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**Energy Penetration into Harmonic and
Anharmonic Disordered Lattices**

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ENERGY PENETRATION INTO HARMONIC AND
ANHARMONIC DISORDERED LATTICES

by

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ABSTRACT

A discussion is given of a computer-generated film which gives a direct graphical representation of the penetration of an energy wave into two-dimensional isotopically disordered lattices. The blockage of energy flow due to low concentrations of light impurities in a host lattice is contrasted with that due to like arrangements of heavy impurities. Similarly, the differences between energy flow into harmonic and anharmonic lattices are considered. The film demonstrates that energy flows more easily through a disordered anharmonic lattice than through an equivalent harmonic lattice and that it is less impeded by light impurities than by heavy ones.

INTRODUCTION

In the course of an investigation of the thermal conductivity of disordered harmonic and anharmonic lattices,¹ we decided that a better understanding of the nature of the energy flow could be obtained by graphically following the propagation of an energy pulse through a lattice. The accompanying film is the development of a technique for direct observation of the lattice motion.

The film contains a number of examples of energy flowing in a two-dimensional square lattice which is 10 atoms wide and 50 atoms long. In every case the lattice is excited from rest by giving an identical impulse to each of the 10 atoms at one

end. The propagation of this energy pulse down the lattice has been followed by numerical integration of the equations of motion for the system. The results are displayed in three-dimensional plots of the energy of the atoms of the array at successive times. The individual frames were obtained from the direct computer output to a SC-4020 plotter.

The film sequences have been arranged to contrast the energy propagation through a region of randomly distributed light impurities with propagation through a heavy impurity region and to show the changes which occur when anharmonic interatomic forces are added to the harmonic lattice. The first two sequences show propagation in monatomic harmonic and anharmonic lattices. These are

followed by situations in which a single light or heavy impurity has been placed one-third of the distance down the lattice. In the remaining sequences, the first one-third of the lattice is monatomic with the following two-thirds containing low concentrations of randomly distributed light or heavy impurities. Results are shown for harmonic and anharmonic lattices with 5 and 15% impurity concentrations.

The first section of this report discusses briefly the equations of motion of the square lattice used in generating the film and the method of calculation employed for their solution. The second section contains a detailed discussion of the film's individual sequences. The Fortran computer code used in making the film is given in the appendix.

THE LATTICE EQUATIONS

The lattice model used in making the film is illustrated in Fig. 1. It consists of a 10 X 50 array of atoms that interact through nearest-neighbor central and noncentral forces. Rigid boundary conditions were used at both ends of the long axis, and periodic boundary conditions were used in the short direction. Displacements of atoms from equilibrium satisfy the relations

$$\begin{aligned} x_{0,j} = y_{0,j} = 0, \quad x_{51,j} = y_{51,j} = 0, \\ j = 1, 2, \dots, 10, \\ x_{i,1} = x_{i,11}, \quad y_{i,1} = y_{i,11}, \\ i = 1, 2, \dots, 50, \end{aligned} \quad (1)$$

where x and y are coordinates relative to the long and short axes, respectively, and the subscripts

Fig. 1. Representation of the binary disordered square lattice model used in making the film. Periodic boundary conditions are used in the j direction.

specify the individual atoms. The lattice can be considered to be cylindrical.

The equations of motion for the lattice atoms are

$$\begin{aligned} m_{1j} \frac{d^2 x_{1j}}{dt^2} &= - \frac{d\Phi}{dx_{1j}}, \quad i = 1, \dots, 50, \\ m_{1j} \frac{d^2 x_{1j}}{dt^2} &= - \frac{d\Phi}{dy_{1j}}, \quad j = 1, \dots, 10. \end{aligned} \quad (2)$$

To decouple the x motion from that in the y direction, it has been assumed that the potential Φ is the sum of two terms

$$\Phi = \Phi_x + \Phi_y, \quad (3)$$

where Φ_x is a function of the x_{ij} displacements only and Φ_y depends only on the y_{ij} displacements. In the film, just the x motions of the lattice were excited. The y motions are identical and independent.

The potential Φ_x is a sum of nearest-neighbor interactions

$$\begin{aligned} \Phi_x &= \sum_{i,j} V_c(x_{1j} - x_{i-1,j}) \\ &+ \sum_{i,j} V_{nc}(x_{1j} - x_{i,j-1}). \end{aligned} \quad (4)$$

The central and noncentral terms V_c and V_{nc} relate to interactions parallel and transverse to the line between equilibrium points of a pair of atoms. The functional forms of V_c and V_{nc} have been taken to be equal. They were obtained from an expansion of a Lennard-Jones potential about the equilibrium spacing r_0 to fourth-order

$$\begin{aligned} V(r) &= \epsilon_0 \left[(r_0/r)^{12} - 2(r_0/r)^6 \right] \\ &\approx -\epsilon_0 + \frac{1}{2} \gamma (r-r_0)^2 - \frac{1}{3} \mu (r-r_0)^3 + \frac{1}{4} \nu (r-r_0)^4. \end{aligned} \quad (5)$$

The magnitudes of μ and ν relative to γ were taken appropriate to noble gas solids for the anharmonic lattice films and were set equal to zero for the harmonic cases. With arbitrary units such that $\gamma = 1$, the potentials used are

$$V_c(x) = \frac{1}{2} x^2 - \frac{1}{3} \mu x^3 + \frac{1}{4} v x^4 \quad (6)$$

with

$$\begin{aligned} \mu = 0.0 \quad v = 0.0 \quad & \text{harmonic} \\ \mu = 0.35 \quad v = 0.069 \quad & \text{anharmonic.} \end{aligned} \quad (7)$$

The equations of motion take on the explicit form

$$\begin{aligned} m_{ij} \frac{d^2 x_{ij}}{dt^2} = & \sum_{\lambda=-1}^1 \left[(x_{ij} - x_{i+\lambda, j}) \right. \\ & \left. - \lambda \mu (x_{ij} - x_{i+\lambda, j})^2 + v (x_{ij} - x_{i+\lambda, j})^3 \right] \\ & + \sum_{\lambda=-1}^1 \left[(x_{ij} - x_{i, j+\lambda}) \right. \\ & \left. - \lambda \mu (x_{ij} - x_{i, j+\lambda})^2 + v (x_{ij} - x_{i, j+\lambda})^3 \right]. \end{aligned} \quad (8)$$

Different methods of numerical integration of the equations of motion were used depending on whether the anharmonic forces were included. A simple iterative procedure was used in the harmonic case. This consisted of rewriting Eq. (8) as a pair of first-order difference equations

$$\begin{aligned} \frac{dv_{ij}}{dt} & \rightarrow \frac{v_{ij}(t+\Delta t) - v_{ij}(t)}{\Delta t} \\ & = - \left\{ \sum_{\lambda=-1}^1 \left[(x_{ij} - x_{i+\lambda, j}) - \lambda \mu (x_{ij} - x_{i+\lambda, j})^2 \right. \right. \\ & \quad \left. \left. + v (x_{ij} - x_{i+\lambda, j})^3 \right] \right. \\ & \quad \left. + \sum_{\lambda=-1}^1 \left[(x_{ij} - x_{i, j+\lambda}) - \lambda \mu (x_{ij} - x_{i, j+\lambda})^2 \right. \right. \\ & \quad \left. \left. + v (x_{ij} - x_{i, j+\lambda})^3 \right] \right\}, \end{aligned} \quad (9)$$

$$\frac{dx_{ij}}{dt} \rightarrow \frac{x_{ij}(t+\Delta t) - x_{ij}(t)}{\Delta t} = \frac{1}{2} v_{ij}(t) + v_{ij}(t+\Delta t). \quad (10)$$

The displacements on the right-hand side of Eq. (9) are assumed to refer to time $t + \frac{1}{2}\Delta t$, and to be defined by

$$x_{ij}(t + \frac{1}{2}\Delta t) \equiv \frac{1}{2} [x_{ij}(t) + x_{ij}(t + \Delta t)]. \quad (11)$$

Taking an initial guess of

$$x_{ij}(t + \Delta t) = x_{ij}(t) + \Delta t v_{ij}(t),$$

new values of the velocities at time $t + \Delta t$ can be obtained from Eq. (9), followed by new displacements using Eq. (10). The procedure gives convergence in two or three iterations for a sufficiently small time step. Convergence was determined by the requirement that no displacement shall change by more than 10^{-6} from one iteration to the next. This method required relatively small amounts of computer time. The total energy within the lattice remained constant to one part in 10^6 throughout a calculation, which served as a check on the overall accuracy of the calculation.

