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One-dimensional mixtures of hard points with stochastic boundary conditions

P L Garrido and J Marro

Departamento de Física Aplicada, Facultad de Ciencias, Universidad de Granada, 18071 Granada, Spain

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Abstract. A one-dimensional mixture system of impenetrable, hard-core particles is analysed numerically. The particles have masses either m_1 or m_2, with $\sigma \equiv m_1/m_2 = 1$ and 1.2. Several realisations of stochastic boundary conditions simulating the contact with thermal walls are considered. We report on the relaxation from initial states with velocities ± 1 and on the properties of the final stationary non-equilibrium state. In particular, we describe the breakdown of Fourier's law when $\sigma = 1$ and the good ergodic properties of the case $\sigma > 1$, and compare with some existing theories for $\sigma = 1$.

1. Introduction

The study of one-dimensional systems of hard points with stochastic boundary conditions (SBC) is of considerable interest as a simple, non-trivial basis for investigating the nature of stationary *non-equilibrium* states (see, e.g., de Groot and Mazur (1984), Glansdorff and Prigogine (1971) and Haken (1975) for the classical theory of stationary states). Moreover, that study may provide some insight into the problem of thermal conductivity (Lebowitz and Spohn 1978, Ciccotti and Tenenbaum 1980, Tenenbaum *et al* 1982, Kipnis *et al* 1982; see also, e.g., Visscher and Gubernatis 1980 and references therein). Unfortunately, exact results are rather scarce here, even for such simple one-dimensional systems. This situation is aggravated in practice by the fact that statistical mechanics has no general formalism for non-equilibrium phenomena which is comparable to the well defined Gibbs ensemble theory for equilibrium states (see, however, for instance, Lebowitz and Bergmann 1957). As a consequence, the simulation of the behaviour of one-dimensional mixtures of hard points in a computer seems nowadays most suitable for extracting relevant information, e.g. that needed to develop a theory.

The prime motivation of the present work is in a paper by Mokross and Büttner (1983) (see also, e.g., Lebowitz and Frisch 1957, Benettin *et al* 1987, Mareschal and Amellal 1988, Erpenbeck and Cohen 1988, and references therein). Mokross and Büttner (1983) studied numerically a (small) diatomic linear chain with exponential nearest-neighbour forces (the so-called Toda lattice) with SBC. They concluded that the system only seems to support a linear temperature gradient, as in Fourier's law, in the case of different masses, i.e. when the system is non-integrable. We analyse in detail that property by considering 'large' linear chains of hard-core particles of masses either m_1 or m_2 with different realisations of SBC simulating the contact with thermal walls. The same system has previously been studied (with a different goal) either with

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periodic boundary conditions (PBC) or in the thermodynamic limit, both numerically (Masoliver and Marro 1983, Marro and Masoliver 1985a, b) and analytically (Aizenman *et al* 1978, Kasperkowitz and Reisenberger 1985a, b, Dickman 1985, Foidl 1986, Foidl *et al* 1987).

2. Description of the model

The model system of interest here is, except for boundary conditions, similar to the one considered previously by Masoliver and Marro (1983) and Marro and Masoliver (1985a, b). It consists of N impenetrable, hard-core points with masses either m_1 or m_2 moving freely, except when they collide, on a line of length L. When two particles collide, the new velocities are computed according to the energy and momentum conservation laws by using a standard algorithm (Masoliver and Marro 1983; see also Alder and Wainwright 1959). Note that in this case, collisions between particles with equal masses just produce an interchange of identity.

The particles are placed initially at random on the line, with masses either m_1 or m_2 and, independently, velocities +1, or −1, both properties also given at random. This allows the study of the system relaxation towards a stationary state in the case of a simple initial condition.

The linear chain ends at two walls, a distance L apart from each other, at temperatures T_1 (right-hand end) and T_2 (left-hand end). The walls are treated in the algorithm as special particles with zero velocity: when a particle collides with a wall, the direction of the particle velocity is reversed and its magnitude is chosen at random from a given distribution $f(v)$. We have investigated two different wall velocity distributions.

Lebowitz and Frisch (1957) studied the case of particles with equal masses, with $f(v) = f_x(v)$,

$$f_{\text{I}}(v) = (m/kT)v\exp(-mv^2/2kT) \qquad v \geq 0 \tag{2.1}$$

where m represents the mass of the particle colliding with the wall at temperature T, and k is Boltzmann's constant. That kind of SBC is known to drive the system with equal masses to a Maxwellian stationary velocity distribution when $T_1 = T_2$; our interest here is on the system's temporal evolution and stationary properties for the mixture when $T_1 \neq T_2$.

It also seems interesting to investigate the behaviour of the mixture in the case of other physically plausible wall velocity distributions lacking, however, some of the good properties of (2.1). Therefore, we have also studied the choice

$$f_{\text{II}}(v) = (2\pi\delta^2)^{-1/2}\{\exp[-(v-v_0)^2/2\delta^2] + \exp[-(v+v_0)^2/2\delta^2]\} \qquad v \geq 0. \tag{2.2}$$

Here, v_0 is fixed (arbitrarily) at $v_0^2 = kT/m\sqrt{2}$, and $\langle v^2\rangle = v_0^2 + \delta^2 = kT/m$ as required by the classical equipartition of energy; thus we have

$$\langle v\rangle = 0.739(kT/m)^{1/2} \qquad \delta^2 = 0.293(kT/m). \tag{2.3}$$

The choice $f_{\text{II}}(v)$ lacks the reversibility or symmetry property discussed by Lebowitz and Frisch (1957) (cf their equation (7)). The latter is known to be a necessary and sufficient condition for the system with equal masses and $T_1 = T_2$ to reach a canonical distribution. Therefore one should perhaps expect $f_{\text{II}}(v)$ to produce a pathological behaviour. It contains, in particular, a singularity at $v = 0$ (cf equations (8) and (5) in Lebowitz and Frisch (1957)) which may imply a slower evolution of the system, thus allowing the detailed observation of transient quasistationary states.

