The One-Dimensional Boltzmann Gas:
The Ergodic Hypothesis and the Phase Portrait of Small Systems

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The concept of ergodicity and its application to microcanonical systems composed of few particles of different masses are clarified. The distribution functions in position and velocity are theoretically derived and numerically verified. Moreover, we deal with a one-dimensional Boltzmann gas where the order relation (connected to the one dimensionality) brings constraints depending on the two classes of boundary conditions enforced (reflecting, periodic). The numerical simulations on a one-dimensional Boltzmann gas act as real experiments and allow us to play on the constraints to which the system is subjected.

1. INTRODUCTION

The study of one-dimensional N-body systems has been a very active field in these last 30 years and has produced many interesting results for the following reasons. The exact treatment on a computer of such system is possible for three interesting cases: the plasma and gravitational gas, hard-core segments, and the Boltzmann gas. The Boltzmann gas, the simplest of the three cases, is fully treated in this paper and gives nontrivial results, as we are going to prove.

A theoretical treatment is also possible due to the existence of an order relation which allows one to perform the integral of statistical mechanics in a telescopic way. This fact, first recognized for the plasma by Lenard,[1]

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was extended to the hard-core segments[2] and is here applied to the Boltzmann gas.

Although one-dimensional systems often have different behaviors compared to three-dimensional ones, they may exhibit features which strain the theory up to its limit. Such is the difference between the evolution of a global population and a test population in plasma physics.[3] Taking a large number of particles ($N \sim 10,000$), we can construct an initial set of velocities which takes into account all the particles and then follow its time evolution. This set of velocities defines the global one-particle distribution function. On the other hand, taking a subset of this global population, for example, initially in a range of velocities, we get, in a similar way, the relevant one-particle distribution function of these "distinguished particles." In the plasma case, the global distribution does not relax, while the distinguished distribution function relaxes to the global one. Of course all particles interact: introducing the "distinguished particles" is only possible in a computer experiment, while from a theoretical point of view this concept is quite interesting. The one-dimensional Boltzmann gas, if constituted of particles of the same mass, shows the same behavior (see Section 2 for the dynamics of the Boltzmann gas). In this case only binary interactions appear and the relaxation of any distinguished distributions toward the global distribution (which does not relax) is rather easy to understand. The surprise comes from the plasma case, where all the particles interact with each other with long-range forces. We add that in the plasma case this is only true to first order in the so-called plasma parameter.

Now, to be more precise, this work was undertaken with the following goals:

1. To test the ergodic hypothesis for microcanonical systems with a low number of particles (two, three, and more). A failure of this hypothesis for the gravitational case was reported by Hohl and Broaddus,[4] Reidl and Miller,[5] and Mineau *et al.*[6]

2. To study the case of particles of different masses. In the one-dimensional Boltzmann gas this hypothesis is needed to avoid trivial global behavior. It turns out that this case points out the correct way to build the uniformly dense energy hypersurface.

3. To check the differences between reflective and periodic boundaries (especially important for small systems).

The remainder of the paper is organized in four sections. Section 2 gives the model and the numerical code. The treatment for reflective boundaries, first of the velocity space, then of the configuration space, is

given in Section 3. The two parts of Section 4 deal with the same questions, but for the periodic boundary case. Finally, our conclusions are given in Section 5.

2. MODEL AND NUMERICAL CODE

The one-dimensional system is composed of points constrained to move on a straight line. The particles are hard-core particles and interact only when they collide. During a collision, kinetic energy and momentum are conserved. Due to the fact that the potential is infinite, particles are not allowed to cross each other. This is the origin of an order relation which will play a central role in the theory.

If the particles have the same mass, they exchange their velocity in the collision. Another point of view is to say that the particles freely pass through each other keeping their velocity. Then all the particles have a free motion. In order to obtain some change, one must consider a system of particles of different masses.

