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A numerical study of one-dimensional systems: Kinetics and equilibrium states

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Abstract. We report on the numerical analysis of the relaxation towards equilibrium in one dimension of a 'large' system of hard cores particles having masses either m_1 or m_2 and velocities ± 1 given at random; a very broad range of values of m_1/m_2 is investigated for the first time. Several quantities such as velocity autocorrelations, diffusion coefficients, relaxation and correlation times are monitored, some times until the system reaches equilibrium. We conclude about new interesting qualitative and quantitative changes in the system relaxation as one considers different values for m_2/m_1.

1. Introduction

The study of one-dimensional systems is nowadays an active area of research given that, in addition to having mathematical interest, they may capture essential physical features or model one-dimensional effects which are sometimes present in real systems (Thouless and Kirkpatrick 1981, Baker and Bragg 1983, Mokross and Büttner 1983, van Beijeren *et al* 1983). Exact results are known in a few cases of interest (Jepsen 1965, Lebowitz and Percus 1967, Lebowitz *et al* 1968, Aizenman *et al* 1978, van Beijeren *et al* 1983) while, more often, one has to rely on approximations and computer simulations (Mokross and Büttner 1983, van Beijeren *et al* 1983, Masoliver and Marro 1983) to extract the relevant information. These facts motivated the computer analysis of binary mixtures of impenetrable particles with different masses, m_1 and m_2 respectively, on a ring (Masoliver and Marro 1983); the main conclusion there is that, unlike the system with $m_2 = m_1$ which is non-ergodic in the velocity distribution function, the system with $m_2 \neq m_1$ relaxes from any initial state towards a Maxwellian velocity distribution. The interesting qualitative features observed in that work suggested the details of the evolution of the system with time should be investigated more closely.

We report in this paper on a series of numerical experiments related to those in our previous work, i.e. we study the relaxation towards equilibrium of a periodic one-dimensional binary mixture of hard-core particles with masses m_1 and m_2. We consider in this case, however, a broader range of m_2/m_1 values, namely $m_2/m_1 = 1, 1.01, 1.03,$

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1.05, 3, 4, 5, 8, 10, 30, 40 and 50 which include smaller and larger mass ratios. In addition, we have followed the evolution of the system to much longer times and, when it was necessary in order to obtain reasonable statistics, e.g. at $m_2/m_1 = 1.01$ and 50, we averaged over three independent histories. This allows us to conclude quantitatively here about specific kinetic properties and equilibrium states for one-dimensional mixtures. In particular, we analyse the nature of the reported 'critical slowing down' in the relaxation of the system when $m_2/m_1 \to 1$ as well as the behaviour for large values of m_2/m_1. The gradual increase of the relaxation time for $m_2/m_2 \gg 1$, compared with the critical divergence in the low-mass-ratio limit, may reveal a sort of local equilibrium when light particles are surrounded by heavy ones; our data, however, seem to extrapolate to correct equilibrium values. We also investigate correlation times and other quantitative observations in the asymptotic relaxation of the Boltzmann H-function and velocity autocorrelation and present a detailed discussion of the nature and dependence with m_2/m_1 of long time tails which may shed some light into a recent related controversy. Our observations certainly encourage us to anticipate exact solutions or more general approximate descriptions of this finite system or its infinite counterpart.

2. Description of model

The system consists of $N = 1000$ hard core particles randomly distributed on a line with periodic boundary conditions. This size can be considered as 'macroscopic' (in one dimension) for many purposes (Alder and Wainwright 1959, 1970). The length of the line, on the contrary, is set $L = 1000$ rather arbitrarily because we do not investigate the dependence on density. Half the particles, selected at random, are assigned masses $m_1 = 1$ while the rest are assumed to have masses m_2. Each particle is also assigned at random either a velocity $+1$ or -1, independently of its mass. The evolution of the system then proceeds according to a slight modification of the method developed by (Alder and Wainwright 1959, 1967, 1970, Masoliver and Marro 1983). The algorithm computes the set of virtual collision times as

$$t_{i,i+1} = \begin{cases} -x_{i,i+1}/v_{i,i+1} & x_{i,i+1} \leqslant 0 \\ (-x_{i,i+1} + L)/v_{i,i+1} & x_{i,i+1} > 0 \end{cases} \tag{1}$$

where $x_{ij} = x_i - x_j$ and $v_{ij} = v_i - v_j$ represent respectively the relative position and velocity of particles i and j (which can only be neighbours due to the hard-core potentials). The second value in (1) holds when the particle at one end of the line is expected to collide with the one at the other end. Particles are then moved to the positions $x_i + v_i t_m$ where $t_m = \min\{t_{i,i+1};\ i = 1, 2, \ldots, N\}$ and the velocities of the colliding particles are changed as implied by momentum and energy conservation. New virtual collision times are computed as $t_{i,i+1} - t_m$ or again from (1) when that happens to be zero. This constitutes the basic step which is repeated T times each run. At the end of each run, the mean free time t_0 is computed as the inverse of the collision frequency; see table 1 for the duration of the runs and for the dependence of t_0 on m_2/m_1.

