A molecular dynamics study of the overpopulation phenomena in a two-region system

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By means of molecular dynamics, we have studied the time evolution of an isolated system composed of Lennard-Jones particles. The system was initially split into two regions, all the particles in the same region having the same speed. The dominant collisions leading to the overpopulation effects have been identified. It has also been shown that the more relevant features of the evolution of the system can be accurately described by means of a local equilibrium distribution function.

I. INTRODUCTION

Usually, in molecular dynamics studies one considers systems which are in steady states, at equilibrium as well as at nonequilibrium. This allows the substitution of ensemble averages by time averages.[1] Nevertheless, if one is interested in the study of the relaxation towards a steady situation from a given initial state,[2–4] time averages are not possible. Instead, one should generate a large number of microstates compatible with the initial macrostate, follow the evolution of each of them, and average over all of them. This would require a great computational effort. Another possibility is to consider a single microstate, but using a coarse-grained description, which is expected to contain the essential features of a statistical average.[2–4] In any case, the results obtained by this procedure will have a highly qualitative character.

The importance of the initial conditions on the evolution of an isolated system towards equilibrium has been shown recently by means of studies carried out with the Boltzmann equation.[5–7] When solving this equation numerically for a highly idealized two-dimension model, Tjon[5] found that the relaxation to equilibrium of the speed distribution function is not monotonous when starting from some initial conditions. The initial state considered by Tjon was homogeneous, isotropic, and with a fraction of particles having speed v_α and the rest v_β. Tjon showed that, for a sufficient "separation" between v_α and v_β,[6] the high speed distribution grows up quickly, crossing the equilibrium value, further decaying towards it from above (Tjon effect).

Recent analysis carried out with molecular dynamics[3] shows that, if one starts from initial conditions of the type described above, real systems present the Tjon effect and, at the same time, an overpopulation effect in the low speed region.

Inhomogeneous systems have also been considered,[4] studying the interrelation between the speed distribution relaxation and the tendency towards homogeneity. An isolated system was simulated starting from an initial isotropic system of uniform density but with a linear gradient of particles with speed v_α along a given direction. It was observed that the tendency towards homogeneity of the kinetic energy gave rise to a density gradient and successive alternate inhomogeneities in both quantities. Moreover, the time scale characterizing the tendency to homogeneity is larger than that of the relaxation of the speed distribution function of the whole system.

The goal of this paper is to explore some of the aspects of the overpopulation effect and to try to understand the essential physical mechanisms governing the system evolution. Initial conditions of the type described above can be approximately achieved in practice by putting in contact two containers with identical gases and at sufficiently different temperatures. It then seems interesting to simulate a system with particles of speeds v_α and v_β spatially separated at the initial time. This type of condition also allows us to follow, at least for some short time, the temporal evolution of the fast and slow particles separately. As we will see, we will be able to separate clearly an effect associated with a flow of particles in the system and another which is due to collisions between particles. Besides, we will be able to analyze which type of collisions contribute to overpopulation effects at high as well as low speeds.

Another very important result is associated with the fact that each "gas" evolves independently, at least during some time, because their initial speeds are very different. This suggests that it is possible to describe the system, to a reasonable approximation, with a distribution of the local equilibrium type. Identification of collisions relevant for the overpopulation effect and the possible accuracy of a description in terms of characteristic relaxation times may open the possibility of extending the present theoretical studies beyond the simple model based on the Boltzmann equation.

II. DESCRIPTION OF THE SYSTEM

We have simulated a system of $N = 864$ particles interacting with a Lennard-Jones potential

$$u(r) = 4\epsilon[(\sigma/r)^{12} - (\sigma/r)^6]. \tag{2.1}$$

These particles are inside a box whose corners are located at $x = \pm L/2, y = \pm L/2, z = \pm L/2$. As we are not interested in the study of the influence of the walls, we have introduced periodic boundary conditions.

Initially, two regions α and β are clearly distinguished in the system (Fig. 1). Region β occupies the central zone in

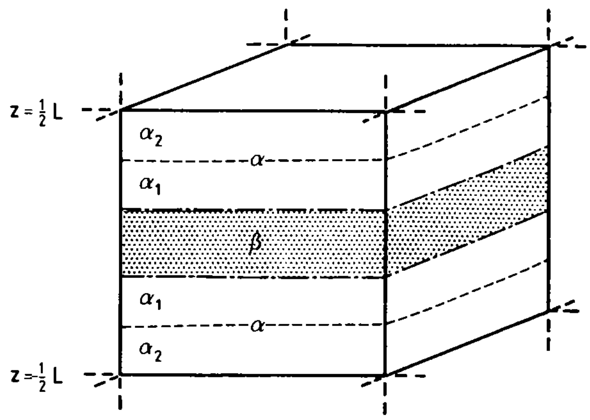


FIG. 1. Sketch of the regions in which the system has been divided. Initially, all the particles inside region α have speed v_α, and the particles in region β have speed v_β. The broken lines at the corners mean that periodic boundary conditions are considered.

the box, while region α corresponds to the zones on top and below the central one. All the particles contained in region β have an initial speed v_β, while those in region α have an initial speed v_α. Namely, the initial distribution of speeds is

$$f_{\alpha,\beta}(v;0) = N^0_{\alpha,\beta}\delta(v - v_{\alpha,\beta}), \tag{2.2}$$

where $N^0_\alpha + N^0_\beta = N$. Furthermore, the initial distribution of velocities is isotropic in region α as well as in β. If the initial kinetic energy per particle of the whole system is taken as $\frac{3}{2}k_B T_0$, it is clear that

$$\frac{N^0_\alpha}{N^0_\beta} = \frac{v^2_\beta - 3k_B T_0/m}{3k_B T_0/m - v^2_\alpha}, \tag{2.3}$$

where m is the mass of each particle and k_B the Boltzmann constant. In order to guarantee that the number density is uniform at the initial time, the ratio of the sizes of regions α and β has been taken equal to N^0_α/N^0_β.

