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GENERALIZED GAUSSIAN DYNAMICS, PHASE-SPACE REDUCTION AND IRREVERSIBILITY: A COMMENT

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A rubric of methods developed in the past decade by various workers, W. G. Hoover, D. J. Evans, G. P. Morriss and others[1,2], have proved to be a really ingenious and efficient set of techniques for non-equilibrium molecular dynamics. In this approach, the Newtonian dynamics is modified by adding "frictional terms" according to a prescription of Gauss[3] in order to keep the total or kinetic energy a constant of the motion when the system is subjected to a thermodynamic or mechanical driving field. A variation of Gauss' modified dynamics was invented by S. Nosé[4], and simplified by Hoover[5], in which only the long-time average of the (total or kinetic) energy is fixed but which is also often employed in practical applications. We shall refer to these modifications of Newtonian dynamics collectively as *generalized Gaussian dynamics*, and to the nonequilibrium simulation technique based upon them as the Gaussian or generalized Gaussian MD method. Especially for problems where it is important to minimize boundary influences, the method seems to have significant advantages. Quite generally, it eliminates the need for any random-number generation and only requires the numerical integration of deterministic dynamics. The method can be expected to work since holding the total or kinetic energy fixed should naturally be equivalent to introducing a coupling to a heat bath or "thermostatting" the system when the number of particles is large. Therefore, it is not surprising if for such large-particle systems the use of the Gaussian method produces a steady state measure which will correctly reproduce the universal (i.e. independent of the reservoir-modeling technique) physical features of the non-equilibrium steady state. The "physical" properties are generally those which depend only on large-scale features and a macroscopic number of particles.

The phenomenon of "phase-space reduction" for this reservoir-modeling method appears to be real. There is an accumulation of numerical evidence which indicates that the "physical" ergodic measures for the Gaussian dynamics will have a multifractal character and that their information dimensions will be strictly less than the total dimension of the phase space. In particularly favorable cases where the "unperturbed dynamics" is strictly hyperbolic, e.g. the Lorentz gas with finite horizon[6,7], such statements are expected to be true for sufficiently small perturbations on rather general theoretical grounds (Y. G. Sinai, private communication). The numerical work indicates that the "dimensional reduction" may exceed the number of additional thermostatting or boundary degrees of freedom added to produce the steady state. On the other hand, we know of no systematic numerics which indicate whether or how the reduction grows asymptotically with the size of the system.

In any case, we are not ready to concede any theoretical relevance of the phase-space reduction for understanding non-equilibrium steady state phenomena in real systems. As we have already indicated, if a reservoir-modeling technique is valid at all, then the physically relevant features of the stationary measure should be independent of the technique employed. This just expresses the fact that a "reservoir" should be identified by a few thermodynamic parameters, e.g. temperature or chemical potential, and all other features should be irrelevant. Now it has been rigorously proved in some cases (and is expected to be true generally) that

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with the modeling technique using stochastic boundary conditions the stationary measures are in fact absolutely continuous with respect to the Liouville measure (see e.g.references 8 and 9). This makes it seem likely that in stationary non-equilibrium situations, fractality of the essential support of the measure has no degree of universality but is just an artifact of a particular simulation method. Of course, it is possible that even with the method of stochastic boundary conditions the "effective" support is "approximately" fractal, e.g. a slightly "thickened" version of a fractal set which becomes more and more fractal-like as the number of particles increases. That would be perfectly consistent with the rigorous theorems and most interesting (if it were true!). Let us just remark that on a certain level one should not be too surprised if the steady state measure should have a support of "vanishing volume" in the large system limit since we know even from Boltzmann and Gibbs that for a given total energy the microcanonical measure has the most entropy(=phase-space volume). All other measures supported on the shell of the same energy should therefore be concentrated in an (exponentially) small relative area. However, even if the "effective" support of the measure is approximately fractal with any modeling-technique, it is still possible to question the physical importance of the observation. Would it be a deep new insight about the non-equilibrium steady state or just a mildly interesting curiosity? *A priori* we are inclined to doubt the importance of detailed phase space features to physical questions. What is definitely missing is any clear theoretical significance of the phase space reduction in the Gaussian method.