The computations were carried in double precision in a CDC CYBER 173 where they took a total of several hundred hours of CPU time. Round-off errors never produced relative differences in the total momentum larger than 10^{-13} after 4×10^5 steps or larger than 10^{-11} after 2×10^7 steps. We have also checked by making independent runs that the evolution of the system is independent in practice of the particular randomisation of

Table 1. Duration of the runs reported here, corresponding mean free time t_0, equilibrium values for the Boltzmann's H-function, for the standard deviation σ and for the kurtosis k of the velocity distribution function, relaxation times t^* and t'^* as defined in the text, and the parameter α and corresponding coefficient of linear regression r when fitting the data with equation (4) and $\beta = 1.2$.

m_2/m_1	Steps	t_0	σ	k	t^*/t_0	H_{eq}	t'^*/t_0	α	r
1	1.6×10^5	2.00	—	—	∞	—	—	—	—
1.01	18.4×10^6	1.97	1.0009	−0.49	15000 ± 500	0.3669	14000	0.0011	0.962
1.03	5.6×10^6	1.86	1.0009	−0.38	3000 ± 200	0.3675	2724	0.0017	0.980
1.05	2.4×10^6	1.79	1.0014	−0.09	1000 ± 100	0.3677	807	0.0064	0.981
1.20	1×10^6	1.77	1.006	−0.09	60 ± 4	0.3681	48.3	0.0064	1.000
2	1×10^5	1.68	1.006	0.28	6 ± 2	0.3734	5.5	0.0021	0.964
5	1×10^5	1.36	1.33	1.305	4 ± 2	0.3919	3.9	0.0129	0.984
8	1×10^5	1.16	1.57	1.70	10 ± 2	0.4052	5.1	0.0189	0.993
10	1×10^5	1.07	1.70	2.10	15 ± 10	0.4100	5.2	0.0140	0.974
30	1×10^5	0.65	2.54	2.61	30 ± 20	0.4376	12.7	0.0116	0.976
50	1×10^5	0.50	2.96	3.08	50 ± 40	0.4387	30.5	0.0040	0.971

the initial state and that the accuracy of individual particle trajectories is good enough in general, as we discuss later on.

3. Relaxation time

The system starts with velocities ± 1 and evolves with time when $m_2 \neq m_1$ towards a velocity distribution which can be approximated by a Maxwellian distribution centred at $v = 0$ (Masoliver and Marro 1983):

$$f(v) = \frac{1}{\sigma(2\pi)^{1/2}} \exp(v^2/2\sigma^2). \tag{2}$$

The standard deviation σ is seen to increase monotonically with increasing mass ratio m_2/m_1 so that the equilibrium distribution of velocities becomes more sharply peaked as $m_2 \to m_1$. The kurtosis, k, related to the fourth moment μ by $k \equiv \mu/\sigma^4 - 3$, also increases with increasing m_2/m_1. See table 1 for values of σ and k.†

The time evolution of the velocity distribution, $f(v, t)$, is qualitatively similar for all mass ratios considered here: the initial distribution ± 1 degenerates, approximately, into two gaussians centred respectively at ± 1 which finally evolve into the curve (2). The time the system takes to reach the maxwellian velocity distribution (2), t^*, increases gradually when $m_2 \gg m_1$ and very dramatically when $m_2/m_1 \to 1$. When $m_2 = m_1$ the initial distribution ± 1 is conserved in time; as a matter of fact, the exact results by Jepsen (1965) show that only the distribution of a specified, test particle (starting at $t = 0$ from the origin with a velocity v) exhibits normal kinetic behaviour, i.e. diffusion and approach to equilibrium. We can estimate visually the 'relaxation time' t^* when $m_2 \neq m_1$ to obtain the values reported in table 1.

† Note that the values for σ and k in table 1 might indicate that the initial times included in the time averaging process to compute them are still outside equilibrium. Should this be the case, however, it does not affect our conclusions here: it only introduces minor numerical inacuracies for $m_2/m_1 \geq 30$ while it notably helps to improve our statistics.

