

Exact Results in Nonequilibrium Statistical Mechanics: Where Do We Stand?*)

J. L. LEBOWITZ

Rutgers University, New Brunswick, New Jersey

Statistical mechanics attempts to account for the observed behavior of macroscopic physical systems on the basis of the microscopic laws which govern the behavior of their "elementary" constituents (particles or molecules). A central fact of the entire endeavor is that the number of particles is very large, so that, of necessity, the concepts of probability theory play an important role. (For large systems a macroscopic statistical description is not only consistent with deterministic 'laws' it is indeed the only one feasible.) The success of the program, at least from the mathematical or rigorous point of view, has so far been largely limited to the realm of equilibrium statistical mechanics, where it explains in particular how even complex systems are susceptible to a complete macroscopic description involving only a small number of parameters (temperature, pressure, energy, entropy, volume,...). The situation with respect to nonequilibrium statistical mechanics is far more tentative. Here one is concerned with why and how systems come to equilibrium: i.e., we would like to account for the experimental fact that starting from a nonequilibrium state the system will evolve, under the action of its time evolution, to the appropriate equilibrium state, and furthermore that this approach to equilibrium satisfies the relevant kinetic (e.g. Boltzmann), hydrodynamic, and transport equations. We shall review briefly the current status of some of these problems and discuss a little more fully some steady state nonequilibrium phenomena, i.e., attempts to rigorously prove the validity of Fourier's law.

Introduction

Statistical mechanics is the link between the world of the atom and the world of the (macroscopic) object. The subject is traditionally split into two parts: equilibrium and nonequilibrium. While the latter is the subject of this meeting it may not be amiss if I start with a few words about equilibrium in order to bring out the contrast between their current status.

Our understanding of equilibrium statistical mechanics is, formally at least, essentially complete. The Gibbs formalism gives a well-specified prescription for computing all the equilibrium properties of a macroscopic system from a knowledge of its microscopic hamiltonian. Furthermore, equilibrium statistical mechanics has various model systems which: a) have a basic structure qualita-

*) Supported in part by NSF Grant No. PHY 77-22302.

tively similar to some real systems and b) exhibit in a precise mathematical form interesting phenomena observed in real systems. I have in mind here particularly the model for ferromagnetism, spins on a lattice, for which the existence of spontaneous magnetization at low temperatures can be proven rigorously.

In contrast, there are at present neither general prescriptions for constructing nonequilibrium ensembles nor realistic model systems for which kinetic laws can be proved to hold. Such well established experimental facts as Fourier's law of heat conduction or Fick's law of diffusion can neither be derived rigorously for general systems nor shown to hold for realistic microscopic models. These deficiencies in the currently available stock of rigorous results in nonequilibrium statistical mechanics while highly regrettable are not surprising. The subject is not only very broad, as the talks at this meeting certainly show, it is also mathematically very hard. Furthermore, the last dozen years have brought some remarkable progress in the field and this makes me feel encouraged about the future.

Since this is a lecture and not a course I will have to content myself with just mentioning briefly a few of these recent developments—before going on to discuss one or two examples in some detail. A final word of caution: The order in which I shall mention things is not necessarily related in any direct way to my estimation of their significance.

(i) Sinai's proof¹⁾ of the very good ergodic properties of a particle moving among fixed scatterers, further extended by I. Kubo²⁾ certainly marks some milestone. The still incomplete proof for real hard spheres is slowly moving forward: It is done for three.³⁾ Sinai's recent work⁴⁾ on calculating the Kolmogorov-Sinai entropy per particle of a system of many (possibly infinite) hard spheres is most interesting.

(ii) The work by Lanford and others⁵⁾ proving the existence of dynamics for infinite classical systems and some similar results for quantum systems.⁶⁾ These works have laid the groundwork necessary for doing nonequilibrium statistical mechanics of infinite systems. This is not just a mathematical curiosity since, as is the case in equilibrium statistical mechanics, the thermodynamic limit is essential for many purposes. (The interesting novel features of macroscopic systems, e.g., phase transitions or transport coefficients, become "mathematically clean" only in this limit.)

(iii) The work by Lanford⁵⁾ and his students on the validity of the Boltzmann equation (at least for short times) in the Boltzmann-Grad limit, $\rho \rightarrow \infty$, $a \rightarrow 0$, $\rho a^3 \rightarrow 0$, $\rho a^2 \rightarrow \lambda^{-1}$ finite $\neq 0$, and its extension to the Lorentz gas by Spohn.⁷⁾ The derivation by Braun and Hepp⁸⁾ of the Vlasov equation by a different limiting procedure.

(iv) The work by Haag, Kastler and Trych-Pohlmeyer⁹⁾ and others¹⁰⁾ on the stability of Gibbs (equilibrium) states for infinite systems which singles

them out among all possible stationary states.¹¹⁾

(v) The work by Sinai, Gurevitch and Suhov¹²⁾ proving that for a certain class of interactions the equilibrium Gibbs state is the only stationary state, among a certain large class of states.

(vi) The proof of good ergodic properties for various simple (infinite) systems¹³⁾ and the introduction by Goldstein¹⁴⁾ of the notion of space-time ergodicity for infinite classical systems.

(vii) The work by Davies¹⁵⁾ and others¹⁶⁾ proving the validity of some old, heuristically derived, and some new Master equations in the van Hove weak coupling limit. The proof of a microscopic minimum entropy production principle for these systems under suitable conditions.¹⁶⁾

(viii) The work by Hepp and Lieb¹⁷⁾ and others¹⁸⁾ on the derivation of deterministic equations for macroscopic variables in certain open systems under appropriate limiting conditions.