This iterative method was unstable when the anharmonic terms were included. A fourth-order Runge-Kutta integration scheme² was used in that case.

DISCUSSION OF THE FILM SEQUENCES

In the film, the atoms of the host lattice were assigned a mass of three. The light and heavy impurities were given masses of one and nine, respectively; the impurity sites are identical in corresponding cases. The initial energy pulse has kinetic energy per atom corresponding to a temperature of about 7° K, and the motion through the first one-third of the lattice is unperturbed in each case. The temperature of the wave front just before striking the impurity region is on the order of 1° . Even at this low temperature, the anharmonic forces are about 10% of the harmonic forces for the interaction used.

Figures 2 through 5, consisting of actual frames selected from the film sequences, illustrate the energy penetrations.

Sequences 1 and 2: Energy Wave

The first sequence shows propagation of an energy pulse through a monatomic harmonic lattice (Fig. 2a). The initial pulse diminishes in amplitude as it moves and is followed by a trail of lesser waves as it deposits energy in the lattice. The pulse builds up again during reflection due to the pileup of energy at the rigid boundary during this process.

Fig. 2. Comparison of the energy waves at equal times in monatomic lattices: (a) harmonic (b) anharmonic.

The second sequence gives a comparison with propagation in a monatomic anharmonic lattice. The principal differences are that the anharmonic wave front is noticeably sharper than the harmonic wave front and that its speed is greater. Figure 2 compares the harmonic and anharmonic energy pulses at equal times with the wave front about two-thirds of the way down the lattice.

Sequences 3 and 4: Single Light Impurity

The third and fourth sequences show monatomic harmonic and anharmonic lattices with a single light impurity placed one-third of the way down the lattice. As shown in Fig. 3a, an indentation appears in the wave front as it passes over the light impurity, indicating that little energy has been transferred to this atom. In these cases the principal mode of excitation of the light impurity is a localized vibrational mode whose amplitude dies off exponentially with distance from the impurity. The initial impulse to the lattice leaves the localized mode practically unexcited, so that the light atom takes almost no part in the general oscillation of the lattice.

Sequences 5 and 6: Single Heavy Impurity

The opposite extreme, a single heavy impurity in an otherwise monatomic lattice, is shown in sequences five and six for harmonic and anharmonic forces, respectively. As shown in Fig. 3b, a sharp spike appears in the energy wave as it crosses the heavy atom. The normal mode decomposition of the heavy atom motion is sharply peaked near the low energy end of the phonon spectrum, and within this narrow frequency range the modes act coherently to give the heavy impurity a large energy. The initial impulse populates all the available normal

Fig. 3. (a) the dip occurring in the energy wave as it passes over a light impurity, and (b) the spike resulting from encounter with a heavy impurity.

modes well, and, since a band of these modes involves large motions of the heavy impurity, a substantial amount of energy can be transferred to this atom when the pulse arrives at its location.

Sequences 7, 8, 9, and 10: 5% Light and Heavy Impurities

The remaining film sequences show results with randomly distributed impurities in the second two-thirds of the lattice: the seventh and eighth illustrate energy penetration into a region containing 5% light impurities for harmonic and anharmonic interaction, respectively; the ninth and tenth give the corresponding results with 5% heavy impurities. Dips are visible in the successive waves as they cross the light impurity sites, while energy spikes occur at the heavy impurity sites. The energy wave can be seen to penetrate more easily into a region of light impurities than into one of heavy defects, as shown for the 15% impurity regions in Fig. 4. The primary point of these sequences is that the energy penetrates into the impurity region more easily when anharmonic forces are present than in the corresponding harmonic cases. This fact supports the observation made previously by the

Fig. 4. Equal time comparison of energy penetration into (a) a harmonic lattice containing 15% heavy impurities with that into (b) a 15% light impurity region. Impurity sites are identical in the two pictures.

authors¹ that the thermal conductivity in a disordered anharmonic lattice is generally greater than in a similar harmonic lattice. In general, anharmonicity increases the energy flow into the disordered region by allowing the high frequency harmonic normal modes--which tend to be localized, and so transport little energy-- to decay into low frequency energy-carrying modes.

Sequences 11, 12, 13, and 14: 15% Light and Heavy Impurities

Film sequences eleven through fourteen are equivalent to sequences 7 through 10, respectively, except that the impurity concentration has been raised to 15%. The energy penetration into the region of disorder is much slower than at the lower impurity concentration in the pure harmonic cases. For heavy impurities, one sees little more than the energy spikes at the impurity sites. The effect of anharmonicity in increasing the energy flow is more noticeable than at the lower impurity concentration. Otherwise, the comments about the 5% impurity cases apply here also. Figure 5 gives a comparison of the energy flow into the disordered heavy impurity region with and without anharmonic forces.

Fig. 5. Comparison at equal times of the energy penetration into a region of 15% heavy impurities for (a) an anharmonic lattice and (b) a harmonic lattice.

REFERENCES

1. D. N. Payton, III, M. Rich, and W. M. Visscher, Phys. Rev. 160, 706 (1967).
2. Fr. A. Willers, Practical Analysis, Dover Publications, Inc., New York, 1948, p. 378.

APPENDIX

The following pages contain a listing of the Fortran IV computer code used to make the film discussed in this report. This program is a modification of a code used for the calculation of lattice thermal conductivities by means of numerical experiments. As such, the program contains a number of parts extraneous to its film-making capability. The integration method given in the listing is the Runge-Kutta; the iteration procedure noted in the text is not shown.

The input data required by the program is as follows:

ISTAR	=	0
IPIC	=	1
PL	=	mass of the impurity atoms
PM	=	mass of the host lattice atoms
FA	=	concentration of impurity atoms of mass PL
SI	=	$\begin{cases} 0 & \text{impurity atoms disordered} \\ 1 & \text{ordered diatomic lattice} \end{cases}$
MRL	=	0.0
MRR	=	0.0
DT	=	time step for integration of the equations of motion (~ 0.05)
PROBL	=	0.0
PROBR	=	0.0
UBARL	=	0.0
UBARR	=	0.0
N	=	width of the lattice + 2
M	=	length of the lattice
JR	=	arbitrary origin of random number sequence
NDP	=	1, number of integration steps between plots
MSTOP	=	total number of integration steps to be run
CC	=	μ , the cubic anharmonic constant
CQ	=	ν , the quartic anharmonic constant

