |
| | 2325 | 448.2 | 2.7 | 2.9 | 2.6 | 3.5 | 2.9 | 3.2 | 3.1 | 3.0 | 3.4 | 3.1 | 2.7 | 3.2 | 2.8 | 2.7 | 2.9 |
| | 3100 | 613.6 | 2.9 | 2.8 | 2.9 | 3.7 | 3.3 | 3.7 | 3.2 | 3.1 | 3.4 | 3.2 | 3.0 | 3.4 | 2.9 | 2.9 | 3.4 |

TABLE A2.13. ENERGIES (A), AND TIME AVERAGES (B), FOR THE SYSTEM 31-2-31.

| | C | Z | I=1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A. | 0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| | 30 | 3.9 | .0 | 7.0 | .0 | 3.5 | .0 | .1 | .1 | .3 | .0 | .0 | .1 | .1 | .2 | .3 | .1 | .0 |
| | 60 | 17.1 | .3 | 13.0 | 2.3 | 2.6 | 4.3 | 4.8 | 2.6 | .1 | 2.8 | .5 | 3.6 | .9 | 3.2 | 2.9 | 9.2 | 3.2 |
| | 90 | 24.9 | 2.5 | 13.1 | 1.1 | .3 | 1.4 | 3.5 | 4.8 | .5 | .2 | 1.0 | .2 | 4.9 | 9.4 | .8 | 4.3 | .8 |
| | 120 | 31.2 | 3.0 | 15.7 | .2 | 3.6 | 5.6 | 11.9 | 2.6 | 1.2 | 7.4 | .2 | 2.5 | 5.4 | 1.1 | 1.2 | 5.5 | .3 |
| | 150 | 38.8 | 4.0 | 8.9 | 2.1 | 2.6 | 3.5 | 3.5 | 3.8 | .3 | 2.4 | .9 | 3.3 | 6.3 | .6 | 4.2 | 5.9 | 3.0 |
| | 310 | 68.0 | 7.5 | 3.9 | .2 | 6.0 | 2.8 | .5 | 1.4 | 3.6 | 8.3 | 5.7 | 5.5 | 1.1 | 1.0 | .9 | 1.0 | 3.4 |
| | 620 | 127.3 | 5.0 | .2 | 4.2 | 2.9 | 4.0 | 6.3 | 3.1 | 1.8 | 1.2 | 1.1 | 9.2 | 10.3 | 1.2 | .0 | 6.1 | 1.5 |
| | 930 | 193.8 | 3.3 | 2.8 | .6 | 1.0 | .1 | 3.3 | 8.7 | 2.9 | 2.9 | .2 | .6 | 1.2 | 4.7 | 3.5 | 4.1 | 5.2 |
| | 1240 | 256.7 | 4.8 | 1.3 | .7 | .5 | 4.1 | 3.2 | 5.9 | 2.4 | 2.9 | 2.2 | 2.2 | .5 | .9 | 2.2 | 7.9 | 3.1 |
| | 1550 | 321.3 | 3.0 | 4.9 | 2.7 | 1.4 | 2.9 | 8.3 | 4.5 | 1.9 | 3.6 | .9 | 1.9 | 5.6 | 6.5 | .6 | .3 | .1 |
| | 1860 | 385.5 | 2.2 | 1.9 | .5 | 1.8 | 9.0 | 4.6 | 3.6 | 8.6 | .1 | .0 | .5 | 12.8 | 3.2 | .0 | .4 | 5.6 |
| | 2170 | 449.3 | 4.6 | .7 | .7 | .8 | 15.9 | .5 | 1.8 | .5 | 2.4 | 4.8 | 9.5 | 3.1 | .3 | 1.2 | .7 | 2.5 |
| | 2480 | 480.5 | .2 | .4 | 3.9 | .5 | .2 | 2.6 | 5.8 | .9 | 8.1 | 2.3 | 7.1 | .2 | 1.7 | 2.5 | 8.3 | 2.2 |
| | 2790 | 577.6 | 2.8 | 5.2 | .8 | 3.6 | 5.3 | .6 | 4.4 | 1.7 | 4.6 | .4 | 1.4 | 3.9 | 3.8 | 10.9 | 8.5 | .5 |
| | 3100 | 647.0 | 2.7 | .9 | .8 | 1.7 | .2 | 1.0 | 2.4 | .1 | .3 | 2.2 | 4.4 | 10.4 | .4 | .4 | 10.0 | 9.9 |
| B. | 0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| | 775 | 160.7 | 5.2 | 5.4 | 2.8 | 3.2 | 2.2 | 4.2 | 2.8 | 4.4 | 2.3 | 3.2 | 3.0 | 3.3 | 2.8 | 2.9 | 2.9 | 2.4 |
| | 1550 | 321.3 | 4.9 | 4.0 | 2.6 | 2.4 | 2.4 | 4.2 | 3.2 | 3.7 | 2.8 | 3.1 | 2.6 | 3.4 | 3.0 | 2.8 | 3.0 | 3.0 |
| | 2325 | 483.7 | 5.3 | 4.2 | 2.2 | 2.7 | 2.8 | 3.7 | 3.0 | 3.2 | 3.0 | 3.1 | 2.7 | 3.1 | 2.9 | 2.8 | 2.9 | 3.3 |
| | 3100 | 647.0 | 5.0 | 3.9 | 2.1 | 2.8 | 2.9 | 3.5 | 3.1 | 3.0 | 2.8 | 3.0 | 2.7 | 3.4 | 3.1 | 2.8 | 3.1 | 3.2 |

TABLE A2.13(CONT). ENERGIES (A), AND AVERAGES (B), FOR THE SYSTEM 31-2-31.

| | C | Z | I=17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A. | 0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | 100 |
| | 30 | 3.9 | .7 | .2 | 1.1 | .1 | 2.6 | .0 | 5.7 | .1 | 14.6 | .0 | 20.3 | .3 | 17.9 | .5 | 24.2 |
| | 60 | 17.1 | 1.7 | 1.4 | 2.9 | 2.6 | 3.6 | .8 | .3 | 2.5 | .1 | .5 | 2.3 | 4.1 | 3.5 | 12.8 | 4.5 |
| | 90 | 24.9 | 3.7 | 2.6 | 8.9 | 6.0 | 4.8 | .6 | 6.3 | 2.8 | .1 | 7.9 | 1.5 | 2.4 | 2.3 | .8 | .4 |
| | 120 | 31.2 | 3.3 | 1.2 | 4.3 | 2.6 | .6 | 1.8 | .1 | 4.4 | 2.7 | 3.3 | 2.1 | 1.1 | 3.0 | .6 | 1.6 |
| | 150 | 38.8 | 1.0 | 6.0 | 1.2 | 2.3 | 6.6 | 2.8 | 8.3 | 3.5 | 3.0 | .3 | 2.7 | 1.6 | 1.0 | 2.3 | 1.9 |
| | 310 | 68.0 | 4.2 | 4.2 | 9.1 | 2.0 | 5.9 | 1.8 | 5.9 | .1 | .0 | 1.2 | 1.6 | 1.3 | 3.1 | 1.8 | 5.0 |
| | 620 | 127.3 | .8 | 3.7 | 2.4 | 7.4 | 1.7 | 1.8 | 7.0 | 1.5 | 1.0 | 4.6 | 4.4 | 3.3 | 1.1 | .7 | .2 |
| | 930 | 193.8 | 4.6 | .8 | 1.6 | 2.8 | 1.7 | 3.2 | 6.9 | 2.4 | 2.0 | 3.4 | 5.6 | 4.6 | 12.8 | 1.2 | 1.4 |
| | 1240 | 256.7 | 7.1 | 1.7 | 1.4 | 11.0 | 3.1 | 5.9 | 8.3 | .1 | 2.9 | .9 | .6 | 3.3 | 2.3 | 4.1 | 2.5 |
| | 1550 | 321.3 | 4.3 | 2.4 | .9 | 2.1 | 1.1 | 1.9 | 3.4 | 1.4 | 6.8 | 11.1 | 4.3 | 4.3 | 1.6 | 3.6 | 2.0 |
| | 1860 | 385.5 | .2 | .3 | 2.3 | 4.4 | .3 | 4.0 | .1 | 3.5 | 4.7 | 4.2 | 10.2 | .0 | 5.3 | 3.3 | 2.6 |
| | 2170 | 449.3 | 7.8 | 2.1 | 1.8 | 5.4 | 1.7 | 1.1 | 5.0 | 5.7 | 1.4 | 1.7 | 4.6 | 1.9 | 5.4 | 1.0 | 3.0 |
| | 2480 | 480.5 | 1.8 | 5.0 | 11.1 | 6.4 | .3 | 13.8 | 1.2 | .7 | 2.1 | .4 | 2.9 | 1.3 | 3.1 | 2.5 | .6 |
| | 2790 | 577.6 | 1.1 | 4.7 | 2.3 | 2.6 | 1.7 | 4.2 | 4.0 | .6 | 1.8 | 1.7 | 8.9 | 2.4 | 2.4 | 2.5 | .7 |
| | 3100 | 647.0 | .7 | 5.0 | 5.4 | 2.7 | 1.8 | 5.4 | .8 | 4.7 | 3.0 | .4 | 11.4 | 5.1 | .5 | .1 | 5.4 |
| B. | 0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | 100 |
| | 775 | 16.1 | 3.1 | 3.0 | 3.3 | 3.0 | 4.0 | 2.7 | 3.9 | 2.7 | 3.2 | 2.6 | 2.9 | 2.1 | 3.9 | 2.4 | 4.3 |
| | 1550 | 321.3 | 3.2 | 2.9 | 3.1 | 3.3 | 3.6 | 2.6 | 3.8 | 3.0 | 3.5 | 3.1 | 3.1 | 2.2 | 4.2 | 3.3 | 4.1 |
| | 2325 | 483.7 | 3.2 | 3.0 | 3.0 | 3.2 | 3.3 | 3.0 | 3.8 | 3.1 | 3.4 | 3.2 | 3.2 | 2.6 | 4.1 | 3.2 | 4.0 |
| | 3100 | 647.0 | 3.0 | 3.3 | 2.9 | 3.1 | 3.3 | 3.3 | 3.8 | 3.2 | 3.2 | 3.3 | 3.3 | 3.0 | 3.9 | 3.3 | 3.9 |

TABLE A2.14. ENERGIES (A), AND TIME AVERAGES (B), FOR THE SYSTEM 32-2-1.