(ix) The work by Holley¹⁹⁾ on the derivation of the Ornstein-Uhlenbeck process (Fokker-Planck eqn.) for a heavy mass particle in a fluid in one dimension.

This list is certainly not meant to be exhaustive even among the rigorous results (which are anyway not necessarily the most interesting). In particular I have not mentioned the exciting work on:

- i) integrable Hamiltonian systems,²⁰⁾
- ii) on the "stochastic" behavior of Hamiltonian and non-Hamiltonian systems (which Ruelle and others will discuss at this meeting),
- iii) the work by Spitzer,²¹⁾ Holley and Stroock and others²²⁾ on infinite systems with stochastic dynamics,
- iv) the recent progress on the solutions of the Boltzmann eqn.,²³⁾
- v) the interesting mathematical developments in ergodic theory.^{19), 24)}

All of these will likely have an impact on future study in the field.

I hope that I have now given you some feeling for the activity in the field of rigorous statistical mechanics and would like to devote the rest of my talk to two examples of the kind of results we would like to prove, how much has actually been proven showing, unfortunately, how discouragingly far we still are from our goal. I believe, however, that the problems I shall describe are solvable and I hope that my talk will act as a challenge. To spur you on I shall offer, as has become somewhat customary at some gatherings, a bottle of champagne (or brandy if you prefer) for each solution. Now to the problems.

Stationary nonequilibrium states: Fourier's law

Consider a box A , say a parallelepiped, of cross sectional area A and height L . Imagine the box filled with fluid or solid at an average density ρ .

Let now the base of the box, at $z=0$, be “kept” at a temperature T_1 and its top, at $z=L$, at a temperature T_2 . We wish to prove; i) that the fluid in the box, the “system,” will approach in time and remain in a stationary state, and ii) that for $T_1 > T_2$ there will be, in this stationary system, a steady heat flux J through the system which, under appropriate conditions, will obey Fourier’s law of heat conduction; that is, J will be proportional to the temperature gradient in the system.

The above problem is quite clear physically, measurements of the heat conductivity of various materials are made every day and neatly tabulated in standard reference books. Mathematically however the problem is not yet well posed—even the dynamics, or the meaning of “state of the system” have not been defined. Let me therefore make the problem precise by considering a mathematically well defined model of the system and of the heat baths. The modeling is of course not unique—there are legitimate physical and even conceptual objections which can be raised about it. It does however, I believe, satisfy two objectives: a) to keep it sufficiently close to the real physical situation so that its solution will give an insight into the latter and b) to keep it simple enough to make a solution in our life time a realistic goal.

The system will be taken to be a classical fluid of hard spheres of diameter a . The microscopic state of the system will therefore be specified by a point X in Γ —the $6N$ dimensional phase space, $N=\rho AL$. If this system were isolated, e.g., free motion between collisions in the interior and specular reflection at the walls, then the time evolution of the microscopic state would be described by the measure (Liouville, microcanonical or canonical) preserving transformation $S_t: X \rightarrow S_t X$. (Possible ambiguities at triple collisions, which make S_t only defined almost everywhere, are an irrelevant and soluble difficulty.) The problems associated with proving an approach to equilibrium of such an isolated system will be discussed later. What I want to do now is to describe how the bottom and top surfaces, A_1 and A_2 at $z=0$ and $z=L$, are to model heat reservoirs at temperatures T_1 and T_2 . I shall do this by assuming a stochastic particle-surface collision.²⁵⁾ One can easily imagine more sophisticated, even purely mechanical, versions of a heat reservoir (see later). But after all the thermal conductivity should be a property of the system independent of the detailed nature of the heat reservoirs.

A simple choice of the stochastic boundary condition is that a particle arriving at A_α is emitted with a “Maxwellian” velocity distribution corresponding to the temperature T_α , $\alpha=1, 2$. More precisely, if a particle arrives at a point $(x, y, 0)$ of the bottom ((x, y, L) at the top) wall then, independently of its incoming velocity, its outgoing velocity at the same point will be in the velocity range dv with probability $v_z \phi_1(v) dv$, $v_z \geq 0$ ($-v_z \phi_2(v) dv$, $v_z < 0$), where

$$\phi_\alpha(v) = (\beta^2/2\pi) \exp[-\beta_\alpha v^2/2], \quad \alpha=1, 2. \quad (1)$$

Here $\beta_\alpha = (kT_\alpha)^{-1}$; the mass of the particles is unity. The factor v_z multiplying ϕ_α is necessary to make the canonical distribution with reciprocal temperature β stationary when $\beta_1 = \beta_2 = \beta$. The constant $\beta^2/2\pi$ has been chosen to properly normalize the flux at the wall

$$\pi \int_0^\infty d|v| |v|^3 \phi_\alpha(v) = 1.$$

Our problem is now well defined. We have as the object of our study a continuous time homogeneous Markov process on the space of all possible phase space trajectories of our system. Let $P_t(dX|X_0)$ denote the (transition) probability that a system started at the point $X_0 \in \Gamma$ at time zero will be in the volume element dX at time t . The first question is then whether $P_t(dX|X_0)$ approaches, as $t \rightarrow \infty$, some stationary distribution $\mu_s(dX)$?