A better quantitative measure of the system relaxation can be obtained through the use of the Boltzmann's H-function:

$$H(t) = \int \mathrm{d}v\, f(v,t) \ln f(v,t). \tag{3}$$

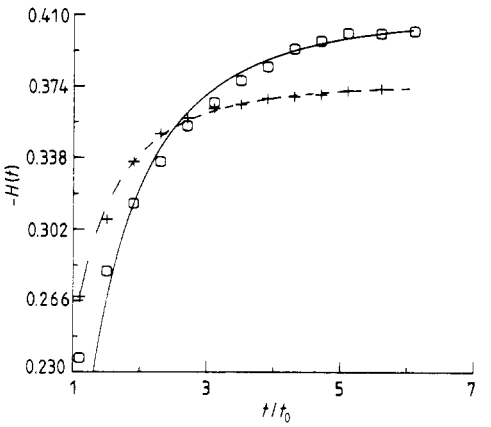

Figure 1. Early time development of the negative of Boltzmann's H-function (time is in units of the mean free time t_0, i.e. it represents the number of collisions per particle) in the cases $m_2/m_1 = 8$ (circles) and 2 (crosses). The full and broken curves are fits to the data of the form (4).

As shown in figure 1, the function H is observed to decrease monotonically with time for all values of m_2/m_1 towards the stationary value H_{eq}; thus $\mathrm{d}H(t)/\mathrm{d}t = 0$ for $t \geqslant t'^*$ showing that the system has indeed reached an equilibrium velocity distribution such as (2) and that the evolution bears an undeniable irreversible character. The values for H_{eq} in table 1 show an increase with increasing m_2/m_1; this behaviour can be understood as a consequence of the approximate validity of description (2) and of the definition (3) which implies a proportionality between H_{eq} and $\ln \sigma$. This proportionality is indeed supported by the data, as figure 2 shows. The data, on the other hand, suggest that a simple relaxation formula should be sought, say

$$H(t) - H_{eq} = \alpha[(t'^*/t) - 1]^{\beta}. \tag{4}$$

This equation fits the data very well (see figure 1) and it allows one to compute α, t'^* and β. We find that $\beta = 1.1 \pm 0.1$. We present in table 1 the values obtained for α and t'^* from the fit in the case $\beta = 1.2$; note that the latter are very close to our estimations t^* (we also obtain values for t'^* which are compatible with those for t^* when requiring, say $\beta = 1.0$ in equation (4)).

The relaxation times depict a quite interesting feature of the system evolution. Any of them, t^* or t'^*, clearly show that $t^* \to \infty$ when $m_2/m_1 \to 1$. This critical behaviour can be fitted very accurately by

$$t^* \sim (m_2/m_1 - 1)^{-\varepsilon} \tag{5}$$

where we find $\varepsilon = 1.9 \pm 0.1$; see figure 3. There is also a clear increase of t^* with m_2/m_1 when $m_2 \gg m_1$, but this is much slower and less dramatic than (5). The limiting case $m_2/m_1 \to \infty$ would again resemble in some sense (Nossal 1965) the situation when $m_2 = m_1$.

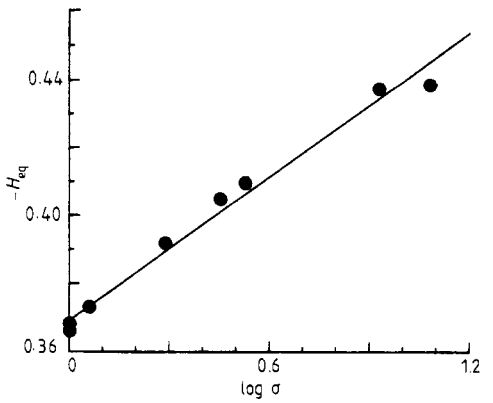

Figure 2. The negative of the equilibrium value H_{eq} of Boltzmann's H-function, obtained as a time average over the stationary part of the evolution of $H(t)$, versus the logarithm of the standard deviation σ of the corresponding velocity distribution.

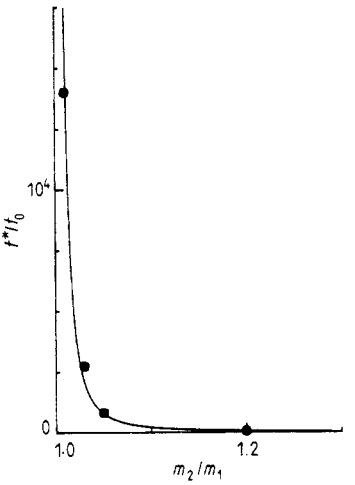

Figure 3. The relaxation time t^* as a function of the mass ratio when $m_2/m_1 \rightarrow 1$. The full curve corresponds to equation (5).