Two kinds of systems have been studied. For the first one, the particles are confined in a box with reflective edges. When a particle reaches one edge, its velocity is inverted. This procedure does not conserve the total momentum, but keeps constant the kinetic energy, which is the only invariant of the motion. In addition, because of the shape of the potential, the first particle is always localized between the left edge and the second particle; this second particle is localized between the first and the third one; and so on. In the second case the system is periodic and when a particle leaves the box through one side, it enters the other side with the same velocity. The system can be visualized as a circle where the edges gathered at a single point can take place anywhere on the circle.

In the case of a one-dimensional system, the motion of the particles is very easy to treat. Between two collisions, the particles have a free motion and the program has just to compute the collision times between all pairs of neighbors, to find the smallest of these collision times, to give the new position and velocities to the corresponding pair of particles (these position and velocities after the collision are now the new initial conditions of motion of these two particles), and to reiterate the calculation. As a collision does not concern all the particles, we do not need to update the positions and velocities of all the particles, provided we keep for each the time at which its position and velocity were recorded. Obviously for each kind of edge a special treatment has to be added to the general scheme. Note that this scheme is exact and introduces no error except the roundoff errors due to the finite number of digits.[7] When N increases, the sorting out of the next smallest collision time very quickly absorbs the quasitotality

of the computer time if special techniques are not used.[8] This is, of course, of no importance for small N.

The subscript i in the variables of position x_i, velocity v_i, and mass m_i is connected to the ith particle by order of increasing position (for all the simulations in the case of reflecting edges and at the initial time in the periodic box case). The positions of the edges are $-x_0$ and x_0, where $x_0 = 0.5$. Twice the total energy is set to one for all the simulations.

3. REFLECTING-EDGE BOX

Let us first consider the case of the reflecting-edge box. Then the only constraint of the system is the total energy.

Numerical simulations have been performed with various numbers N of particles of different masses, which allows us to construct the velocity distribution function for each particle. This is done by collecting the velocities at regular time intervals Δt, where Δt is large enough to ensure a few collisions between two particles preventing two successive samples from being too correlated. Before a particle of mass m collides with its neighbor, it travels a mean distance of $2x_0/N$, with a mean velocity of $(2E/mN)^{1/2}$ (this will be verified by the equipartition of the energy E). Taking the largest amount of time given by the heaviest particle, we roughly consider $\Delta t = 10 \cdot 2x_0(m/2EN)^{1/2}$. The time of the simulations is set to ensure a set of 10,000 data. Initial positions and velocities are taken at random under the constraints of the system (total energy, etc.).

The microcanonical theory tells us that the point must be taken at random with uniform density on the surface of constant total energy, the axis being p (momentum axis). Since usually the masses are equal, we can take v or $p = mv$. Here with different masses we must take as axis the value $p_i/m_i^{1/2}$ (or $m_i^{1/2}v_i$) in order to recover the experimental results. Note that the equipartition of the energy for all particles is consequently automatically obtained. This need of taking $p_i/m_i^{1/2}$ to obtain the uniform density on the constant-energy surface is hardly mentioned in statistical physics books.

In the Boltzmann-gas case, the total energy reduces to kinetic energy. For $N = 3$, the corresponding surface is a sphere of radius equal to the root of twice the total energy E. Taking constant the probability of finding the system at each point on the surface and projecting on each axis, one finds the distribution function in "velocity" of one particle. This calculation is extended to every value of N and reads (see Appendix A for details)

$$f_N(z_i) = \frac{1}{\text{Norm}_{N-2}} (1 - z_i^2)^{(N-3)/2} \tag{1}$$

where Norm_N is a factor of normalization given by

$$\mathrm{Norm}_{2N} = 2\pi \frac{(2N-1)!!}{(2N)!!} z_{max} \tag{2}$$

$$\mathrm{Norm}_{2N+1} = 2 \frac{(2N)!!}{(2N+1)!!} z_{max} \tag{3}$$

using the notation of Gradshteyn and Ryshik[9]: !! means the product of all even (or odd) numbers from the indicated one to two (or one). The normalized variable z_i reads

$$z_i = \frac{m_i^{1/2} v_i}{z_{max}} \tag{4}$$

where z_{max} is the maximum possible value independent, in this case, of the mass of the particle:

$$z_{max} = (2E)^{1/2} \tag{5}$$

Results of numerical simulations for systems containing, respectively, $N = 3$, 4, and 5 particles are given in Figs. 1a–1c. The distribution function of one of the particles of each system is represented with a histogram shape and the theoretical function is drawn as a continuous line. Numerical experiments have been performed for up to six particles showing a very good agreement with the theory.