Table 1. Identification of the most important numerical experiments (N = number of particles, L = length of the system, $\sigma = m_1/m_2$ is the mass ratio, T_1 = temperature of the colder wall, $T_0 \equiv 14.4$, M = total number of collisions) and some properties of the observed stationary state: t_i and m are, respectively, the initial time and number of measurements characterising our stationary averages; t_0 is the mean free time between collisions (the column next to it, denoted Δ, lists the corresponding standard deviation); E represents the total (kinetic) energy of the particles (this is followed by the standard deviation Δ, skewness s, and kurtosis k of the corresponding distribution); C and K are, respectively, the global specific heat (at constant volume) and (isothermal) compressibility defined by using locally fluctuation theorems. Experiments numbered 15 and 16 concern type I SBC, while the rest are for type II; all the data here refer to elastic collisions between particles.

Expt	System						Stationary state												
no	N	N/L	σ	T_1/T_0	$\nabla T/T_0$	$M \times 10^{-6}$	t_i/t_0	m	t_0	$\Delta \times 10^2$	$E \times 10^{-2}$	$\Delta \times 10^{-2}$	s	k	$C \times 10$	$\Delta \times 10$	$K \times 10^2$	$\Delta \times 10^2$
1	1000	1	1	10	0.01	6.5	5333	91	0.26	0.12	379	24.0	−0.02	−0.6	0.16	0.02	0.97	0.23
2	1000	1	1.2	10	0.01	9.9	5677	102	0.20	0.08	530	12.0	0.41	−0.5	0.10	0.02	0.90	0.18
3	1000	1	1	1	0.001	4.1	2154	131	0.65	0.78	43.6	3.2	−0.19	−1.2	0.13	0.02	9.26	2.22
4	1000	1	1.2	1	0.001	3.4	2226	82	0.67	1.18	49.7	1.4	−0.39	−0.6	0.10	0.02	8.64	1.69
5	150	1	1	10	0.016	0.6	2950	158	0.27	0.10	36.5	5.9	0.28	0.2	1.60	0.25	1.83	0.33
6	150	1	1.2	10	0.016	0.6	2843	175	0.21	0.03	58.7	8.2	0	−0.6	0.81	0.16	1.32	0.14
7	150	1	1	10	0.067	1.0	1177	717	0.25	0.49	43.4	7.8	0	−0.3	1.88	0.10	1.67	0.17
8	150	1	1.2	10	0.067	1.0	2420	681	0.19	0.10	77.8	8.9	0.03	−0.1	0.82	0.09	0.93	0.06
9	50	0.05	1	10	0.01	0.2	1903	170	5.3	9.75	14.2	4.5	0.61	0.4	6.90	0.94	35.4	5.16
10	50	0.05	1.2	10	0.01	0.2	1969	169	3.8	2.18	26.1	5.7	0.19	−0.1	6.13	0.48	21.3	2.93
11	150	10	1	10	0.67	0.6	2780	181	0.03	0.01	46.1	7.8	0.29	−0.2	1.71	0.26	0.16	0.02
12	150	10	1.2	10	0.67	0.6	2383	246	0.02	0.01	79.0	8.0	−0.15	−0.7	0.86	0.10	0.09	0.01
13	150	1	1	1	0.007	0.9	2880	457	0.83	1.00	4.14	0.78	0.42	−0.3	2.35	1.34	18.7	5.49
14	150	1	1.2	1	0.007	0.9	2445	274	0.57	0.10	8.03	0.98	−0.13	0.2	0.84	0.12	9.29	0.87
15	1000	1	1	7.1	0.01	7.9	6000	134	0.20	0.44	768	16	−0.17	−0.52	0.10	0.01	0.43	0.15
16	1000	1	1.2	7.1	0.01	9.0	6250	201	0.16	0.17	759	20	0.15	−0.82	0.10	0.01	0.62	0.19

Brief references to inelastic collisions and to SBC other than the ones just described will be made in § 5.

In addition to different lengths L and numbers of particles N, implying different particle densities $n = N/L$ and/or system sizes, we also simulated different non-equilibrium stationary states by varying the wall temperatures, T_1 and T_2, and the mass ratio $\sigma = m_1/m_2$. The parameters defining some of our experiments are given in table 1.

2.1. Some technical details

We have no definite estimate of the influence of a given initial mass and velocity distribution, out of the set we have just defined, on the system behaviour. Nevertheless, that effect should be negligible for the system and stationary ensemble sizes involved here. Actually, no such effects were evident in a previous study with PBC (Marro and Masoliver 1985a, b); we performed each run here with a different initial distribution (and they consistently followed a good set of data), and it is known that, when it exists, the stationary distribution for equal masses in the presence of SBC will be approached in the course of time for almost all initial velocity distributions (Lebowitz and Frisch 1957).

The microscopic time-reversal invariance of the system can be guaranteed within comfortable error limits in the case of PBC (Masoliver and Marro 1983). In the present case of SBC, we updated the estimation of the total system energy each time there was a net contribution from the walls, and we also independently made periodic direct calculations of the total system energy; the two estimations of the total energy agreed within a 10^{-12} error throughout the simulations (most of the reported work was performed on an IBM 370/3083R3 computer where it required some 100 hours of CPU time).

In order to compute local quantities we divided the line into equal segments, usually of length $L/20$. The local density and temperature, for instance, were then evaluated at selected values of the time by counting the number of particles in each cell and computing their kinetic energy, respectively.

Concerning statistical errors, they are typically reasonably small in the case of properties which are independent of the labels of the particles, as they involve an average over particles which is equivalent in some sense to an average over configurations. We also tried to minimise statistical errors by sometimes performing averages over short time intervals during the system evolution, and by always performing averages over large time intervals during the stationary regime. The magnitude of finite-size effects may be estimated by comparing different system sizes, e.g. as reported in table 1. The analysis of table 1 and the rest of the data allows one to conclude that neither statistical nor finite-size errors should influence our main conclusions in this paper.

3. Time relaxation

The system relaxation from the initial state with velocities ± 1 was monitored by measuring the temporal evolution of the velocity distribution, local temperature and density, total system energy, mean particle velocity and mean free time. Most important differences occur when comparing the cases $\sigma = m_1/m_2 = 1$ and 1.2, e.g. the systems numbered 3, 4, 15 and 16 in table 1.