The values in table 1 show that the minimum value for t^* is located in the neighbourhood of $m_2/m_1 = 5$.

The velocity autocorrelation function $\psi(t) = \text{constant} \times \langle v(0)v(t)\rangle$ provides a familiar method to analyse the relaxation of the system. It was computed here by means of the algorithm:

$$\psi_a(t) = \sum_{i=1}^{N_a} v_i(0)v_i(t) \Big/ \sum_{i=1}^{N_a} v_i^2(0) \tag{6}$$

where $a = 1, 2$ refer to species with masses m_1 and m_2 respectively; i.e. we do not make the usual average over different time origins because the statistical behaviour of the quantity (6) is good enough (and most interesting) for many purposes. The case $m_2 = m_1$ is described (Jepsen 1965) by the exact result $\psi(t) = \exp(-2t)$ for $t < 2$ so that it

Table 2. Correlation times as defined in equation (7) and 'diffusion coefficients' as defined in equation (9) as a function of m_2/m_1.

m_2/m_1	τ_1/t_0	τ_2/t_0	$\tilde{D}_1$	$\tilde{D}_2$
1	0.250	0.250	0.490	0.490
1.01	0.335	0.280	0.484	0.486
1.03	0.342	0.281	0.485	0.488
1.05	0.334	0.311	0.482	0.493
1.20	0.326	0.324	0.470	0.507
2	0.293	0.394	0.392	0.603
4	0.171	0.510	0.310	0.700
5	0.159	0.526	0.248	0.742
8	0.199	0.625	0.240	0.781
10	0.189	0.741	0.228	0.824
30	0.364	1.645	0.218	0.855
50	0.489	2.151	0.216	0.884

seems reasonable to make here the Langevin type, short-time assumption:

$$\psi_a(t) \sim \exp(-t/\tau_a) \qquad (a = 1, 2) \tag{7}$$

where τ_a is a correlation time. The relation (7) does indeed describe very well the data in the time range $0 \leqslant t/t_0 \leqslant b$, where b is of order of unity, for any mass ratio m_2/m_1. The values for τ_a obtained from a fit of equation (7) to the data also show an interesting behaviour; they are reported in table 2. Figure 4 displays τ_0/t_0 and τ_2/t_0 as a function of m_2/m_1. Note that τ_1/t_0 decreases with increasing m_2/m_1 in the range $1 < m_2/m_1 \lesssim 5$ while it increases with m_2/m_1 for $m_2 > 5m_1$; τ_1 (i.e. the quantity reported in table 2 times t_0) shows a similar trend. This behaviour might just indicate that τ_1/t_0 has a constant value, say $\tau_1/t_0 \simeq 0.3$. The correlation time τ_2, on the contrary, clearly increases monotonically with m_2/m_1.

The diffusion constant D can be related to the velocity autocorrelation function by the Green–Kubo formula

$$D = \int_0^\infty \mathrm{d}t\, \psi(t). \tag{8}$$

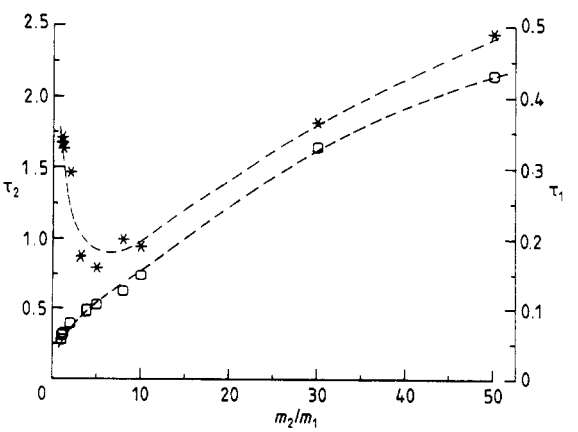

Figure 4. The correlation times τ_a (in units of t_0) for $a = 1$ (asterisks) and 2 (circles) as a function of the mass ratio m_2/m_1. The broken curves are a guide to the eye.