Obviously, increasing in formula (1) the number of particles to infinity while keeping the energy per particle $\varepsilon = E/N$ fixed will yield the Maxwell distribution function. The variable $m^{1/2} v$ appears explicitly.

The case $N = 2$ exhibits a certain lack of ergodicity. The phase portrait in velocity space (see Fig. 2a) shows that after a rather long time the circle
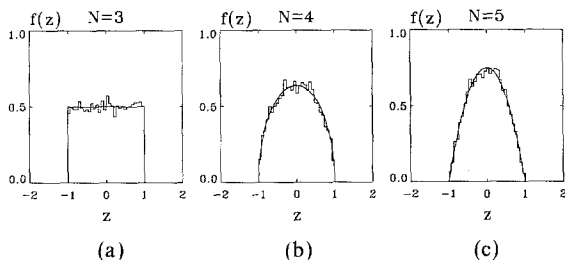

Fig. 1. Velocity distribution function of one particle of a system, confined in a reflecting-edge box, containing (a) $N = 3$ particles of mass $m_1 = 1$, $m_2 = 3$, and $m_3 = 6$; (b) $N = 4$ particles of mass $m_1 = 1$, $m_2 = 3$, $m_3 = 6$, and $m_4 = 11$; (c) $N = 5$ particles of mass $m_1 = 1$, $m_2 = 3$, $m_3 = 6$, $m_4 = 11$, and $m_5 = 19$.

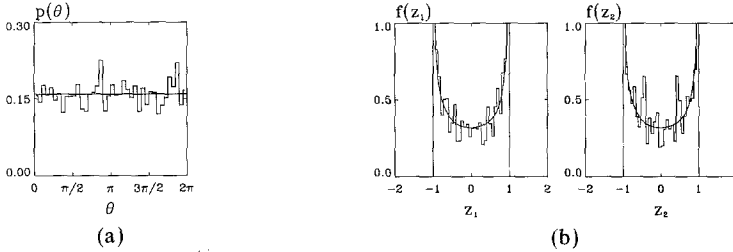(a)   (b)

Fig. 2.   Results for $N = 2$ particles of mass $m_1 = 1$ and $m_2 = 5$, confined in a reflecting-edges box. (a) Histogram of the repartition of the representative point on the circle in volocity space; (b) velocity distribution function for particle 1 and for particle 2.

is not uniformly covered. Figure 2b shows the resulting $f_2(z_1)$ and $f_2(z_2)$. The reason is the following. First, let us define C as a collision between the two particles and I as a collision of one of the particles with an edge (I only changes the sign of one of the velocities). Two successive collisions (CC) between the same two particles will bring back the two velocities to their initial values. Of course this kind of event can only happen with two particles moving in a periodic edge box. In the present case, one particle, at least, must collide with a wall. If only one particle experiences a wall collision, the next particle collision (CIC) will change the velocities. But if both particles collide with the wall (CIIC), the next particle collision will bring back the velocities (or opposite velocities) experienced before the first particle collision,

$$CIIC = \pm 1 \tag{6}$$

Note that the employed notation does not take care of the label of the particle which collides with the edge because it has, in fact, no importance: if the two collisions with the wall (II) concern the two particles, the sequence CIIC is equal to -1, and is equal to 1 if II concerns the same particle. Obviously such a situation never arises in a real simulation, but can be envisaged in the analysis of a given sequence. Consider, for example, the following sequence:

$$\text{CICICIICIC} \tag{7}$$

Since the underlined sequence CIIC $= \pm 1$, ignoring the trivial change of sign, we can simplify by CIIC and obtain

$$\text{CICIIC} \tag{8}$$

The final result for this example is CI, and this sequence gives in fact only two new points in velocity space. This explains briefly the very low efficiency of long sequences.