A little thought shows that this cannot generally be true for every initial point X_0 ; if the density is not too high, $\rho a^3 < 1$, for a cubical box, then we can arrange for all the particles to move perpendicular to the z -axis so that they never hit the top or bottom surfaces. Clearly if X_0 is such an initial state, then $P_t(dX|X_0)$ will not approach any limit. We may, however, rephrase our question in the following way: Does $P_t(dX|X_0) \rightarrow \mu_s(dX)$ for almost all (a.a.) X_0 ? By this we mean that if $\Gamma' \subset \Gamma$ is the set of all initial states X_0 for which the limit does not exist, then the Lebesgue measure of Γ' ,

$$\omega(\Gamma') = \int_{\Gamma'} \omega(dX),$$

equals zero: $\omega(dX) = \prod_{i=1}^N dr_i dv_i$.

If the answer to the above question is yes and if furthermore μ_s is independent of the initial state X_0 then, in analogy with equilibrium statistical mechanics, we can identify the probability measure μ_s with the macroscopic state of our stationary system between the two heat reservoirs. We could then ask what is the nature of this stationary state when $T_1 > T_2$? (If $T_1 = T_2 = T$ then μ_s will clearly be the Gibbs canonical distribution at that temperature.)

In particular let $Q(X)$ be a function on Γ such that

$$J(T_1, T_2, \rho, a, A, L) = \int_\Gamma Q(X) \mu_s(dX) \quad (2)$$

is the amount of energy per unit time transported by the system from the bottom to the top reservoir. We shall then "define" the heat conductivity κ of the hard sphere fluid at density ρ and temperature T by the following sequence of limits: Let $T_1 = T + \frac{1}{2} \Delta T$, $T_2 = T - \frac{1}{2} \Delta T$, then

$$\kappa(\rho, a, T) = \lim_{L \rightarrow \infty} L [\lim_{\Delta T \rightarrow 0} (\Delta T)^{-1} (\lim_{A \rightarrow \infty} J/A)], \quad (3)$$

i.e., κ is the heat flux per unit area divided by the temperature gradient, $\Delta T/L$. The question then is: Do the limits in (3) exist and is the resulting κ positive, i.e., $0 < \kappa < \infty$? As might be expected it is the limit $L \rightarrow \infty$ which is the crux of the matter.

We do expect of course that κ will exist and be an intrinsic property of the hard-sphere system, entirely independent of the model reservoirs we used. Indeed we expect, and this is another problem—to prove, that κ , as defined by Eq. (3), coincides with the Kubo formula for the heat conductivity.²⁶⁾ The latter, as you all know, involves an integral over time of the auto-correlation function of a quantity $j(X)$ (similar to $Q(X)$)

$$\kappa_{\text{(Kubo)}} = \int_0^\infty dt C(t; \rho, a, T), \quad (4)$$

where

$$C = \lim \langle j(X) j(S_t X) \rangle_T \equiv \lim Z^{-1} \int \omega(dX) \exp[-\beta H] j(X) j(S_t X) \quad (5)$$

is an appropriate infinite volume limit²⁷⁾ of the equilibrium expectation value of $j(X) j(S_t X)$ with S_t the isolated system flow defined earlier. The existence of the integral is of course a good hard problem in its own right—but it would be interesting to get even a formal proof of the equivalence of (3) and (4) assuming both to exist.

We remark here that by dimensional analysis $\kappa(\rho, a, T)$, if it exists, will have the form

$$\kappa(\rho, a, T) = \rho \lambda \sqrt{kT} K(\rho a^3), \quad (6)$$

where $\lambda = (\rho a^3)^{-1}$ is (roughly) the mean free path (*mfp*) and K is a dimensionless function of ρa^3 . As a secondary problem we would like to prove that $\rho \lambda \sqrt{kT} K(0)$ coincides with the thermal conductivity obtained from the solution of the Boltzmann equation (via Chapman-Enskog or Hilbert) for a hard sphere gas with fixed *mfp* λ . As we shall see later it is in the Boltzmann Grad limit, $\rho a^3 \rightarrow 0$, with $\rho a^2 = \lambda^{-1}$ fixed that the Boltzmann eqn. may be expected to be exact.^{25), 27)}

What do we know? It is sad to say that, as far as I know at least, there are at present no results in the literature which could be used, more or less directly, to answer any of the questions raised for this particular, or similar, model. Goldstein, Presutti and myself have been working²⁸⁾ on such problems which combine deterministic dynamics with stochastic interactions. I feel confident that we shall soon be able to prove (certainly for the case $T_1 = T_2$ but hopefully also for $T_1 \neq T_2$) that $P_t(dX|X_0) \rightarrow \mu_s(dX)$ *a.a.* I am much less confident, however, that we shall be able, in the next year or two at least, to prove anything about the validity of Fourier's law for such a system—except possibly in the Boltzmann-Grad limit where recent work with Spohn²⁹⁾ strongly

suggests a positive answer.

The model system, which Spohn and I have considered,²⁵⁾ is a simplified version of the one described above. Instead of a hard sphere system we consider a Lorentz gas inside the box A , i.e., the particles have zero diameter and thus move independently of each other but there are *fixed* hard sphere scatterers of diameter R located at positions q_i inside the box, $i=1, \dots, M$, $\{q_i\} = \mathbf{q}$. Since the particles are independent we may as well consider just one and denote its position and velocity by $x = (r, v) \in \Gamma_1 = A \times \mathbf{R}^3$. With the same boundary conditions as before we can find the stationary distribution $\mu_s(dx; \mathbf{q})$ and we have indicated explicitly the dependence of μ_s on the position of the scatterers.