On the other hand, it is not impossible that the Gaussian method may yield interesting new insights. One possibility we find rather intriguing is that the stationary ergodic measures produced by this method may be characterized by a variational principle. It is well- known that ergodic measures for strongly hyperbolic flows, like Axiom A systems, can be characterized by Gibbs-like variational principles involving the dynamical (KS) entropy and phase-space expansion coefficient (e.g. see reference 10.) Since the phase-space contraction, the sum of all the Lyapounov exponents, turns out in the Gaussian method to represent the physical entropy-production, there seems a suggestive similarity to a "principle of minimum entropy production." However, no precise connection is apparent to us at the moment, and one should caution that the rigorous variational principles characterize the "physical" measure only out of the class of all ergodic measures. This is quite different from more traditional variational principles.

Let us remark finally that we are quite impressed with some of the amazing properties exhibited by the Gaussian-type dynamics: the equality of phase-space contraction with physical entropy-production---even in the nonlinear regime, the resulting relation between Lyapounov exponents and transport coefficients, the ease of applying formal linear response methods within this framework, etc. It is a nice method whose mathematical structure should be explored further.

What we very strongly oppose, however, is the notion that the Gaussian dynamics has any relevance to any conceptual or foundational issue of "irreversibility." In a number of published works[11,12] it has been suggested that this dynamics is necessary to resolve the classic Loschmidt reversibility objection against the Boltzmann equation. We believe that Boltzmann's response to Loschmidt was exactly correct, and, in fact, the argument of Boltzmann has been made into a rigorous theorem by Oscar Lanford. For a very lucid discussion of the result and its conceptual implications we recommend the paper of Lanford, "On a Derivation of the Boltzmann Equation," reprinted in reference 13 . Here, let us just say that it has been shown that, out of the phase-space points consistent with an initially prescribed 1-particle distribution, the overwhelmingly larger volume in the phase-space will consist of those for which the subsequent evolution of the empirical 1-particle distribution (a phase-space function!) is given by the Boltzmann equation. This result is presently technically limited to a fraction of a mean-free-time, but that is sufficient for the entropy to increase by a finite amount. We want to emphasize that the only "assumption" in this derivation is that the initial microscopic state, or phase point, is typical for the Liouville measure. This seems very likely to be true since the set of "bad" points can be expected to occupy in the initial region at most a fraction of the volume of order $10^{-10^{20}}$ for a system of 10^{20} particles! Of course, the Loschmidt argument shows there must really be some "bad" phase-space points for which the Boltzmann evolution will not hold. In particular, letting the system evolve a certain amount of time sufficient for the entropy to increase by a positive amount and then reversing all the velocities produces such a "bad" point for which the entropy subsequently decreases.

However, this is just what Newtonian dynamics tells us should happen, and it is just what was seen, for example, in the numerical hard-disk study of Orban and Bellemans[14]. The "bad" points *are* there! However, the argument of Boltzmann and the proof of Lanford show that they are very extremely rare by any reasonable definition and inordinately unlikely to be encountered in practice.

We do not see how Gaussian dynamics makes any contribution to the understanding of irreversibility. In the first place, we think that the reservoir-modeling technique, whatever it is, introduces some built-in irreversibility. In the Gaussian method this is the phase-space contraction one typically sees asymptotically running *forward* in time. What is very special to the Gaussian-type method is that it is a *reversible* dynamics, in the sense that it is a flow on the phase space which runs backwards as well as forwards. Hence, there is a kind of "Loschmidt paradox" which arises in the context of that dynamics itself (not to be confused with the original paradox!) The question there is why the long-time future behavior of the system is for phase-space volume to contract (physical entropy-production to be positive) when, in fact, for every phase-point where there is contraction there is another (its time-reverse) where there is expansion. We believe the resolution proposed by the above authors is essentially correct: the future behavior of the system is governed by an attractive measure with essential support of fractal dimension and thus zero-volume. The behavior in the distant past is governed by a similar measure whose essential support is, however, also of zero-volume and, furthermore, *unstable* to forward evolution. Thus, behavior typical for it will never be seen in the distant future. However, this has *nothing* to do with the original paradox, and only has relevance for the Gaussian dynamics itself.