Finally, for special values of the mass ratio, the points in velocity space will be trapped on a finite number of sites. We have proved, for example, that a ratio of 3 gives only 12 possible sites and $(\sqrt{2}+1)/(\sqrt{2}-1)$ only 16 (the entire proof will be given in a future paper). Consequently, these cases are not relevant to the ergodic theory.

The density of the three-dimensional Boltzmann gas is homogeneous. Such a property cannot be obtained in the one-dimensional system because of the order relation of the positions of the particles.

Nevertheless, supposing that the density of the representation point in the N-dimensional configuration space is homogeneous with respect to the constraint $-x_0 < x_1 < x_2$ and so on, we can obtain the cutoff $x_1 - x_2$, or $x_2 - x_3,...,$ of this configuration space. The distribution in position of one particle can then be deduced. It depends on the relative position of the particle but not on its mass. The position distribution function of particle i in a system containing N particles reads (see Appendix B for details)

$$\rho_i(x) = \frac{N!}{(2x_0)^N} \frac{(x_0 - x_i)^{N-i}}{(N-i)!} \frac{(x_0 + x_i)^{i-1}}{(i-1)!} \tag{9}$$

The results for a simulation containing $N = 3$ particles are given in Fig. 3, with the theoretical value shown as a straight line. The theoretical curve fits the experimental one. The summation of the three distribution functions gives a constant density over all the box as shown in Fig. 4 in the case of the previous simulation.

This fact could be related to a simple thermodynamic result. Consider a box containing three gases (or more) of density n_1, n_2, and n_3 constituted of particles of mass m_1, m_2, and m_3, respectively, and separated by moving, perfectly reflecting walls. These walls ensure that the three gases are not mixed and keep their relative positions as the hard-core particles in
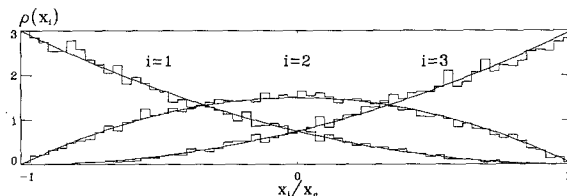

Fig. 3.   Position distribution function of one particle of a system, confined in a reflecting-edge box, containing $N = 3$ particles of mass $m_1 = 1$, $m_2 = 3$, and $m_3 = 6$.
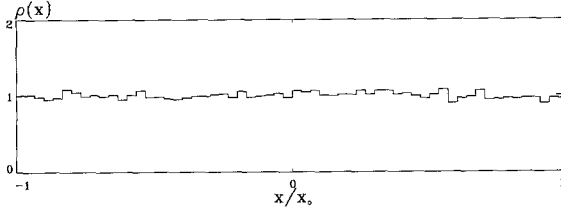
Fig. 4. Sum of the three distribution functions give Fig. 3.

our system do. After a transient time, the different pressures on the walls will be the same, and supposing that the temperatures of the different gases are also equal, i.e., supposing thermodynamic equilibrium (in order to follow the equipartition in energy of the hard-core particle system), the densities will be equal ($n_1 = n_2 = n_3$). Consequently, neglecting the nature of the different gases, the density all over the box will be constant. In our system, the walls are not strictly localized but are symbolized by the collisions between two particles. Nevertheless, one particle mimics the behavior of a very large system. This shows that, in a certain sense, the behaviors of very large and small systems are not so different.

4. PERIODIC BOX

Let us now consider the case of a periodic box. The system is thus subjected to the conservation of both total energy and total momentum.