3.1. *Velocity distribution*

The initial velocities ± 1 are always seen to relax towards a smooth distribution centred around zero (the latter fact just reflects that the walls allow no net movement). That is, in contrast to the case of PBC, where the (non-ergodic) system with $\sigma = 1$ maintains the initial velocities ± 1 (Masoliver and Marro 1983), there is not such a simple evolution for SBC: the interaction between the particles and the (stochastic) walls causes an effective dissipation of information, even in the case of equal masses. This reveals itself to be as efficient in destroying the initial state as the dissipation caused by a non-uniform distribution of particle lengths which was shown (Aizenman *et al* 1978) to be a sufficient condition for the production of a Markovian evolution of the system with $\sigma = 1$ and PBC.

That follows, for instance, from figure 1(*a*), which shows the relaxation of the peaks ± 1 when $\sigma = 1$ for SBC of type II, (equation (2.2)). There is indeed a definite tendency there towards a smooth distribution which may be adjusted by a Gaussian (with a noticeable kurtosis, however). The interpretation of the situation for $\sigma = 1$ is still relatively simple: the particles move freely from one wall to the other, different values of the wall temperature implying different values for $\langle v \rangle$ and σ; cf equation (2.3). This simplicity allows us to evaluate the time it takes for the system interactions to destroy the information concerning the initial state. That is, the number of particles (with initial velocities ± 1) which have already collided with the walls at time t may be written approximately as

$$N(t) = N - N_{\pm 1}(t) \tag{3.1}$$

where $N_{\pm 1}(t)$ represents the number of particles still having velocities ± 1 at time t; that is exact for short enough times. One also has

$$\tilde{N}(t) = 2\Gamma t \tag{3.2}$$

where Γ is the frequency of collisions (for particles with initial velocities ± 1) with any one of the walls. It follows that the initial state is practically destroyed when $\tilde{N}(t') \simeq N$, i.e. at time $t \simeq N/2\Gamma$. We may estimate the parameter Γ from the data by combining equations (3.1) and (3.2) and interpreting $N_{\pm 1}(t)$ as the sum of the heights of the observed peaks at $v = \pm 1$ in the velocity distribution at time t. That data nicely confirms the above expectation; it reveals a linear variation of $N_{\pm 1}(t)$ with t and, in the case of system 3, for instance, one obtains $\Gamma = 0.285$ and $t' \simeq 1750 t_0$ where t_0 represents the mean free time. This helps the visual interpretation of the graphs in figure 1(*a*) and manifests a slow evolution of the system with $\sigma = 1$.

The case $\sigma = 1$ with walls of type I (equation (2.1)) shows a relaxation of the velocity distribution which is indistinguishable from that just described. That is, both types of SBC seem to cause a similar dissipation of information. The system with $\sigma = 1$ finally reaches the stationary velocity distribution predicted by Lebowitz and Frisch (1957); cf figure 2. (Note that the gap revealed by $p(v)$ at $v = 0$ in figure 2 goes to zero as $T_2 \to T_1$, the case considered by Lebowitz and Frisch.)

The evolution of the velocity distribution for $\sigma > 1$ is depicted by figure 1(*b*). This reveals a more decisive tendency towards a smooth distribution than before. Actually, the evolution of the mixture with SBC is a consequence of both the interactions between