We considered then the average of $\mu_s(dx; \mathbf{q})$ over a Poisson distribution of scatterers with mean density n/R^2 , $\overline{\mu_s(dx; \mathbf{q})} = \mu_s(dx; R)$, where we have indicated only the dependence on R . Taking now the Boltzmann-Grad limit appropriate to this problem, $R \rightarrow 0$, $n = \lambda^{-1}$ fixed, we prove that $\lim \mu_s(dx; R) = f_s(x) dx$ where $f_s(x)$ is the stationary solution of the linear Boltzmann equation

$$\begin{aligned} \frac{\partial}{\partial t} f(r, v, t) &= -v \frac{\partial}{\partial r} f(r, v, t) \\ &+ n|v| \left[(4\pi)^{-1} \int d\Omega' f(r, \Omega', |v|, t) - f(r, v, t) \right] \\ &+ \text{stochastic boundary conditions,} \end{aligned} \quad (7)$$

where Ω is the direction of the velocity vector and $|v|$ its magnitude. It is now easy to show that the heat flux obtained from the stationary solution of (7) does indeed satisfy Fourier's law with

$$\kappa_B = \rho \frac{8}{3} \left(\frac{2kT}{\pi} \right)^{1/2} \lambda.$$

We can actually prove a stronger result: The stationary heat flux in the Lorentz gas converges as $R \rightarrow 0$ for almost all configurations of the scatterers, with respect to their Poisson distribution, to that obtained from the stationary solution of (7). That is to say, in the Boltzmann-Grad limit it is not really necessary to average over the distribution of the scatterers to obtain Fourier's law. This is all very nice but it doesn't really go the whole way. It requires that we take the limit $R \rightarrow 0$ *before* taking the limit $L \rightarrow \infty$. We can therefore only say that for fixed L we can make R sufficiently small for the heat flux of the Lorentz gas to be as close as we wish to that obtained from the solution of (7). We cannot, however, prove at the present time that for any fixed R , no matter how small, the limit $L \rightarrow \infty$ defined in (3) would exist. Thus we cannot rule out the possibility that the heat flux per unit area would have a form inconsistent with Fourier's law, e.g.,

$$J_R = [\kappa_B + O(R)\sqrt{L}] 4T/L.$$

In this case, as $L \rightarrow \infty$, the heat flux would go as $L^{-1/2}$ and the conductivity would diverge as $\sqrt{L}$. This kind of situation is exactly what happens for the heat flow in a harmonic chain with random masses.

Heat flow in a harmonic crystal

As you might expect, Fourier's law does not hold for a perfect harmonic crystal. We can set up the problem as before putting a crystal of cross sectional area A and length L between heat reservoirs at temperatures T_1 and T_2 which can be modeled by Langevin forces acting on the bottom and top layer,²⁹⁾ or we may consider reservoirs which are also Hamiltonian systems.³⁰⁾ In either case the heat flux per unit area will have, for large L , the form

$$J = C(T_1 - T_2),$$

where C is a constant independent of L . This means that the heat conductivity κ , defined as in (3), will be proportional to L . This is reasonable since the phonons have an infinite mfp , and all phonons participate in the energy transport, the heat flux does not vanish as $L \rightarrow \infty$.

The situation should be different, however, when the crystal is anharmonic and/or there is isotopic disorder. The anharmonic case is at the present time too difficult to treat in a rigorous mathematical way. The isotopically disordered harmonic crystal—which might not be a bad approximation to a real crystal at low temperatures—appears more within reach. Still we have no results for the two and three dimensional case, where I do expect Fourier's law to hold. For the one dimensional case, however, we do have a complete solution to the conductivity, at least for the case of dynamical reservoirs. We find that J is asymptotically proportional to $\sqrt{L}$,³¹⁾ as conjectured by Visscher.³²⁾ There is a technical, presumably unimportant, restriction on the probability distribution of the masses (assumed the same at each site) in the rigorous derivation of the above result. Furthermore it is not known at present whether J for the chain with stochastic reservoirs also behaves asymptotically like $\sqrt{L}$ or vanishes as $L^{-1/2}$.^{29)~31)}

Let me now describe a little more precisely the two different models of reservoirs mentioned above: The system will always consist of $2L+1=N$ particles with coordinates and momenta $\{q_j, p_j\} = X$, $X \in \Gamma = R^{2N}$, masses m_j and interaction energy $U = \frac{1}{2} \sum_j (q_{j+1} - q_j)^2$.

Stochastic reservoirs: Particles $-L$ and L are "tied down" by an additional potential energy term $\frac{1}{2}[q_{-L}^2 + q_L^2]$ and at the same time are in contact with heat reservoirs at temperatures T_1 and T_2 . This is specified further by saying that particles $-L$ and L are, in addition to being acted on by the harmonic

forces, also undergoing Brownian motion, i.e., an Ornstein-Uhlenbeck process, characterised by friction constants γ and temperatures T_1 and T_2 . The system now has again a Markovian transition kernel $P(dX|X_0)$.

