EXPERIMENT 2

Apparatus
RML Nimbus computer

Ten sheets of graph paper.

Please complete synopsis sheet in addition to answering this experimental problem.

THIS IS A TWO AND A HALF HOUR EXAMINATION

INFORMATION

The microcomputer has been programmed to solve the Newtonian equations of motion for a two-dimensional system of 25 interacting particles, in the *xy* plane. It is able to generate the positions and velocities of all particles at discrete, equally spaced time intervals. By depressing appropriate keys (which will be described), access to dynamic information about the system can be obtained.
The system of particles is confined to a box which is initially (at time $t = 0$) arranged in a two-dimensional square lattice. A picture of the system is displayed on the screen together with the numerical data requested. All particles are identical; the colours are to enable the particles to be distinguished. As the system evolves in time the positions and velocities of the particles will change. If a particle is seen to leave the box the program automatically generates a new particle that enters the box at the opposite face with the same velocity, thus conserving the number of particles in the box.
Any two particles i and j, separated by a distance r_{ij} interact with a well-defined potential U_{ij},

It is convenient to use dimensionless quantities throughout the computation. The quantities given below are used throughout the calculations.

Variable	**Symbol**
Distance	r^*
Velocity	v^*
Time	t^*
Energy	E^*
Mass of particle	$M^* = 48$
Potential	U_{ij}^*
Temperature	T^*
Kinetic Energy	$E_k^* = \frac{1}{2} m^* v^{*2}$

INSTRUCTIONS

The computer program allows you to access three distinct sets of numerical information and display them on the screen. Access is controlled by the grey function keys on the left-hand side of the keyboard, labelled F1, F2, F3, F4, and F10. These keys should be pressed and released - do not hold down a key, nor press it repeatedly. The program may take up to 1 second to respond.

FIRST INFORMATION SET. PROBLEMS 1 – 5

$$< v_x, n >= \frac{1}{25} \sum_{i=1}^{25} \left(v_{ix}^* \right)^n$$

$$< v_y, n >= \frac{1}{25} \sum_{i=1}^{25} \left(v_{iy}^* \right)^n$$

and

$$< U >= \frac{1}{25} \sum_{j=1}^{25} \sum_{i=1}^{25} U_{ij}^* \quad (i \neq j)$$

where

v_{ix}^* is the dimensionless x – component of the velocity for the i'th particle,

v_{iy}^* is the dimensionless y – component of the velocity for the i'th particle,

and n is and integer with $n \geq 1$.

[Note: the summation over U_{iy}^* excludes the cases in which $i = j$]

After depressing F1 it is necessary to input the integer $n\,(n \geq 1)$ by depressing one of the white keys in the top row of the keyboard, before the information appears on the screen.

The information is displayed in dimensionless time intervals Δt at dimensionless times

S Δt^{**} (S = 0, 1, 2, ...)

Δt^{**} is set by the computer program to the value $\Delta t^{**} = 0{\bullet}100000$.

The value of S is displayed at the bottom right hand of the screen. Initially it has the value S = 0. The word "waiting" on the screen indicates that the calculation has halted and information concerning the value of S is displayed.

Depressing the long bar (the "space" bar) at the bottom of the keyboard will allow the calculation of the evolution of the system to proceed in time steps $\Delta^{**}t$. The current value of S is always displayed on the screen. Whilst the calculation is proceeding the word "running" is displayed on the screen.

Depressing F1 again will stop the calculation at the time integer indicated by S on the screen, and display the current values of

$$< v_x, n >, \; < v_y, n > \text{ and } < U >$$

after depressing the integer n. The evolution of the system continues on pressing the long bar.
The system can, if required, be reset to its original state at S = 0 by pressing F10 TWICE.

SECOND INFORMATION SET: PROBLEM 6

Depressing F2 initiates the computer program for the compilation of the histogram in problem 6. This program generates a histogram table of the accumulated number ΔN, of particle velocity components as a function of dimensionless velocity. The dimensionless velocity components, v_x and v_y are referred to collectively by v_c. The dimensionless velocity range is divided into equal intervals $\Delta v_c = 0.05$. The centres of the dimensionless velocity "bins" have magnitudes

$$v_c^* = \mathrm{B}\Delta v_c^* \qquad (\mathrm{B} = 0, \pm 1 \pm 2, ...)$$

When the long bar on the keyboard is pressed the 2 x 25 dimensionless velocity components are calculated at the current time step, and the program adds one, for each velocity component, into the appropriate velocity 'bin'. This process is continued, for each time step, until F3 is depressed. Once F3 is depressed the (accumulated) histogram is displayed. The accumulation of counts can then be continued by pressing the long bar. (Alternatively if you wish to return to the initial situation, with zero in all bins, press F2).