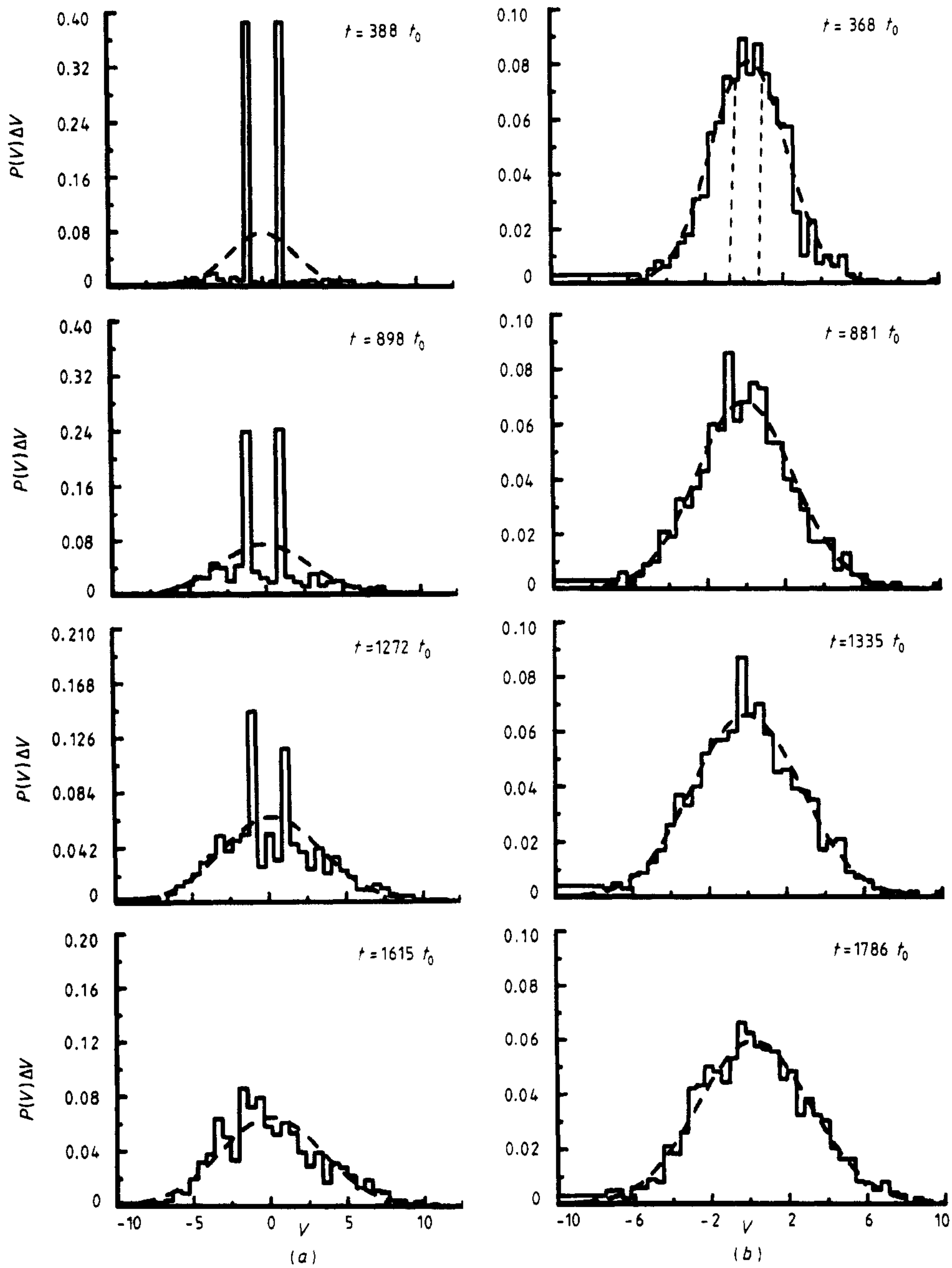

Figure 1. The time evolution of the velocity distributions of two systems: (*a*) System 3 ($\sigma = 1$); (*b*) System 4 ($\sigma > 1$). The walls are defined as in equation (2.2). The times appear on the graphs.

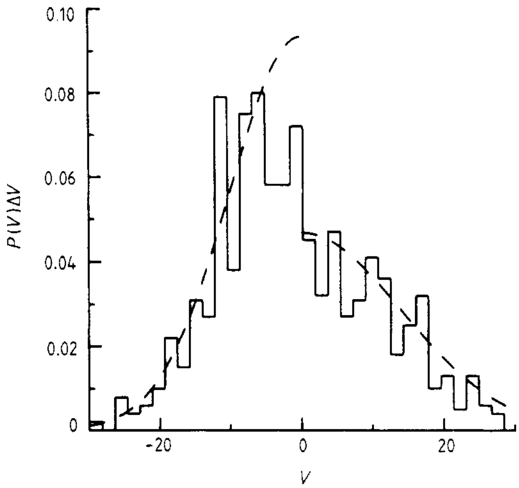

Figure 2. Stationary velocity distribution for system 15 ($\sigma = 1$, and walls defined as in equation (2.1)) at $t = 7126t_0$. The broken curve is the prediction of Lebowitz and Frisch (1957).

particles and walls and the interactions between the particles themselves. This results in a relatively complex dissipation of information for which there is no quantitative theory at hand, e.g. a theory similar to that for $\sigma = 1$ discussed in the last two paragraphs. Some qualitative reasoning, however, is consistent with our observations. As the characteristic times for those two mechanisms of dissipation differ by an order of magnitude or so, the ('ergodic') interactions between particles first tend to produce (in relatively short times) smooth distributions of velocities which are then modulated (more slowly) again and again, as a consequence of the interactions with the walls, until the system reaches the final distribution. The time the system takes to destroy the initial state is now shorter than before, because it is controlled by the ergodic mechanism which has a shorter characteristic time; nevertheless, the system takes a time comparable to that in the case $\sigma = 1$ before it reaches the final, stationary velocity distribution. Again, we found no sensible differences on the temporal evolution of the system with $\sigma > 1$ which can be associated with the type of SBC.

3.2. *Density and temperature profiles*

The present SBC simulate two walls at different temperature, i.e. the action of an external agent on the particles. Initially these have velocities ± 1, which corresponds to a uniform temperature $T = 1$ in units of $(m_1 + m_2)/2k$, i.e. the particles are 'cold' as compared to the usual wall temperatures (cf table 1). Consequently, the external agent will heat up the particle system during the evolution. More unexpected is the fact that the external agent can induce a certain non-uniform distribution of particles and kinetic energy during the system relaxation. Such an extraordinary effect was observed for $\sigma = 1$ and walls of type II; cf figure 3.

Figure 3(a) describes the time evolution of the temperature profile. This behaves in a very peculiar manner indeed: at intermediate times the temperature profile clearly tends to be bent upward around the centre of the line, thus revealing that the most energetic particles are near the centre. The corresponding density profiles in figure