When $0 < m_j < \infty$, then it can be shown that

$$P_t(dX|X_0) \rightarrow \mu_s(dX) = Z^{-1} \exp[-\frac{1}{2} X \mathbf{B}^{-1} X] \omega(dX). \quad (8)$$

That is, the stationary state μ_s is a Gaussian measure with a $2N$ by $2N$ covariance matrix $\mathbf{B}$ (and normalization Z) whatever the masses m_j or temperatures T_1 and T_2 .²⁹⁾ For $T_1 = T + \frac{1}{2} \Delta T$, $T_2 = T - \frac{1}{2} \Delta T$, $\mathbf{B}^{-1} = \mathbf{B}_{\text{eq}}^{-1}(T) + \Delta T \mathbf{G}$ so that for $T_1 = T_2 = T$ we recover the Gibbs state at that temperature.

The heat flux J is the average of $q_j p_{j+1}$ in the stationary ensemble μ_s . We find that when the m_j are periodic in j then, $J = c(T_1 - T_2)$, and $c \neq 0$ as $L \rightarrow \infty$. If on the other hand, the masses m_j are independent random variables with a distribution $g(dm)$, e.g., $m_j = m, M$ with probabilities p and $1-p$, then, for almost all sequences of masses $\{m_j\}$, $J \rightarrow 0$ as $L \rightarrow \infty$.²⁹⁾

The results for the regular chain go over, essentially unchanged, to higher dimensional crystals. Furthermore these stationary states have a well defined limit $\hat{\mu}_s$ as $L \rightarrow \infty$; they are actually stationary (nonequilibrium if $T_1 \neq T_2$) states of the time evolution operator $\hat{S}_t$ of the *infinite* crystal. The existence of this operator can be proven very generally, c.f. Lanford and Lebowitz in Ref. 13). We may consider these $\hat{\mu}_s$ as heat "superconducting" states; there is a flux but no gradient, c.f. Spohn and Lebowitz in Ref. 30).

Dynamical reservoirs: In this model the reservoirs themselves consist of semi-infinite harmonic chains—the left reservoir is the set of particles with index $j \in (-\infty, -L-1)$ and the right reservoir is the set of particles with index $j \in (L+1, \infty)$, i.e., the system plus reservoirs is just an infinite harmonic chain with nearest neighbor interactions $\frac{1}{2}(q_{j+1} - q_j)^2$, $j \in \mathbb{Z}$. The masses of the reservoir particles are unity, $m_j = 1$ for $j \in (-\infty, -L-1)$ or $j \in (L+1, \infty)$. At $t=0$ these reservoirs are assumed to be in thermal equilibrium at temperatures T_1 and T_2 respectively. The time evolution of system plus reservoirs is of course now governed by $\hat{S}_t$.

When the masses of the system are also equal to unity, which implies in particular that the frequency spectrum of the infinite chain is absolutely continuous, then it is possible to prove³⁰⁾ that whatever the initial state of the system the probability distribution of the infinite chain, $\hat{\mu}(t)$, will evolve in time toward a stationary Gaussian (superconducting if $T_1 \neq T_2$, equilibrium if $T_1 = T_2$) state $\hat{\mu}_s$. (Again this holds also in higher dimensions and does not depend on the interactions being nearest neighbor only).

When the masses m_j , $j \in (-L, L)$ are not equal to unity, such an approach to stationarity has not been proven independent of the initial state of the system. (It probably follows, however, from the results in Ref. 30) despite the fact that when there are isolated frequencies, as would occur if some of the

systems masses are small, then the equilibrium state of the infinite chain, for $T_1 = T_2$, is not even ergodic.¹³⁾ Nevertheless it can be shown that the heat flux through the chain has an asymptotic form given by³⁰⁾

$$J(N) = (4\pi)^{-1} (T_1 - T_2) \int_0^2 d\omega |t_N(\omega)|^2, \quad (9)$$

where $t_N(\omega)$ is the transmission coefficient, through the system, of a plane wave with frequency ω .

The proof now that the heat flux in (9), averaged over the probability distribution of the independent identically distributed sequences of masses $\{m_j\}$, $j \in (-L, L)$, each m_j having the distribution $g(dm)$, behaves, for large N as $\sqrt{N}$ depends on the behavior of products of random matrices: c.f. Ruelle in Ref. 33).

Let D_j be the two by two matrix with determinant one,

$$D_j = \begin{pmatrix} 2 - \lambda_j x & -1 \\ 1 & 0 \end{pmatrix}, \quad (10)$$

where j is a positive integer and $\{\lambda_j\}$ are independent random variables, $\bar{\lambda}_j = 1$; $\lambda_j, x > 0$. (For our problem, $\lambda_j = (m_{j-(L+1)})/\bar{m}$, $\bar{m} = \int m g(dm)$, $x = \bar{m} \omega^2$). Let now

$$\rho_N(x) = \frac{1}{N} \ln \left| \left[\prod_{j=1}^N D_j(x) \right] u \right|, \quad (11)$$

where u is a unit vector in $\mathbf{R}^2$. Then loosely stated,

$$\lim_{N \rightarrow \infty} \rho_N(x) = I(x), \quad (12)$$

where $I(x) > 0$ for $x > 0$, is continuous and behaves for small x as $(\bar{\lambda}^2 - 1)x/8$, and

$$\text{Prob}\{|\rho_N(x) - I(x)| > \varepsilon\} \leq C \exp[-N\varepsilon\phi(x)], \quad (13)$$

where $\phi(x) > 0$ for $x > 0$ and also goes as x for $x \rightarrow 0$.