The total momentum is equal to zero and the center of mass of the system is put initially in the center of the periodic box. As in previous cases, the representative point of the system is supposed to be uniformly distributed on the allowed surface (or hypersurface) which is the intersection between the sphere (or hypersphere), due to the conservation of energy, and the plane (or hyperplane), due to the second invariant. Supposing that the reflective edges of the previously studied system play the role of one particle of infinite mass, one can deduce from (1) the theoretical value of the distribution function in the case of a periodic box:

$$f_N(z_i) = \frac{1}{\text{Norm}_{N-3}} (1 - z_i^2)^{(N-4)/2} \tag{10}$$

Norm_N is the normalization factor defined by (2) or (3) and $z_{i\max}$, the maximal value of z_i defined by (4), is given by the technique of Lagrange multipliers (see Appendix C for details):

$$z_{i\max}^2 = \frac{\sum_{j=1, j \neq i}^{N} m_j}{\sum_{j=1}^{N} m_j} 2\varepsilon \tag{11}$$

Formula (10) is similar to formula (1) except for the power $(N-4)/2$ and the value of $z_{i\max}$, as a result of the conservation of momentum. The same shape of the distribution function is obtained in both cases if the periodic system contains one more particle than the reflective-edges system. As in the previous case, upon increasing N to infinity while keeping $\varepsilon = E/N$ constant, one recovers the Maxwellian.

Numerical simulations have been performed for different numbers of particles and masses. The data have been collected in the same way as previously and the results for $N=3$, 4, and 5 particles are respectively given in Figs. 5a–5c. The agreement with theory is quite good, as shown by the fitting between theoretical and experimental curves. Notice that the theory is valid even for $N=3$, which corresponds to $N=2$ in the case of a reflective-edge box, where a lack of ergodicity appears in the previous section.

For the density, the situation is a little more complicated than for the reflective-edges system. Particles can freely pass from one edge to the other and although all combinations of positions are not possible, the previous order relation is no longer preserved. Considering the steadiness of the center of mass, as long as no particles have reached an edge, or when one or two particles have passed from one edge to the other, one can obtain the phase portrait of $x_1 - x_2$ or $x_2 - x_3$.

In the case $N=3$ the phase portrait is easily obtained by considering the different cases where zero, one, or two particles have crossed the system.

If no particles have reached the edges, the constraints are

$$\sum_{i=1}^{3} m_i x_i = 0, \qquad -x_0 < x_1 < x_2 < x_3 < x_0 \qquad (12)$$
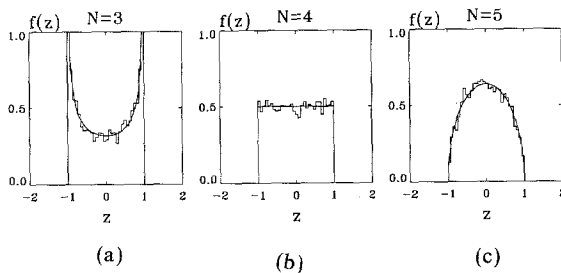

Fig. 5. Velocity distribution function of one particle of a system, confined in a periodic box, containing (a) $N=3$ particles of mass $m_1 = 1$, $m_2 = 3$, and $m_3 = 6$; (b) $N=4$ particles of mass $m_1 = 1$, $m_2 = 3$, $m_3 = 6$, and $m_4 = 11$; (c) $N=5$ particles of mass $m_1 = 1$, $m_2 = 3$, $m_3 = 6$, $m_4 = 11$, and $m_5 = 19$.

and give the allowed area of the representative point:

$$-\frac{m_1}{m_2+m_3}\,x_1 < x_3 < -\frac{m_1+m_2}{m_3}\,x_1 \tag{13}$$

If, for example, particle 1 crosses the left side and consequently enters the box through the right side, the constraints are

$$\sum_{i=1}^{3} m_i x_i = 2m_1 x_0, \qquad -x_0 < x_2 < x_3 < x_1 < x_0 \tag{14}$$

The allowed area, in this case, reads

$$-\frac{m_1}{m_2+m_3}\,x_1 + 2\,\frac{m_1}{m_2+m_3}\,x_0 < x_3 < x_1 \tag{15}$$

The different cases have to be studied, but it can be proved that only two particles at most can cross the edges, whatever the relative values of the masses of the three particles are. If $m_1 < m_2 + m_3$ and $m_3 < m_1 + m_2$, particle 1 can leave the box through the right side and particle 3 through the left side. If $m_3 > m_1 + m_2$, particles 1 and 2 can leave the box through the left side and if $m_1 > m_2 + m_3$, particles 2 and 3 can leave the box through the right side.