| | C | Z | I=1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A. | 0 | .0 | 100 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| | 30 | 1.5 | 92.4 | 1.1 | 1.4 | 1.1 | .5 | .1 | .0 | .0 | .0 | .1 | .2 | .4 | .3 | .1 | .0 | .1 |
| | 60 | 2.2 | 83.9 | 4.8 | 4.0 | 1.3 | .1 | .3 | .3 | .1 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .1 |
| | 90 | 3.2 | 77.7 | 8.4 | 2.7 | .6 | 1.6 | .4 | .4 | .7 | .1 | .4 | .4 | .0 | .3 | .4 | .3 | .5 |
| | 120 | 4.7 | 74.8 | 11.1 | 2.0 | 1.3 | .6 | .9 | .7 | .2 | .5 | .0 | 1.2 | 1.1 | .2 | .1 | .1 | .0 |
| | 160 | 7.3 | 75.2 | 10.8 | 2.2 | 1.2 | .8 | .2 | .4 | .2 | .2 | .2 | .1 | .6 | .0 | 1.1 | 1.0 | .3 |
| | 240 | 28.8 | 32.5 | 17.0 | 2.5 | 1.2 | .0 | 1.0 | 1.3 | .6 | 1.5 | 3.7 | .8 | .9 | 1.2 | 4.0 | 1.0 | 2.2 |
| | 320 | 36.4 | 29.7 | 8.4 | 4.1 | 1.7 | 6.8 | 6.5 | 1.5 | 2.3 | .2 | 1.6 | 1.6 | .1 | .5 | 1.1 | .8 | .3 |
| | 480 | 66.6 | 17.0 | 10.0 | 2.4 | 1.1 | 4.7 | .1 | 1.0 | .3 | .1 | 2.7 | 5.4 | .9 | .5 | 3.4 | 2.6 | 1.4 |
| | 640 | 99.6 | 10.2 | 7.7 | 8.9 | 4.2 | 1.0 | 4.5 | .2 | 1.8 | .3 | 2.4 | .8 | .5 | 2.7 | .4 | 2.4 | 2.4 |
| | 800 | 130.9 | 1.7 | 1.3 | 2.9 | 1.1 | 3.7 | 1.2 | 6.2 | 3.7 | 1.0 | 5.2 | 1.6 | 5.7 | 1.3 | 2.0 | 1.0 | 2.4 |
| | 960 | 165.7 | 2.0 | 2.6 | 14.4 | 14.0 | .6 | 10.1 | .7 | .6 | .7 | 4.4 | .5 | 4.3 | 1.8 | 2.5 | 2.0 | 4.0 |
| | 1120 | 195.8 | .8 | .2 | .6 | 2.7 | 5.9 | 5.1 | 1.3 | 4.1 | .8 | .9 | .3 | 4.2 | 3.6 | 5.7 | 4.9 | 2.1 |
| | 1280 | 231.2 | 4.6 | .3 | .1 | 1.2 | 6.9 | 2.0 | 4.1 | .9 | 7.6 | .7 | 4.6 | 2.1 | 1.0 | 8.7 | 1.9 | 11.6 |
| | 1440 | 266.3 | .5 | 9.3 | .4 | 1.1 | 1.6 | 1.5 | .8 | 7.6 | 2.2 | 3.1 | .2 | .0 | .3 | 4.7 | 6.6 | 1.4 |
| | 1600 | 299.5 | 1.7 | 13.1 | 5.1 | 2.4 | 5.5 | .0 | 1.9 | 1.2 | .5 | 2.3 | .8 | .3 | .8 | 5.7 | 5.5 | .4 |
| B. | 0 | .0 | 100 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| | 400 | 55.5 | 51.2 | 9.3 | 2.8 | 1.3 | 1.8 | 1.4 | .8 | 1.3 | .8 | .7 | 1.0 | .7 | 1.1 | .9 | 1.1 | .8 |
| | 800 | 130.9 | 26.9 | 8.8 | 3.0 | 1.7 | 2.4 | 2.3 | 1.6 | 2.5 | 1.2 | 2.2 | 2.6 | 1.5 | 2.5 | 2.0 | 1.5 | 2.1 |
| | 1200 | 212.0 | 17.6 | 6.1 | 4.0 | 3.8 | 2.4 | 2.8 | 1.9 | 2.6 | 2.0 | 2.4 | 2.5 | 2.1 | 2.7 | 2.8 | 2.2 | 2.3 |
| | 1600 | 299.5 | 13.0 | 6.3 | 3.2 | 3.6 | 2.7 | 2.5 | 1.9 | 2.4 | 2.6 | 2.3 | 2.5 | 2.2 | 2.7 | 2.9 | 2.3 | 2.6 |

TABLE A2.14(CONT). ENERGIES (A), AND AVERAGES (B), FOR THE SYSTEM 32-2-1.

| | C | Z | I=17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A. | 0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| | 30 | 1.5 | .3 | .2 | .0 | .0 | .2 | .5 | .5 | .3 | .1 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| | 60 | 2.2 | .3 | .4 | .1 | .0 | .0 | .1 | .6 | 1.3 | 1.1 | .3 | .0 | .2 | .1 | .1 | .4 | .3 |
| | 90 | 3.2 | 1.3 | 1.7 | .7 | .0 | .3 | .2 | .0 | .1 | .0 | .0 | .0 | .0 | .0 | .1 | .3 | .3 |
| | 120 | 4.7 | .2 | .5 | .1 | .2 | .0 | .2 | .3 | .0 | .7 | .8 | .6 | .5 | .4 | .0 | .2 | .3 |
| | 160 | 7.3 | .6 | .4 | .0 | .1 | .0 | .4 | .2 | .1 | .2 | .3 | .1 | 1.4 | .1 | 1.0 | .2 | .3 |
| | 240 | 28.8 | 1.1 | .5 | .8 | 3.3 | 2.7 | 1.9 | 4.2 | 2.4 | 2.3 | 5.1 | .6 | 1.3 | 1.0 | .2 | .9 | .2 |
| | 320 | 36.4 | 1.6 | 1.4 | .0 | 2.1 | 2.0 | 3.3 | .0 | .2 | 3.5 | 5.4 | 4.9 | .1 | .3 | 1.3 | .3 | 6.3 |
| | 480 | 66.6 | 4.7 | 1.2 | 4.3 | 2.9 | .6 | 5.0 | 3.3 | 5.4 | 3.0 | 1.7 | .9 | 3.7 | 2.9 | 3.3 | 2.8 | .9 |
| | 640 | 99.6 | 1.7 | 5.7 | 13.4 | .7 | 9.4 | 2.4 | 1.5 | .1 | .2 | .5 | 5.1 | .9 | 2.0 | .8 | .8 | 4.1 |
| | 800 | 130.9 | 3.8 | 1.8 | 3.6 | 5.8 | 3.3 | 4.1 | 4.4 | 2.3 | 3.8 | 2.1 | 15.5 | .3 | 1.0 | .9 | 5.0 | .5 |
| | 960 | 165.7 | .4 | 4.2 | .3 | .8 | .7 | .1 | 7.9 | .5 | 4.2 | 1.2 | .2 | 2.9 | .7 | 2.1 | 5.9 | 2.5 |
| | 1120 | 195.8 | 3.7 | .8 | 1.0 | 2.2 | 8.1 | .9 | 1.1 | 4.2 | 9.0 | 2.7 | 1.0 | .3 | 2.6 | 1.2 | 14.3 | 3.5 |
| | 1280 | 231.2 | 1.0 | .2 | 3.5 | 1.2 | 2.2 | 4.5 | 5.7 | .9 | 4.5 | 3.1 | 4.1 | 1.5 | .2 | 2.5 | 3.1 | 3.4 |
| | 1440 | 266.3 | 2.3 | 5.0 | 2.8 | 7.8 | .4 | 1.1 | 4.5 | 6.0 | 4.8 | .4 | 1.0 | .9 | 11.4 | 1.1 | 4.2 | 5.3 |
| | 1600 | 299.5 | .1 | .6 | 5.1 | 1.9 | 9.2 | .8 | 3.7 | .9 | 4.5 | 2.7 | 1.8 | 1.8 | 2.5 | 1.3 | 13.0 | 2.8 |
| B. | 0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| | 400 | 55.5 | 1.3 | 1.1 | 1.3 | .9 | 1.6 | 1.5 | .8 | 2.0 | 1.4 | 1.3 | 2.5 | 1.2 | 1.0 | 1.9 | .9 | 2.1 |
| | 800 | 130.9 | 1.9 | 2.1 | 2.7 | 2.3 | 2.6 | 2.5 | 1.7 | 2.3 | 1.7 | 1.9 | 2.7 | 2.1 | 1.9 | 2.5 | 1.9 | 2.3 |
| | 1200 | 212.0 | 2.5 | 2.2 | 3.0 | 2.5 | 2.8 | 3.2 | 2.1 | 2.2 | 2.3 | 2.0 | 2.7 | 2.5 | 2.3 | 2.6 | 2.4 | 2.7 |
| | 1600 | 299.5 | 2.5 | 2.7 | 2.8 | 2.8 | 2.9 | 3.2 | 2.7 | 2.6 | 2.9 | 2.5 | 2.9 | 2.8 | 2.9 | 2.9 | 2.8 | 2.7 |

TABLE A2.15. ENERGIES (A), AND TIME AVERAGES (B), ANTISYM SYSTEM 32-2-32.