Equation (12) is Furstenberg's Theorem³⁴⁾ first introduced into study of random chains by Matsuda and Ishii.²⁹⁾ Equation (13) as well as the completion of the proof about the $N^{-1/2}$ dependence of $\bar{J}(N)$ is due to Verhaggen.³¹⁾ It makes use of the work of Papanicolaou³⁵⁾ and of Pastur and Feldman.³⁶⁾

We are now exploring what happens to the heat conduction in a strip of a disordered harmonic system. The random matrix will now be of dimension $2n$ by $2n$ where n is the number of chains in the strip and it is possible that the behavior of the heat flow will change drastically when $n \rightarrow \infty$, leading to the validity of Fourier's law. This is by no means certain, however: For a two dimensional lattice in which the disorder is one dimensional, i.e. the masses

are the same in each column but vary randomly from column to column, the heat flow behaves as in the one dimensional chain.^{29), 30)}

Remark: It may be worth remarking, apropos the lecture by Araki, that for a regular harmonic crystal the stationary Gaussian states $\hat{\mu}_s$ have the same good ergodic properties as the equilibrium states but, since they do not satisfy the KMS conditions when $T_1 \neq T_2$, are not stable against perturbations in the Hamiltonian.³⁰⁾ This means that while a heat conducting state $\hat{\mu}_s$ will, if perturbed locally, return as $t \rightarrow \infty$ to its original form there may be no “nearby” stationary state when the Hamiltonian of the system is changed—even if the change is local and small. This is very reasonable physically since a small change in the interaction energy, say an additional term of the form $\varepsilon \exp [-(q_1 - q_2)^2]$ between the first and second particle, would probably lead to a change in the amount of heat flowing through the system in the steady state. This would then have to correspond to a global change in the state of the system, since the heat flux must be constant everywhere, even for very small ε .

The big problem

I have talked earlier about heat transport in the steady state of realistic systems where Fourier's law is expected to hold. There are of course also other, more microscopic, measurements which one can and does make on real systems in a steady state, i.e., x -ray scattering from a current carrying system. What we would like to have, therefore, is, in analogy with equilibrium, a prescription for finding the whole steady state μ_s of such a system. We expect that for macroscopic systems this state will be, in the “appropriate” thermodynamic limit, an intrinsic property of the system independent of the boundary conditions giving rise to the transport. More precisely, if we consider again the hard sphere gas, then we would like to know at least the linear corrections to the equilibrium state at temperature T and density ρ , i.e., does

$$\lim_{A \rightarrow \infty} \lim_{L \rightarrow \infty} \lim_{\Delta T \rightarrow 0} \left[\frac{L}{\Delta T} (\mu_s - \mu_e) \right] = \phi \quad (14)$$

exist as a linear functional, not necessarily a measure, on the appropriate space of the infinite system? If it does exist, then we could use it to calculate, in principle at least, all experimentally measured quantities in a system with a steady heat flux (at least to linear order in the gradients). Under appropriate circumstances the result should coincide with what is obtained from the solution of the Boltzmann equation. Furthermore if ϕ exists; is there any general way, in analogy with the KMS conditions, the variational principle or the DLR equation for equilibrium states, which would characterize it?

Kinetic equations: the Boltzmann-Grad limit

I would like to conclude my talk with a brief and thus necessarily rough statement of Lanford's results on the validity of the Boltzmann equations.²⁷⁾ This is a prototype of the kind of results we are after, but again we are still far from our goal.

Lanford considers a cube Λ with periodic (or reflecting) boundary conditions containing N hard spheres of diameter a . Consider now a sequence of particle numbers $N \rightarrow \infty$ and particle diameters $a \rightarrow 0$ such that $Na^2 \rightarrow \lambda^{-1}$ finite, nonzero. For each N and a we have at time zero a probability measure $\mu^{(a)}$ which has reduced distribution functions $\rho_1^{(a)}, \rho_2^{(a)}, \dots, \rho_N^{(a)}$, $\int \rho_j^{(a)} dx_1 \dots dx_j = N(N-1) \dots (N-j+1)$. Here $x_j = (q_j, p_j)$ is the position and momentum of the j th particle. The $\{\rho_j^{(a)}\}$ satisfy the ordinary BBGKY hierarchy. Define now the rescaled distributions

$$f_j^{(a)}(x_1, \dots, x_j) = N^{-j} \rho_j^{(a)}(x_1, \dots, x_j)$$

and assume that the initial states $\mu^{(a)}$ are chosen in such a way that $f_j^{(a)} \rightarrow f_j^{(0)}(x_1, \dots, x_j)$ in a "strong sense" as $a \rightarrow 0$ ($N \rightarrow \infty$). Let $f_j^{(a)}(t; x_1, \dots, x_j)$ be the distribution functions at time t obtained from the solution of the Liouville eqn. or the BBGKY hierarchy (with fixed N). Then for $0 < t < \tau$ (where τ is approximately .2 of the mean free time between collisions) Lanford finds the following: $f_j^{(a)}(t; x_1, \dots, x_j)$ converges as $a \rightarrow 0$ ($N \rightarrow \infty$) almost everywhere to $f_j^{(0)}(t; x_1, \dots, x_j)$ where the latter are solutions of a "Boltzmann hierarchy".

In particular if $f_j^{(0)}(x_1, \dots, x_j) = \prod_{i=1}^j [f_1^{(0)}(x_i)]$, then $f_j^{(0)}(t; x_1, \dots, x_j) \doteq \prod_{i=1}^j [f_1^{(0)}(t; x_i)]$ where $f_1^{(0)}(t; x)$ is the solution of the Boltzmann equation with initial condition $f_1^{(0)}(x)$. I refer you for all details, including the definition of the Boltzmann hierarchy, to Lanford's paper. This hierarchy has a structure similar to the BBGKY hierarchy for $f_j, j=1, \dots, \infty$, is irreversible and has the property that starting at $t=0$ with f_j 's which are products of the one particle distribution f_1 they remain products for all $t > 0$ with $f_1(t)$ evolving according to the Boltzmann equations.