As our system is initially symmetric with respect to the plane $z = 0$ and we are taking periodic boundary conditions, there is no reason to expect a breaking of this symmetry in the course of time. Thus, we will assume that two layers located symmetrically with respect to $z = 0$ can be considered as equivalent in their time evolution. Moreover, it is convenient to distinguish in region α two subregions α_1 and α_2, in order to give account of a zone where region β has a stronger influence.

Let us describe next the way in which we have generated in the computer a microstate compatible with the initial desired macrostate. It is customary to simulate a uniform system in molecular dynamics starting from a spatial localization of the particles according to a given lattice structure, e.g., fcc. Because the potential energy of that initial distribution is smaller than that of a disordered one, there is a rapid decay of the kinetic energy, for very short times, associated with the destruction of the initial structure.[3,4] This effect is of no importance when one is interested in steady situations, where the initial time can be taken arbitrarily. Nevertheless, when one is interested in the study of the relaxation of the system from given initial conditions, it is convenient to eliminate as much as possible the effects due to the simulation procedure.

In this work, we have started from a fcc spatial localization and a Maxwellian distribution of velocities. We have allowed the system to evolve during a certain time interval t_0, big enough so the rigid distribution of particles is destroyed and the kinetic energy reaches a practically steady value. The velocities of the particles are then redefined, assigning speed v_α to the particles located in region α and v_β to those in region β. The isotropy of the distribution is achieved assigning two random numbers to each particle to determine its velocity direction.[3] In this way, we have already generated the initial microstate of the system.

Actually, in order to study the macroscopic evolution of the system, one should follow the evolution of a large number of microstates, and average over all of them. A form of generating different initial microstates would be to consider different spatial configurations (varying the time t_0) and different directions to the velocities of the particles (choosing different sets of random numbers). This is a formidable task beyond the present computational capabilities available to us. Nevertheless, we think[3] that the evolution of a single microstate is sufficiently representative of the more relevant aspects of the evolution of the corresponding macrostate when one uses a coarse-grained description of the type considered here. Therefore, the results shown here, obtained with a single "experiment", must be understood in an essentially qualitative way.

Henceforth, our velocity unit will be taken as $(k_B T_0/m)^{1/2}$. We have considered the case $v_\alpha = 1$, $v_\beta = 3$; then, $N^0_\alpha/N^0_\beta = 3$. The number density is $\rho = 0.60\ \sigma^{-3}$ and $T_0 = 3.00\ \epsilon/k_B$. The initial condition preparation time is $t_0 = 150$ h, where

$$h = 0.032\ (m\sigma^2/48\epsilon)^{1/2}$$

is the time step used in the integration of the equations of motion.

III. RESULTS

As discussed in the previous section, we have tried to avoid in our simulation the abrupt conversion of kinetic energy into potential energy observed when one starts from a lattice distribution. To check this point, we have plotted in Fig. 2 the kinetic energy per particle $K(t)$ for the whole system. Let us recall that the time origin is taken at the time when the velocities are redefined. It is observed that, indeed, the rapid initial decay of $K(t)$ does not exist (compare with Fig. 1 in Ref. 4). The quantity $K(t)$ fluctuates about a steady value reached for times of the order of 400 h. We have taken as the equilibrium temperature of the system the value $T^{\rm eq} = 2.83\ \epsilon/k_B$, obtained from the relation $\bar{K} = \frac{3}{2}k_B T^{\rm eq}$, where $\bar{K}$ is the average value of $K(t)$ between $t = 400$ h and $t = 1000$ h. In Fig. 2, we also plot the total energy per particle $E(t)$ of the whole system. It remains practically constant as it should be for an isolated system.

Let us remember that the initial state, although of uniform density, is highly inhomogeneous: All particles in region β have speed v_β, while those in region α have v_α. As we are dealing with an isolated system, we expect a relaxation towards a homogeneous equilibrium state. This is studied in Fig. 3, where we show the evolution of $K_j(t)$ and $N_j(t)/N_j^{\rm eq}$.

