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A Computer Program for Molecular Dynamics of Dilute Gases

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A general flexible program for computer experiments with dilute gases approaching equilibrium is described. The program uses the Alder–Wainwright algorithm between collisions, and solves the Newton equations for binary and multiple collisions, making use of the conservation laws in the binary case. The program may be used for both central and noncentral interactions, and time-irreversible or multiple-particle interactions can simply be added. Examples of results, for 100 particles in a 2-dimensional box and for 125 particles in a 3-dimensional box, are described, and the time symmetry of the calculation is checked and discussed.

1. INTRODUCTION

In the last fifteen years, the techniques of high speed computer experiments for studying the behavior of molecular and atomic systems has been extensively used [1]. The works in this field may be divided into two main groups. One group, represented, e.g., in the work of Rahman and collaborators [2] or in those of Vineyard and coworkers [3], consists of works in which all $6N$ differential equations

$$d\mathbf{r}_i/dt = \mathbf{v}_i\,,$$
$$d\mathbf{v}_i/dt = \mathbf{F}_i = \sum_{j\neq i} \mathbf{F}_{ij}\,, \qquad i = 1, 2,..., N. \tag{1}$$

(N is the number of particles, $\mathbf{r}_i$ and $\mathbf{v}_i$ the position and velocity of the i-th particle, $\mathbf{F}_i$ the force on this particle (the masses are taken as 1)) are simultaneously solved, with a fixed time step. In all these works, only binary interactions are considered, the force $\mathbf{F}_{ij}$ being computed from a radially symmetric potential

$$\mathbf{F}_{ij} = -\nabla V(|\,\mathbf{r}_i - \mathbf{r}_j\,|). \tag{2}$$

The second approach, due to Alder and Wainwright [4], deals with systems of hard spheres. In these calculations, successive binary collision points are connected

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by straight-line molecular trajectory segments. The veclocity changes at each collision are calculated simply from conservation laws, and no use of Newton's equations (1) is needed.

The first group of calculations has been very successful in investgations of dense matter behavior [2], and of lattice radiation damage [3]. The second has described beautifully the approach to equilibrium of dilute gases, when each particle interacts at most with one neighbor in a simplified binary collision.

Clearly, the model of hard spheres, with or without an attractive square-well potential, is not realistic and very restrictive. The question of the approach to equilibrium of a gas is of great interest in many aspects, and a more detailed research on different factors which affect this approach might clarify many points. For example, the use of various realistic central potentials, such as the Lennard–Jones potential, instead of the hard sphere model, will make clear the effect of the specific form of the interaction on the approach to equilibrium. Other kinds of interaction which have not yet been used are those of noncentral, nonbinary and nonlocal forces. Most statistical theories use central local binary interactions, and find it difficult to include more general forces, although these exist in nature. Noncentral forces, such as the Stockmayer potential [5], are important for studying the behavior of polar molecules, e.g., H_2O. Nonbinary forces, such as the 3-body Axilrod–Teller potential [6], are important for calculations related with the dynamics of noble gas atoms [7] and for nuclear matter problems [8]. Nonlocal forces, or equivalently, velocity dependent forces [9], appear, e.g., in connection with the pseudopotential in solid state physics [10], or in relation with time reversal violating potentials [11]. Some microscopically irreversible effects, such as in the neutral kaon decay [12] or in atomic inelastic collisions, may also have an important effect on the macroscopic behavior of the gas.

Of course, a Rahman technique can be used to solve such problems, but the solution might not be very precise and would waste computer time due to the fact that in a dilute gas only very few particles are interacting at a given moment.

Therefore, a flexible program to compute the approach to equilibrium of a dilute gas, with a general short-range interaction, has been written. This program combines the "hard sphere" Alder–Wainwright method [4], for the description of the molecular trajectories between collisions, with a realistic general solution of the equations of motion for the colliding particles. The program is very flexible; the type of interaction can easily be changed, and its effect may be studied.[1]

[1] After this work was completed, a work by H. W. Harrison and W. S. Schieve [13] appeared, in which 2-dimensional computer calculations for dilute gases with the Lennard–Jones potential are described. These authors combine the Alder–Wainwright and the Rahman techniques, for pair collisions (I thank Dr. Harrison for a private communication, clarifying this point). Still, it seems that our procedure for dealing with the pair collision, and the possibility for multiple collisions in three dimensions, have not yet been described in any published work.