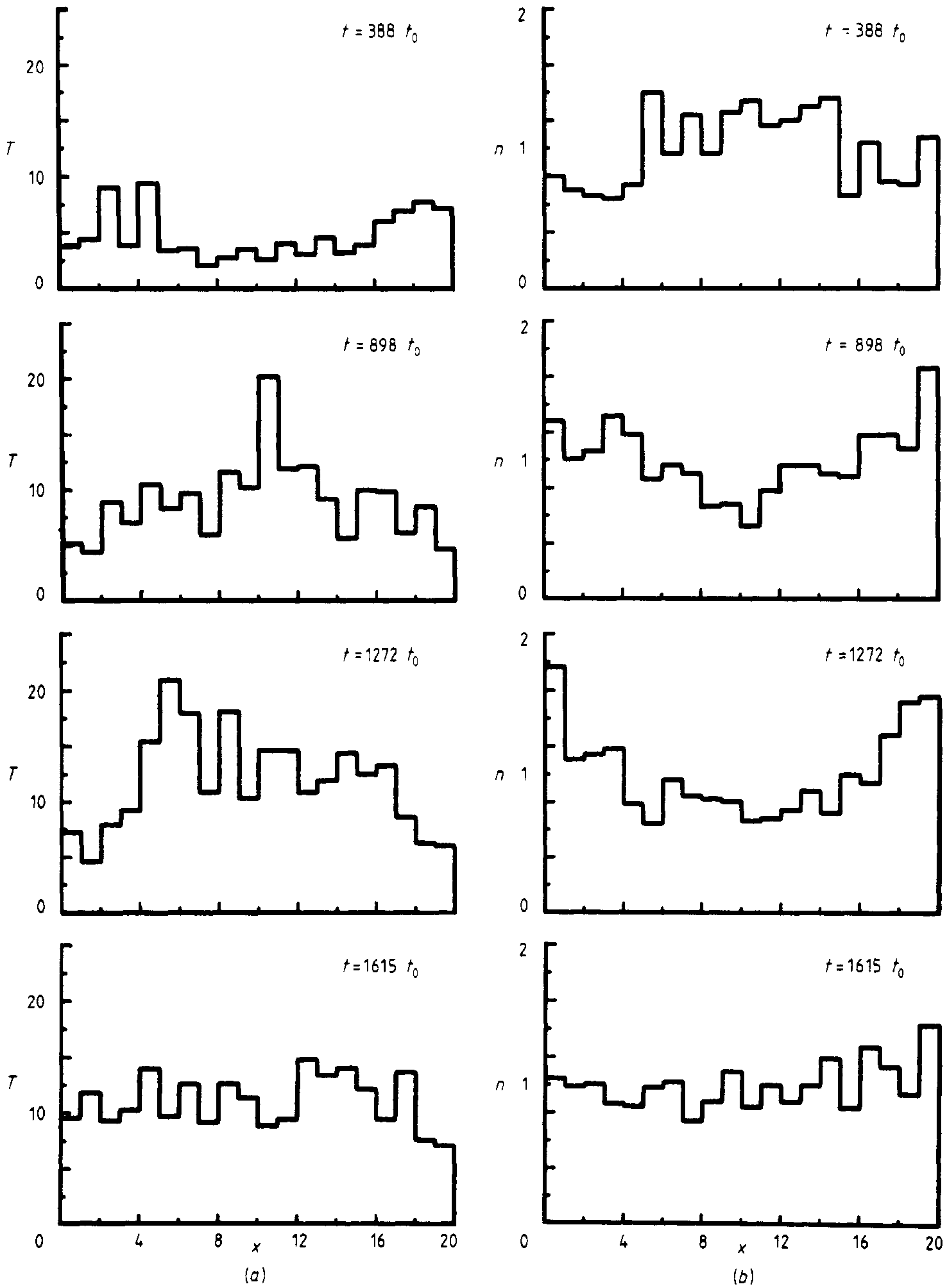

Figure 3. The time development of (a) the temperature profile and (b) the density profile of system 3 ($\sigma = 1$). The times appear on the graphs.

3(b) denote a tendency to the accumulation of particles near the ends. Having in mind that a cold particle may take more than $10^3 t_0$ to travel from one part of the system to the other, this is to be interpreted as a transient effect characteristic of type II of SBC which, contrary to type I, reject (with a high probability) particles having arbitrarily small (even zero) velocities. It should be emphasised that this is indeed a transient effect. After large enough times, as suggested by the $t = 1615 t_0$ graphs in figures 3(a) and 3(b) (see a more conclusive proof in § 4), the system tries to reach a uniform distribution of local temperatures and densities which seems to characterise the systems with $\sigma = 1$ independently of the type of SBC.

System 4, i.e. $\sigma > 1$ and type II SBC, was observed to have a more 'conventional' behaviour. That is, in addition to the fact that fluctuations are now less dramatic, the system is observed to heat up monotonously at each point of the line, presenting a regular tendency towards the stationary state, and (excluding perhaps the very initial stage of the evolution) the local temperature (local density) at any given value of the time increases (decreases) approximately linearly as one moves from T_1 to $T_2 > T_1$. We observed no noticeable (transient) effects here which can be associated with the 'pathologies' of the SBC involved: they are absent in the presence of a rich, ergodic dissipation of information. Furthermore, comparison between different experiments reveals the irrelevance of the wall properties when $\sigma > 1$, i.e. the macroscopic irrelevance of the (important) microscopic differences we consider here.

3.3. *Total system energy*

The typical time evolution of the total (kinetic) energy of the particles is depicted by figures 4 (type II SBC) and 5 (type I). The systems with unequal masses show, independently of the nature of the walls, the expected monotonous increase of the total energy which finally reaches the stationary value. Since the temperature gradient is then a constant (cf § 4), and the heating of the system has finally ceased, so that the energy flow is then the minimum necessary to maintain the stationary non-equilibrium state, the behaviour shown by the systems $\sigma > 1$ in figures 4 and 5 is compatible with the minimum entropy production which sometimes serves to characterise those states (de Groot and Mazur 1984, Glansdorff and Prigogine 1971). The systems with equal

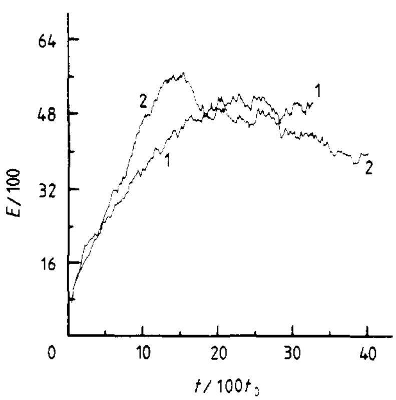

Figure 4. The total particle kinetic energy as a function of time for system 4 (curve 1) and system 3 (curve 2).

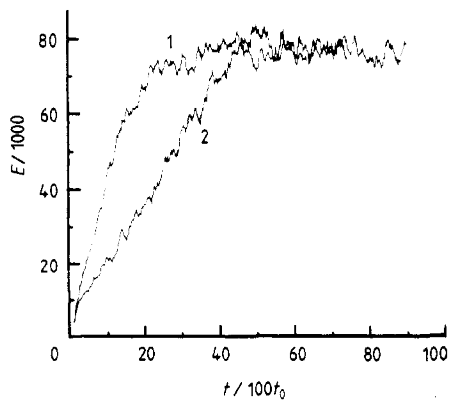

Figure 5. The total particle kinetic energy as a function of time for system 16 (curve 1) and system 15 (curve 2).

masses, on the contrary, again exhibit here differences during the evolution which may be associated with the SBC. That is, the case $\sigma = 1$ in figure 4 is rather untypical: the total energy first increases, shows a maximum around t' as computed before (after equation (3.2)), and then decreases since, in the absence of the ergodic mechanism, the transmission of energy from the high-temperature wall to the low-temperature one is faster than in the opposite direction. The observed decrease seems to stabilise in the case of small systems, while we never observed such stabilisations during the evolutions of systems 1 and 3, for instance. The behaviour of the case $\sigma = 1$ in figure 5 (type I SBC) is not so surprising, but still one may detect some decreasing behaviour during the late evolution of the energy. We interpret this as related to the failure of the minimum entropy production principle when $\sigma = 1$, a fact which can be demonstrated (Lebowitz and Frisch 1957) for small temperature gradients.