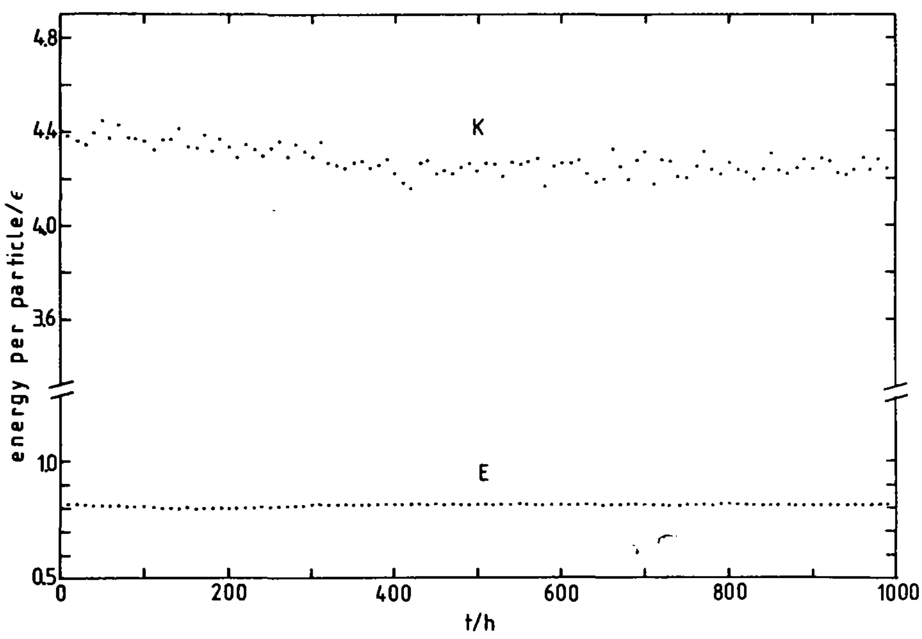


FIG. 2. Time evolution of the kinetic energy per particle (K) and of the total energy per particle (E) for the whole system.

Here, $K_j(t)$ and $N_j(t)$ represent the kinetic energy per particle and the number of particles in layer j, respectively. Moreover, N_j^{eq} is the number of particles that would be in that layer if the number density were constant. Let us recall that the system is considered as separated into the three layers of Fig. 1, i.e., $j = \alpha_1$, α_2, or β. The fact that $N_j(0)/N_j^{eq}$ is not strictly one for all layers is associated with our definition of the initial microstate and it shows that this microstate is not strictly uniform.

It is observed that $K_j(t)$ tends, in a first stage (until $t \approx 200$ h), to relax towards a homogeneous value, independent of j. At the same time, layer β is depopulated due to an increase in the density of, basically, layer α_2. We can distinguish a second stage (until $t \approx 400$ h), where the tendency of the density towards homogenization gives rise to an increase in the difference between temperatures of layers β and α_2. In the figure, it is observed that these two stages alternate in the further evolution of the system. In that way, for $t \approx 600$ h the density is clearly inhomogeneous, while for $t \approx 800$ h a small difference between the temperatures of regions α and β can be noticed. In other words, in the equilibrium relaxation, a competition between the tendency towards homogeneity of the density and that of the kinetic energy is established. This gives rise to successive inhomogeneities in both quantities, dephased and of decreasing amplitude. The characteristic times of the different stages are practically the same as those observed in Ref. 4. Nevertheless, the inhomogeneity amplitudes were appreciably smaller in the cases studied in Ref. 4 and, therefore, the fluctuations did not allow a clear observation of the last stages. Let us notice that layer α_1 relaxes more

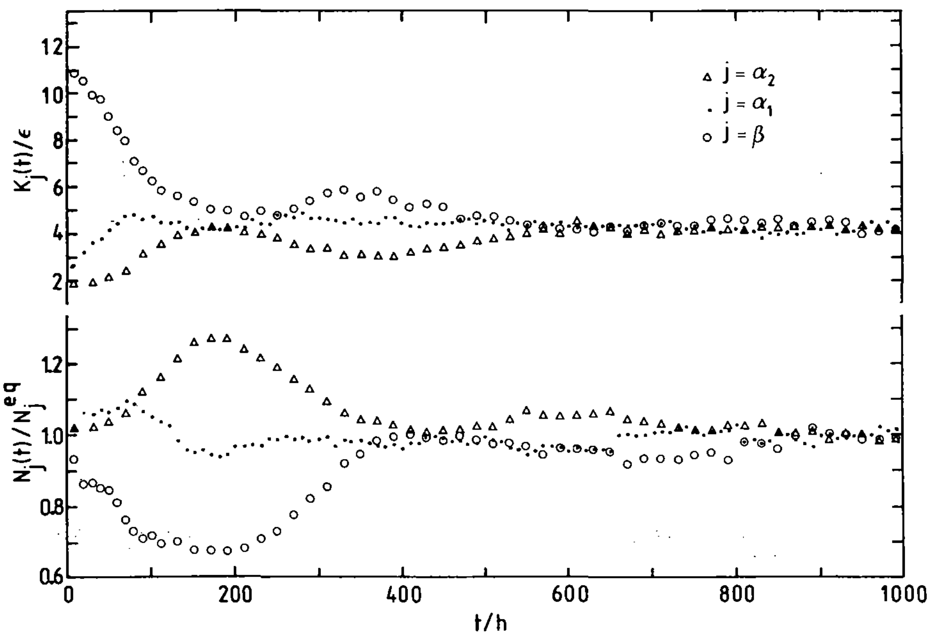


FIG. 3. Time evolution of the kinetic energy per particle in layer j, $K_j(t)$, and of the ratio $N_j(t)/N_j^{eq}$, where $N_j(t)$ is the number of particles in layer j, and N_j^{eq} is the number of particles corresponding to a uniform density.

rapidly than the other two and besides that the density and the kinetic energy per particle in this layer remain close to the equilibrium values. In this sense, layer α_1 evolves in a qualitatively different way than layer α_2 and this is the reason why we have considered them separately.