Section 2 gives a general outline of the program. In Section 3, our version of the Alder–Wainwright algorithm for arranging the time steps is described. Section 4 describes the method of calculating a binary collision, and Section 5 that of dealing with a multiple collision. Section 6 gives examples of results and a discussion of the precision of the calculation. Further examples are hoped to be discussed in future publications.

2. Description of the Program

The main parts of the program are as follows:

2.1. *Input*

The main input data are

NX, NY, NZ = the dimensions of the initial lattice,

a, b, c = the unit lengths of the lattice,

a_0, b_0, c_0 = the distances of the walls from the lattice,

v_0 = the magnitude of the initial velocity,

Δv = the velocity interval for calculating the velocity distribution, the H-function, etc.,

ϵ, β, etc. = the parameters of the binary potentials (e.g., in the Lennard–Jones case the potential is $\epsilon[(\beta/r)^{12} - (\beta/r)^6]$),

RMX = the cutoff radius of the potential.

2.2. *Equilibrium Distribution*

For comparison with the final results, the equilibrium Maxwell–Boltzmann distribution is calculated:

$$n_{\text{eq}}(v) = NX \cdot NY \cdot NZ \left(\frac{3}{2\pi {v_0}^2}\right)^{3/2} e^{-3/2(v/v_0)^2}. \tag{3}$$

2.3. *Initial Conditions*

The particles can either be arranged on a cubic lattice:

$$\begin{aligned} X(N) &= a_0 + (I-1)\,a, \qquad I = 1, 2, \ldots, NX, \\ Y(N) &= b_0 + (J-1)\,b, \qquad J = 1, 2, \ldots, NY, \\ Z(N) &= c_0 + (K-1)\,c, \qquad K = 1, 2, \ldots, NZ, \\ N &= NZ \cdot NY \cdot (I-1) + NZ \cdot (J-1) + K, \end{aligned} \tag{4}$$

or randomly distributed in the box.

The directions of the velocities, all of magnitude v_0, are randomly distributed.

2.4. *Initial Arrangement of Time Steps*

For each particle, the shortest time interval after which it is going to collide either with another particle or with a wall of the box is recorded. The procedure of finding these time intervals will be described in Section 3. The time intervals are then arranged in increasing order, in the vector $DTT(I)$. The numbers of the particles which are going to collide at these times are recorded in the vector $IT(I)$, and the number of the particle or of the wall (the walls are given negative indices) with which particle N is going to collide is recorded in the vector $IJ(N)$.

2.5. *Output*

For chosen time intervals, and after each collision, the physical time, number of collisions, H-function, kinetic and potential total energies, etc., are printed. The velocity distribution and the detailed positions and velocities of all the particles may also be printed, or written on a file (or a magnetic tape) for future uses (e.g., the calculation of velocity correlations etc.)

2.6. *Main Part*

At the beginning of each time step, $NN = IT(1)$ is recorded, and $DT = DTT(1)$ is taken as the running time step (unless printing time is approaching). The vector $DTT(I)$ is afterwards moved:

$$\begin{aligned} DTT(I) &= DTT(I+1) - DT, \\ IT(I) &= IT(I+1). \end{aligned} \tag{5}$$

Now, a loop over all the particles is done. All particles which are not undergoing collisions are moved on straight lines:

$$\begin{aligned} X(N) &= X(N) + DT \cdot VX(N), \\ Y(N) &= Y(N) + DT \cdot VY(N), \\ Z(N) &= Z(N) + DT \cdot VZ(N). \end{aligned} \tag{6}$$

The vector $II(N)$ contains information concerning the "state of collision" of each particle: If $II(N) = 0$, the particle is not in the middle of any collision, and Eqs. (6) are used. If $N < II(N) \leqslant NT$ (NT is the total number of particles), then particle N is undergoing a collision with particle $II(N)$, and subroutine PAIR is used to calculate their final positions and velocities (see Section 4). If $0 < II(N) < N$, then particles N and $II(N)$ are undergoing a collision, and their final positions are velocities have already been calculated [when the loop was at particle II(N)].