In addition, a number of Los Alamos film plotting routines, called for in the main body of the code, would be needed to operate this program.


```

C      PROGRAM SQUAR(INPUT,OUTPUT,FILM,TAPE,2=FILM,TAPE5)
C
C      SQUAR IS A PROGRAM TO PRODUCE TIME STUDIES OF A SQUARE LATTICE
C      BY PRODUCING A SEQUENCE OF TIME RELATED PLOTS OF INTERESTING
C      QUANTITIES ON A SC4020 PLOTTER
C
C      THE SQUARE LATTICE IS COMPOSED OF AN ARRAY OF NXM ATOMS OF MASSES
C      PM AND PL WITH A CONCENTRATION OF THE PL ATOMS BEING FA. THE
C      DEGREE OF ORDERING OF THESE ATOMS IS GIVEN BY SI(SI=0, DISORDER
C      AND SI=1, ORDERED DIATOMIC). THE ENDS OF THE LATTICE IN THE M
C      DIRECTION ARE ATTACHED TO RIGID WALLS AND CAN BE IN CONTACT WITH
C      THERMAL RESERVOIRS. PROBL AND PROBR ARE THE PROBABILITIES OF
C      COLLISION WITH THE RESERVOIR ATOMS( PROBL=0 MEANS NO INTERACTION).
C      MRL AND MRR ARE THE MASSES OF THE RESERVOIR ATOMS, AND UBARL AND
C      UBARR ARE THE RMS VELOCITIES OF THE ATOMS IN THE RESERVOIRS. THE
C      BOUNDARIES IN THE N DIRECTION ARE CYCLIC. JR IS A RANDOM START
C      VARIABLE. NDP AND NSTOP ARE THE NUMBER OF CYCLES BETWEEN PLOTS
C      AND TOTAL NUMBER OF CYCLES TO BE RUN, RESPECTIVELY. DT IS THE
C      TIME STEP. IPIC ALLOWS ONLY PRINTOUT DATA TO BE OBTAINED.
C
C      DIMENSION MASS(12,50), VI(12,50), X(12,50), E(500,5), ER(1000), EL
1      1(1000), ECH(1000), TIME(1000), DX(1000), XI(12,50), XF(12,50), ENG
2      2(1000), DY(100), VT(100), VP(100), VE(100), A1(200), A2(401), XA(4
3      301), D(200), Y(12,100), YP(12,100), YPA(12,100), YPB(12,100), YPC(
4      412,100), TEMP(12,100)
5      REAL MASS,MRL,MRR,MU,KEL,KER
6      COMMON PL,PM,FA,SI,MRL,MRR,DT,JR,PROBL,PROBR,UBARR,UBARL,TMAX,NCYC
7      COMMON IONE
8      EXTERNAL KICK
9      I1=272
10
11      THIS PROGRAM IS EQUIPPED WITH A RESTART CAPABILITY TO GUARD
12      AGAINST MACHINE INTERRUPTS.
13
14      READ 46, ISTAR,IPIC
15      IF (ISTAR.EQ.1) GO TO 44
16      READ 47, PL,PM,FA,SI,MRL,MRR,DT,PROBL,PROBR,UBARL,UBARR,N,M,JR,NDP
17      1,NSTOP,CC,CQ
18      MN=M*M
19      NN=N
20      NCYC=0
21      IC=0
22      NP=1
23      I1=1
24      MN=M*NN
25      IONE=1
26      ERROR=1.E-06
27      NC=N/2+1
28      NP1=N+1
29      DT2=.25*DT**2
30      NM1=N-1
31
32      GENERATE THE MASSES IN THE ARRAY.
33
34      CALL CHAGEN (MN,PL,PM,FA,JR,SI,MASS)
35      DO 1 J=1,M
36      MASS(1,J)=MASS(NM1,J)
37      MASS(N,J)=MASS(2,J)
38      UBAR=0.5*(UBARL**2+UBARR**2)
39      UBAR=SQRT(UBAR)
40
41      GENERATE THE INITIAL DISPLACEMENTS AND VELOCITIES OF THE LATTICE.
42
43      CALL INIT (VI,X,MN,MASS,N)
44      DO 2 J=1,M
45      VI(1,J)=VI(NM1,J)
46      X(1,J)=X(NM1,J)
47      VI(N,J)=VI(2,J)
48      X(N,J)=X(2,J)
49      EL(1)=0.
50      ER(1)=0.

```

	ENG(1)=1.	72
	TIME(1)=0.	73
	ECH(1)=0.	74
C		75
C	CALCULATE THE INITIAL ENERGY CONTAINED IN THE CHAIN	76
C		77
	DO 3 I=2,NM1	78
	DO 3 J=2,M	79
3	ECH(1)=ECH(1)+0.5*MASS(I,J)*VI(I,J)**2+.5*(X(I,J)-X(I-1,J))**2+.5*	80
	1(X(I,J)-X(I,J-1))**2+CC*((X(I,J)-X(I-1,J))**3+(X(I,J)-X(I,J-1))**3	81
	2)/3.0+CQ*((X(I,J)-X(I-1,J))**4+(X(I,J)-X(I,J-1))**4)/4.0	82
	DO 4 I=2,NM1	83
4	ECH(1)=ECH(1)+.5*MASS(I,1)*VI(I,1)**2+.5*(X(I,1)-X(I-1,1))**2+.5*X	84
	1(I,1)**2+CC*((X(I,1)-X(I-1,1))**3+X(I,1)**3)/3.0+CQ*((X(I,1)-X(I-1	85
	2,1))**4+X(I,1)**4)/4.0	86
	DO 5 I=2,NM1	87
5	ECH(1)=ECH(1)+.5*X(I,M)**2-CC*X(I,M)**3/3.0+CQ*X(I,M)**4/4.0	88
	ELL=0.	89
	ERR=0.	90
	DO 6 I=1,M	91
	VI(I)=0.	92
6	VP(I)=0.	93
	DO 7 I=2,1000	94
7	ECH(I)=0.	95
8	JMAX=20	96
	CC=-.35	
	CQ=.07	
	DT=.05	
	ESTAR=ECH(1)	97
	DO 9 JJ=1,200	98
9	D(JJ)=JJ	99
	ITWO=1	100
	IONE=1	101
	VMAX=1.5*AMAX1(UBARL,UBARR)	102
	ERROR=1.E-06	103
	NC=N/2+1	104
	NM1=N-1	105
	DT2=.25*DT**2	106
	MN2=M*(N-2)	107
	NM2=N-2	108
	MM1=M-1	109
	NM4=N-4	110
	DO 10 J=1,5	111
	DO 10 I=1,MN2	112
10	E(I,J)=0.	113
	DO 11 I=1,M	114
11	DX(I)=I-1	115
	DO 12 I=1,N	116
12	DY(I)=I-1	117
	KEL=.5*MRL*UBARL**2	118
	KER=.5*MRR*UBARR**2	119
	TMAX=1.25*AMAX1(KEL,KER)	120
	IF (TMAX.EQ.0.) TMAX=1.0	
	PRINT 48	122
	PRINT 49	123
	PRINT 50	124
	PRINT 52, PL,PM,FA,SI,MRL,MRR,DT,N,M,JR,PROBL,PROBR,UBARL,UBARR	125
	PRINT 51, CC,CQ	126
	PRINT 53, (I,I=1,10)	127
	DO 13 J=1,M	128
	PRINT 54, J,(MASS(I,J),I=2,NM1)	129
13	CONTINUE	130
C		131
C	BEGIN THE MAIN ITERATION LOOP.	132
C		133
14	IPP=1	134
15	NCYC=NCYC+1	135
C		136
C	TREAT THE COLLISIONS WITH THE RESERVOIRS, IF ANY.	137
C		138

	DO 16 I=2,NM1	139
	P=RANDOM(T)	140
	IF (PROBL.LT.P) GO TO 16	141
	CALL KICK (IONE,UBARL,UZERU)	142
	CALL IMP (I,1,VI,UZERO,MRL,N,M,MASS,ELL)	143
16	CONTINUE	144
	DO 17 I=2,NM1	145
	P=RANDOM(T)	146
	IF (PROBR.LT.P) GO TO 17	147
	CALL KICK (IONE,UBARR,UZERU)	148
	CALL IMP (I,M,VI,UZERO,MRR,N,M,MASS,ERR)	149
17	CONTINUE	150
C		151
C	DO THE RUNGE-KUTTA INTEGRATION OF THE EQUATIONS OF MOTION TO	152
C	ADVANCE THE TIME.	153
C		154
	DO 18 J=1,M	155
	DO 18 I=1,N	156
	K=J+M	157
	Y(I,J)=X(I,J)	158
18	Y(I,K)=V1(I,J)	159
	CALL ZVR (N,M,DT,CC,CQ,Y,YP,MASS)	160
	DO 19 J=1,MM	161
	DO 19 I=1,N	162
19	TEMP(I,J)=Y(I,J)+0.5*YP(I,J)	163
	CALL ZVR (N,M,DT,CC,CQ,TEMP,YPA,MASS)	164
	DO 20 J=1,MM	165
	DO 20 I=1,N	166
20	TEMP(I,J)=Y(I,J)+0.5*YPA(I,J)	167
	CALL ZVR (N,M,DT,CC,CQ,TEMP,YPB,MASS)	168
	DO 21 J=1,MM	169
	DO 21 I=1,N	170
21	TEMP(I,J)=Y(I,J)+YPB(I,J)	171
	CALL ZVR (N,M,DT,CC,CQ,TEMP,YPC,MASS)	172
	DO 22 J=1,M	173
	DO 22 I=1,N	174
	K=J+M	175
	X(I,J)=Y(I,J)+(YP(I,J)+YPC(I,J))/6.0+(YPA(I,J)+YPB(I,J))/3.0	176
22	VI(I,J)=Y(I,K)+(YP(I,K)+YPC(I,K))/6.0+(YPA(I,K)+YPB(I,K))/3.0	177
C		178
C	CALCULATE THE AVERAGE KINETIC AND POTENTIAL ENERGIES OF EACH ROW	179
C	OF ATOMS IN THE LATTICE.	180
C		181
	VTT=0.	182
	DO 24 J=1,M	183
	DO 23 I=2,NM1	184
23	VTT=VTT+0.5*MASS(I,J)*VI(I,J)**2	185
	VT(J)=VTT/10.+VT(J)	186
	VIT=0.	187
24	CONTINUE	188
	VPP=0.	189
	DO 26 J=2,MM1	190
	DO 25 I=2,NM1	191
	VPP=VPP+0.25*((X(I,J+1)-X(I,J))**2+(X(I,J)-X(I,J-1))**2+(X(I+1,J)-	192
	1X(I,J))**2+(X(I,J)-X(I-1,J))**2)+CC*((X(I,J+1)-X(I,J))**3+(X(I,J)-	193
	2X(I,J-1))**3+(X(I+1,J)-X(I,J))**3+(X(I,J)-X(I-1,J))**3)/6.0+CQ*((X	194
	3(I,J+1)-X(I,J))**4+(X(I,J)-X(I,J-1))**4+(X(I+1,J)-X(I,J))**4+(X(I,	195
	4J)-X(I-1,J))**4)/8.0	196
25	CONTINUE	197
	VP(J)=VPP/10.+VP(J)	198
	VPP=0.	199
26	CONTINUE	200
	DO 27 I=2,NM1	201
	VPP=VPP+0.25*((X(I,1)-X(I-1,1))**2+(X(I+1,1)-X(I,1))**2+X(I,1)**2)	202
	1+CC*((X(I,1)-X(I-1,1))**3+(X(I+1,1)-X(I,1))**3+X(I,1)**3)/6.0+CQ*(	203
	2X(I,1)-X(I-1,1))**4+(X(I+1,1)-X(I,1))**4+X(I,1)**4)/8.0	204
27	CONTINUE	205
	VP(1)=VPP/10.+VP(1)	206
	VPP=0.	207
	DO 28 I=2,NM1	208
	VPP=VPP+0.25*((X(I,M)-X(I-1,M))**2+(X(I+1,M)-X(I,M))**2+X(I,M)**2)	209