Figure 6a gives the theoretical phase portrait of the position of particle 3 versus particle 1 for $m_3 = m_1 = m_2/3$ (particles 1 and 3 can leave the box) and Fig. 6b gives the experimental one.

The position distribution function can be easily derived from the phase portrait such as those given in Fig. 6b for each of the three particles,
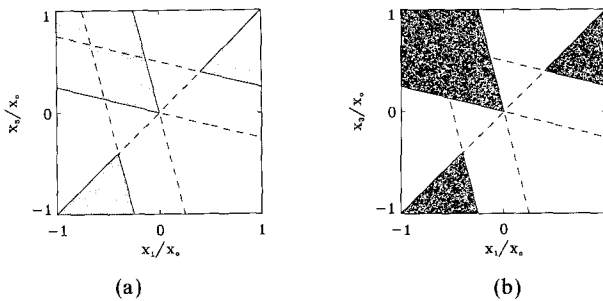

(a)   (b)

Fig. 6. Position x_2 versus position x_1 for a system containing $N = 3$ particles of mass $m_1 = 1$, $m_2 = 3$, and $m_3 = 1$ confined in a periodic box. (a) Theoretical phase portrait. The shaded area gives the allowed surface. (b) Experimental phase portrait.
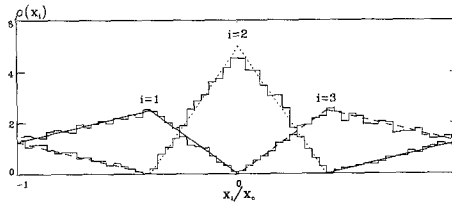
Fig. 7.   Position distribution function of one particle of a system, confined in a periodic box, containing $N = 3$ particles of mass $m_1 = 1$, $m_2 = 3$, and $m_3 = 1$.

supposing the probability of the point to be uniform in the shaded area (see Fig. 7).

The results of the simulation for the case $m_1 = 1$, $m_2 = 3$, $m_3 = 6$ (particles 1 and 2 can leave the box), previously studied, with reflective edges (Section 3), are given in Figs. 8a and 8b (theoretical and experimental phase portraits) and Fig. 9 (position distribution function).

Contrary to the previous case, the summation of the three distributions does not give a constant. Nevertheless, when the three masses are nearly equal this distribution goes to a constant.

On the other hand, if the total momentum is not initially set to zero, the distributions of each of the particles are constant all over the box.

5. CONCLUSION

The study of this very simple system, the Boltzmann gas, allows us to obtain theoretical results as well as to perform exact numerical simulations.

In both cases, with reflective edges and a periodic box, ergodicity is obtained. Nevertheless, for two particles moving in a reflective-edge box,
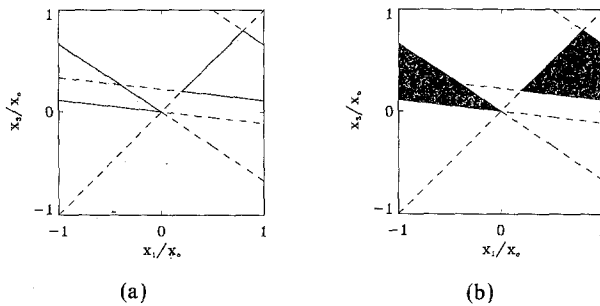

(a)

(b)

Fig. 8.   Position x_2 versus position x_1 for a system containing $N = 3$ particles of mass $m_1 = 1$, $m_2 = 3$, and $m_3 = 6$ confined in a periodic box. (a) Theoretical phase portrait. The shaded area gives the allowed surface. (b) Experimental phase portrait.
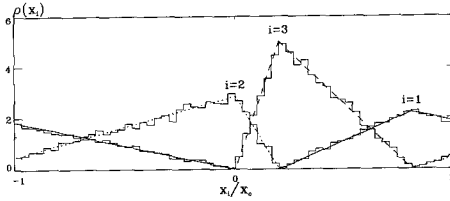
Fig. 9.   Position distribution function of one particle of a system, confined in a periodic box, containing $N = 3$ particles of mass $m_1 = 1$, $m_2 = 3$, and $m_3 = 6$.

the dynamical process does not drive so easily toward ergodicity, while for special values of the mass ratio the system is not ergodic at all.