Let us study next the relaxation towards equilibrium of the distribution function of the system, which is expected to depend on z. Just as above, in order to reduce the effect of fluctuations associated with the limited number or particles, we have divided the system in layers β, α_1, and α_2. We define $\varphi_j(v_1,v_2;t)$ as the number of particles in layer j with speeds between v_1 and v_2 at time t. At equilibrium, for a Maxwell–Boltzmann distribution,

$$\varphi_j^{\text{eq}}(v_1,v_2) = N_j^{\text{eq}}\{(2T_0/\pi T^{\text{eq}})^{1/2}[v_1 \exp(-v_1^2 T_0/2T^{\text{eq}}) - v_2 \exp(-v_2^2 T_0/2T^{\text{eq}})] + \operatorname{erf}(v_2\sqrt{T_0/2T^{\text{eq}}}) - \operatorname{erf}(v_1\sqrt{T_0/2T^{\text{eq}}})\}, \quad (3.1)$$

where the speeds are expressed in terms of $(k_B T_0/m)^{1/2}$ and $\operatorname{erf}(x)$ is the error function.

It is useful to introduce a "local equilibrium" distribution function $\varphi_j^{\text{LE}}(v_1,v_2;t)$ defined by means of an expression equivalent to the right-hand side of Eq. (3.1) but replacing N_j^{eq} *by* $N_j(t)$ and T^{eq} by

$$T_j(t) \equiv \tfrac{2}{3}K_j(t)/k_B.$$

It is, of course, a coarse-grained version of the local equilibrium concept used in kinetic theory, in the sense that neither $N_j(t)$ nor $T_j(t)$ are truly local quantities, but they represent values averaged over layer j.

To characterize the system evolution towards equilibrium, we introduce the normalized populations

$$R_j(v_1,v_2;t) = \frac{\varphi_j(v_1,v_2;t)}{\varphi_j^{\text{eq}}(v_1,v_2)}, \quad (3.2)$$

$$R_j^{\text{LE}}(v_1,v_2;t) = \frac{\varphi_j^{\text{LE}}(v_1,v_2;t)}{\varphi_j^{\text{eq}}(v_1,v_2)}. \quad (3.3)$$

It is clear that as we consider just a single microstate, both functions will oscillate around unity once equilibrium has been reached. Nevertheless, for $t = 0$, R_j is substantially different from R_j^{LE}. In particular, for $v_\alpha = 1$, $v_\beta = 3$, we get $R_\beta^{\text{LE}}(0.0,0.9;0) \simeq 0.21$, $R_\beta^{\text{LE}}(3.1,\infty;0) \simeq 20$, $R_\alpha^{\text{LE}}(0.0,0.9;0) \simeq 3.1$, and $R_\alpha^{\text{LE}}(3.1,\infty;0) \simeq 1.4\times 10^{-4}$, while $R_j(v_1,v_2;0)$ is identically zero when neither v_α nor v_β lie in the interval (v_1,v_2).

For all the layers, we will study the relaxation of the speed distribution function in the zone of speeds smaller than v_α, and in the zone of speeds greater than v_β. Besides, due to the reduced number of particles of the system, we will consider globally the populations corresponding to each zone. To have an idea of the order of magnitudes, let us notice that

$$\varphi_j^{\text{eq}}(0.0,0.9)/N_j^{\text{eq}} \simeq 0.1645,$$

$$\varphi_j^{\text{eq}}(3.1,\infty)/N_j^{\text{eq}} \simeq 1.709\times 10^{-2},$$

$$N_\beta^{\text{eq}} = 216,\ N_{\alpha_1}^{\text{eq}} = N_{\alpha_2}^{\text{eq}} = 324.$$

First of all, we analyze the evolution of the distribution function in the first of the stages discussed in relation with Fig. 3. In Fig. 4, we represent $R_j(3.1,\infty;t)$ and $R_j(0.0,0.9;t)$ vs t for the layers β, α_1, α_2, and for the whole system. We have also plotted R_j^{LE}. Let us start with the analysis of $R_j(t)$. As