Remarks:

i) The theorem has been extended by King²⁸⁾ to particle interactings with a more general pair potential of range a .

ii) The limitation to short times is a serious defect but is believed to be "technical" rather than fundamental. It would of course be very nice to overcome this technical difficulty so that the approach to equilibrium as $t \rightarrow \infty$ could be studied for the $f_j^{(a)}(t)$.

iii) It is not necessary to keep the region Λ fixed as $N \rightarrow \infty$. We can let $\Lambda \rightarrow \infty$ but keep ρa^2 fixed as $a \rightarrow 0$ where ρ is the average density.

iv) The appearance of an irreversible equation from the reversible dynamics is here tied up with the difference in the nature of the convergence of

the $f_j^{(a)}$ to $f_j^{(0)}$ at $t=0$ and at $t>0$. A stronger convergence is required at $t=0$, which restricts our choice of initial measures (ensemble densities) $\mu^{(a)}$, than is obtained at $t>0$. We cannot, therefore, after we have let $a\rightarrow 0$ and obtained $f_j^{(a)}(t)\rightarrow f_j^{(0)}(t)$ at some $t>0$, reverse the velocities and go back after a time t to the distributions $f_j^{(0)}(0)$.

A very crucial problem is to obtain corrections to the Boltzmann equation and show that they are "small", in some reasonable sense, when $\rho a^3 \ll 1$. To be entirely explicit consider the case where $\mu^{(a)}$ is a product of a configurational part given by the equilibrium Gibbs ensemble for hard spheres and a velocity part of the form $\prod_{i=1}^N [h(p_i)]$, with $h(p) = \exp[-\alpha p^4]$. We would then like to show that $f_i^{(a)}(t; q, p)$ can, for fixed t and p be made close to the solution of the Boltzmann equation when ρa^3 is sufficiently small (with ρa^2 fixed).

References

- 1) Ya. G. Sinai, Russ. Math. Surveys **25** (1970), 137.
See also G. Gallavotti, in *LNP 38* (Springer-Verlag, 1975), ed. J. Moser, where the proof is given in detail.
- 2) I. Kubo, *LNP 39* (Springer-Verlag, 1975), ed. H. Araki; *Lecture Notes, University of Erlangen, 1975*.
- 3) Ya. G. Sinai, Soviet Math. Doklady **4** (1963), 1818; *Stat. Mech. Found. and App.*, ed. T. A. Bak (Benjamin, 1967).
Afterword by Sinai to book by N. S. Krylov, *Foundations of Stat. Phys.* (Princeton University Press, 1978).
- 4) Ya G. Sinai, "On the Entropy per Particle for the Dynamical System of Hard Spheres", Harvard University preprint, to appear in J. Rat. Mech.
- 5) O. E. Lanford, in *LNP 38* (Springer-Verlag, 1975) and reference there in.
R. L. Dobrushin and J. Fritz, Comm. Math. Phys. **55** (1977), 275; **57** (1977), 67.
O. E. Lanford, J. L. Lebowitz and E. H. Lieb, J. Stat. Phys. **16** (1977), 453.
C. Marchiero, A. Pellegrinotti and M. Pulvirenti, Comm. Math. Phys. **58** (1978), 113.
- 6) D. Robinson, Comm. Math. Phys. **7** (1968), 337.
D. Robinson and O. E. Lanford, Comm. Math. Phys. **24** (1972), 193.
D. Ruelle, Helv. Phys. Acta.
- 7) H. Spohn, Comm. Math. Phys. **60** (1978), 277.
- 8) W. Braun and K. Kepp, Comm. Math. Phys. **56** (1977), 101.
- 9) R. Haag, D. Kastler and E. Trych-Pohlmeyer, Comm. Math. Phys. **38** (1974), 173.
H. Araki, K. Kastler, M. Takesaki and R. Haag, Comm. Math. Phys. **53** (1977), 97.
G. L. Sewell, Comm. Math. Phys. **55** (1977), 53, 63.
- 10) M. Aizenman, G. Gallavotti, S. Goldstein and J. L. Lebowitz, Comm. Math. Phys. **48** (1976), 1.
See also H. Araki, this volume for further references.
- 11) c.f. A. Lenard, J. Stat. Phys. to appear.
- 12) B. M. Gurevich, Ya. G. Sinai and Ju. Suhov, Uspekhi Mat. Nauk SSSR **28** (1973), 45.
B. M. Gurevich and Ju. M. Suhov, Comm. Math. Phys. **56** (1977), 225.
- 13) O. de Pazzis, Comm. Math. Phys. **22** (1971), 121.
Ya. G. Sinai, Funkts. Analiz. **6** (1972), 1, 41.
O. E. Lanford and J. L. Lebowitz, in *LNP 38* (Springer-Verlag, 1975), ed. J. Moser.
M. Aizeman, S. Goldstein and J. L. Lebowitz, in *LNP 38* (Springer-Verlag, 1975), ed. J. Moser.