The accurate estimation of transport coefficients (Erpenbeck and Wood 1982, for instance) is difficult in practice, however, due to the very slow asymptotic behaviour we discuss next. Thus, in order to gain some qualitative idea we have computed the quantities:

$$\tilde{D}_a \equiv \int_0^{3\tau_a} \mathrm{d}t\, \psi_a(t) \qquad (a = 1, 2) \tag{9}$$

where τ_a is the correlation time associated with $\psi_a(t)$. The corresponding values are shown in table 2. These are described very well by linear relations:

$$\tilde{D}_1 = -0.61\,\mu + 0.79 \qquad \tilde{D}_2 = 0.82\,\mu + 0.07 \tag{10}$$

with $\mu = m_1 m_2/(m_1 + m_2)$ the reduced mass, which intersect at $\mu \simeq \frac{1}{2}(m_1 = m_2)$ when $\tilde{D}_1 = \tilde{D}_2 \simeq 0.49$ as one should expect. The behaviour (10) is illustrated in figure 5.†

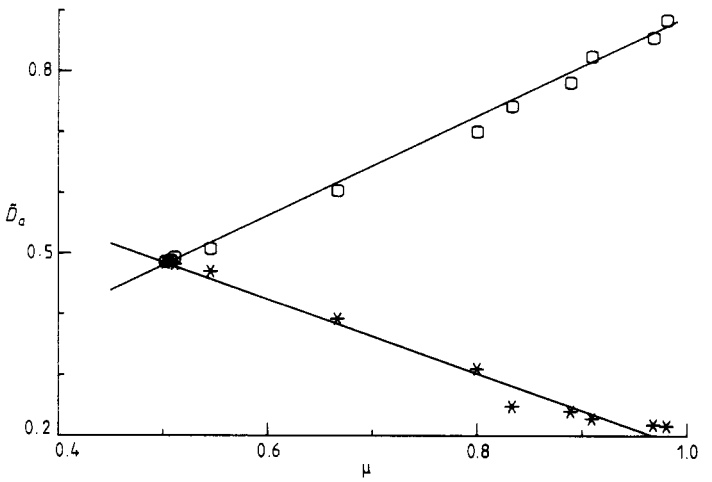

Figure 5. The 'diffusion coefficients' $\tilde{D}_a$ as defined in equation (9) versus the reduced mass of the system, $\mu = m_1 m_2/(m_1 + m_2)$. The lines correspond to equations (10).

4. Long-time tails

The computer simulation of hard-spheres and hard-discs systems revealed years ago (Alder and Wainwright 1967, 1970) that the 'classical' exponential decay (7) is replaced at large values of the time by a much slower relaxation or long-time tail

$$\psi(t) \sim t^{-\delta} \qquad t \to \infty \tag{11}$$

where $\delta = d/2$ and $d = 2, 3$ is the dimension of the system considered. This effect was subsequently explained in the context of linear kinetic and mode-coupling theories (Hauge and Martin-Lof 1973, Ernst *et al* 1976, Pomeau and Résibois 1975, Dorfman and Cohen 1975) as well as observed in scattering experiments (Paul and Pusey 1981; Ohbayashi *et al* 1983). On the other hand, exact results on the one-dimensional system

† Note that the values for $\tilde{D}_a$ probably differ significantly from the corresponding diffusion constants D_a, as defined in equation (8), due to long-time effects.

of hard rods (Jepsen 1965, Lebowitz and Percus 1967) also provide some partial confirmation of the behaviour (11); namely, they show that the relaxation of a specified test particle in an infinite system with maxwellian or very long-range velocity distributions deviates for $t \geqslant 2$ from the short-time form $\psi(t) = \exp(-2t)$, which then becomes negative, very small and can be represented by a long-time limit expansion $\psi(t) \sim t^{-3} - \alpha t^{-5}$, $\alpha > 0$. Thus, one seems to have $\delta = 3$ when $d = 1$ which is in contradistinction to the $\delta = d/2$ behaviour found in two and three dimensions. Furthermore, the observed tail is negative for $d = 1$ whereas it is positive for $d = 2, 3$. Bishop and Berne (1974) compared computer experiment results with the exact analytical solution of the hard-rods system but a positive noisy tail prevented them from observing the expected negative t^{-3} tail. Haus and Raveché (1978) observed in the same system the negative part of the velocity autocorrelation function in both single and multiple trajectory time averages but their data were insufficient to conclude about its particular dependence on time; this was also the case in our earlier work (Masoliver and Marro 1983) on the mixture system. In addition, general interest in asymptotic behaviours such as (11) has increased after the recent work by Fox (1983) arguing that our understanding of long-time tails is not satisfactory from the theoretical point of view nor from the viewpoint of experiments, including computer experiments. In relation to the latter, Fox (1983) heuristically claims that the propagation of round-off errors takes the numerical trajectory off a true Newtonian trajectory so that the autocorrelations are changed into mutual or cross correlations; were this the case, the computed long-time tails would rather correspond to hydrodynamic-like numerical noise. We believe, however, that the accuracy shown by our individual particle trajectories and the reported continuous changeover from our observations to the exact results for $m_2 = m_1$ certainly imply that we are analysing a real effect.