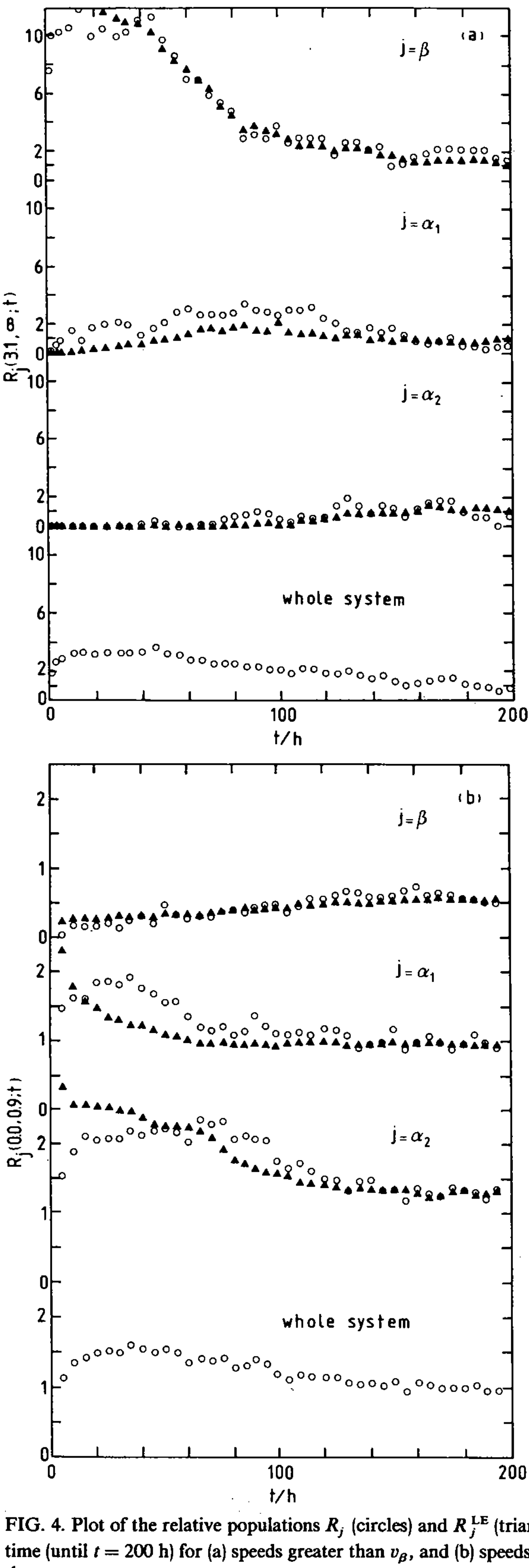


FIG. 4. Plot of the relative populations R_j (circles) and R_j^{LE} (triangles) vs time (until $t = 200$ h) for (a) speeds greater than v_β, and (b) speeds smaller than v_α.

for region $v > v_\beta$, Fig. 4(a), it is observed that the layer β (where all particles have initially speed v_β) shows an abrupt overpopulation effect, with a maximum which is maintained until $t \simeq 45$ h and, later on, the population tends to relax slowly to equilibrium. The layer α_1 (next to layer β) also presents an overpopulation of particles with speeds greater than v_β, although it is less intense than in layer β. This effect has its origin, basically, in the flow of fast particles coming from layer β. This explains why the overpopulation in layer α_1 is maintained until $t \simeq 120$ h. Layer α_2 does not present an appreciable overpopulation except for small time intervals ($t \simeq 130$ h and $t \simeq 170$ h), due presumably to particles coming from α_1. As was expected, the whole system has an overpopulation in the region of high speeds. This effect is greater and much more persistent than in the case of homogeneous systems.[3] We then see that the type of inhomogeneous initial conditions considered here, in which the particles with speeds v_α are spatially separated from particles with speeds v_β, favors the production of fast particles.

In the low speed zone, Fig. 4(b), $R(t)$ increases slowly and monotonously in layer β towards the equilibrium value, while in α_1 and α_2 it very quickly goes over that value. Although α_1 and α_2 are initially equivalent, the overpopulation is less intense and it lasts less in α_1 than in α_2. This is because of the influence of the flow of high speed particles coming from β. As for the whole system, overpopulation exists for $v < v_\alpha$ and with a maximum value comparable to the homogeneous case,[3] although it lasts longer.

Let us now compare the evolution of the actual population $R_j(t)$ with that of a local equilibrium one $R_j^{\mathrm{LE}}(t)$ for each layer. Going back to Fig. 4(a) and with respect to layer β, we see that, after an initial period (until $t \simeq 40$ h), the local equilibrium function gives a good description of the further evolution of R_β. This good agreement also exists in the low speed zone, as observed in Fig. 4(b). According to this, the first few collisions between high speed particles in β make the distribution function tend to approach a Maxwellian distribution. The further behavior of the distribution function may be described with a good approximation by the Maxwellian distribution.

With respect to α_1, we do not get such a good agreement between R_{α_1} and $R_{\alpha_1}^{\mathrm{LE}}$ neither for $v < v_\alpha$ nor for $v > v_\beta$. We think that this is essentially due to the flow of fast particles coming from β. This gives rise to a double effect. On one hand, even if one expects that collisions between particles with speeds close to v_α tend to generate a Maxwellian distribution, the population of particles with high speed is increased due to those coming from β. This explains why $R_{\alpha_1}(3.1,\infty;t)$ lies above $R_{\alpha_1}^{\mathrm{LE}}(3.1,\infty;t)$ until $t \simeq 150$ h. On the other hand, the presence of fast particles coming from layer β increases the computed temperature of α_1 and this provokes a shift towards the right of the local equilibrium distribution with respect to that obtained in the absence of the flow. This explains why, except in the very first few times, $R_{\alpha_1}(0.0,0.9;t)$ is greater than $R_{\alpha_1}^{\mathrm{LE}}(0.0,0.9;t)$, at least until $t \simeq 130$ h.

In the layer α_2, the influence of the flow of more energetic particles is slightly smaller and it appears later than in α_1, and it is basically associated with the second of the effects mentioned above. Namely, once $R_{\alpha_2}^{\mathrm{LE}}(0.0,0.9;t)$ has crossed over $R_{\alpha_2}(0.0,0.9;t)$, the temperature increase in the layer makes the actual population of particles with speeds $v < v_\alpha$ greater than the value given by the local equilibrium distribution function, until $t \simeq 130$ h.

In the analysis we have just carried out, we have neglected the influence of the flow of particles with speeds close to v_α. In the initial stage, we are considering that (until $t \simeq 200$ h) the most important flow is that of fast particles coming from layer β. This is precisely the flow giving rise to the depopulation of that layer observed in Fig. 3 in this stage. In spite of this depopulation, the local equilibrium distribution function represents a good description of the speed distribution in layer β, because the most important collisions are still those between particles that were initially in that layer.