	1+CC*((X(I,M)-X(I-1,M))**3+(X(I+1,M)-X(I,M))**3-X(I,M)**3)/6.0+CQ*(	210
	2*(X(I,M)-X(I-1,M))**4+(X(I+1,M)-X(I,M))**4*X(I,M)**4)/8.0	211
28	CONTINUE	212
	VP(M)=VPP/10.+VP(M)	213
	VPP=0.	214
	VIII=VI(7,23)	215
	CALL MAXWEL (II,A1,VIII,ITWO,VMAX)	216
	IF (NCYC.LT.NP) GO TO 15	217
	IC=IC+1	218
	IE=0	219
C		220
C	CALCULATE THE KINETIC ENERGY OF EACH ATOM AND STORE IT TO BE	221
C	PLOTTED LATER.	222
C		223
	DO 29 J=1,M	224
	DO 29 I=2,NM1	225
	IE=IE+1	226
	E(IE,1)=X(I,J)	
29	E(IE,2)=VI(I,J)	
	IF (IC.NE.1) GO TO 32	
	P=NCYC	229
	IT=IT+1	230
	TIME(IT)=P*DT	231
	ER(IT)=ERR	232
	EL(IT)=ELL	233
C		234
C	CALCULATE THE TOTAL ENERGY OF THE LATTICE TO USE IN CHECKING	235
C	THE ENERGY CONSERVATION OF THE SYSTEM	236
C		237
	ECH(IT)=0.	238
	DO 30 J=2,M	239
	DO 30 I=2,NM1	240
	ECH(IT)=ECH(IT)+.5*MASS(I,J)*VI(I,J)**2+.5*((X(I,J)-X(I-1,J))**2+(	241
	1*(X(I,J)-X(I,J-1))**2)+CC*((X(I,J)-X(I-1,J))**3+(X(I,J)-X(I,J-1))**3	242
	2)/3.0+CQ*((X(I,J)-X(I-1,J))**4+(X(I,J)-X(I,J-1))**4)/4.0	243
30	CONTINUE	244
	DO 31 I=2,NM1	245
	ECH(IT)=ECH(IT)+.5*MASS(I,1)*VI(I,1)**2+.5*(X(I,1)**2+X(I,M)**2+(X	246
	1(I,1)-X(I-1,1))**2)+CC*((X(I,1)-X(I-1,1))**3+X(I,1)**3)/3.0+CQ*((X	247
	2(I,1)-X(I-1,1))**4+X(I,1)**4)/4.0-CC*X(I,M)**3/3.0+CQ*X(I,M)**4/4.	248
	30	249
31	CONTINUE	250
32	IF (IC.NE.1) GO TO 15	
	NP=NP+NDP	252
	IC=0	253
C		256
C	CALCULATE THE ENERGY CONTAINED IN A CENTRAL REGION OF THE LATTICE.	257
C		258
	ENG(IT)=0.	259
	DO 34 J=23,27	260
	DO 34 I=4,NM4	261
	ENG(IT)=ENG(IT)+.5*MASS(I,J)*VI(I,J)**2+.5*(X(I,J)-X(I,J-1))**2+.5	262
	1*(X(I,J)-X(I-1,J))**2+CC*((X(I,J)-X(I,J-1))**3+(X(I,J)-X(I-1,J))**	263
	23)/3.0+CQ*((X(I,J)-X(I,J-1))**4+(X(I,J)-X(I-1,J))**4)/4.0	264
34	CONTINUE	265
C		266
C	CALCULATE THE TOTAL ENERGY OF THE LATTICE BY SUMMING THE ENERGY	267
C	FLOW INTO AND OUT OF THE LATTICE AND THE INITIAL ENERGY.	268
C		269
	ETOT=EL(IT)+ER(IT)+ESTAR	270
C		273
C	ASSEMBLE AND PLOT THE ENERGIES FOR THE MOVIE SEQUENCE.	274
C		275
	GO TO 41	
33	CONTINUE	
	IPP=IPP+1	277
	IF (NCYC/500*500-NCYC.EQ.0) GO TO 45	
	IF (NCYC.LT.NSTOP) GO TO 15	279
C		280
C	THIS CONCLUDES THE MAIN ITERATION CYCLE.	281

C	EMAX=0.	282
	DO 35 I=1,IT	283
	IF (EMAX.LT.ABS(EL(I))) EMAX=ABS(EL(I))	284
	IF (EMAX.LT.ABS(ER(I))) EMAX=ABS(ER(I))	285
35	CONTINUE	286
C		287
C	PLOT ENERGY FLOWS AT THE RESERVOIRS.	288
C		289
	CALL ADV (1)	290
	CALL DGA (120,980,50,910,TIME(1),TIME(IT),EMAX,-EMAX)	291
	CALL DLNLN (10,10)	292
	CALL SHLIN (10,03)	293
	CALL SLLIN (10,13)	294
	CALL PLOT (IT,TIME,1,EL,1,42,1)	295
	CALL PLOT (IT,TIME,1,ER,1,16,1)	296
	CALL LINCNT (2)	297
	WRITE (12,49)	298
	CALL LINCNT (32)	299
	WRITE (12,57)	300
	CALL LINCNT (60)	301
	WRITE (12,58)	302
	CALL LINCNT (61)	303
	WRITE (12,59)	304
	CALL LINCNT (62)	305
	WRITE (12,50)	306
	CALL LINCNT (63)	307
	WRITE (12,52) PL,PM,FA,SI,MRL,MRR,UT,N,M,JR,PHOHL,PROBR,UBARL,UBAR	308
1R	PRINT 60, (ENG(IT),I1=1,IT)	309
	A2(2)=A1(1)	310
	A2(1)=A1(1)	311
	A2M=A1(1)	312
	XA(1)=0.	313
	DO 36 I=1,200	314
	I1=2*I	315
	A2(I1)=A1(I)	316
36	XA(I1)=I	317
	DO 37 I=3,400,2	318
	A2(I)=A2(I+1)	319
37	XA(I)=XA(I-1)	320
	XA(401)=XA(400)	321
	A2(401)=0.	322
	NA2=401	323
C		324
C	PLOT THE VELOCITY DISTRIBUTION FOR THE PARTICLE I1.	325
C		326
	CALL ADV (1)	327
	CALL LINCNT (61)	328
	WRITE (12,61) I1	329
	CALL LINCNT (62)	330
	WRITE (12,50)	331
	CALL LINCNT (63)	332
	WRITE (12,52) PL,PM,FA,SI,MRL,MRR,UT,N,M,JR,PHOHL,PROBR,UBARL,UBAR	333
1R		334
	AM=0.	335
	DO 38 I=1,200	336
	IF (A1(I).GT.AM) AM=A1(I)	337
38	CONTINUE	338
	CALL DGA (120,980,50,910,XA(1),XA(401),AM,0.)	339
	CALL DLNLN (2,4)	340
	CALL SHLIN (2,02)	341
	CALL SLLIN (4,12)	342
	CALL PLOT (401,XA,1,A2,1,42,1)	343
	FIT=NCYC	344
	DO 39 I=1,M	345
	VP(I)=VP(I)/FIT	346
39	VT(I)=VT(I)/FIT	347
	PRINT 62	348
	PRINT 63, (VT(I),I=1,M)	349
C		350
		351
		352