The main result of the simulation is that uniform-density surface theory is valid if applied to the "right" variable $P/\sqrt{m}$, where P is the momentum and m the mass of a particle. Consequently, whatever masses the particles take (except if all are equal), the theoretical distribution functions are recovered, depending only on the number of particles the system contains.

The equipartition of the kinetic energy, a property of the canonical ensemble, is consequently automatically recovered in this case, a consequence of the equiprobability of finding the representative point on the sphere (or hypersphere). Sometimes the concepts of ergodicity and nonintegrability are vaguely associated. Consequently, it may be interesting to underline that the system is piecewise integrable (see the numerical code, Section 2), but nevertheless ergodic. Only the succession of the collision times, although it is exactly calculated by the code, gives an idea of a random process which changes the velocities of the particles (but only if the masses are different). On the other hand, some systems (for example, reflective edges, $N = 2$, mass ratio of 3) exhibit a nonergodicity which comes from the special property of the collision matrix, while they are no more or less piecewise integrable than the others.

The Boltzmann gas is usually associated with a uniform distribution of position. This is valid for the three-dimensional case. Nevertheless, the one-dimensionality imposes an order relation which keeps the memory of the initial values of the positions. However, for a periodic box, invariance by translation is recovered if the momentum is not strictly zero.

Due to the infinity of the potential, the constraint of the order relation between particles imposes the position distribution functions shown above. Nevertheless, a system in which particles are allowed to cross each other (and consequently interact with a finite potential) can be introduced to obtain constant values of the position distribution functions.

At least this paper has given a good demonstrative illustration of the computer approach of ergodic theory and of phase space properties for a system that finally is not so trivial.

APPENDIX A

Here were calculate the theoretical 'velocity" distribution function in the case of a reflective-edge box. The representative point of the system containing n particles is on a hypersphere. The projection on an axis of the element dV_n of the total hypersurface V_n of the hypersphere gives the contribution dz, and then one writes

$$f(z)\, dz = p(V_n)\, dV_n \qquad (A.1)$$

where $p(V_n)$ is assumed to be a constant which much normalize to 1 the probability of finding the point on the total surface:

$$p(V_n) = \frac{1}{V_n} \qquad (A.2)$$

Then

$$f(z) = \frac{1}{V_n}\frac{dV_n}{dz} \qquad (A.3)$$

For $N = 2$ particles, the representative point is on a circle of radius $R = (2E)^{1/2}$. The coordinates are $z_i = m_i^{1/2}v_i$ for $i = 1, 2$. With the notations of Fig. 10 one writes

$$\cos\theta = \left[1 - \left(\frac{z}{R}\right)^2\right]^{1/2} \qquad (A.4)$$
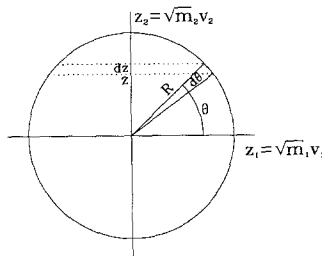
$$dR\sin\theta = R\cos\theta\, d\theta = dz \qquad (A.5)$$

Fig. 10.

and

$$dV_2 = R\, d\theta \tag{A.6}$$

$$V_2 = 2\pi R \tag{A.7}$$

so

$$f(z) = \frac{1}{\pi R} \frac{1}{[1 - (z/R)^2]^{1/2}} \tag{A.8}$$

For $N = 3$ particles:

$$dV_3 = 2\pi(R \cos \theta) R\, d\theta \tag{A.9}$$

$$V_3 = 4\pi R^2 I_1 = 4\pi R^2 \tag{A.10}$$

with

$$I_n = \int_0^{\pi/2} \cos^n \theta\, d\theta \tag{A.11}$$

For N particles:

$$dV_n = 2^{(n-1)}\pi I_{n-3}(R \cos \theta)^{n-2} R\, d\theta \tag{A.12}$$

$$V_n = 2^n \pi R^{n-1} I_{n-3} \cdot I_{n-2} \tag{A.13}$$

With the help of Eqs. (A.4) and (A.5), (A.12) reads

$$dV_n = 2^{n+1}\pi I_{n-3}\, R^{n-2} \left[1 - \left(\frac{z}{R}\right)^2\right]^{(n-3)/2} dz \tag{A.14}$$