Next, we analyze the evolution for greater times. In Fig. 5 we plot the same quantities as in Fig. 4, except that for $t > 200$ h. The inhomogeneities of the kinetic energy and the number of particles (see Fig. 3) do now show up in the actual distribution function of the system. So, layer β presents a new overpopulation of particles with speeds greater than v_β, reaching a maximum value for $t \simeq 400$ h. Also at this time, an appreciable difference of temperature between layers exists. At approximately the same time, we observe a minimum in $R_{\alpha_2}(3.1,\infty;t)$ and a maximum in $R_{\alpha_2}(0.0,0.9;t)$. Let us notice that the "excess" of particles with $v > v_\beta$ in layer β for $t \simeq 400$ h is greater than the "defect" in layer α_2, in such a way that the whole system presents a slight overpopulation. The fluctuations of R_j, due to the reduced number of particles, do not allow us to follow so clearly the influence of the inhomogeneities in the following stages on the speed distribution.

The above results can also be analyzed using the local equilibrium distribution function which, again, describes the state of the system with an acceptable precision. In Fig. 3 we observe that, for times between $t \approx 200$ h and $t \approx 400$ h, the temperature and the number of particles increases (decreases) for layer $\beta(\alpha_2)$. The opposite happens between $t \approx 400$ h and $t \approx 600$ h. The temperature and density changes affect additively the number of particles present with $v > v_\beta$ in the local equilibrium. This fact explains why, for $t \simeq 400$ h, $R_\beta^{\mathrm{LE}}(3.1,\infty;t)$ has a maximum and $R_{\alpha_2}^{\mathrm{LE}}(3.1,\infty;t)$ a minimum, as can be seen in Fig. 5(a).

On the other hand, the temperature and density changes between $t \approx 200$ h and $t \approx 600$ h affect the local equilibrium population with $v < v_\alpha$ in an opposite sense. An increase (decrease) of the temperature implies a decrease (increase) of the probability for finding a particle with speed smaller than v_α. It follows from Fig. 5(b) that for 200 h $< t < 400$ h, the effect associated with the increase of particles is dominant in layer β, while in layer α_2 the decrease in temperature is the dominant one. More quantitatively, the increase in temperature (14%) in layer β gives rise to a decrease of about 16% in the local equilibrium probability for the region $v < v_\alpha$, while the net population has increased by 53%. During this same stage, the net population in layer α_2 decreases by 18% and the probability, due to a decrease in temperature of about 23%, increases by 39%. For times between 400 and 600 h, the temperature variation is, in abso-

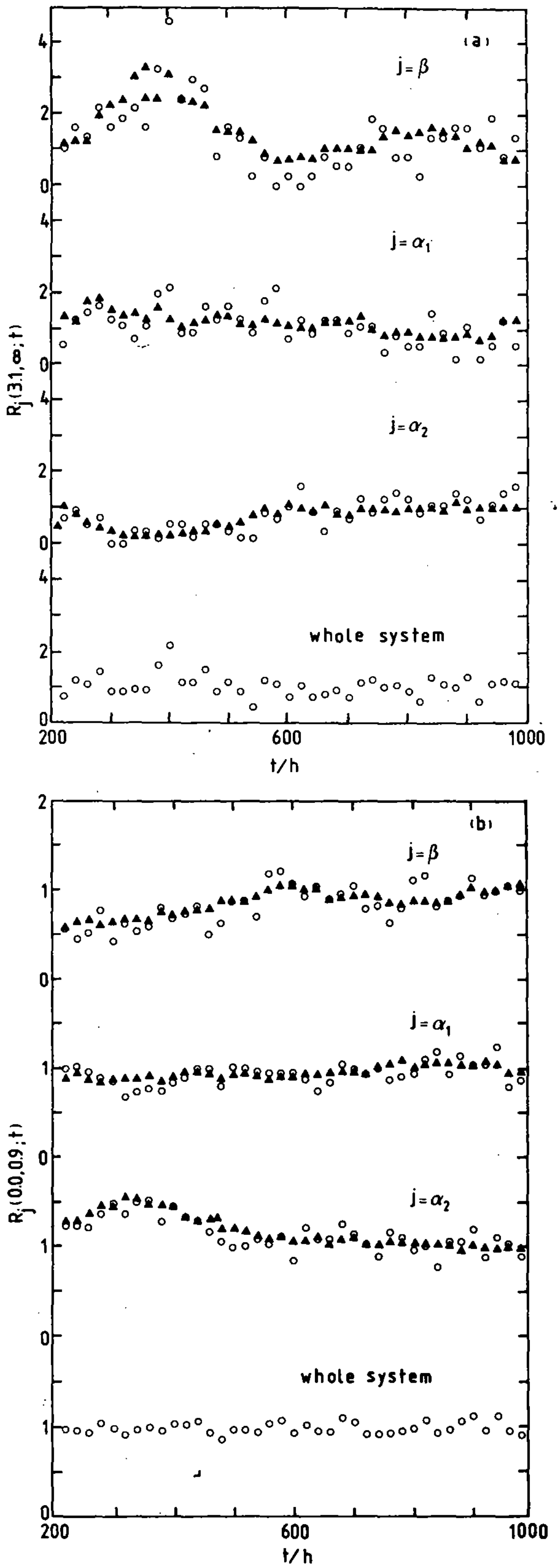


FIG. 5. The same as in Fig. 4, but for times greater than 200 h.

lute value, approximately the same as in the previous stage, while the density variation is smaller. For this reason, during this stage, the dominant effect in layer β as well as in layer α_2 is that one related with the variation in temperature, as observed in Fig. 5(b).