C	PLOT TIME-AVERAGED KINETIC ENERGIES.	353
C		354
	CALL ADV (1)	355
	CALL LINCNT (60)	356
	WRITE (12,62)	357
	CALL LINCNT (62)	358
	WRITE (12,50)	359
	CALL LINCNT (63)	360
	WRITE (12,52) PL,PM,FA,SI,MRL,MRR,DT,N,M,JR,PROBL,PROBR,UBARL,UBAR	361
	1R	362
	CALL DGA (120,980,50,910,D(1),D(M),TMAX,0.)	363
	CALL DLNLN (10,10)	364
	CALL SLLIN (10,13)	365
	CALL SBLIN (10,04)	366
	CALL PLOT (M,D,1,VT,1,42,1)	367
	DO 40 I=1,M	368
40	VE(I)=VT(I)+VP(I)	369
	PRINT 64	370
	PRINT 63, (VE(I),I=1,M)	371
C		372
C	PLOT TIME-AVERAGED TOTAL ENERGIES.	373
C		374
	CALL ADV (1)	375
	CALL LINCNT (60)	376
	WRITE (12,64)	377
	CALL LINCNT (62)	378
	WRITE (12,50)	379
	CALL LINCNT (63)	380
	WRITE (12,52) PL,PM,FA,SI,MRL,MRR,DT,N,M,JR,PROBL,PROBR,UBARL,UBAR	381
	1R	382
	CALL DGA (120,980,50,910,D(1),D(M),TMAX,0.)	383
	CALL DLNLN (10,10)	384
	CALL SLLIN (10,13)	385
	CALL SBLIN (10,04)	386
	CALL PLOT (M,D,1,VE,1,42,1)	387
	CALL EMPTY	388
	CALL EXIT	389
41	IF (IPIC.EQ.0) GO TO 42	390
	CALL BEDSPR (M,N,MN2,E,NN,MASS)	391
42	DO 43 J=1,5	392
	DO 43 I=1,MN2	393
43	E(I,J)=0.	394
	CALL SSWTCH (1,III)	395
	IF (III.EQ.1) GO TO 45	396
	GO TO 33	
44	READ (5) PL,PM,FA,SI,MRL,MRR,DT,PROBL,PROBR,UBARL,UBARR,N,M,JR,NDP	398
	1,NSTOP,MN,ELL,ERR	399
	READ (5) IT,NCYC,NP,IC,NN	400
	READ (5) (TIME(I),I=1,IT),(ECH(I),I=1,IT),(ER(I),I=1,IT),(EL(I),I=	401
	1,IT),(ENG(I),I=1,IT),((MASS(I,J),I=1,N),J=1,M),(VT(I),I=1,M),(VP(	402
	2(I),I=1,M)	403
	READ (5) ((X(I,J),I=1,N),J=1,M),((VI(I,J),I=1,N),J=1,M)	404
	REWIND 5	405
	GO TO 8	406
45	WRITE (5) PL,PM,FA,SI,MRL,MRR,DT,PROBL,PROBR,UBARL,UBARR,N,M,JR,ND	407
	1P,NSSTOP,MN,ELL,ERR	408
	WRITE (5) IT,NCYC,NP,IC,NN	409
	WRITE (5) (TIME(I),I=1,IT),(ECH(I),I=1,IT),(ER(I),I=1,IT),(EL(I),I=	410
	1,IT),(ENG(I),I=1,IT),((MASS(I,J),I=1,N),J=1,M),(VT(I),I=1,M),(VP	411
	2(I),I=1,M)	412
	WRITE (5) ((X(I,J),I=1,N),J=1,M),((VI(I,J),I=1,N),J=1,M)	413
	REWIND 5	414
	CALL EXIT	415
C		416
46	FORMAT (2I5)	417
47	FORMAT (7E10.5/4E10.5/5I5/2E10.5)	418
48	FORMAT (1H1)	419
49	FORMAT (40X16H EDICT II CYCLIC)	420
50	FORMAT (2X5H PL,6X2HPM,6X2HFA,6X2HSI,6X3HMRL,5X3HMRR,5X2HDT,6X1H	421
	IN,6X1HM,7X2HJR,4X5HPROBL,3X5HPROBR,3X5HUBARL,3X5HUBARR)	422
51	FORMAT (/4H CC=1P1E15.5,4H CQ=1P1E15.5)	423

52	FORMAT (7(1XF7.2),3(2XI6),4(1AF7.2))	424
53	FORMAT (//8H MASSES//4H I=.I10,9I12)	425
54	FORMAT (1XI3,1PE12.2)	426
55	FORMAT (////7H TIME=1PE12.4,7H CYCLE=16,18H LEFT ENERGY FLOW=.1	427
	1PE12.4,19H RIGHT ENERGY FLOW=1PE12.4,20H CHAIN TOTAL ENERGY=.1PE12	428
	2.4,6H ETOT=1PE12.4/12H ITERATIONS=15,10X22H ENERGY OF SUBSECTION=.	429
	31PE14.5//8(15H NO. K.E.(AV))/)	430
56	FORMAT (8(1XI4,1PE10.2))	431
57	FORMAT (12H ENERGY FLOW)	432
58	FORMAT (40X5H TIME)	433
59	FORMAT (5X41H . INDICATES ENERGY FLOW AT LEFT END AND,39H * INDI	434
	ICATES ENERGY FLOW AT RIGHT END.)	435
60	FORMAT (//19H ENG(II),II=1,IT.../10(1PE14.3))	436
61	FORMAT (10X39H VELOCITY DISTRIBUTION FOR PARTICLE NO.,I3)	437
62	FORMAT (20X25H AVERAGE KINETIC ENERGIES)	438
63	FORMAT (1P8E14.3)	439
64	FORMAT (20X17H AVERAGE ENERGIES)	440
	END	441-

	SUBROUTINE CHAGEN (N,PL,PM,FA,JR,SI,P)	CHA	1
C		CHA	2
C	CHAGEN GENERATES AN ARRAY OF MASSES PM AND PL WITH THE FRACTION	CHA	3
C	FA OF THESE BEING PL. THIS ARRAY IS ORDERED TO THE DEGREE SI,	CHA	4
C	I.E.. SI=0 DISORDER AND SI=1 ORDERED DIATOMIC.	CHA	5
C		CHA	6
	DIMENSION P(N)	CHA	7
	DO 1 J=1,JR	CHA	8
1	R=RANDOM(T)	CHA	9
	IF (FA.GE.0.5) GO TO 2	CHA	10
	P(1)=PM	CHA	11
	GO TO 3	CHA	12
2	P(1)=PL	CHA	13
3	DO 10 J=2,N	CHA	14
	R=RANDOM(T)	CHA	15
	JM=J-1	CHA	16
	IF (P(JM)-PM) 4,7,7	CHA	17
4	PAA=FA*(1.0-SI)	CHA	18
	IF (PAA-R) 5,5,6	CHA	19
5	P(J)=PM	CHA	20
	GO TO 10	CHA	21
6	P(J)=PL	CHA	22
	GO TO 10	CHA	23
7	PBR=(1.0-FA)*(1.0-SI)	CHA	24
	IF (PBR-R) 8,9,9	CHA	25
8	P(J)=PL	CHA	26
	GO TO 10	CHA	27
9	P(J)=PM	CHA	28
10	CONTINUE	CHA	29
	RETURN	CHA	30
	END	CHA	31-

	SUBROUTINE INIT (V,X,N,MASS,NN)	INT	2
C		INT	3
C	INITIALIZATION FOR TEMPERATURE WAVE STUDIES.	INT	4
C		INT	5
C	INIT INITIALIZES THE VELOCITIES (V) AND DISPLACEMENTS (X) SO THAT	INT	6
C	ALL ARE ZERO EXCEPT THE VELOCITIES OF THE END ROW.	INT	7
C		INT	8
	REAL MASS	INT	9
	DIMENSION V(N), X(N), MASS(N)	INT	10
	COMMON PL,PM	INT	11
	DO 1 I=1,N	INT	12
1	V(I)=0.		
	X(I)=0.		