| | C | Z | I=1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A. | 0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| | 31 | 3.7 | .0 | 6.3 | .0 | 3.9 | .0 | .0 | .0 | .7 | .0 | .5 | .0 | .4 | .0 | .4 | .0 | 1.2 |
| | 60 | 16.1 | .0 | 11.5 | .0 | 5.2 | .0 | 9.7 | .0 | 11.8 | .0 | 6.2 | .0 | 4.0 | .0 | 2.1 | .0 | 2.1 |
| | 90 | 23.7 | .0 | 28.4 | .0 | 3.8 | .0 | .1 | .0 | 2.0 | .0 | 7.4 | .0 | 1.4 | .0 | 8.4 | .0 | .1 |
| | 121 | 27.7 | .0 | 20.8 | .0 | 3.6 | .0 | 6.1 | .0 | 7.7 | .0 | 3.4 | .0 | 5.9 | .0 | .0 | .0 | 5.6 |
| | 150 | 36.1 | .0 | 18.9 | .0 | 1.7 | .0 | 6.9 | .0 | .1 | .0 | 3.3 | .0 | 1.8 | .0 | 11.3 | .0 | .9 |
| | 200 | 46.2 | .0 | 6.3 | .0 | 2.9 | .0 | 1.5 | .0 | 7.8 | .0 | 5.3 | .0 | 5.5 | .0 | 5.6 | .0 | 13.4 |
| | 251 | 54.1 | .0 | .9 | .0 | 2.9 | .0 | 2.6 | .0 | .1 | .0 | 7.0 | .0 | 7.3 | .0 | 11.8 | .0 | 2.6 |
| | 300 | 65.7 | .0 | 4.7 | .0 | 2.9 | .1 | 2.7 | .0 | 2.2 | .0 | 3.8 | .0 | 4.0 | .1 | 4.0 | .0 | 4.3 |
| | 350 | 76.0 | .0 | 5.0 | 1.1 | 1.0 | 1.3 | 2.7 | 1.6 | 3.8 | 5.3 | 1.6 | 2.6 | 2.3 | 1.8 | 8.0 | 2.7 | 1.1 |
| B. | 0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| | 31 | 3.7 | .0 | 3.1 | .0 | 1.9 | .0 | .1 | .0 | .4 | .0 | .2 | .0 | .3 | .0 | .3 | .0 | .5 |
| | 60 | 16.1 | .0 | 8.8 | .0 | 3.6 | .0 | 2.4 | .0 | 2.8 | .0 | 3.2 | .0 | 3.3 | .0 | 3.0 | .0 | 3.2 |
| | 90 | 23.7 | .0 | 13.5 | .0 | 4.9 | .0 | 2.8 | .0 | 3.1 | .0 | 4.2 | .0 | 3.0 | .0 | 4.5 | .0 | 2.8 |
| | 121 | 27.7 | .0 | 14.8 | .0 | 4.7 | .0 | 2.8 | .0 | 3.6 | .0 | 4.0 | .0 | 3.1 | .0 | 4.5 | .0 | 3.0 |
| | 150 | 36.1 | .0 | 17.5 | .0 | 4.2 | .0 | 2.7 | .0 | 3.8 | .0 | 3.8 | .0 | 2.7 | .0 | 4.3 | .0 | 4.2 |
| | 200 | 46.2 | .0 | 16.7 | .0 | 4.0 | .0 | 3.9 | .0 | 3.5 | .0 | 3.7 | .0 | 2.9 | .0 | 4.3 | .0 | 4.9 |
| | 251 | 54.1 | .0 | 14.7 | .0 | 3.9 | .0 | 3.5 | .0 | 3.6 | .0 | 4.7 | .0 | 3.6 | .0 | 5.0 | .0 | 4.6 |
| | 300 | 65.7 | .0 | 12.9 | .0 | 4.2 | .0 | 3.1 | .0 | 3.7 | .0 | 4.3 | .0 | 4.0 | .0 | 4.4 | .0 | 4.3 |
| | 350 | 76.0 | .0 | 12.0 | .0 | 4.0 | .0 | 2.9 | .1 | 3.7 | .1 | 4.4 | .1 | 4.5 | .2 | 4.1 | .1 | 4.2 |

TABLE A2.15(CONT). ENERGIES (A), AND AVERAGES (B), ANTISYM SYSTEM 32-2-32.

| | C | Z | I=17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A. | 0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | 100 |
| | 31 | 3.7 | .0 | 1.6 | .0 | 1.4 | .0 | 5.5 | .0 | 7.2 | .0 | 10.7 | .0 | 19.0 | .0 | 17.1 | .0 | 24.1 |
| | 60 | 16.1 | .0 | 6.9 | .0 | 7.3 | .0 | 1.9 | .0 | .6 | .0 | 2.2 | .0 | 19.3 | .0 | 6.7 | .0 | 2.5 |
| | 90 | 23.7 | .0 | 13.0 | .0 | 1.7 | .0 | 1.7 | .0 | 7.5 | .0 | 2.7 | .0 | 3.7 | .0 | .4 | .0 | 17.6 |
| | 121 | 27.7 | .0 | .7 | .0 | 5.6 | .0 | 10.0 | .0 | 2.0 | .0 | 12.4 | .0 | .2 | .0 | 4.7 | .0 | 11.2 |
| | 150 | 36.1 | .0 | 3.9 | .0 | 3.3 | .0 | 2.3 | .0 | 16.6 | .0 | 2.8 | .0 | 5.7 | .0 | 2.4 | .0 | 18.1 |
| | 200 | 46.2 | .0 | 12.2 | .0 | 6.5 | .0 | 2.5 | .0 | 3.8 | .0 | 1.3 | .0 | .3 | .0 | 21.2 | .0 | 4.1 |
| | 251 | 54.1 | .0 | 5.0 | .0 | 5.4 | .0 | 18.7 | .0 | 1.7 | .0 | .8 | .0 | 5.6 | .0 | 25.5 | .0 | 2.2 |
| | 300 | 65.7 | .0 | 2.1 | .0 | 4.0 | .1 | .1 | .2 | 20.1 | .1 | 26.9 | .3 | 3.6 | .1 | 3.6 | .4 | 9.7 |
| | 350 | 76.0 | 1.8 | 2.0 | 6.5 | 1.7 | 2.4 | 1.7 | 3.2 | 3.0 | 7.2 | .9 | .5 | 11.7 | 5.3 | 6.8 | 1.9 | 1.6 |
| B. | 0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | 100 |
| | 31 | 3.7 | .0 | .8 | .0 | .9 | .0 | 2.2 | .0 | 3.4 | .0 | 8.9 | .0 | 11.8 | .0 | 34.9 | .0 | 30.2 |
| | 60 | 16.1 | .0 | 4.1 | .0 | 4.4 | .0 | 5.8 | .0 | 6.0 | .0 | 7.1 | .0 | 9.6 | .0 | 15.5 | .0 | 17.4 |
| | 90 | 23.7 | .0 | 4.1 | .0 | 5.3 | .0 | 4.7 | .0 | 5.6 | .0 | 5.7 | .0 | 8.4 | .0 | 13.5 | .0 | 14.2 |
| | 121 | 27.7 | .0 | 4.5 | .0 | 5.5 | .0 | 5.0 | .0 | 5.2 | .0 | 6.1 | .0 | 7.9 | .0 | 12.2 | .0 | 13.2 |
| | 150 | 36.1 | .0 | 4.2 | .0 | 5.4 | .0 | 4.7 | .0 | 5.3 | .0 | 5.9 | .0 | 7.8 | .0 | 10.5 | .0 | 12.8 |
| | 200 | 46.2 | .0 | 3.9 | .0 | 4.8 | .0 | 5.3 | .0 | 6.3 | .0 | 6.2 | .0 | 7.1 | .0 | 10.2 | .0 | 12.3 |
| | 251 | 54.1 | .0 | 4.4 | .0 | 5.2 | .0 | 5.5 | .0 | 6.0 | .0 | 7.2 | .0 | 6.8 | .0 | 10.2 | .0 | 11.2 |
| | 300 | 65.7 | .0 | 4.8 | .0 | 5.3 | .0 | 6.4 | .0 | 6.4 | .0 | 7.4 | .0 | 6.3 | .0 | 9.6 | .0 | 12.6 |
| | 350 | 76.0 | .2 | 4.7 | .1 | 5.0 | .3 | 6.0 | .2 | 8.2 | .1 | 7.4 | .1 | 5.9 | .2 | 9.3 | .1 | 11.8 |

TABLE A2.16. ENERGIES (A), AND TIME AVERAGES (B), PERTURBED SYSTEM 32-2-32.

| | C | Z | I=1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A. | 0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| | 31 | 3.7 | .0 | 6.3 | .0 | 3.8 | .0 | .0 | .0 | .7 | .0 | .5 | .0 | .4 | .0 | .4 | .0 | 1.2 |
| | 60 | 16.0 | .0 | 11.5 | .0 | 5.4 | .0 | 10.0 | .0 | 11.8 | .0 | 6.3 | .0 | 3.5 | .0 | 2.3 | .0 | 2.7 |
| | 90 | 23.3 | .0 | 27.8 | .0 | 3.7 | .1 | .3 | .3 | 1.0 | .2 | 11.4 | .4 | .7 | 1.5 | 15.8 | .1 | .2 |
| | 120 | 26.9 | .0 | 19.6 | .0 | 1.5 | .4 | 6.8 | .7 | 5.8 | .5 | 6.0 | 1.4 | 6.6 | .4 | 7.3 | 1.4 | 7.7 |
| | 150 | 31.1 | .0 | 28.4 | .0 | 4.6 | .1 | .6 | .5 | 3.7 | .1 | .4 | 2.2 | .5 | .7 | 1.2 | .3 | 3.2 |
| | 180 | 36.4 | .1 | 9.4 | .2 | 4.9 | .4 | 1.0 | 1.1 | 6.9 | .2 | 1.5 | 4.8 | 1.7 | 1.5 | 1.5 | 1.1 | 3.8 |
| | 210 | 40.7 | .1 | 11.0 | .7 | 3.5 | .7 | 2.1 | .1 | 2.8 | 2.6 | 2.8 | 2.6 | 5.9 | 3.3 | 4.2 | .8 | 4.2 |
| | 240 | 46.5 | .0 | 4.0 | 1.6 | .2 | .2 | .2 | 2.3 | 7.4 | .3 | 3.9 | .4 | .6 | .0 | 4.1 | .1 | 3.9 |
| | 270 | 51.8 | .1 | 2.8 | 2.8 | .6 | 2.8 | 5.3 | .4 | 7.6 | 1.1 | .4 | 4.1 | 1.4 | .6 | 4.0 | .6 | 2.8 |
| | 300 | 58.2 | .2 | .6 | 3.1 | .1 | 5.6 | 6.9 | 1.0 | .9 | 1.2 | 1.1 | .8 | 6.7 | 2.7 | 5.3 | 1.9 | .7 |
| | 400 | 76.1 | .3 | 6.5 | 1.5 | 1.2 | .5 | 12.5 | 4.2 | 7.9 | .2 | 1.3 | 6.1 | 10.4 | 3.9 | 1.9 | .2 | 1.9 |
| | 500 | 96.5 | .9 | 11.3 | 1.1 | 4.3 | 2.9 | 2.8 | .5 | 11.4 | .7 | .9 | .5 | 1.1 | 13.4 | .6 | 2.0 | .0 |
| B. | 0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 |
| | 50 | 13.3 | .0 | 8.2 | .0 | 3.8 | .0 | 1.0 | .0 | 1.4 | .0 | 1.7 | .0 | 2.3 | .0 | 2.7 | .0 | 3.4 |
| | 100 | 24.6 | .0 | 13.8 | .0 | 4.8 | .0 | 2.6 | .1 | 3.1 | .1 | 4.0 | .1 | 2.9 | .3 | 4.8 | .1 | 2.8 |
| | 200 | 39.2 | .0 | 16.2 | .0 | 4.4 | .1 | 2.4 | .2 | 3.7 | .3 | 3.6 | 1.3 | 3.2 | .5 | 4.1 | .5 | 3.6 |
| | 300 | 58.2 | .0 | 12.7 | .7 | 3.4 | .7 | 3.0 | .9 | 4.0 | .7 | 3.4 | 2.1 | 3.5 | .9 | 4.1 | 1.0 | 3.3 |
| | 400 | 76.1 | .1 | 10.5 | 1.0 | 3.0 | 1.4 | 2.9 | 1.7 | 4.2 | 1.2 | 3.4 | 2.0 | 4.0 | 1.1 | 3.8 | 1.6 | 3.1 |
| | 500 | 96.5 | .2 | 10.6 | 1.0 | 3.3 | 2.1 | 3.4 | 2.0 | 3.8 | 1.1 | 3.3 | 2.1 | 3.6 | 1.7 | 4.0 | 1.6 | 2.8 |