If $NT < II(N)$, then particle N interacts with more than one particle. To save

room in the memory, the numbers of these particles are stored in $II(N)$ in the form

$$II(N) = N1 + (1 + N)\,N2 + (1 + NT)^2\,N3 + (1 + NT)^3 \cdot N4 \tag{7}$$

(no more than five particles per collision are allowed). The positions and velocities after the multiple collision are calculated by subroutine *COL* (Section 5). All N's in $II(N)$ are larger than N, hence the collision is computed when the particle with smallest index N is approached in the loop. The $II(N)$'s of all other particles are equal to this first N, and the above rule for $0 < II(N) < N$ applies here too.

If after DT the collision is terminated, namely, the particles leave the range of each other's force, the values of their $II(N)$'s are again set equal to zero.

At the end of the main loop, the time intervals for the next collisions for all particles which were undergoing collisions are found (Section 3), and put in their proper places in the vector $DTT(I)$.

Now, the particle NN is separately treated: If it is going to collide in the next time with a particle ($IJ(NN) > 0$), then the values of $II(NN)$ and of $II(IJ(NN))$ are properly set, so that II of the lower index is set to include the higher index [Eq. (7)], and II of the higher index is set equal to the lower index. If $IJ(NN) < 0$, then particle NN has now approached the wall number $-IJ(NN)$, and the proper boundary conditions are applied. In the present version, we use rigid walls, e.g.,

$$VX(NN) = -VX(NN), \tag{8}$$

for a collision with a wall perpendicular to the x axis, but these can easily be changed to periodic boundary conditions.

2.7. *Error Exits*

At the end of each time steps, the value of total energy

$$E = E_k + V = \tfrac{1}{2} \sum_{i=1}^{NT} \mathbf{v}_i^2 + V \tag{9}$$

is compared with its former value. The time step is repeated if energy is not conserved within a given error. (The positions and velocities, etc., are stored at the beginning of the main loop, for this purpose).

The time step is also repeated if subroutines PAIR or COL are entered with particles which are not in each other's range of force.

The run is stopped if the time step must be repeated more than once, or if the integration in subroutines PAIR or COL do not converge.

3. Arrangement of Time Steps

This part of the calculation is used at the beginning of a run (Section 2.4) and after each time step (for colliding particles, Section 2.6).

The time interval for the particle N to approach the wall $X = 0$, if $VX(N) < 0$, is

$$\Delta t = -X(N)/VX(N), \tag{10}$$

and to approach the opposite wall, $X = A$, if $VX(N) > 0$,

$$\Delta t = (A - X(N))/VX(N)\,(A = (NX - 1)\,a + 2a_0). \tag{11}$$

Similar calculations give the minimal time interval for the particle to approach any wall.

The main part of this routine is a loop on all other particles, except N. The procedure is similar to that of Alder and Wainwright [4], but with a few significant differences: For each pair of particles n and m we define

$$\mathbf{r}_{nm} = \mathbf{r}_n - \mathbf{r}_m\,, \tag{12}$$

$$C_{nm} = r_{nm}^2 - RMX^2, \tag{13}$$

$$\mathbf{v}_{nm} = \mathbf{v}_n - \mathbf{v}_m\,, \tag{14}$$

$$B_{nm} = \mathbf{r}_{nm} \cdot \mathbf{v}_{nm}\,, \tag{15}$$

$$D_{nm} = B_{nm}^2 - C_{nm} v_{nm}^2\,, \tag{16}$$

$$\Delta t = -(B_{nm} + \sqrt{D_{nm}})/v_{nm}^2\,. \tag{17}$$

The flow chart in Fig. 1 describes the logic of checking the state of collision of these two particles: If $C_{nm} \leqslant 0$, then n and m are inside the range of each other's force, and a collision must be undergoing. The values of $II(N)$ and $II(M)$ are thus checked and reset if necessary (See Section 2.6). If $C_{nm} > 0$, B_{nm} is checked. If $B_{nm} < 0$ then the particles are approaching each other, and will reach the range RMX after a time interval Δt if the equation

$$(\mathbf{r}_{nm} + \mathbf{v}_{nm}\Delta t)^2 = RMX^2 \tag{18}$$

has a real positive solution, given by Eq. (17).