The accumulation of histogram data should continue for about 200 time steps after initiation.

In the thermodynamic equilibrium the histogram can be approximated by the relation

$$\Delta N = Ae^{\left[\frac{-24(v_c^*)^2}{\alpha}\right]}$$

where α is a constant associated with the temperature of the system, and A depends on the total number of accumulated velocity components.

THIRD INFORMATION SET: PROBLEM 7

Depressing F4 followed by the long bar at any time during the evolution of the system will initiate the program for Problem 7. The program will take some 30 seconds, in real time, before displaying a table containing the two
Quantities

$$< RX,2 >= \frac{1}{25}\sum_{i=1}^{25}\left[x_i^*(S) - x_i^*(SR)\right]^2$$

and

$$< RY,2 >= \frac{1}{25}\sum_{i=1}^{25}\left[y_i^*(S) - y_i^*(SR)\right]^2$$

where x_i^* and y_i^* are the dimensionless position components for the i'th particle. S is the integer time unit and SR is the fixed initial integer time at which the programme is initiated by depressing F4. It is convenient to introduce integer

$SZ = S - SR.$.

The programme displays a table of $<RX,2>$ and $<RY,2>$ for

SZ = 0, 2, 4.……24.

Prior to the display appearing on the screen a notice 'Running' will appear on
the screen indicating that a computation is proceeding. Depressing F4, followed by the long bar, again will initiate a new table with SR advanced to the point at which F4 was depressed.

COMPUTATIONAL PROBLEMS

1 Verify that the dimensionless total linear momentum of the system is conserved for the times given by

S = 0, 40, 80, 120, 160.

State the accuracy of the computer calculation.

2. Plot the variation in dimensionless kinetic energy of the system with time using the time sequence

S = 0, 2, 4, 6, 12, 18, 24, 30, 50, 70, 90, 130, 180.

3. Plot the variation in dimensionless potential energy of the system with time using the time sequence in 2.

4. Obtain the dimensionless total energy of the system at times indicated in 2. Does the system conserve energy? State the accuracy of the total energy calculation.

5. The system is initially (at $S = 0$) NOT in thermodynamic equilibrium. After a period of time the system reaches thermodynamic equilibrium in which the total dimensionless kinetic energy fluctuates about a mean value of E_k^*. Determine this value of E_k^* and indicate the time, *SD*, after which the system is in thermodynamic equilibrium.

6. Using the dimensionless accumulated velocity data, during thermodynamic equilibrium, draw up a histogram giving the number ΔN of velocity components against dimensionless velocity component, using the constant velocity component interval $\Delta V_c^* = 0.05$, specified in the table available from the SECOND INFORMATION SET. Data accumulated from approximately 200 time steps should be used and the starting time integer *S* should be recorded.

Verify that ΔN satisfies the relation

$$\Delta N = Ae^{-\left[\frac{24\left(v_C^*\right)^2}{\alpha}\right]}$$

where *C* and *A* are constants. Determine the value of α.

7. For the system of particles in thermodynamic equilibrium evaluate the average value of R^2, $< R^2 >$, where *R* is the straight line distance between the position of a particle at a fixed initial time number *SR* and time number *S*. The time number difference *SZ* = (*S* - *SR*) takes the values

SZ = O, 2, 4, ….. 24.

Plot $<R^2>$ against *SZ* for any appropriate value of *SR*. Calculate the gradient of the function in the linear region and specify the time number range for which this gradient is valid.
In order to improve the accuracy of the plot repeat the previous calculations for three (additional) different values of SR and determine the AVERAGE $<R^2>$ for the four sets of results together with the 'linear' gradient and time number range.
Deduce, with appropriate reasoning, the thermodynamic equilibrium state of the system, either solid or liquid.