TABLE A2.16(CONT). ENERGIES (A), AND AVERAGES (B), PERTURBED SYSTEM 32-2-32.

| | C | Z | I=17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A. | 0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | 100 |
| | 31 | 3.7 | .0 | 1.6 | .0 | 1.3 | .0 | 5.4 | .0 | 7.2 | .0 | 10.5 | .0 | 19.6 | .0 | 17.5 | .0 | 23.4 |
| | 60 | 16.0 | .0 | 6.7 | .0 | 7.6 | .1 | 1.3 | .1 | 1.0 | .0 | 3.2 | .0 | 17.6 | .0 | 5.7 | .0 | 3.4 |
| | 90 | 23.3 | .3 | 14.2 | .0 | .7 | .3 | .6 | .4 | 1.9 | .3 | 3.2 | .1 | 2.4 | .1 | .1 | .5 | 11.5 |
| | 120 | 26.9 | .1 | 2.9 | 1.2 | 1.8 | 1.5 | 2.5 | .4 | 2.5 | 1.0 | 5.0 | 1.2 | 6.5 | 1.7 | 2.6 | .0 | 2.9 |
| | 150 | 31.1 | .9 | 6.9 | 1.6 | 10.1 | .8 | 1.5 | 2.7 | 9.3 | .3 | 4.9 | 1.8 | 5.2 | 1.8 | 2.9 | 1.1 | 1.6 |
| | 180 | 36.4 | 2.2 | 4.8 | 8.3 | .5 | 3.4 | 2.4 | 3.4 | .3 | 5.4 | 2.9 | 12.2 | 8.7 | 1.9 | .1 | .7 | 2.9 |
| | 210 | 40.7 | 3.8 | .1 | .0 | .9 | .2 | .1 | .8 | 18.3 | 2.7 | 4.6 | 5.2 | 5.0 | .5 | 6.5 | .6 | 3.3 |
| | 240 | 46.5 | 9.6 | 2.4 | 2.8 | .2 | 2.5 | 2.9 | 9.3 | 8.4 | .6 | 2.9 | 4.6 | 1.3 | 16.1 | 3.9 | 1.2 | 2.4 |
| | 270 | 51.8 | .0 | .9 | 14.5 | 5.1 | .5 | 4.2 | .2 | 1.6 | 7.1 | 9.3 | 4.7 | 1.4 | 2.2 | 3.6 | 4.8 | 2.4 |
| | 300 | 58.2 | 2.4 | 3.7 | 1.0 | 2.9 | .2 | 4.6 | 9.9 | 5.3 | 1.5 | 2.4 | 3.2 | 9.3 | 8.5 | 4.3 | 1.3 | .7 |
| | 400 | 76.1 | .3 | .5 | .2 | 2.8 | .1 | 4.5 | 10.3 | 1.0 | 2.3 | 1.8 | 1.2 | 8.5 | 2.3 | 2.0 | .0 | 1.5 |
| | 500 | 96.5 | .2 | .3 | .4 | .2 | 2.4 | 3.2 | 1.1 | 1.7 | 1.3 | 1.3 | 15.2 | .5 | 3.6 | 6.2 | 1.0 | 7.0 |
| B. | 0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | .0 | 100 |
| | 50 | 13.3 | .0 | 4.3 | .0 | 4.4 | .0 | 5.8 | .0 | 7.1 | .0 | 7.7 | .0 | 9.1 | .0 | 17.1 | .0 | 19.6 |
| | 100 | 24.6 | .1 | 4.3 | .1 | 5.3 | .1 | 4.6 | .1 | 5.4 | .2 | 6.0 | .1 | 7.8 | .1 | 12.6 | .2 | 13.4 |
| | 200 | 39.2 | .6 | 4.4 | .9 | 5.1 | .8 | 3.7 | .9 | 5.1 | .7 | 5.7 | .9 | 6.7 | .8 | 9.7 | .7 | 9.1 |
| | 300 | 58.2 | 1.3 | 3.4 | 1.8 | 3.9 | 1.0 | 3.7 | 1.7 | 5.5 | 1.4 | 5.0 | 2.5 | 5.3 | 2.7 | 7.7 | 1.9 | 6.8 |
| | 400 | 76.1 | 1.4 | 3.7 | 1.7 | 3.8 | 1.5 | 3.6 | 2.3 | 4.8 | 1.7 | 4.7 | 3.1 | 4.6 | 2.6 | 6.8 | 2.4 | 6.0 |
| | 500 | 96.5 | 1.6 | 3.5 | 2.2 | 3.5 | 1.9 | 3.3 | 2.8 | 4.5 | 1.9 | 4.3 | 3.1 | 4.5 | 2.8 | 5.8 | 2.3 | 5.4 |

# APPENDIX III

## THE 7090 FORTRAN II PROGRAMME FOR THE COMPUTATIONS

Considerable effort was devoted to achieving an efficient computer programme for carrying out the calculations on the model. The programme in its final form is listed in the following pages. Many other subsidiary programmes were developed to test the accuracy of the numerical procedures, to prepare data for the starting configuration of each system, to derive theoretical energy-pressure-temperature tables, and many other calculations. It is impracticable to list all these programmes here. The computations were carried out on IBM 1620 and IBM 7090 computers. The 1620, which was readily available in the University, was used for most of the development of the programmes. It was even possible to compute the motion of systems of up to 16 particles on a minimum configuration 1620, with information at each collision being output on cards for further processing to obtain the numerical results. However, when access to a 7090 was obtained, most of the computations were transferred to that computer. In all, over 800 hours of computing was done on the 1620, and about 100 hours on the 7090.

The 'comments' which appear in the listing indicate each main phase of the programme. The relationship between the variables used in the preceding theory and those employed in the programme is as follows:

| | | |
|---|---|---|
| N | N | number of degrees of freedom; |
| M | WW | mass of each particle; |
| $\gamma$ | U | spring constant; |
| $\ell$ | DL | mean free path; |
| a | DA | natural length of spring is a - d; |

| | | |
|---|---|---|
| $d$ | DD | diameter of each particle; |
| $x_j$ | X(J+5) | displacement of j-th particle; |
| $\dot{x}_j$ | XX(J+5) | velocity of j-th particle; |
| $h_i$ | T(I) | i-th iteration interval; |
| $\underset{\sim}{A}(h_i)$ | A(I+J) | i-th iteration matrix, J = 18*(I-1); |
| $K$ | KN | number of different iteration intervals; |
| $I$ | NNIT | total number of iterations; |
| $C$ | NCØLL | total number of collisions; |
| $t$ | TT | time system has been in motion; |
| $(\gamma/M)$ | UW | the inverse square of the basic time unit; |
| $\underset{\sim}{S}$ | S(I) | transformation matrix, only N elements necessary; |
| $\omega_i$ | W(I) | normal mode frequency; |
| $q_i$ | Q(I) | normal coordinate; |
| $\dot{q}_i$ | QQ(I) | normal velocity coordinate; |
| $\epsilon$ | EE | mean energy per degree of freedom; |
| $J$ | INCØLN | collision index j; |
| $E_i$ | EN(I,J) | energy in i-th mode, second index permits storage of these for up to 100 collisions; |
| $\langle E_i \rangle$ | ENM(I,2) | time average of $E_i$, as a percentage of E; |
| <KE>/N | ENKE | time average of kinetic energy/N; |
| $k$ | BØLTZ | Boltzmann's constant; |
| $T$ | TNP | instantaneous temperature; |
| $\langle T \rangle$ | TMP | time average of temperature; |
| $\sigma_T^2$ | FLT | temperature fluctuations; |
| $\langle P \rangle$ | P | time average of pressure; |
| $\overline{\langle P \rangle}$ | PA | mean time average; |
| $\sigma_{\langle P \rangle}^2$ | FP | pressure fluctuations; |
| | PH | $P - \beta'$, where $\beta'$ is an estimate for $\beta$ in Eq. (6.15); |
| | PHA | mean, or average, value of PH; |
| $x$ | XT | variable defined by Eq. (5.19); |
| $y$ | YP | variable defined by Eq. (5.17); |
| $\beta(\gamma kT)^{-\frac{1}{2}}$ | YPC | estimate for $\beta$ in dimensionless form; |
| | R | (XT+YP)F(YP), where F(y) is given by Eq. (5.16); |
| $\rho_{N,1}(mh)$ | ACC(M+1) | estimates for the autocorrelation function. |

Following the listing we give a typical sample of the output obtained from the programme. The computations are for the system N = 16, $\epsilon = \epsilon'$, $E_i \simeq \delta_{i1} E$ at t = 0. The frequency and quantity of the output is determined by the parameters NC1,NC2,...,NC9, values for which are read in with the input data at the start of each run. In the first line of output in each group TMP = T, while in the second line TMP = <T>. The last two quantities in the first line are values for <KE>/N, and the average number of iterations per collision. The remaining information in the first two lines is obvious if reference is made to the list of variables above. The third line gives values for the time averages $\langle E_i \rangle$ for the interval 0 - t = TT, and in the fourth line the time, and mode energies $E_i$, for the interval between the last two collisions are given. The above are always given when output of numerical results occurs. Additional output, which may include the position and velocity coordinates at that instant, and / or the times and mode energies for the intervals between every other pair of collisions since the last output, is optional. In the sample, the positions and velocities were given only at the 500-th collision. Estimates for the autocorrelation function for 200 intervals of $h_1$ are given periodically.