In all other cases, no collision occurs.

After finding the minimal value of Δt for the particle N, this time interval is put in its proper place in the vector $DTT(I)$, N is put in the same place in $IT(I)$, and the event (collision with M or with a wall) is recorded in $IJ(N)$.

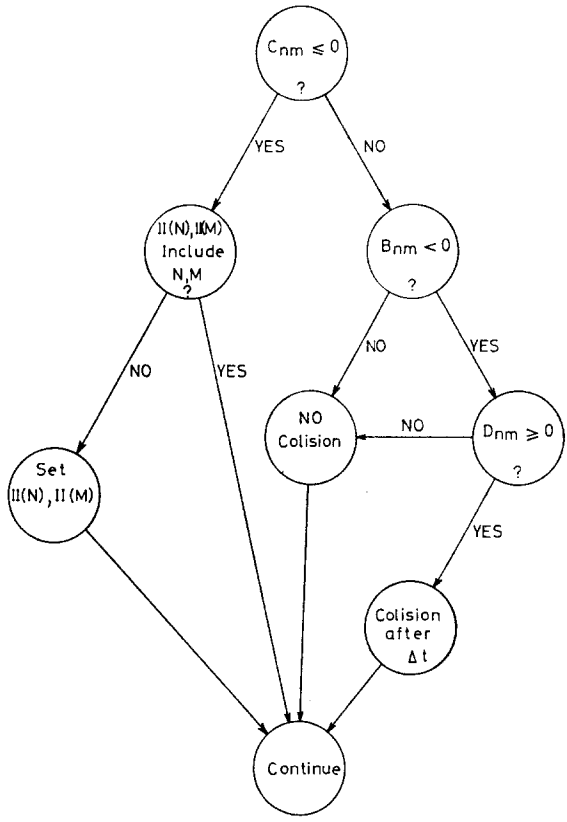

FIG. 1. Flow chart for collision calculation.

4. SUBROUTINE PAIR

This subroutine is used to calculate the new positions and velocities of two colliding particles, after a given time interval *DT*.

The simplest method of solution is, of course, to solve the 12 differential Eqs. (1) for the six coordinates and six velocities of the two particles. This method is used by Rahman [2] for the many-particle case. Clearly, this procedure is both time consuming and not very accurate, due to the large number of equations. Obviously, this subroutine is the most used in the program, and therefore special attention must be given to any possible reduction in the time of calculations in it. The simplest way to reduce the number of differential equations to be solved is to use the conservation laws which hold for the binary collision. In all cases with no

external forces, the total linear momentum is conserved, and therefore the center of mass moves on a straight line. Defining

$$\mathbf{R} = \tfrac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2), \qquad \mathbf{V} = \tfrac{1}{2}(\mathbf{v}_1 + \mathbf{v}_2), \tag{19}$$

we have

$$\mathbf{R}(DT) = \mathbf{R}(0) + DT \cdot \mathbf{V} \tag{20}$$

(we take all masses equal to 1). The number of differential equations is thus reduced to six, in the relative position and velocity

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2\,, \qquad \mathbf{v} = \mathbf{v}_1 - \mathbf{v}_2\,: \tag{21}$$

$$d\mathbf{r}/dt = \mathbf{v}, \qquad d\mathbf{v}/dt = 2\mathbf{F}, \tag{22}$$

with the force $\mathbf{F}$ derivable from the given potential.

In most cases, the center of mass energy E and the relative angular momentum $\mathbf{L}$ are also conserved. These conservation laws enable us to further reduce the number of differential equations to 2, in the distance between the particles r and the azimuthal angle around $\mathbf{L}$, θ. Especially, for a central potential $V(r)$ we have [14]

$$dr/dt = \pm 2[E - V(r) - (l^2/r^2)]^{1/2} \tag{23}$$

$$d\theta/dt = 2l/r^2, \tag{24}$$

where l is the magnitude of $\mathbf{L}$,

$$l = |\,\mathbf{L}\,| = \tfrac{1}{2}\,|\,\mathbf{r} \times \mathbf{v}\,|\,. \tag{25}$$