	NMO=NN*17	
	DO 2 I=1,NMO	INT 14
2	MASS(I)=PM	INT 15
	T=2.0/SQRT(PM)	
	DO 3 I=1,NN	
3	V(I)=T	
	RETURN	INT 18
	END	INT 19-

	SUBROUTINE IMP (II,JJ,VI,UZERO,MR,N,M,MASS,EE)	IMP 1
C		IMP 2
C	IMP TAKES AN ATOM (II,JJ) WHICH HAS COLLIDED WITH A RESERVOIR	IMP 3
C	ATOM WITH VELOCITY UZERO AND MASS MR AND FINDS THE RESULTANT	IMP 4
C	VELOCITY VI AND COMPUTES THE ENERGY FLOW INTO THE SYSTEM.	IMP 5
C		IMP 6
	REAL MASS,MR	IMP 7
	DIMENSION VI(N,M), MASS(N,M)	IMP 8
	P=VI(II,JJ)	IMP 9
	RATIO=MASS(II,JJ)/MR	IMP 10
	VI(II,JJ)=VI(II,JJ)+2.*(UZERO-VI(II,JJ))/(1.+RATIO)	IMP 11
	EE=EE+.5*MASS(II,JJ)*(VI(II,JJ)**2-P**2)	IMP 12
	RETURN	IMP 13
	END	IMP 14-

	SUBROUTINE KICK (IONE,UBAR,UZERO)	KIC 1
C		KIC 2
C	KICK PROVIDES A RANDOM VELOCITY (UZERO) FROM A MAXWELLIAN DISTRI-	KIC 3
C	BUTION ABOUT UBAR FOR THE COLLISION ATOM IN THE RESERVOIR.	KIC 4
C		KIC 5
	DIMENSION U0(1000)	KIC 6
	GO TO (1.6), IONE	KIC 7
C		KIC 8
C	IF IONE IS ONE, SET UP TABLE.	KIC 9
C		KIC 10
1	DO 5 I=1,999	KIC 11
	ZMAX=2.5	KIC 12
	ZMIN=0.	KIC 13
	Z=1.	KIC 14
	RI=.001	KIC 15
2	ERF=ERR169(Z)	KIC 16
	FI=I	KIC 17
	R=RI*FI	KIC 18
	IF (ABS(ERF-R).LT.1.0E-04) GO TO 4	KIC 19
	IF (ERF.GE.R) GO TO 3	KIC 20
	ZMIN=Z	KIC 21
	Z=(Z+ZMAX)/2.	KIC 22
	GO TO 2	KIC 23
3	ZMAX=Z	KIC 24
	Z=(Z+ZMIN)/2.	KIC 25
	GO TO 2	KIC 26
4	U0(I)=Z	KIC 27
5	CONTINUE	KIC 28
	IONE=2	KIC 29
	U0(1000)=1.0E+33	KIC 30
6	R=RANDOM(T)	KIC 31
	IR=R*999.	KIC 32
	IR=IR+1	KIC 33
	UZERO=U0(IR)*UBAR	KIC 34
	R=RANDOM(T)	KIC 35
	IF (R.GT.0.5) UZERO=-UZERO	KIC 36
	RETURN	KIC 37
	END	KIC 38-

	SUBROUTINE BEDSPR (M,N,MN2,C,NN,MASS)	BED	1
C		BED	2
C	BEDSPR TAKES THE ENERGIES FOR NN PLOTS IN THE ARRAY C AND PLOTS	BED	3
C	THEM IN ISOMETRIC FORM IN STEREOPAIRS IF DESIRED.	BED	4
	REAL MASS	BED	5
	DIMENSION C(MN2,NN), MASS(N,M)	BED	6
	DIMENSION Y(50), X(12), IX(4), IV(3), ZO(12,50), Z(12,50)	BED	7
	DIMENSION XYZ(2,3), XB(8), YB(8), ZB(8)	BED	8
	DIMENSION ZYX(6)	BED	9
	DIMENSION IVY(4)		
	COMMON PL,PM,FA,SI,MRL,MRR,DT,JR,PROBL,PROBR,UBARR,UBARL,TMAX,NCYC	BED	10
	DATA (IXY(I),I=1,4)/0.600,423,1023/		
	DATA (IVY(I),I=1,4)/423,1023,0.600/		
	DATA (IV(I),I=1,3)/-1.,-1.,1./	BED	12
	DATA (ZYX(I),I=1,6)/0.,10.,0.,50.,0.,01/	BED	13
	EQUIVALENCE (XYZ(1),ZYX(1))	BED	14
	NM1=N-1	BED	15
	NM2=N-2	BED	16
	XYZ(2,3)=TMAX	BED	17
	NCYC1=NCYC		
	DO 1 I=1,N	BED	19
1	X(I)=I-1	BED	20
	DO 2 I=1,M	BED	21
2	Y(I)=I-1	BED	22
C		BED	23
C	SET UP BOUNDARIES FOR THE ARRAY.	BED	24
C		BED	25
	DO 3 J=1,M	BED	26
	DO 3 I=1,N	BED	27
3	ZO(I,J)=0.	BED	28
	LB=0	BED	29
	DO 4 I=1,2	BED	30
	DO 4 J=1,2	BED	31
	DO 4 K=1,2	BED	32
	LB=LB+1	BED	33
	XB(LB)=XYZ(I,1)	BED	34
	YB(LB)=XYZ(J,2)	BED	35
4	ZB(LB)=XYZ(K,3)	UCU	36
	IE=0	BED	37
	CALL STEREO (IE,IXY,UV,0.,1.,1.,0.,XB,1,YB,1,ZB,1,42,1)	BED	38
C		BED	39
C	PLOT THE ARRAY FOR EACH SET OF DATA.	BED	40
C		BED	41
	DO 12 L=1,2		
	IE=-1	BED	43
	JI=0	BED	44
	DO 5 J=1,M	BED	45
	DO 5 I=2,NM1	BED	46
	JI=JI+1	BED	47
5	Z(I,J)=C(JI,L)*10.		
	DO 6 J=1,M	BED	51
	CALL STEREO (IE,1,1,1,1,1,NM2,X(2),1,Y(J),0,Z(2,J),1,42,1)		
6	CONTINUE	BED	53
	DO 7 I=2,NM1	BED	54
	CALL STEREO (IE,1,1,1,1,1,M,X(I),0,Y,1,Z(I,1),N,42,1)	BED	55
7	CONTINUE	BED	56
	CALL SSWTCH (2,I,2)	BED	57
	IF (I12.NE.1) GO TO 10	BED	58
C		BED	59
C	PLOT AN ARRAY OF SYMBOLS AT THE ZERO POSITIONS INDICATING WHETHER	BED	60
C	EACH ATOM IS PL(L) OR PM(H).	BED	61
C		BED	62
	IJ=0	BED	63
	DO 9 J=1,M	BED	64
	DO 9 I=2,NM1	BED	65
	IF (MASS(I,J).NE.PL) GO TO 8	BED	66
	CALL STEREO (IE,1,1,1,1,1,1,X(I),0,Y(J),0,ZO(I,J),0,35,0)	BED	67
	GO TO 9	BED	68
8	CALL STEREO (IE,1,1,1,1,1,1,X(I),0,Y(J),0,ZO(I,J),0,24,0)	BED	69
9	CONTINUE	BED	70
10	CONTINUE		