Some of the output parameters are used to prevent the computation from running for too long between 'normal' outputs at given collision intervals. The computation is also terminated if the estimate of the temperature goes outside specified bounds. At the end of a run the data necessary to restart the run is output onto cards in octal form, if required.

```
*      CARDS COLUMN
C      MAIN PROGRAMME
C      NON LINEAR GAS MODEL - SERIES METHOD
C      THE FUNCTION OF THE MAIN PROGRAMME IS TO READ IN THE
C      INITIAL DATA, INITIALIZE, TRANSFER CONTROL TO SUBROUTINE
C      COLLN, AND PUNCH OUT DATA AT THE FINISH OF THE RUN IN
C      ORDER TO RESTART IF NECESSARY.
       COMMON X,XX,N,NN,PN,U,WW,DLL,DA,DD,KN,NTST,W,S,EN,ENM,
      1EE,A,T,UW,Q,QQ,NNIT,NCOLL,NC0,NC1,NC2,NC3,NC4,NC5,NC6,
      2NC7,IN,TE,TT,TLAST,C,INCOLN,TMP,TMP1,TMP2,NCOL,TLST,
      3TF,UM,UK,UU,UC,P,PH,ENKET,VENK,PT,PHT,GP,GVP,GPH,
      4GVPH,XDOT,XXDOT,T1,NOTE,NC8,NC9,NIT1,NAUTO,AC,AV,ENKETT
D      DIMENSION X(50),XX(50),W(40),S(40),A(180),T(11),UW(1)
       DIMENSION EN(40,101),ENM(40,2),TE(101),Q(40,2),QQ(40,2),
      1AV(201),AC(201)
   50 FORMAT(3I2,5E10.4,2E8.4)
   51 FORMAT(14I5)
   52 FORMAT(4E18.8)
   53 FORMAT(E18.8)
   54 FORMAT(4018)
   55 FORMAT(6012)
   60 FORMAT(1H032HINITIAL POSITION-VELOCITY VECTOR//
     1(1X8E16.8))
   61 FORMAT(1H24X17HMODEL STATUS FOR I5,2H (I3,2H )I5,
     112H COLLISIONS.//4XI3,2X24HEMERGENCY PRINT-OUTS AT I5,
     221H ITERATION INTERVALS.//)
   63 FORMAT(1H042HPARTITION OF THE ENERGIES OF NORMAL MODES.
     1//(16F8.3))
   64 FORMAT(1H1)
   65 FORMAT(1H032HFINAL   POSITION-VELOCITY VECTOR//(1X8E16.8))
   66 FORMAT(1X8E16.8)
      READ INPUT TAPE 2,50,N,KN,NTST,U,WW,DLL,DA,DD,TMP1,TMP2
      NTS=1
      PUNCH 50,N,KN,NTS ,U,WW,DLL,DA,DD,TMP1,TMP2
      NN=N+5
      PN=N
      DL=DLL-DD
      UU=-U*(DLL-DA)
      UC=WW/(PN+1.)
      UK=WW/(4.*PN)
      UM=UK*DL
      CALL MATRIX
      DO 19 I=1,KN
      PP=1.E-10
   17 PP=.1*PP
      IF(PP-T(I))18,18,17
D  18 AAA=T(I)+PP*.9E-7
   19 PUNCH 53,AAA
      NNP=N+10
      DO 7 I=1,NNP
D     X(I)=0.0
D    7 XX(I)=0.0
```

```
C       READ IN PARAMETERS TO DETERMINE THE LENGTH OF THE RUN,
C       AND SPECIFY WHAT OUTPUT IS REQUIRED.
     1  READ INPUT TAPE 2,51,NCOLL,NC1,NC2,NC3,NC4,NC5,NC6,NC7,
       1NC8,NC9
        WRITE OUTPUT TAPE 3,61,NCOLL,NC1,NC2,NC3,NC4
        NOTE=0
        NCOL=NCOLL+NC1
        NC=NC2-NCOLL
        NC0=NCOLL+NC1*NC5-1
        IF(NC8)12,12,13
    12  NC8=1
    13  IN=1
        T1=0.0
C       IF NTST LTE ZERO THIS IS FIRST RUN, OTHERWISE THIS IS A
C       CONTINUATION RUN.
        IF(NTST)3,3,4
     3  READ INPUT TAPE 2,52,(X(I),I=6,NN),(XX(I),I=6,NN)
        WRITE OUTPUT TAPE 3,60,(X(I),I=6,NN)
        WRITE OUTPUT TAPE 3,66,(XX(I),I=6,NN)
        CALL NORMEN(IN,T1)
        WRITE OUTPUT TAPE 3,63,(EN(I,1),I=1,N)
        DO 6 I=1,201
        AV(I)=0.0
     6  AC(I)=0.0
        DO 8 I=1,N
     8  ENM(I,1)=0.0
        TT=0.0
        TLAST=0.0
        NNIT=0.0
        ENKET=0.0
        ENKETT=0.0
        VENK=0.0
        PT=0.0
        GP=0.0
        GVP=0.0
        PHT=0.0
        GPH=0.0
        GVPH=0.0
        TF=0.0
        CALL AUTOCN
C       CHECK COLLISION INEQUALITIES INITIALLY TO ENSURE THAT NO
C       PARTICLES OVERLAP.
        CALL VCRTST(DL,K)
        GO TO (2,1),K
C       READ IN CONTINUATION RUN DATA IF NISI GT ZERO.
     4  READ INPUT TAPE 2,54,(X(I),I=6,NN),(XX(I),I=6,NN)
        READ INPUT TAPE 2,54,(ENM(I,1),I=1,N),TT,NNIT,ENKET,
       1VENK,PT,GP,GVP
       1,PHT,GPH,GVPH,TF,TLAST,ENKETT
        READ INPUT TAPE 2,55,AV,AC
        P=UU+PT/TT
        PH=UU+(UC*PHT)/TT
        TE(1)=0.0
        CALL NORMEN(IN,T1)
```

```
      IN=2
      CALL NORMEN(IN,T1)
      CALL OUTPUT
      IF(NC5)2,2,11
   11 WRITE OUTPUT TAPE 3,60,(X(I),I=6,NN)
      WRITE OUTPUT TAPE 3,66,(XX(I),I=6,NN)
    2 WRITE OUTPUT TAPE 3,64
      TLST=TT
      NAUTO=TT/T(1)
      NAUTO=(NAUTO/NC9+1)*NC9+200
      CALL XDXXD(XDOT,XXDOT)
C     TRANSFER CONTROL TO SUBROUTINE COLLN FOR MAIN COMPUTATION.
      CALL COLLN
C     DETERMINE WHETHER TO PUNCH CARDS FOR A CONTINUATION RUN.
      IF(NTST)15,14,16
   16 IF(NTST-1)14,14,15
   14 NC2=NC2+NC
      PUNCH 51,NCOLL,NC1,NC2,NC3,NC4,NC5,NC6,NC7,NC8,NC9
      PUNCH 54,(X(I),I=6,NN),(XX(I),I=6,NN)
      PUNCH54,(ENM(I,1),I=1,N),TT,NNIT,ENKET,VENK,PT,GP,GVP,
     1PHT,GPH,GVPH,TF,TLAST,ENKETT
      PUNCH 55,AV,AC
   15 WRITE OUTPUT TAPE 3,65,(X(I),I=6,NN)
      WRITE OUTPUT TAPE 3,66,(XX(I),I=6,NN)
      WRITE OUTPUT TAPE 3,63,(EN(I,IN),I=1,N)
      WRITE OUTPUT TAPE 3,64
C     END OF RUN FOR THIS SYSTEM, START A NEW SYSTEM.
      GO TO 1
      END


*     CARDS COLUMN
      SUBROUTINE OUTPUT
C     OUTPUTS RESULTS REQUIRED AS DETERMINED BY THE PROGRAMME
C     PARAMETERS NC0 - NC9.
      COMMON X,XX,N,NN,PN,U,WW,DLL,DA,DD,KN,NTST,W,S,EN,ENM,
     1EE,A,T,UW,Q,QQ,NNIT,NCOLL,NC0,NC1,NC2,NC3,NC4,NC5,NC6,
     2NC7,IN,TE,TT,TLAST,C,INCOLN,TMP,TMP1,TMP2,NCOL,TLST,
     3TF,UM,UK,UU,UC,P,PH,ENKET,VENK,PT,PHT,GP,GVP,GPH,
     4GVPH,XDOT,XXDOT,T1,NOTE,NC8,NC9,NIT1,NAUTO,AC,AV,ENKETT
D     DIMENSION X(50),XX(50),W(40),S(40),A(180),T(11),UW(1)
      DIMENSION EN(40,101),ENM(40,2),TE(101),Q(40,2),QQ(40,2),
     1AV(201),AC(201)
   60 FORMAT(/ 1X4HNCOLI4,4H,TT=E12.5,8HSEC,TMP=F7.2,3H,P=
     1E12.5,8HDYNE,PH=E13.5,5H,E/N=E13.6,10HERGS,KE/N=E13.6,
     210H,ITN/COLN=I3)
   61 FORMAT(1X4HTMP=F7.2,4H,FL=F7.4,4H,PA=E12.5,4H,FL=F7.4,
     15H,PHA=E13.5,4H,FL=F7.4,3H,X=F6.3,3H,Y=F7.3,3H,R=F7.3,
     25H,YPC=F6.3,9H,COLLN J= I3)
   62 FORMAT(1X16F8.3)
   63 FORMAT( 1XE11.4,16F7.3/(12X16F7.3))
   64 FORMAT(1X10E11.4)
   65 FORMAT(1X16F8.3)
```

```
 66 FORMAT(1X8E16.8)
 67 FORMAT(5X12E10.3)
    BOLTZ=1.3805E-16
    FNIT=NNIT
    FNCOL=NCOLL
    NIT=FNIT/FNCOL+.5
    ENKE=.5*EE+ENKET/TT
    TMP=(2.*ENKE)/BOLTZ
    EKE=ENKE
    IF(NCOLL-NC7)12,12,9
  9 TTT=TT-TF
    ENKE=ENKETT/TTT
    VAR=VENK/TTT-ENKE*ENKE
    FLT=VAR/(ENKE*ENKE)
    PA=GP/TTT
    VAR=GVP/TTT-PA*PA
    FP=VAR/(PA*PA)
    PHA=GPH/TTT
    VAR=GVPH/TTT-PHA*PHA
    FPH=VAR/(PHA*PHA)
    GO TO 10
 12 P=UU+PT/TT
    PA=P
    PH=UU+(UC*PHT)/TT
    PHA=PH
    FLT=0.0
    FP=0.0
    FPH=0.0
 10 DO 13 I=1,N
 13 ENM(I,2)=ENM(I,1)/TT
    CALL KE(TNP)
    WRITE OUTPUT TAPE 3,60,NCOLL,TT,TNP,P,PH,EE,EKE,NIT
    CALL GRAPH(TMP,PA,PHA,YP,YPC,XT,XXX)
    WRITE OUTPUT TAPE 3,61,TMP,FLT,PA,FP,PHA,FPH,XT,YP,XXX,
   1YPC,INCOLN
    WRITE OUTPUT TAPE 3,62,(ENM(I,2),I=1,N)
    IND=IN-1
    WRITE OUTPUT TAPE 3,63,TE(IND),(EN(I,IND),I=1,N)
    INN=IND-1
    IF(INN)205,205,200
200 IF(NC6)205,205,202
202 WRITE OUTPUT TAPE 3,64,(TE(I),I=1,INN)
    WRITE OUTPUT TAPE 3,65,((EN(I,J),I=1,N),J=1,INN)
205 IF(NCOLL-NC0)203,203,201
201 NC0=NC0+NC1*NC5
    WRITE OUTPUT TAPE 3,66,(X(I),I=6,NN)
    WRITE OUTPUT TAPE 3,66,(XX(I),I=6,NN)
203 T1=0.0
    NIT1=0
    DO 8 I=1,N
  8 EN(I,1)=EN(I,IN)
    IN=1
    RETURN
    END
```

```
*       CARDS COLUMN
        SUBROUTINE MATRIX
        COMMON X,XX,N,NN,PN,U,WW,DLL,DA,DD,KN,NTST,W,S,EN,ENM,