In the plane orthogonal to $\mathbf{L}$ we define two orthogonal unit vectors

$$\mathbf{i} = \mathbf{r}/r, \qquad \mathbf{j} = [r^2\mathbf{v} - (\mathbf{r}\cdot\mathbf{v})\,\mathbf{r}]/|\,r^2\mathbf{v} - (\mathbf{r}\cdot\mathbf{v})\,\mathbf{r}\,| \tag{26}$$

(the values of $\mathbf{r}$ and $\mathbf{v}$ are taken at $t = 0$). The initial value of θ is taken as zero. The final values of $\mathbf{r}$ and of $\mathbf{v}$ are then given by

$$\begin{aligned} \mathbf{r}(DT) &= r(DT)[\cos\theta(DT)\cdot\mathbf{i} + \sin\theta(DT)\cdot\mathbf{j}], \\ \mathbf{v}(DT) &= \frac{\dot{r}(DT)}{r(DT)}\cdot\mathbf{r}(DT) + \dot{\theta}(DT)\cdot r(DT)\cdot[-\sin\theta(DT)\mathbf{i} + \cos\theta(DT)\mathbf{j}] \end{aligned} \tag{27}$$

($\dot{r}$ and $\dot{\theta}$ are given by (23) and (24)).

The values of $\mathbf{r}_1$, $\mathbf{r}_2$, $\mathbf{v}_1$ and $\mathbf{v}_2$ are then found by

$$\begin{aligned} \mathbf{r}_1 &= \mathbf{R} + \tfrac{1}{2}\mathbf{r}, \qquad \mathbf{r}_2 = \mathbf{R} - \tfrac{1}{2}\mathbf{r}, \\ \mathbf{v}_1 &= \mathbf{V} + \tfrac{1}{2}\mathbf{v}, \qquad \mathbf{v}_2 = \mathbf{V} - \tfrac{1}{2}\mathbf{v}. \end{aligned} \tag{28}$$

Although Eq. (23) has been written for a central potential, it may be extended to more general potentials which conserve angular momentum. In all the cases where V may be written as a function of r and of $\dot{r}$ ($\dot{\theta}$ may be replaced using l), $\dot{r}$ of Eq. (23) may be replaced by a solution of the equation

$$E = \tfrac{1}{4}\dot{r}^2 + (l^2/r^2) + V(r, \dot{r}) \tag{29}$$

in $\dot{r}$.

Obviously, there is an ambiguity in the sign in Eq. (23). This sign is found as follows: The initial sign is equal to that of $(\mathbf{r}(0) \cdot \mathbf{v}(0))$. This sign is used until the argument $(E - V - l^2/r^2)$ receives a negative value. At this point, the value of r corresponding to the zero value of the above argument (closest approach of the particles if the initial sign is negative) is found by interpolation, and the sign in Eq. (23) is changed. If the time of this closest approach (which is also found by interpolation) is shorter than $\frac{1}{2} \cdot DT$, then the solution of the differential equations is stopped, the values of r, θ and t are set at $r(0)$, 2θ and $2t$ (using the symmetry property of the motion), and the solution is continued from this point. If not, the solution is continued. If the value of r at any time t becomes larger than RMX, the solution is stopped, and the final values of $\mathbf{r}$ and $\mathbf{v}$ are obtained by

$$\begin{aligned} \mathbf{r}(DT) &= \mathbf{r}(t) + \mathbf{v}(t) \cdot (DT - t) \\ \mathbf{v}(DT) &= \mathbf{v}(t). \end{aligned} \tag{30}$$

Many procedures may be used for the actual solution of Eqs. (23)–(24). The preliminary results presented in Section 6 have been obtained using the Runge–Kutta–Gill method, with

$$\Delta t = \epsilon r_m / \dot{r}_{\max}, \tag{31}$$

where r_m is a typical radius (e.g., RMX), $\dot{r}_{\max}$ is the maximum value of $\dot{r}$, of the order

$$\dot{r}_{\max} = 2\left(E - V_{\min} - \frac{l^2}{RMX^2}\right)^{1/2} \tag{32}$$

and ϵ is of the order 10^{-2}. This method has proved to be quite satisfactory, especially with the high demands for accuracy which we discuss in Section 6.