3.4. *Mean free time and particle velocity*

The behaviour of the mean free time between collisions, t_0, which is the unit of time we used for the evolutions, also distinguishes the cases $\sigma = 1$ and $\sigma > 1$ and, to some extent, the type of SBC; cf figures 6 and 7. When $\sigma > 1$, t_0 first shows a rapid decrease, and tends asymptotically to a constant value in a way which is practically independent of the SBC. When $\sigma = 1$, however, $t_0(t)$ seems to increase slowly after reaching a shallow minimum, in accordance with the behaviour of the total energy. There are some obvious differences in the behaviour shown by $t_0(t)$ in figures 6 and 7 which can be associated with the nature of the walls. Note also that t_0, involving an average over all the particles in the system, shows no short-wavelength fluctuations.

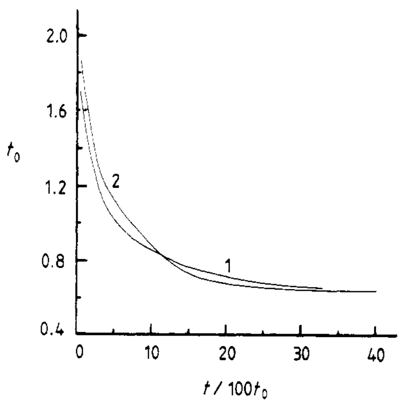

Figure 6. The mean free time between collisions as a function of time when the SBC are of type II and $\sigma > 1$ (curve 1) or $\sigma = 1$ (curve 2).

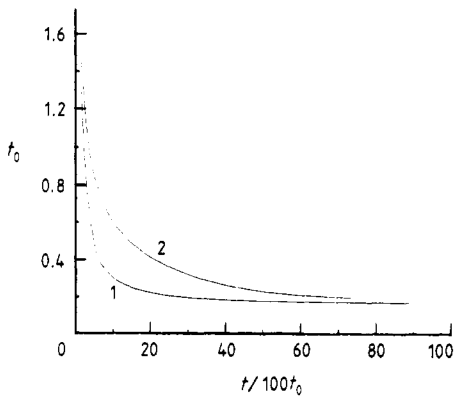

Figure 7. The mean free time between collisions as a function of time for type I SBC and $\sigma > 1$ (curve 1) or $\sigma = 1$ (curve 2).

Finally, we mention that the evolution of the mean particle velocity $\langle v \rangle$ allows us to clearly distinguish two different stages in most experiments. Typically, the centre of mass first moves from one wall to the other according to a well defined periodic oscillation implied by the temperature difference between the walls. Then, after a few such oscillations, when the local temperatures are more evenly distributed and the evolution is independent of the initial state, the motion of the centre of mass is more chaotic with no clear periodicity. The transition between those two stages occurs around $2000t_0$ in the case of system 2, for instance.

4. Stationary non-equilibrium states

Every system we have investigated seems to reach a stationary state independently of the value of σ and of the type of SBC. Table 1 lists the corresponding stationary values for some characteristic quantities as obtained by performing time averages during the final part of the evolutions (it also lists the initial time t_i we used to perform those averages). The reader should be warned that since the type II thermal walls tends to produce a slower evolution, this effect being more dramatic when $\sigma = 1$, our stationary values in table 1 for systems 3, 7 and 9 (and to a lesser extent those for systems 5, 11 and 13 as well) are less reliable than the rest. This seems to be the only clear influence of the nature of the SBC on the properties of the reported stationary states. The value of σ, on the contrary, plays a fundamental role: while the stationary state for $\sigma > 1$ has the expected 'canonical' properties, that for $\sigma = 1$ is rather anomalous.

4.1. Mean free time

The mean free time depends strongly on the density $n = N/L$ and, less dramatically, on T_1 and T_2; table 1 also reveals weak finite-size effects. There is also some evidence indicating that $t_0(\sigma = 1) > t_0(\sigma > 1)$ for given n, N, T_1 and T_2, in accordance with previous comments. Note that the standard deviations from the mean values of t_0 in table 1 are rather small; in particular, they are compatible with a good estimation of the stationary properties.

4.2. Total system energy

The mean stationary values for the system energy are denoted as E in table 1 which also lists the values for the corresponding standard deviations Δ, skewness (i.e., $s = \mu_3/\Delta^3$), and kurtosis ($k \equiv \mu_4/\Delta^4 - 3$) ($\mu_3$ and μ_4 represent respectively the third and fourth moments of the energy distribution). The values for s and k are usually small enough as to indicate that the distributions are approximately normal. On the other hand, the dependence of E (as given in table 1) on n, σ, T_1 and T_2 seems to confirm our qualitative discussion in § 3.

What seems noticeable now is the behaviour of the energy fluctuations Δ_E. On the one hand, we observe that Δ_E is affected by strong finite-size effects when, say $N \ll 1000$ as expected. On the other hand, Δ_E for large systems depends on both σ and the type of thermal walls: fluctuations are larger for $\sigma = 1$ than for $\sigma > 1$ when the system is bounded by SBC of type II, while that effect is less evident for systems with SBC of type I. That is, as the only exchange of energy with the exterior occurs through the SBC, their nature may affect the fluctuations, at least in the case of a non-canonical nature. This effect is also present in our estimations below for the 'specific heat' and 'isothermal compressibility'.

4.3. Temperature profiles

The investigation of the spatial distribution of local quantities involves the *a priori* assumption that equilibrium thermodynamics holds locally—actually at each cell (of length $L/20$). The local temperature then follows by computing the mean kinetic energy of the particles at each cell and assuming an equipartition of the energy.