       1EE,A,T,UW
D       DIMENSION X(50),XX(50),W(40),S(40),A(180),T(11),C(14),
       1D(14),UW(1)
        DIMENSION EN(40,101),ENM(40,2)
   52 FORMAT(E18.8)
D       PI2=1.570796326794897
D       PI=3.141592653589793
        UU=U
        WWW=WW
D       UW=UU/WWW
        PPN=PN+1.
D       PIN=PI2/PPN
D       PINN=PI/PPN
C       COMPUTE NORMAL FREQUENCIES W(I), AND ONLY NECESSARY
C       ELEMENTS OF TRANSFORMATION MATRIX S.
D       SQR=2.*SQRTF(UW)
D       SQRR=SQRTF(2./PPN)
        DO 1 I=1,N
        WI=I
D       W(I)=SQR*SINF(WI*PIN)
D     1 S(I)=SQRR*SINF(WI*PINN)
C       DEFINE CHEBYSHEV CONSTANT COEFFICIENTS.
D       C(1)=.9440024315364695
D       C(2)=2.552557924804532
D       C(3)=-.4994032582704071
D       C(4)=-.2852615691810360
D       C(5)=.02799207961754762
D       C(6)=.9118016006651803E-02
D       C(7)=-.5966951965488465E-03
D       C(8)=-.1365875135419667E-03
D       C(9)=.670439486991684E-05
D       C(10)=.1184961857661 69E-05
D       C(11)=-.4653229589732E-07
D       C(12)=-.670279160383E-08
D       C(13)=.21934576590E-09
D       C(14)=.2667278599E-10
C       COMPUTE COEFFICIENTS OF THE ECONOMIZED POLYNOMIALS IN X.
        DO 2 I=1,2
D       D(I+12)=2048.*C(I+12)
D       D(I+10)=-6144.*C(I+12)+512.*C(I+10)
D       D(I+8)=6912.*C(I+12)-1280.*C(I+10)+128.*C(I+8)
D       D(I+6)=-3584.*C(I+12)+1120.*C(I+10)-256.*C(I+8)+32.*C(I+6)
D       D(I+4)=840.*C(I+12)-400.*C(I+10)+160.*C(I+8)-48.*C(I+6)
       1+8.*C(I+4)
D       D(I+2)=-72.*C(I+12)+50.*C(I+10)-32.*C(I+8)+18.*C(I+6)
       1-8.*C(I+4)+2.*C(I+2)
D     2 D(I)=C(I+12)-C(I+10)+C(I+8)-C(I+6)+C(I+4)-C(I+2)+.5*C(I)
D       C(1)=D(1)
D       PP=1.
```

```
      DO 3 I=2,14
D     PP=PP*PI2
D   3 C(I)=D(I)/PP
C     EVALUATE ITERATION MATRICES A(T) FOR KN VALUES OF T INPUT.
      K=0
    4 READ INPUT TAPE 2,52,DT
      K=K+1
      J=(K-1)*18
D     T(K)=DT
D     B=UW*DT*DT
D     BB=B*B
D     A(J+1)=(((((((924.*C(13)*B+252.*C(11))*B+70.*C(9))*B+20.*
     1C(7))*B+6.*C(5))*B+2.*C(3))*B+C(1))
D     A(J+2)=-(((((792.*C(13)*B+210.*C(11))*B+56.*C(9))*B+15.*
     1C(7))*B+4.*C(5))*B+C(3))*B
D     A(J+3)=((((495.*C(13)*B+120.*C(11))*B+28.*C(9))*B+6.*
     1C(7))*B+C(5))*BB
D     A(J+4)=-(((220.*C(13)*B+45.*C(11))*B+8.*C(9))*B+C(7))*B*BB
D     A(J+5)=((66.*C(13)*B+10.*C(11))*B+C(9))*BB*BB
D     A(J+6)=-(12.*C(13)*B+C(11))*B*BB*BB
D     A(J+7)=(((((924.*C(14)*B+252.*C(12))*B+70.*C(10))*B+
     120.*C(8))*B+6.*C(6))*B+2.*C(4))*B+C(2))
D     A(J+8)=-(((((792.*C(14)*B+210.*C(12))*B+56.*C(10))*B+
     115.*C(8))*B+4.*C(6))*B+C(4))*B
D     A(J+9)=((((495.*C(14)*B+120.*C(12))*B+28.*C(10))*B+6.*
     1C(8))*B+C(6))*BB
D     A(J+10)=-(((220.*C(14)*B+45.*C(12))*B+8.*C(10))*B+C(8))
     1*B*BB
D     A(J+11)=((66.*C(14)*B+10.*C(12))*B+C(10))*BB*BB
D     A(J+12)=-(12.*C(14)*B+C(12))*B*BB*BB
D     A(J+13)=-(((((3432.*C(14)*B+924.*C(12))*B+252.*C(10))*B
     1+70.*C(8))*B+20.*C(6))*B+6.*C(4))*B+2.*C(2))*B
D     A(J+14)=(((((3003.*C(14)*B+792.*C(12))*B+210.*C(10))*B
     1+56.*C(8))*B+15.*C(6))*B+4.*C(4))*B+C(2))*B
D     A(J+15)=-(((((2002.*C(14)*B+495.*C(12))*B+120.*C(10))*B
     1+28.*C(8))*B+6.*C(6))*B+C(4))*BB
D     A(J+16)=((((1001.*C(14)*B+220.*C(12))*B+45.*C(10))*B+8.
     1*C(8))*B+C(6))*B*BB
D     A(J+17)=-(((364.*C(14)*B+66.*C(12))*B+10.*C(10))*B+C(8))
     1*BB*BB
D     A(J+18)=((91.*C(14)*B+12.*C(12))*B+C(10))*B*BB*BB
      DO 5 I=7,12
      IK=I+J
D     A(IK)=A(IK)*DT
D   5 A(IK+6)=A(IK+6)/DT
      IF(K-KN)4,6,6
C     ROUND MATRIX ELEMENTS TO EIGHT DECIMAL FIGURES.
    6 DO 8 I=1,18
      DO 8 K=1,KN
      IK=(K-1)*18+I
D     PP=10.
      B=ABSF(A(IK))
```

```
D    7 PP=.1*PP
       IF(PP-B)14,14,7
     14 IF(A(IK))15,15,16
D    15 A(IK)=A(IK)-PP*5.E-8
       GO TO 8
D    16 A(IK)=A(IK)+PP*5.E-8
     8 CONTINUE
       RETURN
       END



*      CARDS COLUMN
       SUBROUTINE COLLN
C      THE MAIN COMPUTATION TO DETERMINE WHEN COLLISIONS OCCUR.
       COMMON X,XX,N,NN,PN,U,WW,DLL,DA,DD,KN,NTST,W,S,EN,ENM,
      1EE,A,T,UW,Q,QQ,NNIT,NCOLL,NC0,NC1,NC2,NC3,NC4,NC5,NC6,
      2NC7,IN,TE,TT,TLAST,C,INCOLN,TMP,TMP1,TMP2,NCOL,TLST,
      3TF,UM,UK,UU,UC,P,PH,ENKET,VENK,PT,PHT,GP,GVP,GPH,
      4GVPH,XDOT,XXDOT,T1,NOTE
D      DIMENSION X(50),XX(50),W(40),S(40),A(180),T(11),UW(1),
      1Y(50),YY(50)
       DIMENSION EN(40,101),ENM(40,2),TE(101),Q(40,2),QQ(40,2)
    64 FORMAT(/1X14HTEMPERATURES ,3E18.8)
       DL=DLL-DD
       TAF=TLAST+T(1)-TT
       C=0.0
    16 K=3
       L=0
       IN=IN+1
       NIT=0
       T1=0.0
       GO TO 25
C      COMPUTE NEW POSITION COORDINATES BY ITERATION.
    17 KK=K-KN
       JK=(K-1)*18
       DO 20 I=6,NN
       B=0.0
       DO 32 J=1,N
       IJ=I+J-4
       IF(IJ-5)31,31,33
    31 IJ=JK+IJ
       II=J+5
    32 B=B-A(IJ)*X(II)-A(IJ+6)*XX(II)
    33 DO 35 J=1,N
       IJ=N+7+J-I
       IF(IJ-5)34,34,18
    34 IJ=JK+IJ
       II=N+6-J
    35 B=B-A(IJ)*X(II)-A(IJ+6)*XX(II)
    18 DO 19 J=1,4
       IJ=JK+6-J
```

```
      II=I+5-J
      III=I-5+J
   19 B=B+A(IJ)*(X(II)+X(III))+A(IJ+6 )*(XX(II)+XX(III))
      B=B+A(JK+1)*X(I)+A(JK+7)*XX(I)
C     CHECK COLLISION INEQUALITIES.
      IF(B-Y(I-1)+DL)6,20,20
   20 Y(I)=B
      I=NN+1
      IF(-Y(NN)+DL)6,1,1
    1 IF(L-1)2,70,4
    2 L=1
      IF(K-3)3,3,70
    3 K=2
      GO TO 25
    4 L=1
      IF(K-3)5,5,70
    5 K=1
      GO TO 17
    6 IF(KK)7,40,40
    7 K=K+1
      GO TO 17
C     COMPUTE VELOCITY COORDINATES IF NO COLLISION INDICATED.
   70 DO 78 I=6,NN
      B=0.0
      DO 72 J=1,N
      IJ=I+J-4
      IF(IJ-5)71,71,73
   71 IJ=JK+IJ
      II=J+5
   72 B=B-A(IJ+12)*X(II)-A(IJ)*XX(II)
   73 DO 75 J=1,N
      IJ=N+7+J-I
      IF(IJ-5)74,74,76
   74 IJ=JK+IJ
      II=N+6-J
   75 B=B-A(IJ+12)*X(II)-A(IJ)*XX(II)
   76 DO 77 J=1,4
      IJ=JK+6-J
      II=I+5-J
      III=I-5+J
   77 B=B+A(IJ+12)*(X(II)+X(III))+A(IJ)*(XX(II)+XX(III))
   78 YY(I)=B+A(JK+13)*X(I)+A(JK+1)*XX(I)
      DO 79 J=6,NN
      X(J)=Y(J)
   79 XX(J)=YY(J)
      TT=TT+T(K)
      T1=T1+T(K)
      NIT=NIT+1
      TAF=TAF-T(K)
      IF(K-1)28,28,21
   21 IF(KK)22,25,40
   22 K=K+1
```

```
   25 DO 27 J=K,KN
      IF(TAF-T(J))27,26,26
   26 K=J
      GO TO 17
   27 CONTINUE
      DT=TAF
      KK=-1
      GO TO 42
   28 CALL FLUCTN
      CALL AUTOCN
      C=0.0
      TAF=T(1)
      K=3
      L=2
      IF(NOTE-NC3)17,99,99
C     THE FINAL EXTRAPOLATION PROCEDURE TO DETERMINE COLLISIONS.
   40 KK=1
D     A3=X(I)-X(I-1)
D     A2=XX(I)-XX(I-1)
D     A1=(.5*(X(I+1)-X(I-2))-1.5*A3)*UW
D     A0=((XX(I+1)-XX(I-2))/6.-.5*A2)*UW
D     A3=A3+DL
      IF(I-6)46,46,47
D  46 A0=((XX(I+1)-2.*XX(I))*UW)/6.
D     A1=(.5*X(I+1)-X(I))*UW
      GO TO 49
   47 IF(I-NN)49,49,48
D  48 A0=((2.*XX(I-1)-XX(I-2))*UW)/6.
D     A1=(X(I-1)-.5*X(I-2))*UW
D  49 DT=-A3/A2
D  41 FT=((A0*DT+A1)*DT+A2)*DT+A3
D     FDT=(3.*A0*DT+2.*A1)*DT+A2
D     DDT=-FT/FDT
D     DT=DT+DDT
      IF(ABSF(DDT)-1.E-22)42,42,41
   42 K=11
      T(K)=DT
D     B=UW*DT*DT
D     A0=-B+1.
D     A1=.5*B
D     A2=(-.33333333*B+1.)*DT
D     A3=.16666667*B*DT