For less restrictive demands of accuracy, other difference schemes may be used. Special attention must be paid to the time reversibility of the scheme, since we do not want any irreversibility property of the system due to numerical causes [15].

It should be noted that Eq. (23) does not depend on θ, and therefore may be

solved separately, with higher accuracy restrictions. After obtaining the values of $r(t_i)$, we may solve (24) simply by any integration procedure, e.g.,

$$\theta(t_{i+1}) - \theta(t_i) = l(t_{i+1} - t_i)\left(\frac{1}{r(t_i)^2} + \frac{1}{r(t_{i+1})^2}\right) \tag{33}$$

(note that this scheme is time reversible!)

A possible procedure of finding $r(t_i)$ is the following: Eq. (23) may be written in the form

$$dt = \pm dr/2\left(E - V(r) - \frac{l^2}{r^2}\right)^{1/2}, \tag{34}$$

and hence

$$t_{i+1} - t_i = \pm\tfrac{1}{2}(r_{i+1} - r_i)\left(\frac{1}{[E - V(r_i) - l^2/r_i^2]^{1/2}} + \frac{1}{[E - V(r_{i+1}) - l^2/(r_{i+1}^2)]^{1/2}}\right). \tag{35}$$

r_i may be changed in equal steps, chosen properly, and t_i may be calculated through Eq. (35). This way, no iterations are necessary. After finding $t_i(r_i)$, Eq. (33) may be used to calculate the values of $\theta(t_i)$. All other details of the procedure (choosing the sign of Δr according to the proper sign in Eq. (34), stopping the calculation at the point of closest approach, etc.) remain unchanged.

Special attention must be given to the choice of r_i near the point of closest approach, at which the denominator of Eq. (34) vanishes, If for some value of i, $[E - V(r_{i+1}) - l^2/r_{i+1}^2]$ becomes negative, smaller values of Δr are used until the absolute value of this expression becomes small enough, and then the motion is reversed. This usually wastes some computation time if high accuracy is demanded. For usual purposes, however (without the high demands mentioned in Section 6), this procedure is much less time-consuming than the Runge–Kutta–Gill procedure. For our purposes, however, the Runge–Kutta proved to be better.

5. Subroutine COL

This subroutine is used to calculate the new positions and velocities of more than two colliding particles, after a given time interval DT.

Since the main purpose of the program is to deal with dilute gases, multiple collisions are relatively rare (although statistically they may occur, and the program must be prepared to calculate them). Therefore, the question of the length of run-time is less important. Also, the actual usage of the conservation laws is more difficult, and the reduction in the number of differential equations to be obtained by

it is less impressive. Therefore, we preferred here to solve the $6n$ Eqs. (1) for the n colliding particles, and to do this by the simplest method, namely,

$$\mathbf{r}_i^{\text{new}} = \mathbf{r}_i^{\text{old}} + \mathbf{v}_i^{\text{old}} \cdot \Delta t,$$
$$\mathbf{v}_i^{\text{new}} = \mathbf{v}_i^{\text{old}} + \mathbf{F}_i^{\text{old}} \cdot \Delta t, \tag{36}$$

with the accuracy obtained by taking Δt small enough (e.g., of the order $10^{-5}a/v_0$ in our units). After each step Δt, the conservation of energy is checked, and the time step is repeated, with a smaller value of Δt, if energy is not conserved within a given error.

Of course, if multiple collisions are expected to occur frequently, or if multiple-particle interactions (e.g., three-body forces) are to be investigated, this scheme may easily be modified, e.g., to the Rahman scheme [2] or to an extension of our scheme (Section 4) using some conservation laws. This is being done in a new version of the program.

6. Results and Discussion

Our main purpose in writing the present program has been to investigate the irreversible approach of a system of particles to equilibrium, and to study the effects of several factors on the H-function during this approach. Therefore, the most important property the program must have is time reversal symmetry of the numerical procedure, as already discussed in length by Buneman [15]. Even in programs with dilute gases of hard spheres, where it is much easier to control the accuracy, irreversible effects due to numerical reasons have been observed [16, 17].