The case $\sigma = 1$ (figure 8(*a*)) is, in accordance with the study by Lebowitz and Frisch (1957), anomalous in the sense that $T(x)$, $x = 1, 2, \ldots, 20$, is practically constant. This reveals that Fourier's law does not hold for $\sigma = 1$ (independently of the type of thermal walls). The case $\sigma > 1$ is illustrated by figure 8(*b*) where the temperature profile is not constant but, rather, one has

$$\tilde{T} = a_0 + a_1 x \qquad \sigma > 1 \tag{4.1}$$

where $\tilde{T} \equiv (T(x) - \langle T \rangle)/\langle T \rangle$ and $\langle T \rangle$ represents the mean value of $T(x)$ over the system. Higher-order corrections to equation (4.1), e.g. terms of order x^2, are quite negligible in practice; i.e. the linear approximation, Fourier's law, is valid to high accuracy. Table 2 lists values for a_0 and a_1, the latter intimately related to the thermal conductivity coefficient (one has from equation (4.1) that $a_1 = (\mathrm{d}\tilde{T}/\mathrm{d}x)\langle T \rangle^{-1}$ and $\lambda = -\dot{Q}/a_1\langle T \rangle$ after using Fourier's law). Note also from the values in table 2 that $a_0 > 0$ and $a_0 \simeq -10a_1$ in every case and that the result (4.1) is independent of the type of thermal walls.

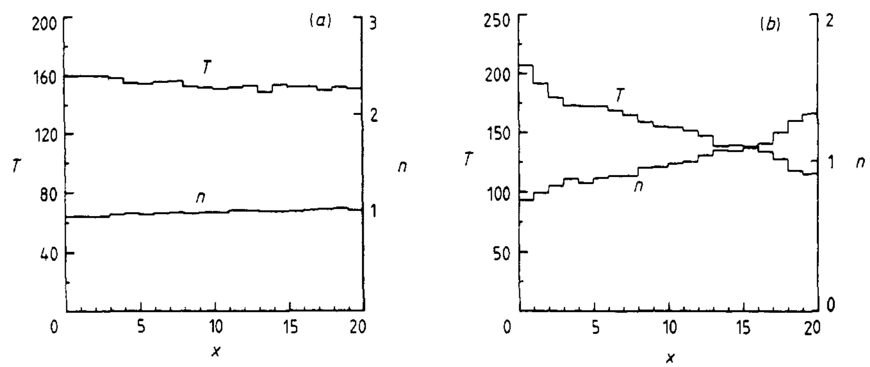

Figure 8. The stationary temperature (T) and density (n) profiles for (a) $\sigma = 1$ and (b) $\sigma > 1$.

4.4. Density profiles

The local density profiles during the stationary regime are $n(x) = \text{constant}$ for $\sigma = 1$, while

$$\tilde{n} = b_0 + b_1 x \qquad \sigma > 1. \tag{4.2}$$

Here $\tilde{n} \equiv (n(x) - \langle n \rangle)/\langle n \rangle$ where one has the sum rule $\langle n \rangle = 1$. The values for b_0 and b_1, which are listed in table 2, always satisfy $b_0 < 0$ and $b_0 = -10b_1$. No significant differences which can be associated with the nature of the walls are observed.

4.5. Local equilibrium

The local product $n(x)T(x)$ is always measured independent of x to a great accuracy. Having in mind that, in the case of the ideal-gas equation of state, nT is proportional to the pressure, this is consistent with the fact that the stationary regime requires a constant local pressure throughout the system. It also provides some *a posteriori*

Table 2. Values for the parameters in (4.1) and (4.2) describing the stationary temperature and density profiles, and mean value of $n(x)$ $T(x)$ in the system, for the cases defined in table 1.

Expt	Equation (4.1)			Equation (4.2)		nT	
no	$\langle T\rangle$	a_0	a_1	b_0	b_1	$\langle nT\rangle$	Δ
1	78.01	0	0	0	0	75.5	1.47
2	107.7	0.205	−0.020	−0.222	0.022	106	1.61
3	8.90	0	0	0	0	8.71	0.08
4	10.15	0.267	−0.027	−0.230	0.023	9.93	0.21
5	48.25	0	0	0	0	48.1	2.93
6	78.25	0.042	−0.004	−0.027	0.003	78.2	3.37
7	57.87	0	0	0	0	57.7	1.36
8	104.3	0.182	−0.018	−0.192	0.019	103	1.85
9	54.92	0	0	0	0	2.73	0.23
10	93.34	0.055	−0.006	−0.118	0.012	4.65	0.37
11	61.24	0	0	0	0	610	36.3
12	105.9	0.195	−0.019	−0.204	0.020	1044	43.1
13	5.54	0	0	0	0	5.37	0.58
14	10.73	0.170	−0.017	−0.192	0.019	10.6	0.44
15	153.3	0	0	0	0	153	1.64
16	155.3	0.212	−0.020	−0.269	0.026	151	1.72

verification of the local equilibrium hypothesis, i.e. the local magnitudes are consistent with the global ones, a fact which is confirmed below. Also interesting is the fact that the mean values of nT in the system, which are reported in table 2, are practically independent of σ in the case of the 'canonical' (type I) SBC, while we measured larger $\langle nT\rangle$ values for $\sigma>1$ than for $\sigma=1$ in the case of the type II thermal walls; this is similar to the effect on the energy fluctuations we described above.

Under the local equilibrium hypothesis, we may compute a local specific heat according to the Einstein formula, $C(x)=\Delta_T^2/4T^2$, where T represents the local temperature and Δ_T is the corresponding standard deviation. The resulting values for $C(x)$ are independent of x; table 1 lists the stationary values $C\equiv\langle C\rangle$. Those values just confirm some of our previous comments, e.g. finite-size effects and larger energy fluctuations for $\sigma=1$ than for $\sigma>1$ in the case of the type II SBC, as well as some other expected facts, e.g. their independence of the temperatures T_1 and T_2 and a strong dependence on N/L.

One may also estimate local isothermal compressibilities as $K(x)=L_c\Delta_n^2/20Tn^2$ where $L_c\equiv L/20$, $\Delta_n^2\equiv\langle n^2\rangle-n^2$ and Δ_n^2, T and n represent local quantities at each cell. Table 1 reports values for K, the mean value of $K(x)$ throughout the system, which turns out to be practically independent of x. That global 'compressibility' depicts a clear dependence on global temperature, density and system size following the expected trends.