D     A4=((B-2.)*B)/DT
D     A5=((-.66666667*B+1.)*B)/DT
D     A6=(.16666667*B*B)/DT
      DO 43 J=6,NN
      B=X(J-1)+X(J+1)
      G=XX(J-1)+XX(J+1)
      D=X(J)
      E=XX(J)
      Y(J)=(((A1*B)+A3*G)+A0*D)+A2*E
   43 YY(J)=((((A6*(X(J-2)+X(J+2)))+A5*B)+A1*G)+A4*D)+A0*E
```

```
      YY(6)=YY(6)-A6*X(6)
      YY(NN)=YY(NN)-A6*X(NN)
      DO 44 J=6,NN
      X(J)=Y(J)
   44 XX(J)=YY(J)
      TT=TT+T(K)
      T1=T1+T(K)
      TAF=TAF-T(K)
      IF(KK)28,28,10
C     CHECK THAT NO COLLISION HAS OCCURRED FOR LARGER J.
   10 II=I+1
      NI=NN+1
      IF(II-NI)95,95,14
   95 DO 97 J=II,NI
      IF(X(J)-X(J-1)+DL)96,97,97
   96 I=J
      GO TO 40
   97 CONTINUE
C     COLLISION FOUND, ALTER VELOCITIES AND COMPUTE CONTRIBS
C     TO THE TEMPERATURE AND PRESSURE.
      IF(I-6)12,12,13
   12 XX(I)=-XX(I)
      C=C+2.*XX(I)
      INCOLN=I-5
      GO TO 15
   13 G=XX(I)
      XX(I)=XX(I-1)
      XX(I-1)=G
      C=C+XX(I)-G
      INCOLN=I-5
      GO TO 15
   14 I=NN
      XX(I)=-XX(I)
      C=C-2.*XX(I)
      INCOLN=NN-4
   15 NCOLL=NCOLL+1
      NNIT=NNIT+NIT
      TΞ(IN-1)=T1
      CALL NORMEN(IN,T1)
C     CHECK TO SEE IF OUTPUT NOW REQUIRED.
      IF(NCOLL-NCOL)16,86,86
   86 NCOL=NCOL+NC1
      CALL FLUCTN
      CALL OUTPUT
      C=0.0
C     CHECK THAT TEMPERATURE IS WITHIN A SPECIFIED RANGE.
      IF(TMP1-TMP)87,87,90
   87 IF(TMP-TMP2)88,88,90
   88 IF(NCOLL+1-NC2)16,16,99
   90 WRITE OUTPUT TAPE 3,64,TMP1,TMP2,TMP
   99 RETURN
      END
```

```
*       CARDS COLUMN
        SUBROUTINE AUTOCN
C       COMPUTES THE ESTIMATE FOR THE AUTOCORRELATION FUNCTION.
        COMMON X,XX,N,NN,PN,U,WW,DLL,DA,DD,KN,NTST,W,S,EN,ENM,
       1EE,A,T,UW,Q,QQ,NNIT,NCOLL,NC0,NC1,NC2,NC3,NC4,NC5,NC6,
       2NC7,IN,TE,TT,TLAST,C,INCOLN,TMP,TMP1,TMP2,NCOL,TLST,
       3TF,UM,UK,UU,UC,P,PH,ENKET,VENK,PT,PHT,GP,GVP,GPH,
       4GVPH,XDOT,XXDOT,T1,NOTE,NC8,NC9,NIT1,NAUTO,AC,AV,ENKETT
D       DIMENSION X(50),XX(50),W(40),S(40),A(180),T(11),UW(1)
        DIMENSION EN(40,101),ENM(40,2),TE(101),Q(40,2),QQ(40,2),
       1A(201),AC(201),ACC(201)
   60 FORMAT(/1X22HAUTOCORRELATIONS, TT =E16.8/(1X20F6.3))
   67 FORMAT(1H0/1X16HEMERGENCY EXIT, I6,
       149H ITERATIONS WITH K = 1 SINCE LAST OUTPUT. NCOLL = I5,
       21H./)
        TLAST=TT
        NIT1=NIT1+1
        DO 1 I=1,200
    1 AV(I)=AV(I+1)
        AV(201)=XX(6)
        IF(AV(1))2,6,2
    2 DO 3 I=NC8,200,NC8
    3 AC(I)=AC(I)+AV(1)*AV(I+1)
        AC(201)=AC(201)+AV(1)*AV(1)
        NIT=TT/T(1)
        IF(NIT-NAUTO)6,4,4
    4 NAUTO=NAUTO+NC9
        DO 5 I=NC8,200,NC8
    5 ACC(I)=AC(I)/AC(201)
        WRITE OUTPUT TAPE 3,60,TT,(ACC(I),I=NC8,200,NC8)
    6 IF(NIT1-NC4)9,7,7
    7 WRITE OUTPUT TAPE 3,67,NIT1,NCOLL
        NOTE=NOTE+1
        TE(IN-1)=T1
        CALL NORMEN(IN,T1)
        CALL OUTPUT
        IN=2
    9 RETURN
        END



*       CARDS COLUMN
        SUBROUTINE KE(TNP)
C       COMPUTES THE INSTANTANEOUS KE.
        COMMON X,XX,N,NN,PN,U,WW
D       DIMENSION X(50),XX(50)
        ENRGYK=0.0
        DO 1 I=6,NN
    1 ENRGYK=ENRGYK+XX(I)*XX(I)
        TNP=(WW*ENRGYK)/(PN*1.3805E-16)
        RETURN
        END
```

```
*       CARDS COLUMN
        SUBROUTINE VCRTST(DL,K)
C       CHECKS THE POSITION COORDINATES AT START OF A FIRST RUN.
        COMMON X,XX,N,NN
D       DIMENSION X(50),XX(50)
   65 FORMAT(1H2/(1X8E16.8))
   66 FORMAT(5X39HINEQUALITIES UNSATISFIED INITIALLY, I =I3,
     17H , DL = E16.8)
        DO 1 I=5,NN
        IF(X(I+1)-X(I)+DL)2,1,1
    1 CONTINUE
        K=1
        RETURN
    2 K=2
        J=I-5
        WRITE OUTPUT TAPE 3,65,(X(I),I=6,NN)
        WRITE OUTPUT TAPE 3,66,J,DL
        RETURN
        END



*       CARDS COLUMN
        SUBROUTINE XDXXD(XDOT,XXDOT)
C       QUANTITIES REQUIRED IN THE EVALUATION OF THE TMP AND PRESS
        COMMON X,XX,N,NN,PN
D       DIMENSION X(50),XX(50)
        XDOT=0.0
        XXDOT=0.0
        PPN=PN+1.0
        DO 1 I=6,NN
        SI=I-5
        XDOT=XDOT+(PPN-2.*SI)*XX(I)
    1 XXDOT=XXDOT+X(I)*XX(I)
        RETURN
        END



*       CARDS COLUMN
        FUNCTION ENERGY(X)
C       COMPUTES E/N
        COMMON X,XX,N,NN,PN,U,WW
D       DIMENSION X(50),XX(50)
        ENERGY=U*(X(6)*X(6)+X(NN)*X(NN))+WW*XX(NN)*XX(NN)
        IF(NN-6)3,3,1
    1 IN=NN-1
        DO 2 I=6,IN
    2 ENERGY=ENERGY+U*(X(I+1)-X(I))*(X(I+1)-X(I))+WW*XX(I)*XX(I)
    3 ENERGY=(.5*ENERGY)/PN
        RETURN
        END
```

```
*       CARDS COLUMN
        SUBROUTINE FLUCTN
C       COMPUTES THE TEMPERATURE AND PRESSURE, AND THEIR FLUCS.
        COMMON X,XX,N,NN,PN,U,WW,DLL,DA,DD,KN,NTST,W,S,EN,ENM,
       1EE,A,T,UW,Q,QQ,NNIT,NCOLL,NC0,NC1,NC2,NC3,NC4,NC5,NC6,
       2NC7,IN,TE,TT,TLAST,C,INCOLN,TMP,TMP1,TMP2,NCOL,TLST,
       3TF,UM,UK,UU,UC,P,PH,ENKET,VENK,PT,PHT,GP,GVP,GPH,
       4GVPH,XDOT,XXDOT,T1,NOTE,NC8,NC9,NIT1,NAUTO,AC,AV,ENKETT
D       DIMENSION X(50),XX(50),W(40),S(40),A(180),T(11),UW(1)
        DIMENSION EN(40,101),ENM(40,2),TE(101),Q(40,2),QQ(40,2),
       1AV(201),AC(201)
        TTT=TT-TLST
        TLST=TT
        EE=ENERGY(X)
        PH=-XDOT
        ENKE=-XXDOT
        CALL XDXXD(XDOT,XXDOT)
        ENKE=UK*(ENKE+XXDOT)+UM*C
        PH=0.5*(PH+XDOT)
        P=UC*(PH+C)
        ENKET=ENKET+ENKE
        PT=PT+P
        PHT=PHT+PH
        IF(NCOLL-NC7)3,1,2
    1   TF=TT
        GO TO 3
    2   ENKE=(0.5*EE+ENKE/TTT)*1.E+20
        ENKETT=ENKETT+ENKE*TTT
        VENK=VENK+ENKE*ENKE*TTT
        P=UU+PT/TT
        GP=GP+P*TTT
        GVP=GVP+P*P*TTT
        PH=UU+(UC*PHT)/TT
        GPH=GPH+PH*TTT
        C/PH=GVPH+PH*PH*TTT
    3   RETURN
        END



*       CARDS COLUMN
        SUBROUTINE GRAPH(TMP,P,PH,YP,YPC,XT,XXX)
C       COMPUTES QUANTITIES RELATED TO THE EQUATION OF STATE.
        COMMON X,XX,N,NN,PN,U,WW,DLL,DA,DD
D       DIMENSION X(50),XX(50)
        BOLTZ=1.3805E-16
        ROOTP2=1.2533141
        ROOT2=1.4142136
        UK=U*BOLTZ
        UAD=U*(DA-DD)
        ULD=U*(DLL-DD)
        RTUKT=SQRTF(UK*TMP)
        FCT=1./RTUKT
```

```
      YP=(P-UAD)*FCT
      YPC=(P-PH)*FCT
      XT=ULD*FCT
      YYY=YP/ROOT2
      ERFN=ERRF(YYY)
      ZZZ=ROOTP2*(1.-ERFN)*EXPF(YYY*YYY)
      IF(YYY)88,89,89
   88 ZZZ=2.*ROOTP2*EXPF(YYY*YYY)-ZZZ
   89 XXX=(XT+YP)*ZZZ
      RETURN
      END



*     CARDS COLUMN
      SUBROUTINE NORMEN(IN,T1)
C     COMPUTES NORMAL MODE ENERGIES, AND THEIR TIME AVERAGES.
      COMMON X,XX,N,NN,PN,U,WW,DLL,DA,DD,KN,NTST,W,S,EN,ENM,
     1EE,A,T,UW,Q,QQ
D     DIMENSION X(50),XX(50),W(40),S(40),A(180),T(11),UW(1)
      DIMENSION EN(40,101),ENM(40,2),Q(40,2),QQ(40,2)
      EE=ENERGY(X)
      FCT=(50.*WW)/(PN*EE)
      DO 5 I=1,N
      D1=0.0
      D2=0.0
      DO 4 J=6,NN
      IJ=I*(J-5)
      SS=1.
    1 JJ=IJ-N-1
      IF(JJ)3,4,2
    2 IJ=JJ
      SS=-SS
      GO TO 1
    3 SS=SS*S(IJ)
      D1=D1+SS*X(J)
      D2=D2+SS*XX(J)
    4 CONTINUE
      Q(I,1)=Q(I,2)
      Q(I,2)=D1
      QQ(I,1)=QQ(I,2)
      QQ(I,2)=D2
      EN(I,IN)=FCT*(W(I)*W(I)*D1*D1+D2*D2)
    5 ENM(I,1)=ENM(I,1)+EN(I,IN-1)*T1
      RETURN
      END
```