Therefore, the best check for the accuracy of the program has been chosen as the calculation of the "antikinetic" evolution of the gas, as discussed by Balescu [18] and by Orban and Bellemans [17]: After a time t_0, all velocities are reversed, and the backwards evolution of the gas to its initial state, with the H-function increasing, is followed.

Naturally, if t_0 is large enough, the gas will not return to its exact initial state. Still, if this t_0 is not much smaller than the time at which the number of collisions is of the order of the number of particles, the program may be considered appropriate for our type of investigations.

As preliminary results, mainly to show the possibilities, we present here two cases. In Fig. 2, the Boltzmann H-function for 100 particles, in a two-dimensional box, with the interaction potential

$$V(r) = e^{-r/\beta}, \qquad \beta = 0.01, \qquad RMX = 5\beta \tag{36}$$

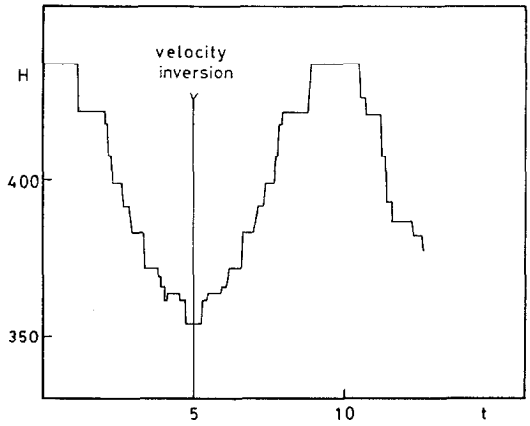

FIG. 2. The Boltzmann H-function for 100 particles in a 2-dimensional box, with an exponential potential and with the velocities inverted after 5 time units.

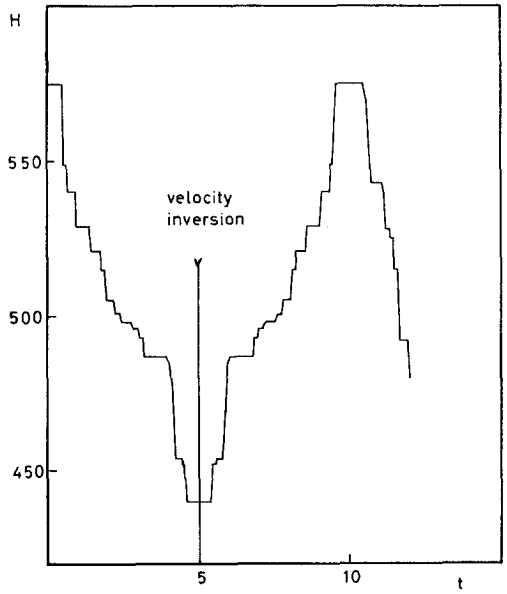

FIG. 3. The Boltzmann H-function for 125 particles in a 3-dimensional box, with a Lennard–Jones potential and with the velocities inverted after 5 time-units.

and with $a = b = 1, v_0 = 1$ (the potential is set equal to zero at RMX, and reduced linearly to this value from the point $RMXX = 0.98 \cdot RMX$). The time t_0 of the velocity inversion has been chosen as $t_0 = 5$ in our units, corresponding to 18 binary collisions (no multiple collisions). As may be seen from the figure, the

H-function retraces its path to its initial value at $2t_0$. The mean velocity returns to its initial value (1) to within 10^{-9}, and the particles return to their initial lattice points to within 10^{-4}.

Figure 3 presents another example. Here, 125 particles were run in a 3-dimensional box, with a Lennard–Jones potential,

$$V(r) = \epsilon[(\beta/r)^{12} - (\beta/r)^6], \qquad \epsilon = 100, \qquad \beta = 0.1, \qquad RMX = 2.25\beta. \tag{37}$$

Again, the velocities are inverted after $t_0 = 5$ units, corresponding here to 25 collisions, and the results are obvious from the figure.

The program was run on a *CDC*-6600 computer, and the runtime has been of the order of 1.5 secs/collision in the 2-dimensional case and 7secs/collision in the 3-dimensional case.

These results seem quite satisfactory, and the program is thus ready for the comparison of different types of potentials, for the use of noncentral or time-irreversible potentials, etc. These will be described in future publications. A listing of the program, for similar purposes, may be obtained from the author.

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