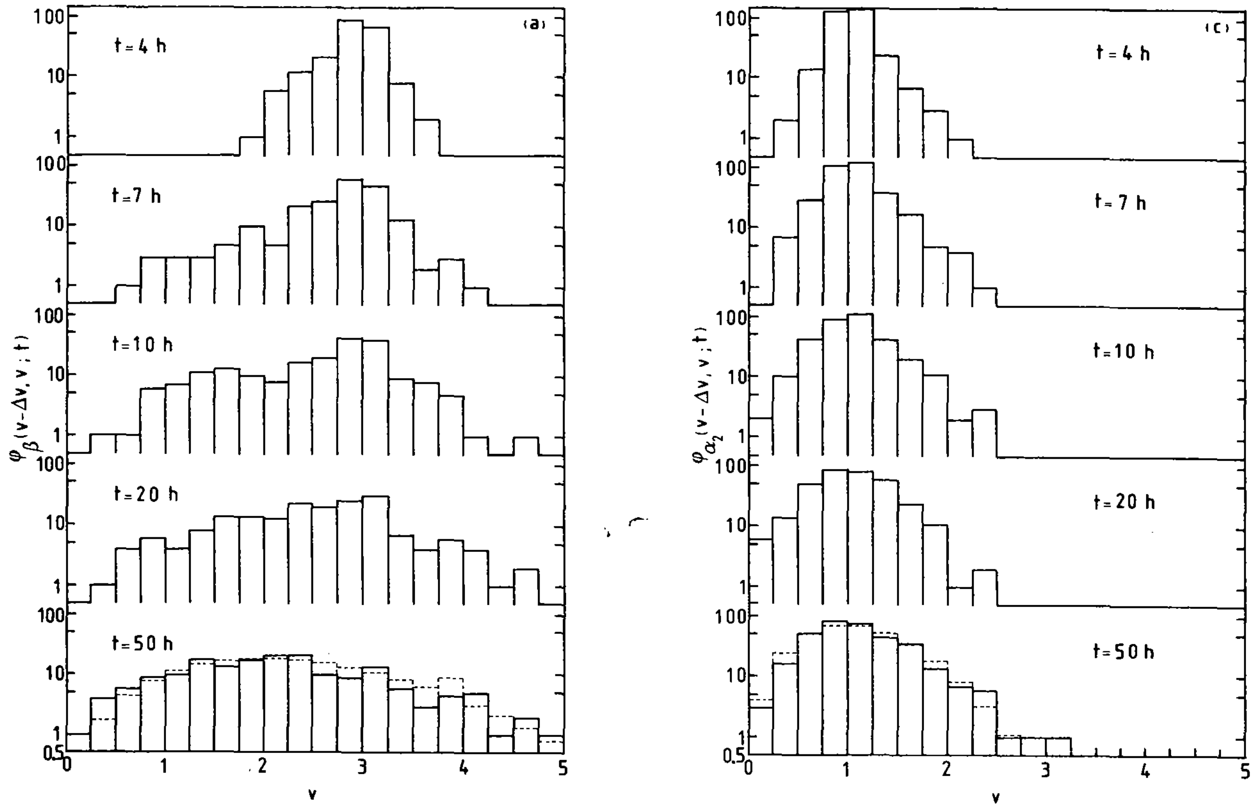
In Fig. 3, it is observed that at $t \simeq 200$ h, the inhomogeneity in density is much more important than that in the kinetic energy. One could then think that $R_\beta^{\mathrm{LE}}(v_1,v_2;200\ \mathrm{h})$ should be less than one and $R_{\alpha_2}^{\mathrm{LE}}(v_1,v_2;200\ \mathrm{h})$ greater than one. Nevertheless, Fig. 5 shows that this is true for $v < v_\alpha$, but not for $v > v_\beta$. The explanation of this fact is that at $t = 200$ h, the temperature of layer β is about 15% higher than that of equilibrium and the temperature of α_2 is 10% smaller than that of equilibrium. A simple calculation shows that the probability for finding a particle in layer β with speed higher than v_β is about 84% higher than that of equilibrium, while, also with respect to equilibrium, the probability is 45% smaller in layer α_2.

Up to now, we have restricted ourselves in our study to speeds smaller than v_α and higher than v_β. Next, we consider with more detail the time evolution of the full speed distribution function. Our interest is centered on the relaxation of the initial delta-peaked distribution and so we will consider times up to $t = 50$ h. For this time, overpopulation effects both in the high and low speed regions have taken place. In Fig. 6 we have represented the population $\varphi_j(v - \Delta v, v;t)$ with $\Delta v = 0.125$ in layers β, α_1, and α_2. Notice that at $t = 4$ h the distribution function is already much broader than at the initial time. Besides, at this time, an appreciable flow towards α_1 of particles with speeds close to v_β has taken place, while in layer β there are not yet particles with speeds close to v_α. At further times, the flow of fast particles towards α_1 is increased. So, at $t = 10$ h we can distinguish two superposed distributions centered on $v \simeq v_\alpha$ and $v \simeq v_\beta$, respectively. The influence of the flows of particles is harder to see in layers β and α_2. In layer β, particles with speed close to v_α coming from α_1 are indistinguishable from those generated by collisions between particles already present in β. As expected, there are no particles with speed v_β reaching layer α_2, but they arrive with lower speeds, being then indistinguishable from those generated by collisions inside their own layer.