A sample of the numerical results obtained during the computations

```
NCOL 500,TT= 0.21567E-09SEC,TMP=  23.67,P= 0.54969E-07DYNE,PH= -0.20746E-07,E/N= 0.399929E-14ERGS,KE/N= 0.211298E-14,ITN/COLN= 14
TMP=  30.61,FL= 0.0458,PA= 0.41775E-07,FL= 0.1306,PHA= -0.20022E-07,FL= 0.0324,X= 1.846,Y= -1.798,R=  0.578,YPC= 0.048,COLLN J= 15
  28.934   5.279   3.466   4.429   4.170   4.779   4.029   4.019   4.290   4.619   4.331   4.980   4.813   5.951   6.362   5.552
 0.9688E-12  3.405 10.310  6.374  1.917  7.251  2.363  0.301  8.918  6.790  6.517 15.481  0.023  6.798  5.289  9.648  8.614

 0.79027084E-08  0.42378733E-08  0.44301339E-08  0.61337679E-08  0.44745839E-08  0.40747233E-08  0.43485099E-08  0.12818058E-08
-0.26653715E-09 -0.43180653E-09 -0.33769759E-08 -0.51046598E-08 -0.51011089E-08  0.13048385E-09 -0.58695161E-08 -0.16381735E-08
-0.17574807E 05 -0.11523236E 05  0.21169861E 04 -0.10974638E 05 -0.81485207E 04  0.34277651E 04 -0.10118859E 05  0.19817955E 04
-0.13355014E 05  0.10497471E 05  0.48236094E 04  0.94607025E 04 -0.17586083E 05 -0.99757252E 04 -0.10367221E 04 -0.13425917E 05

NCOL 505,TT= 0.21728E-09SEC,TMP=  29.97,P= 0.57270E-07DYNE,PH= -0.19107E-07,E/N= 0.399929E-14ERGS,KE/N= 0.211445E-14,ITN/COLN= 14
TMP=  30.63,FL= 0.0458,PA= 0.41891E-07,FL= 0.1294,PHA= -0.20042E-07,FL= 0.0321,X= 1.845,Y= -1.798,R=  0.579,YPC= 0.048,COLLN J=  2
  28.745   5.300   3.485   4.405   4.184   4.765   4.009   4.045   4.316   4.629   4.424   4.961   4.844   5.964   6.365   5.562
 0.5624E-13  4.105  3.011  0.851  1.375  9.387  1.001  2.736  2.702  7.695 18.873 13.114 12.499  9.675 11.005  0.081  1.891


AUTOCORRELATIONS, TT =  0.22004691E-09
 0.924 0.781 0.600 0.389 0.171-0.035-0.214-0.360-0.459-0.510-0.512-0.472-0.399-0.303-0.197-0.094-0.005 0.067 0.116 0.142
 0.146 0.133 0.107 0.071 0.034 0.001-0.026-0.042-0.047-0.041-0.027-0.009 0.010 0.028 0.043 0.051 0.053 0.047 0.035 0.019
 0.001-0.015-0.028-0.035-0.037-0.032-0.021-0.005 0.013 0.030 0.044 0.053 0.055 0.050 0.039 0.021-0.001-0.024-0.046-0.065
-0.080-0.089-0.090-0.085-0.074-0.058-0.040-0.021-0.002 0.014 0.027 0.034 0.036 0.034 0.027 0.017 0.005-0.007-0.018-0.029
-0.037-0.043-0.047-0.051-0.054-0.053-0.051-0.042-0.032-0.021-0.010-0.001 0.007 0.013 0.016 0.018 0.016 0.012 0.005-0.003
-0.012-0.020-0.026-0.031-0.033-0.033-0.031-0.027-0.021-0.014-0.006 0.002 0.008 0.011 0.007 0.001-0.008-0.020-0.035-0.047
-0.056-0.061-0.060-0.054-0.043-0.029-0.012 0.004 0.016 0.024 0.026 0.023 0.015 0.003-0.011-0.026-0.040-0.052-0.058-0.057
-0.049-0.036-0.017 0.002 0.024 0.046 0.065 0.082 0.094 0.097 0.090 0.073 0.050 0.020-0.008-0.036-0.065-0.088-0.101-0.101
-0.092-0.072-0.044-0.010 0.025 0.060 0.088 0.107 0.113 0.107 0.090 0.066 0.036 0.006-0.019-0.038-0.047-0.043-0.029-0.009
 0.019 0.050 0.083 0.115 0.143 0.164 0.174 0.175 0.168 0.153 0.131 0.103 0.071 0.035-0.004-0.039-0.069-0.094-0.113-0.123

NCOL 510,TT= 0.22005E-09SEC,TMP=  23.57,P= 0.56199E-07DYNE,PH= -0.20090E-07,E/N= 0.399928E-14ERGS,KE/N= 0.211412E-14,ITN/COLN= 14
TMP=  30.63,FL= 0.0457,PA= 0.42142E-07,FL= 0.1279,PHA= -0.20028E-07,FL= 0.0317,X= 1.845,Y= -1.798,R=  0.581,YPC= 0.048,COLLN J= 14
  28.435   5.285   3.456   4.429   4.236   4.723   4.010   3.999   4.298   4.664   4.483   5.141   4.972   5.940   6.389   5.541
 0.3873E-12  3.966  4.866  2.313  6.279  7.521  3.814  3.946  0.438  6.420  6.366  9.906 21.046  6.484  6.938  1.667  8.031


NCOL 515,TT= 0.22189E-09SEC,TMP=  30.97,P= 0.57619E-07DYNE,PH= -0.18766E-07,E/N= 0.399927E-14ERGS,KE/N= 0.211479E-14,ITN/COLN= 14
TMP=  30.64,FL= 0.0455,PA= 0.42278E-07,FL= 0.1267,PHA= -0.20043E-07,FL= 0.0314,X= 1.845,Y= -1.797,R=  0.582,YPC= 0.048,COLLN J= 14
  28.226   5.285   3.467   4.435   4.273   4.693   3.995   3.979   4.307   4.715   4.542   5.215   4.986   5.915   6.353   5.614
 0.3183E-12  2.267  5.267  7.078  5.607  7.437  0.420  0.316  2.397  6.240 17.071 16.814  5.983  4.568  2.141  1.273 15.121


NCOL 520,TT= 0.22284E-09SEC,TMP=  20.27,P= 0.58224E-07DYNE,PH= -0.18318E-07,E/N= 0.399927E-14ERGS,KE/N= 0.211511E-14,ITN/COLN= 14
TMP=  30.64,FL= 0.0456,PA= 0.42369E-07,FL= 0.1263,PHA= -0.20031E-07,FL= 0.0313,X= 1.845,Y= -1.797,R=  0.582,YPC= 0.048,COLLN J= 14
  28.114   5.288   3.476   4.426   4.313   4.682   3.981   3.973   4.300   4.745   4.580   5.211   5.017   5.894   6.356   5.646
 0.2692E-12  1.854  6.381  5.420  1.963 13.920  1.652  1.238  3.974  1.692 10.586 14.307  2.264 10.889  1.028  3.320 19.514


NCOL 525,TT= 0.22424E-09SEC,TMP=  22.53,P= 0.56190E-07DYNE,PH= -0.20435E-07,E/N= 0.399926E-14ERGS,KE/N= 0.211493E-14,ITN/COLN= 14
TMP=  30.64,FL= 0.0458,PA= 0.42488E-07,FL= 0.1255,PHA= -0.20027E-07,FL= 0.0311,X= 1.845,Y= -1.797,R=  0.583,YPC= 0.048,COLLN J= 16
  27.950   5.294   3.484   4.405   4.361   4.678   3.973   3.978   4.306   4.780   4.617   5.186   5.087   5.872   6.338   5.692
 0.1881E-12  1.888  6.097  4.195  0.084 12.668  5.933  4.457  4.293  7.791  8.150 10.128  0.613 21.161  1.180  3.068  8.293


NCOL 530,TT= 0.22573E-09SEC,TMP=  26.22,P= 0.56665E-07DYNE,PH= -0.20361E-07,E/N= 0.399925E-14ERGS,KE/N= 0.211591E-14,ITN/COLN= 14
TMP=  30.65,FL= 0.0456,PA= 0.42598E-07,FL= 0.1246,PHA= -0.20038E-07,FL= 0.0308,X= 1.845,Y= -1.797,R=  0.584,YPC= 0.048,COLLN J=  4
  27.777   5.291   3.500   4.379   4.406   4.679   3.977   3.969   4.310   4.824   4.625   5.181   5.222   5.851   6.328   5.683
 0.3492E-12  0.497  2.557  6.675  1.129 12.110  4.424  1.371  0.281  7.829 21.294  0.421  8.147 22.520  0.769  6.052  3.923
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