The above situation brings in any case an undeniable expectation about the long-time behaviour of the function $\psi(t)$ in the one-dimensional mixture studied here. The direct inspection of our relatively long-time data does not reveal any interesting fact except fluctuations of $\psi(t)$ apparently around a constant value which is hardly distinguishable from zero; see figure 6. Nevertheless, performing the appropriate running average of $\psi(t)$ over the time it clearly shows up that, for any value of m_2/m_1, $\psi(t)$ stays negative and it slowly goes to zero. The effect is small enough to prevent a clear direct evidence so that we have investigated the details by computing the time-dependent functions

$$D_a(t) = \int_0^t \mathrm{d}t' \; \psi_a(t') \qquad (a = 1, 2). \tag{12}$$

We observe that, apart from fluctuations, the functions $D_1(t)$ computed in all systems, i.e. for different values of m_2/m_1, are very close to each other when m_2/m_1 is not very far from unity. Thus, we have averaged $D_1(t)$ corresponding to different values of m_2/m_1. The result is shown in figure 7 where we have also included $D_2(t)$ when $m_2/m_1 = 8$ for comparison. The functions $D_2(t)$ when $m_2/m_1 \neq 8$, which are not included in the graph for clarity, only seem to differ from the one shown there by a shift in the vertical direction; see figure 8. Summing up, it seems we should conclude as shown by figures 6–8 that the qualitative behaviour of $D_a(t)$ is practically the same in any case: it decreases with time, usually becoming negative for very small values of m_2/m_1, while presenting large-period oscillations.

In order to conclude more precisely we note that assuming a short-time exponential

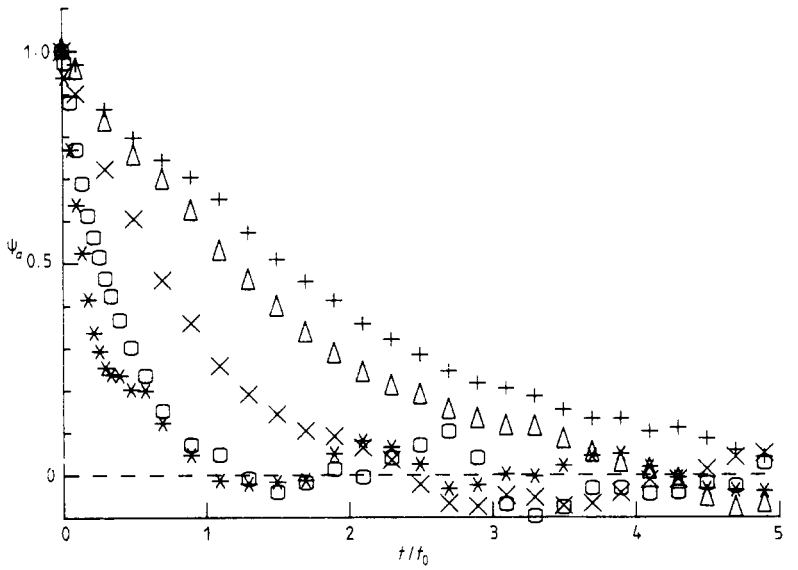

Figure 6. Early time evolution of the velocity autocorrelation function ψ_a. Symbols from the bottom to the top of the graph are as follows: asterisks ($a = 1$, $m_2/m_1 = 1.03$), circles ($a = 2$, $m_2/m_1 = 2$), crosses ($a = 2$, $m_2/m_1 = 10$), triangles ($a = 2$, $m_2/m_1 = 30$) and pluses ($a = 2$, $m_2/m_1 = 50$).

decay (7) and a negative long-time tail (11), both in agreement with the situation in figures 6–8, it follows that:

$$D_a(t) = \alpha_a - \beta_a \begin{cases} \ln t & \text{when } \delta = 1 \\ t^{1-\delta} & \text{otherwise} \end{cases} \tag{13}$$

where the negativity of the tail requires $\beta_a > 0$ and one should also expect $\alpha_a > 0$ given