For $t = 50$ h, we have also plotted the local equilibrium distribution function $\varphi_j^{\mathrm{LE}}(v - \Delta v, v;t)$. As φ_j only takes discrete values and we use a logarithmic scale, the value $\varphi_j = 0$ can not be plotted. We have then assigned the value 0.5 to those populations smaller than or equal to that value. In the figure, we see an acceptable agreement between the actual distribution and that of local equilibrium, especially if one takes into account that we are dealing with the results of a single experiment and the reduced number of particles at hand, particularly with speeds $v < v_\alpha$ and $v > v_\beta$.

The time evolution of the distribution function illustrates how collisions tend to approximate the distribution in each layer to a Maxwellian one. This tendency is opposed by the flow of particles from other layers. Both processes are clearly distinguishable. The fact that for $t \simeq 50$ h the actual and the local equilibrium distributions are very close is not surprising if one considers that an estimation of the mean time between collisions is about 30 h.

We now summarize some of the main physical conclusions arising from the results presented here. Firstly, the presence of inhomogeneities in the system does not seem to



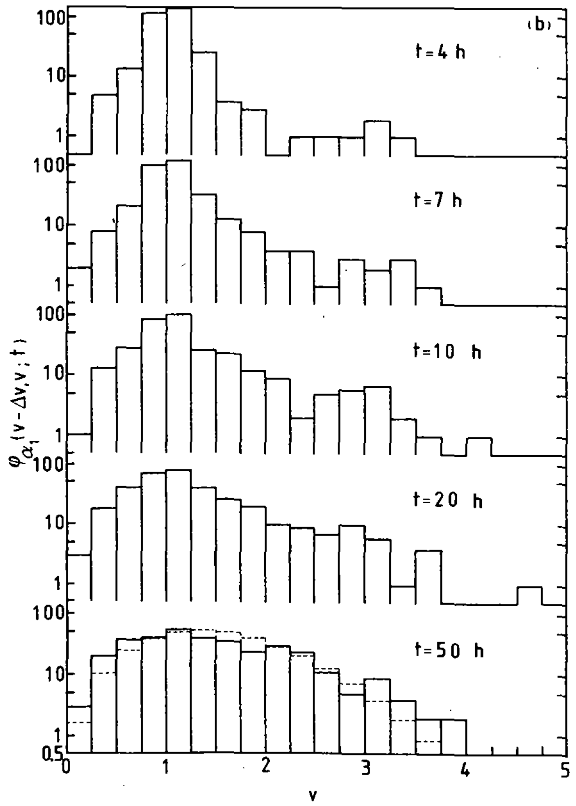


FIG. 6. Actual population for several speed intervals at different times in layers (a) β, (b) α_1, and (c) α_2. The broken lines at $t = 50$ h indicate the populations obtained from the local equilibrium distribution.

affect significantly the overpopulation effects at high and low speeds. This confirms the theoretical predictions[8] that the determining cause of the overpopulation effect is the type of initial distribution of speeds. Of course, in the inhomogeneous case, there exists a net flow of particles also contributing to the evolution of the system. Nevertheless, its influence on the speed distribution does not seem to be very significant. In particular, the overpopulation at high speeds (Tjon effect) is associated with collision between particles that had initially the biggest of the two speeds present. Analogously, overpopulation at low speeds comes from collisions between particles that had initially the smallest speed. This suggests the possibility of analyzing the overpopulation effects with a simple model, where the system is considered as divided into two independent fluids having initially particles with speeds v_α and v_β, respectively. The overpopulation effect at high (low) speeds should appear associated with the equilibrium relaxation of the more (less) energetic fluid. Evidently, the model may be improved by introducing a simple interaction term between the fluids. Work is now in progress along these lines and will be reported shortly.

[1]R. Zwanzig and N. K. Ailawadi, Phys. Rev. **182**, 280 (1969).
[2]B. J. Alder and T. E. Wainwright, in *International Symposium on Statistical Mechanical Theory of Transport Processes, Brussels, 1956*, edited by I. Prigogine (Interscience, New York, 1958), p. 97; J. Orban and A. Bellemans, Phys. Lett. A **24**, 620 (1967); A. Aharony, Phys. Lett A **37**, 45 (1971).
[3]J. J. Brey, J. Gómez Ordóñez, and A. Santos, Phys. Rev. A **26**, 2817 (1982).
[4]J. J. Brey, J. Gómez Ordóñez, and A. Santos, Mol. Phys. **50**, 1163 (1983).
[5]J. A. Tjon, Phys. Lett. A **70**, 369 (1979).
[6]E. H. Hauge and E. Praestgaard, J. Stat. Phys. **24**, 21 (1981).
[7]M. H. Ernst, in *Fundamental Problems in Statistical Mechanics V*, edited by E. G. D. Cohen (North-Holland, Amsterdam, 1980), p. 249; Phys. Rep. **78**, 1 (1981).
[8]G. Turchetti and M. Paolilli, Phys. Lett. A **90**, 123 (1982).