12	CALL STEREO(0,IVY,DV,0.0,1.0,1.0,8,XB,1,YB,1,ZB,1,42,1)	BED	83
	CONTINUE		
	CALL LINCNT (2)	BED	72
	WRITE (12,13)	BED	73
	CALL LINCNT (3)	BED	74
	WRITE (12,14) NCYC1	BED	75
	CALL LINCNT (60)	BED	76
	WRITE (12,15)	BED	77
	CALL LINCNT (61)	BED	78
	WRITE (12,16) PL,PM,FA,SI,MRL,MRR,DT,N,M,JR,PROBL,PROBR,UBARL,UBARR	BED	79
1R	CALL FRAME (0,1023,0,1023)	BED	50
	CALL ADV(1)		
	RETURN	BED	84
C		BED	85
13	FORMAT (45X9H EDICT II)	BED	86
14	FORMAT (40X10H CYCLE NO.15)	BED	87
15	FORMAT (2X5H PL,6X2HPM,6X2HFA,6X2HSI,6X3HMRL,5X3HMRR,5X2HDT,6X1HMBED	BED	88
	1N,7X1HM,7X2HJR,4X5HPROBL,3X5HPROBR,3X5HUBARL,3X5HUBARR)	BED	89
16	FORMAT (7(1XF7.2),3(2X16),4(1XF7.2))	BED	90
	END	BED	91-

	SUBROUTINE MAXWEL (II,A,V,ITWO,VMAX)		1
C			2
C	MAXWELL ARRANGES A VELOCITY DISTRIBUTION A FOR THE ATOM II.		3
C			4
	DIMENSION A(200)		5
	GO TO (1,3), ITWO		6
1	DO 2 I=1,200		7
2	A(I)=0.		8
	ITWO=2		9
3	VM=V*100./VMAX		10
	IV=VM		11
	IV=IV*100		12
	IF (IV.GT.200) IV=200		13
	IF (IV.LT.0) IV=0		14
	A(IV)=A(IV)+1.		15
	RETURN		16
	END		17-

	SUBROUTINE STEREO (IEYE,JXY,DV,A,SF,FWF,N,X,MX,Y,MY,Z,MZ,ICHAR,ICOJEL		1
	IN)		2
C		JEL	3
C	STEREO PROVIDES A MEANS OF PRODUCING TWO PLANE PROJECTIONS SUCH	JEL	4
C	THAT,WHEN ONE IS LOOKED AT WITH ONE EYE AND THE OTHER VIEWED WITH	JEL	5
C	WITH THE OTHER EYE, A THREE-DIMENSIONAL EFFECT IS ACHIEVED. THE	JEL	6
C	PROJECTIONS ARE PUT ON 35MM FILM BY THE SC4020.	JEL	7
C		JEL	8
	DIMENSION JXY(4), DV(3), X(2), Y(2), Z(2), IXY(4), E(3,3), R(3,2),	JEL	9
1	R0(3), RP(3,2), D(3)	JEL	10
C		JEL	11
C	STANDARD EYE SEPARATION IS .25*W, WHERE W IS WIDTH OF WINDOW	JEL	12
C	USED. STANDARD LATERAL FIELD WIDTH IS .3	JEL	13
C		JEL	14
	DATA SS,SFW/.25,.3/	JEL	15
C		JEL	16
C	IF IEYE=0, COMPUTE POSITION VECTORS OF EYE POSITIONS.	JEL	17
C		JEL	18
	IF (IEYE) 1,3,2	JEL	19
1	K=1	JEL	20
	GO TO 43	JEL	21
2	K=2	JEL	22
	GO TO 43	JEL	23
C		JEL	24

C	IF N IS LESS THAN 2, EXIT	JE1	25
C		JE1	26
3	IF (N-2) 4,5,5	JE1	27
4	RETURN	JE1	28
C		JE1	29
C	COMPUTE THE THREE ORTHOGONAL UNIT VECTORS, E1, E2, E3.	JE1	30
C	E1 POINTS ALONG VIEWERS LINE OF SIGHT.	JE1	31
C	E2 POINTS FROM LEFT EYE TOWARD RIGHT EYE.	JE1	32
C	E3 POINTS UP (FROM FEET TOWARD HEAD).	JE1	33
C		JE1	34
5	DP=SQRT(DV(1)**2+DV(2)**2+DV(3)**2)	JE1	35
	IF (DP) 7,6,7	JE1	36
6	DP=1.	JE1	37
	DV(1)=1.	JE1	38
7	DO 8 I=1,3	JE1	39
	E(I,1)=-DV(I)/DP	JE1	40
	E(I,2)=0.	JE1	41
C		JE1	42
C	FIRST COMPUTE E2 AND E3 SUCH THAT E2 IS IN X-Y PLANE, AND	JE1	43
C	E3 = E1 CROSS E2 HAS NON NEGATIVE Z-COMPONENT	JE1	44
C		JE1	45
	IF (E(2,1)) 10,9,10	JE1	46
9	E(2,2)=-1.	JE1	47
	GO TO 11	JE1	48
10	B=-E(1,1)/E(2,1)	JE1	49
	E(1,2)=1./SQRT(1.+B**2)	JE1	50
	E(2,2)=B*E(1,2)	JE1	51
11	E(1,3)=E(2,1)*E(3,2)-E(3,1)*E(2,2)	JE1	52
	E(2,3)=E(3,1)*E(1,2)-E(1,1)*E(3,2)	JE1	53
	E(3,3)=E(1,1)*E(2,2)-E(2,1)*E(1,2)	JE1	54
	IF (E(3,3)) 12,14,14	JE1	55
12	DO 13 I=1,3	JE1	56
	E(I,2)=-E(I,2)	JE1	57
13	E(I,3)=-E(I,3)	JE1	58
C		JE1	59
C	ROTATE E2 AND E3 ABOUT E1 THROUGH THE ANGLE A. POSITIVE ROTA-	JE1	60
C	TION IS COUNTERCLOCKWISE WHEN LOOKING IN DIRECTION E1 IS POINTING.	JE1	61
C		JE1	62
14	IF (A) 15,18,15	JE1	63
15	XC=COS(A)	JE1	64
	YC=SIN(A)	JE1	65
	DO 16 I=1,3	JE1	66
	R(I,1)=XC*E(I,2)-YC*E(I,3)	JE1	67
16	R(I,2)=YC*E(I,2)+XC*E(I,3)	JE1	68
	DO 17 I=1,3	JE1	69
	E(I,2)=R(I,1)	JE1	70
17	E(I,3)=R(I,2)	JE1	71
C		JE1	72
C	DETERMINE WHICH OF THE N POINTS IS NEAREST TO VIEWER.	JE1	73
C		JE1	74
18	I1=1	JE1	75
	I2=1	JE1	76
	I3=1	JE1	77
	DO 22 I=1,N	JE1	78
	DPJ=X(I1)*E(1,1)+Y(I2)*E(2,1)+Z(I3)*E(3,1)	JE1	79
	IF (I-1) 20,20,19	JE1	80
19	IF (DP1=DP) 20,21,21	JE1	81
20	DP=DP1	JE1	82
	K1=I1	JE1	83
	K2=I2	JE1	84
	K3=I3	JE1	85
21	I1=I1+MX	JE1	86
	I2=I2+MY	JE1	87
22	I3=I3+MZ	JE1	88
C		JE1	89
C	FIND THE PROJECTION OF EACH OF THE N POINTS ON THE PLANE	JE1	90
C	PERPENDICULAR TO LINE OF SIGHT AND CONTAINING NEAR POINT.	JE1	91
C	FIND THE MINIMUM SIZE OF A WINDOW THAT WILL CONTAIN ALL	JE1	92
C	THESE POINTS OF PROJECTION.	JE1	93
C		JE1	94