- 14) S. Goldstein, *Comm. Math. Phys.* **39** (1975), 303.
- 15) E. B. Davies, *Comm. Math. Phys.* **33** (1973), 171; **39** (1974), 31; *J. Math. Phys.* **15** (1974), 2036; *Quantum Theory of Open Systems* (Academic Press, 1976).
- 16) c.f. H. Spohn and J. L. Lebowitz, in *Adv. Phys. Chem.* (Wiley, 1978).
- 17) K. Hepp and E. Lieb, in *LNP 38* (Springer-Verlag, 1975), ed. J. Moser.
- 18) Ph. Martin, *J. Stat. Phys.* **16** (1977), 149 and references there.
- 19) R. Holley, *Trans. Am. Math. Soc.* **144** (1969), 523.
- 20) F. Calagero, *J. Math. Phys.* **12** (1971), 419; c.f. "Dynamical Systems", in *LNP 38* (Springer-Verlag, 1975), ed. J. Moser; *Nonlinear Dynamics*, Amer. Inst. Phys. Conf. Proc. series, vol. 44 (1978).
- 21) F. Spitzer, *J. Math. Mech.* **18** (1969), 973; *Bull. Am. Math. Soc.* **83** (1977), 880.
- 22) R. Holley and D. W. Stroock, *Comm. Math. Phys.* **48** (1976), 249; **55**, (1977), 37.
T. M. Liggett, *Lecture Notes Math.* (Springer-Verlag), to appear.
J. Fritz, *J. Stat. Phys.* to appear.
- 23) c.f. C. Cercignani, *Theory and Applications of the Boltzmann Eqn.* (Elsevier, 1975).
S. Kaniel and M. Shinbrot, *Comm. Math. Phys.* **58** (1978), 65.
- 24) c.f. D. Ornstein, *Randomness, Ergodic Theory and Dynamical Systems* (Yale University Press, 1973).
c.f. also J. L. Lebowitz and O. Penrose, *Phys. Today*, p. 23, Feb. 1973.
A. Hajian and Y. Ito, *Bull. Am. Math. Soc.* **84** (1978), 417.
- 25) J. L. Lebowitz and H. Spohn, *J. Stat. Phys.* to appear.
- 26) R. Kubo, *J. Phys. Soc. Japan* **12** (1957); *Reports Prog. Phys.* **29** (1966), 255.
- 27) O. E. Lanford, in Ref. 3).
H. Grad, in *Handbuch der Physik*, ed. S. Flugge, **12** (Springer, 1958).
- 28) S. Goldstein, J. L. Lebowitz and E. Presutti, in preparation. c.f. Ya. G. Sinai, *Russ. Math. Surveys* **166** (1972), 21.
Yu. I. Kifer, *Math. U. S. S. R. Izvestia*, **8** (1974), 1083.
J. Fritz, in Ref. 22).
- 29) Z. Rieder, J. L. Lebowitz and E. Lieb, *J. Math. Phys.* **8** (1967), 1073.
H. Matsuda and K. Ishii, *Prog. Theor. Phys. Suppl. No. 45* (1970), 231.
A. Casher and J. L. Lebowitz, *J. Math. Phys.* **12** (1971), 1701.
A. J. O'Connor and J. L. Lebowitz, *J. Math. Phys.* **15** (1974), 692.
- 30) R. J. Rubin and W. L. Greer, *J. Math. Phys.* **12** (1971), 1686.
H. Spohn and J. L. Lebowitz, *Comm. Math. Phys.* **54** (1977), 97.
A. J. O'Connor and J. L. Lebowitz, in Ref. 29).
- 31) T. Verheggen, to be published.
- 32) W. M. Visscher, *Prog. Theor. Phys.* **46** (1971), 729.
J. B. Keller, G. C. Papanicolaou and J. Wielenman, *Comm. Pure and Appl. Math.*
- 33) D. Ruelle, in *Annals of N. Y. Academy of Sciences*; Conference on Bifurcation, 1978, to appear.
- 34) H. Furstenberg, *Trans. Am. Math. Soc.* **108** (1963), 377.
- 35) G. C. Papanicolaou, to appear.
- 36) L. A. Pasteur and E. P. Feldman, *Soviet Phys.-JETP* **40** (1975), 241.
- 37) F. King, Thesis, University of California, Berkeley (1976).

Discussion

R. Kubo: In your model of heat conduction there is no mechanism to establish local equilibrium for the velocity distribution. Is the temperature established in the stationary state varying in space?

J. L. Lebowitz: Yes, in some sense. The distribution at any point $\mathbf{r}$ in space

is a superposition of particles whose last collision was with wall No. one and those which last collided with wall No. two. The essence of the validity of Fourier's law for the solution of the linear Boltzmann equation is that the contribution of each of these particles decays as the distance from the wall, i.e., $\phi_1(x) \sim (1 - (x/L))\psi_1$, $\phi_2(x) = (x/L)\psi_2$ where x measures the distance from wall No. one.

M. S. Green: There is another model similar to the model of fixed hard sphere scatterers in the Boltzmann-Grad limit, which might be useful in deriving rigorous results, this is the model of independent particles moving in a weak random potential in the van Hove limit ($\lambda^2 t \rightarrow \text{constant}$).

J. L. Lebowitz: Yes, it can indeed be done but I personally don't like the time rescaling necessary in this limit.

M. S. Green: In Lanford's proof may the initial correlations be long-ranged, perhaps as long as the size of the vessel or of the mean free path?

J. L. Lebowitz: Yes, but the correlations at later times are then equal to the solution of the "Boltzmann hierarchy" which does not factor either.