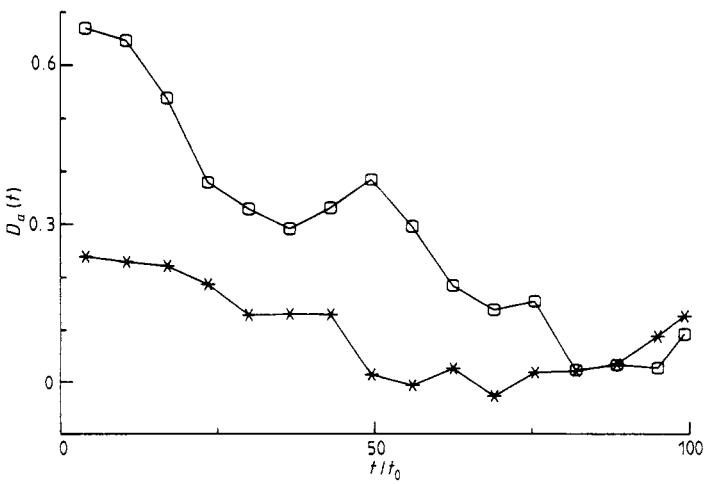

Figure 7. The function $D_a(t)$ as defined in equation (12) versus the time in units of t_0. The asterisks correspond to an average of $D_1(t)$ as computed in the cases $m_2/m_1 = 2$, 5 and 8. The circles represent the data for $D_2(t)$ when $m_2/m_1 = 8$.

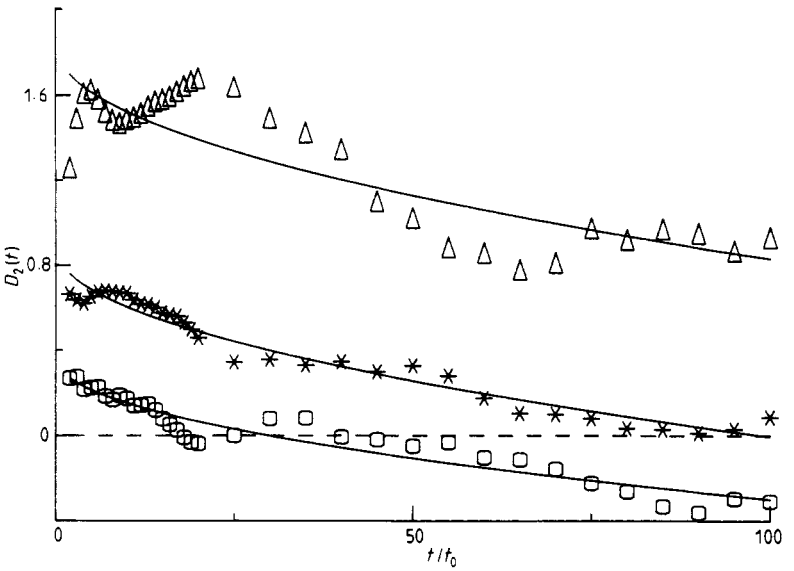

Figure 8. The function $D_2(t)$ defined in equation (12) versus time when $m_2/m_1 = 1.03$ (circles), 8 (asterisks) and 40 (triangles). The full curves correspond respectively to the fits $D_2 = 0.360 - 0.066t^{1/2}$ ($r = 0.95$), $D_2 = 0.885 - 0.089\ t^{1/2}$ ($r = 0.98$) and $D_2 = 1.841 - 0.101\,t^{1/2}$ ($r = 0.89$). A semilogarithmic fit is slightly worse giving $D_2 = 0.486 - 0.115 \ln t$ ($r = 0.90$), $D_2 = 1.043 - 0.205 \ln t$ ($r = 0.91$) and $D_2 = 1.966 - 0.214 \ln t$ ($r = 0.74$) respectively. A fit $D_2 = \alpha_2 - \beta_2 t^{-2}$ is not appropriate, e.g. gives coefficients of linear regression r much smaller: $r = 0.80$, 0.72, 0.70 respectively; see the text for an interpretation of this fact.

that after the exponential decay $\psi(t)$ becomes only slightly negative (compared with the area enclosed by $\psi(t)$ versus t when $\psi(t)$ is positive). As a consequence, we made log–log and semilogarithmic plots of $D_a(t)$ versus t to conclude that only $\delta = 1$ or $\delta = \frac{1}{2}$ are consistent with most of the data; as a matter of fact, the fit of the data to a power law t^m *with* $m < 0$ is very bad and produces negative values for the constants α_a and β_a (see caption for figure 8). We also find that a fit $D_2(t)$ versus t^{-2} (implying $\delta = 3$), which is not supported by the data when $m_2 \gg m_1$, seems to become slightly better when m_2 decreases, i.e. it seems that $\delta \to 3$ when $m_2/m_1 \to 1$ but it is difficult to make a definite statement about because the data become very noisy when $m_2/m_1 \to 1$. Figure 8 presents some examples of the general behaviour of $D_2(t)$ and fits to the data of the from $D_2 = \alpha_2 - \beta_2 t^{1/2}$.