Using Eq. (A.13), one finds

$$f(z) = \frac{1}{2R I_{n-2}} \left[1 - \left(\frac{z}{R}\right)^2\right]^{(n-3)/2} \tag{A.15}$$

APPENDIX B

Here we calculate the theoretical position distribution function in the case of a reflective-edge box containing N particles.

The distribution function $\rho(x_i)$ for particle i is found by cutting the configuration space at $x_i = \text{const}$, then applying successive integrations and taking into account the relation order

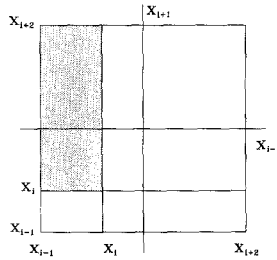$$-x_0 < x_1 \cdots x_{i-1} < x_i < x_{i+1} \cdots x_N < x_0 \tag{B.1}$$

Fig. 11.

This leads to Fig. 11 and the following telescopic integral, where it has been supposed that the available area (shaded area in Fig. 11) is uniformly distributed:

$$\rho(x_i) = \int_{-x_0}^{x_i} \cdots \int_{x_i-4}^{x_i} \int_{x_i-3}^{x_i} (x_i - x_{i-2})\, dx_{i-2}\, dx_{i-3} \cdots dx_1$$

$$\times \int_{x_i}^{x_0} \cdots \int_{x_i}^{x_{i+3}} \int_{x_i}^{x_{i+2}} (x_{i+2} - x_i)\, dx_{i+2}\, dx_{i+3} \cdots dx_N \qquad \text{(B.2)}$$

After a little algebra, one finds

$$\rho(x_i) = \frac{1}{S_N} \frac{(x_0 - x_i)^{N-i}}{(N-i)!} \frac{(x_0 + x_i)^{i-1}}{(i-1)!} \qquad \text{(B.3)}$$

with $S_N = (2x_0)^N/N!$, which corresponds to the total available volume of the hypercube of dimension N, taking account of relation (B.1).

APPENDIX C

Here we calculate the maximal value of $z_i = z_{i\max}$ for a system of N particles enclosed in a periodic edge box.

It is given by the equation

$$\sum_{j=1}^{N} z_j^2 = 2E \qquad \text{(C.1)}$$

under the constraint

$$\sum_{j=1}^{N} m_j^{1/2} z_j = 0 \qquad \text{(C.2)}$$

Applying a small perturbation dz_j to each variable and supposing $dz_i = 0$, since we are looking for the maximum value of z_i, (C.1) and (C.2) read, respectively,

$$\sum_{j=1, j \neq i}^{N} z_j \, dz_j = 0 \tag{C.3}$$

$$\sum_{j=1, j \neq i}^{N} m_j^{1/2} \, dz_j = 0 \tag{C.4}$$

Multiplying (C.3) by μ (Lagrange multiplier) and summing with (C.4), one obtains

$$\sum_{j=1, j \neq i}^{N} (\mu z_j + m_j^{1/2}) \, dz_j = 0 \tag{C.5}$$

which gives the value of

$$z_j = -\frac{m_j^{1/2}}{\mu} \tag{C.6}$$

for each value of $j = 1, 2, ..., N$ (with $j \neq i$). The value of μ is given by putting Eq. (C.6) into Eq. (C.2), which gives the value of z_j with the help of Eq. (C.6). Putting the value of z_j in Eq. (C.1), one finds

$$z_{i\max}^2 = \frac{\sum_{j=1, j \neq i}^{N} m_j}{\sum_{j=1}^{N} m_j} 2E \tag{C.7}$$

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