5. Inelastic collisions and further types of SBC

We also performed a series of experiments involving inelastic collisions. When two particles, say i and j (with $j=i+1$ or $j=i-1$), with respective velocities v_i and v_j

collide, the new velocities are, as implied by momentum conservation:

$$\begin{aligned} v_i' &= (1+\sigma_{ji})^{-1}[v_i(1-\sigma_{ji}\varepsilon)+\sigma_{ji}v_j(1+\varepsilon)] \\ v_j' &= (1+\sigma_{ji})^{-1}[v_i(1+\varepsilon)+v_j(\sigma_{ji}-\varepsilon)]. \end{aligned} \tag{5.1}$$

Here σ_{ij} represents the relation between the masses involved, and $\varepsilon \equiv -(v_i'-v_j')/(v_i-v_j)$. That is, $\varepsilon=1$ for the experiments described above and $\varepsilon>1$ corresponds to inelastic collisions. The main conclusion from this study is that the differences between the pure and mixed cases only seem dramatic, as described above, when the collisions are elastic. On the contrary, the increase of ε tends to cancel out those differences and the system with $\sigma=1$ presents an apparently 'good' (ergodic) behaviour for $\varepsilon>1$.

We also considered further types of SBC. For instance, (elastic) walls which constantly emit particles such that they disappear when they first collide with one of the system particles, have the velocity distributions given by (2.1) and (2.2), and are emitted with a given frequency ν; the product $\nu T^{1/2}$, where T represents the wall temperature, is then a measure of the pressure exerted by the walls. Therefore, the latter mechanism allows the evaluation of the influence of the pressure in the system evolution. Otherwise, the only conclusion is that those emitting walls produce a slower system evolution in the computer than the contact walls described above. It may be noted, however, that such emitting walls may be quite appropriate when trying to simulate an infinite system, e.g. a few particles immersed in an infinite bath.

6. Conclusions

One-dimensional mixtures of hard points with masses either m_1 or m_2, enclosed by stochastic walls evolve as a consequence of two well defined mechanisms. There is always an effective dissipation of information caused by the interactions between the particles and the walls which, in the case $\sigma=m_1/m_2>1$, adds up to the more familiar relaxation mechanism associated with the interactions between particles. The latter mechanism has a shorter characteristic time. As a consequence, there are some qualitative as well as quantitative differences in the system relaxation (e.g. from initial states having particle velocities ± 1) when one compares the cases $\sigma=1$ and $\sigma>1$. Those differences tend to become less dramatic, or they disappear, when the collisions are inelastic ($\varepsilon>1$).

The most outstanding differences between the systems $\sigma=1$ and $\sigma>1$ with elastic collisions are seen, however, in contrast to the case of periodic boundary conditions (Marro and Masoliver 1985a, b), in the properties of the final stationary state. As expected, this is a non-equilibrium state consistent with a minimum entropy production and with linear relations such as Fourier's law when $\sigma>1$. The pure case $\sigma=1$, however, is rather untypical, for instance the total kinetic energy decreases during the final stage of the evolution, the local density and temperature are independent of position, and the minimum entropy production principle fails. In either case, $\sigma=1$ or $\sigma>1$, the local equilibrium hypothesis is well verified in the sense that some local quantities such as the pressure, specific heat and isothermal conductivity computed on that assumption are practically constant throughout the system. It is also noticeable that stochastic walls having pathologies in a sense defined by Lebowitz and Frisch (1957) do not seem to influence the stationary state. They may, however, affect the fluctuations and induce the presence of certain unexpected transient states during the system relaxation.

The peculiar, simple evolution of the system with $\sigma = 1$ and periodic boundary conditions explains that it can be solved exactly (e.g. Jepsen 1965, Lebowitz and Percus 1967), while the task is more difficult otherwise, except in certain special cases (e.g. Aizenman *et al* 1978). It thus remains a challenge to develop a complete theory for the (relatively simple) one-dimensional system considered here with either periodic or stochastic boundary conditions.

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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
Benettin G, Galgani L and Giorgilli A 1987 *Phys. Lett.* **120A** 23
Ciccotti G and Tenenbaum A 1980 *J. Stat. Phys.* **23** 767
Dickman R 1985 *J. Stat. Phys.* **41** 607
Erpenbeck J J and Cohen E G D 1988 *Phys. Rev.* A **38** 3054
Foidl Ch 1986 *J. Chem. Phys.* **85** 410
Foidl Ch, Kasperkowitz P and Eder O J 1987 *J. Phys. A: Math. Gen.* **20** 2497
Glansdorff P and Prigogine I 1971 *Structure, Stability and Fluctuations* (New York: Wiley)
de Groot S R and Mazur P 1984 *Nonequilibrium Thermodynamics* (New York: Dover)
Haken H 1975 *Rev. Mod. Phys.* **47** 67
Jepsen D W 1965 *J. Math. Phys.* **6** 405
Kasperkowitz P and Reisenberger 1985a *Phys. Rev.* A **31** 2639
—— 1985b *J. Math. Phys.* **26** 2601, 2617
Kipnis C, Marchioro C and Presutti E 1982 *J. Stat. Phys.* **27** 65
Lebowitz J L and Bergmann P G 1957 *Ann. Phys., NY* **1** 1
Lebowitz J L and Frisch H L 1957 *Phys. Rev.* **107** 917
Lebowitz J L and Percus J K 1967 *Phys. Rev.* **155** 122
Lebowitz J L and Spohn H 1978 *J. Stat. Phys.* **19** 633
Mareschall M and Amellal A 1988 *Phys. Rev.* A **37** 2189
Marro J and Masoliver J 1985a *Phys. Rev. Lett.* **54** 731
—— 1985b *J. Phys. C: Solid State Phys.* **18** 4691
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
Tenenbaum A, Ciccotti G and Gallico R 1982 *Phys. Rev.* A **25** 2778
Visscher W M and Gubernatis J E 1980 *The Dynamical Properties of Solids* vol 3, ed G K Horton and A A Maraudin (Amsterdam: North-Holland)