5. Conclusions

Our results clearly confirm (Masoliver and Marro 1983) that the system evolves, except for $m_2 = m_1$, to a maxwellian velocity distribution. The relaxation time t^* the system takes to reach this velocity distribution diverges as $m_2 \to m_1$ according to equation (5) with $\varepsilon \simeq 1.9$ (figure 3) and it increases slowly with m_2/m_1; t^* presents a minimum around $m_2 \simeq 5m_1$.

The short-time behaviour of the velocity autocorrelation function shows the Lan-

gevin decay (7) with an interesting dependence of the correlation time on m_2/m_1 (figure 4). Concerning the long-time behaviour, we find for the first time experimental evidence for the existence of slowly decaying 'tails' in one-dimensional mixtures. Our results seem to indicate that the conjecture by Fox (1983) is doubtful while they extend previous exact results for $m_2 = m_1$ (Jepsen 1965, Lebowitz and Percus 1967, Lebowitz *et al* 1968). The tail we observe here is negative (figures 6–8) in agreement with the exact results and in contradiction with previous computations in two and three dimensions (Adler and Wainwright 1959, 1967, 1970). The data for $m_2 \neq m_1$ seem consistent with a characteristic exponent $\delta = 1$ in equation (11), which is in turn consistent with some results for one-dimensional lattice gases (van Beijeren *et al* 1983), but they slightly favour $\delta = \frac{1}{2}$ thus apparently following in this point the trend observed in higher dimensions, $\delta = d/2$. We also find some evidence that $\delta \to 3$ as $m_2 \to m_1$, say $m_2 \lesssim 1.01\, m_1$ (Marro and Masoliver 1985), a result which was proved rigorously in one dimension when $m_2 = m_1$ and also seems to hold for one-dimensional one-component Lennard-Jones systems (Bishop 1981).

Finally, we evaluate other interesting quantities, such as Boltzmann's H-function and correlation times, and report on their dependence on m_2/m_1.

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References

Aizenman M, Lebowitz J L and Marro J 1978 *J. Stat. Phys.* **18** 179
Alder B J and Wainwright T E 1959 *J. Chem. Phys.* **31** 459
—— 1967 *Phys. Rev. Lett.* **18** 988
—— 1970 *Phys. Rev.* A **1** 18
Baker D F and Bragg R H 1983 *Phys. Rev.* B **28** 2219
van Beijeren H, Kehr K W and Kutner R 1983 *Phys. Rev.* B **28** 5711 and references therein
Bishop M 1981 *J. Chem. Phys.* **75** 4741
Bishop M and Berne B J 1974 *J. Chem. Phys.* **60** 893
Dorfman J R and Cohen E G D 1975 *Phys. Rev.* A **12** 292
Ernst M H, Hauge E H and van Leeuwen J M J 1976 *J. Stat. Phys.* **15** 7
Erpenbeck J J and Wood W W 1982 *Phys. Rev.* A **26** 1648
Fox R F 1983 *Phys. Rev.* A **27** 3216
Hauge E H and Martin-Lof A 1973 *J. Stat. Phys.* **7** 259
Haus J W and Raveché H J 1978 *J. Chem. Phys.* **68** 4969
Jepsen D W 1965 *J. Math. Phys.* **6** 405
Lebowitz J L and Percus J K 1967 *Phys. Rev.* **155** 122
Lebowitz J L, Percus J K and Sykes J 1968 *Phys. Rev.* **171** 224
Marro J and Masoliver J 1985 *Phys. Rev. Lett.* **54** 731
Masoliver J and Marro J 1983 *J. Stat. Phys.* **31** 565
Mokross F and Büttner H 1983 *J. Phys. C: Solid State Phys.* **16** 4539
Nossal R 1965 *J. Math. Phys.* **6** 201
Ohbayashi K T, Kohno T and Utiyama H 1983 *Phys. Rev.* A **27** 2632
Paul G L and Pusey P N 1981 *J. Phys. A: Math. Gen.* **14** 3301
Pomeau Y and Résibois R 1975 *Phys. Rep.* C **19** 63
Thouless D J and Kirkpatrick K 1981 *J. Phys. C: Solid State Phys.* **14** 235