	I1=1	JE1 95
	I2=1	JE1 96
	I3=1	JE1 97
	DO 33 I=1,N	JE1 98
	DP=(X(K1)-X(I1))*E(1,1)+(Y(K2)-Y(I2))*E(2,1)+(Z(K3)-Z(I3))*E(3,1)	JE1 99
	PX=DP*E(1,1)+X(I1)	JE1 100
	PY=DP*E(2,1)+Y(I2)	JE1 101
	PZ=DP*E(3,1)+Z(I3)	JE1 102
	XC=-PX*E(1,2)-PY*E(2,2)-PZ*E(3,2)	JE1 103
	YC=PX*E(1,3)+PY*E(2,3)+PZ*E(3,3)	JE1 104
	IF (I-1) 23,23,24	JE1 105
23	XMIN=XC	JE1 106
	XMAX=XC	JE1 107
	YMIN=YC	JE1 108
	YMAX=YC	JE1 109
	GO TO 32	JE1 110
24	IF (XC-XMIN) 25,28,26	JE1 111
25	XMIN=XC	JE1 112
	GO TO 28	JE1 113
26	IF (XC-XMAX) 28,28,27	JE1 114
27	XMAX=XC	JE1 115
28	IF (YC-YMIN) 29,32,30	JE1 116
29	YMIN=YC	JE1 117
	GO TO 32	JE1 118
30	IF (YC-YMAX) 32,32,31	JE1 119
31	YMAX=YC	JE1 120
32	I1=I1+MX	JE1 121
	I2=I2+MY	JE1 122
33	I3=I3+MZ	JE1 123
C		JE1 124
C	COMPUTE CENTER POINT AND DISTANCE EYE POSITIONS MUST BE	JE1 125
C	FROM WINDOW.	JE1 126
C		JE1 127
	X0=.5*(XMIN+XMAX)	JE1 128
	Y0=.5*(YMIN+YMAX)	JE1 129
	DO 34 I=1,4	JE1 130
34	IXY(I)=JXY(I)	JE1 131
	DX=IXY(2)-IXY(1)	JE1 132
	DY=IXY(4)-IXY(3)	JE1 133
	W=XMAX-XMIN	JE1 134
	XL=YMAX-YMIN	JE1 135
	IF (FWF) 35,35,36	JE1 136
35	FWF=1.	JE1 137
36	FW=FWF*SF	JE1 138
	IF (SF) 37,38,38	JE1 139
37	SF=1.	JE1 140
38	DIST=W*(1.+SS*SF)/FW	JE1 141
	FW1=FW*DY/DX	JE1 142
	IF (XL-FW1*DIST) 40,40,39	JE1 143
39	DIST=XL/FW1	JE1 144
	W=FW*DIST/(1.+SS*SF)	JE1 145
40	DP=X(K1)*E(1,1)+Y(K2)*E(2,1)+Z(K3)*E(3,1)	JE1 146
	DO 41 I=1,3	JE1 147
41	R0(I)=DP*E(I,1)-X0*E(I,2)+Y0*E(I,3)	JE1 148
C		JE1 149
C	DETERMINE POSITION VECTOR FOR EACH EYE.	JE1 150
C		JE1 151
	S=SS*SF*W/2.	JE1 152
	DO 42 I=1,3	JE1 153
	RR=R0(I)-DIST*E(I,1)	JE1 154
	RP(I,1)=RR+S*E(I,2)	JE1 155
42	RP(I,2)=RR-S*E(I,2)	JE1 156
	XS=FW/2.	JE1 157
	YS=FW1/2.	JE1 158
	RETURN	JE1 159
C		JE1 160
C	IF N IS LESS THAN 1, EXIT	JE1 161
C		JE1 162
43	IF (N) 58,58,44	JE1 163
44	IJ=0	JE1 164
	IJ=1	JE1 165

	I2=1	JE1 166
	I3=1	JE1 167
	DO 57 I=1,N	JE1 168
	D(1)=X(I1)-RP(1,K)	JE1 169
	D(2)=Y(I2)-RP(2,K)	JE1 170
	D(3)=Z(I3)-RP(3,K)	JE1 171
	SUM=E(1,1)*D(1)+E(2,1)*D(2)+E(3,1)*D(3)	JE1 172
	IF (SUM) 55,55,45	JE1 173
45	DO 46 J=1,3	JE1 174
46	D(J)=D(J)/SUM-E(J,1)	JE1 175
	X2=-E(1,2)*D(1)-E(2,2)*D(2)-E(3,2)*D(3)	JE1 176
	Y2=E(1,3)*D(1)+E(2,3)*D(2)+E(3,3)*D(3)	JE1 177
	IX=.5*(1.+(X2+XS)*DX/XS)	JE1 178
	IX=IXY(1)+IX	JE1 179
	IY=.5*(1.+(Y2+YS)*DY/YS)	JE1 180
	IY=IXY(4)-IY	JE1 181
	IF (IY-IXY(4)) 47,47,55	JE1 182
47	IF (IY-IXY(3)) 55,48,48	JE1 183
48	IF (IX-IXY(2)) 49,49,55	JE1 184
49	IF (IX-IXY(1)) 55,50,50	JE1 185
50	IF (ICON) 52,51,51	JE1 186
51	CALL PLT (IX,IY,ICHR)	JE1 187
	IF (ICON) 52,56,52	JE1 188
52	IF (IJ) 55,54,53	JE1 189
53	CALL DRV (IX,IY,IX,IY)	JE1 190
54	IX=IX	JE1 191
	IY=IY	JE1 192
	IJ=1	JE1 193
	GO TO 56	JE1 194
55	IJ=0	JE1 195
56	I1=I1+MX	JE1 196
	I2=I2+MY	JE1 197
57	I3=I3+MZ	JE1 198
58	RETURN	JE1 199
	END	JE1 200-

	FUNCTION ERR169 (X)	C32 1
C		C32 2
C	ERROR FUNCTION APPROXIMATION (ACCURATE WITHIN .00000015)	C32 3
C		C32 4
1	IF (X,NE,0.0) GO TO 2	C32 5
	ERR169=0.0	C32 6
	RETURN	C32 7
2	E=1.0/(1.0+.3275911*X)	C32 8
	S=(((((940646070*E)-1.287822453)*E+1.259695130)*E-.252128668)*E+.1225836846)*E	C32 9
	S=S*EXP(-X**2)*(1.1283791679551)	C32 10
	ERR169=1.0-S	C32 11
	RETURN	C32 12
	END	C32 13
		C32 14-

	SUBROUTINE ZVR (N,M,DT,CC,CQ,Y,YP,MASS)	ZVR 1
C		ZVR 2
C	ZVR PROVIDES A MODIFIED RUNGE-KUTTA INTEGRATION SCHEME TO BE USED	ZVR 3
C	TO ADVANCE THE TIME IN THE EQUATIONS OF MOTION.	ZVR 4
C		ZVR 5
	DIMENSION Y(12,100), YP(12,100), MASS(12,50), AA(12), AB(12)	ZVR 6
	REAL MASS	ZVR 7
	K=N-1	ZVR 8
	L=M+1	ZVR 9
	DO 1 I=2,K	ZVR 10
	YP(I,1)=Y(I,L)*DT	ZVR 11
1	AB(I)=Y(I,1)*(1.0+Y(I,1)*(CC+CQ*Y(I,1)))	ZVR 12
	YP(I,1)=YP(K,1)	ZVR 13

	YP(N,1)=YP(2,1)	ZVR	14
	DO 3 J=2,M	ZVR	15
	L=M+J-1	ZVR	16
	IL=J-1	ZVR	17
	S=Y(2,IL)-Y(1,IL)	ZVR	18
	BC=S*(1.0+S*(CC+CQ*S))	ZVR	19
	DO 2 I=2,K	ZVR	20
	BB=BC	ZVR	21
	S=Y(I+1,IL)-Y(I,IL)	ZVR	22
	BC=S*(1.0+S*(CC+CQ*S))	ZVR	23
	AA(I)=AB(I)	ZVR	24
	S=Y(1,J)-Y(I,IL)	ZVR	25
	AB(I)=S*(1.0+S*(CC+CQ*S))	ZVR	26
	YP(I,J)=Y(I,L+1)*DT	ZVR	27
2	YP(I,L)=(AB(I)-AA(I)+BC-BB)*DT/MASS(I,IL)	ZVR	28
	YP(1,J)=YP(K,J)	ZVR	29
	YP(N,J)=YP(2,J)	ZVR	30
	YP(1,L)=YP(K,L)	ZVR	31
3	YP(N,L)=YP(2,L)	ZVR	32
	L=M+M	ZVR	33
	S=Y(2,M)-Y(1,M)	ZVR	34
	BC=S*(1.0+S*(CC+CQ*S))	ZVR	35
	DO 4 I=2,K	ZVR	36
	BB=BC	ZVR	37
	S=Y(I+1,M)-Y(I,M)	ZVR	38
	BC=S*(1.0+S*(CC+CQ*S))	ZVR	39
	S=-Y(I,M)*(1.0-Y(I,M)*(CC-CQ*Y(I,M)))	ZVR	40
4	YP(I,L)=(S-AB(I)+BC-BB)*UT/MASS(I,M)	ZVR	41
	YP(1,L)=YP(K,L)	ZVR	42
	YP(N,L)=YP(2,L)	ZVR	43
	RETURN	ZVR	44
	END	ZVR	45-