Of course, there is ABSOLUTELY no reason to believe that particles in the real world move according to a Gauss-type dynamics rather than according to Newton's laws! We want to stress this fact---despite its apparent obviousness---since it is the most essential objection against any relevance of the Gaussian motion to fundamental conceptual issues. How could one possibly believe that simply because a group of atoms is embedded in a heat-conducting state or a shear flow that their dynamics is altered from Newton (or Schrödinger) evolution? We know of absolutely no evidence or theoretical argument that would support such a radical claim, and it is easy to see that it is really impossible to consistently maintain. (Do system particles move along one set of trajectories if one just ignores the behavior of reservoir particles, and along another set of trajectories if one considers the evolution of the entire collection of system+reservoir particles?!) To believe in the actuality of the Gaussian motion would be to suffer a severe confusion between what is a convenient and interesting modeling technique and what actually happens in the real world.

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ROUND-TABLE DISCUSSIONS (II): IRREVERSIBILITY AND LYAPUNOV SPECTRA

COHEN (chairman)

The organizers in Brussels had already planned a round table on Lyapunov exponents. However, we will try and I think we will succeed in getting other topics in, also. But first, let us do the Lyapunov exponents. Now, Denis Evans already gave a talk about one aspect of it, namely a connection in a stationary state between the viscosity in particular and the sum of pairs of Lyapunov exponents which refer to a stationary state subject to a shear. About the same time, completely independently, in Brussels, Gaspard and Nicolis also found a relation between a transport coefficient, in this case a diffusion coefficient, and a Lyapunov exponent but a different kind of relation and one of the issues is "Is there any connection between these two relations, the Brussels one and the one with Denis Evans?" But since none of you has heard yet what they have done in Brussels, we thought it might be a good idea to ask Pierre Gaspard first to give a little exposé, twenty minutes, to tell us all what the Brussels' result is.

The talk by Pierre Gaspard is not reproduced here: it can be found as an article in these proceedings.

COHEN

Thank you very much. Let us ask if anybody has any comments or questions on this presentation.

EGGERS

I have got lost in in the comparison between non-equilibrium state and equilibrium state. Even in the equilibrium state, the local reflections go and they are chaotic, the trajectories are unstable. So what is meant by being stable there, in the equilibrium state?

GASPARD

In the case of equilibrium, the equilibrium will occur when the system is closed for instance. Then the escape rate is equal to zero and there will be equality between the Kolmogorov-Sinai entropy and the sum of the Lyapunov exponents which is based on formula Eq.(1.6)[1]. And because the escape rate is equal to zero, it means that the number of particles is constant in the system which means the stability of the system.

HOOVER

Could you just comment a little bit on the sensitivity of the dimensionality to the density of the scatterers?

GASPARD

By the density, do you mean the distance between the disks?

HOOVER

Yes.

GASPARD

We do not have any result on this for the moment.

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[1] the equation and figure numbers refer to those in the article by P. Gaspard.

COHEN

Well they have to be sufficiently close together, right?

GASPARD

I can give you some relationships. Here is the information dimension, D_I, which is

$$3 - 2D/\lambda\,(\frac{2.67}{R})^2$$

where 3 is the dimension of the phase space, D is the diffusion coefficient and λ is th Lyapunov exponent[2]. Let us consider a system of finite size, R fixed. We observe that th Lyapunov exponents do not change very much with the size of the gap, so the distanc between the disks. On the other hand from the work by Machta and Zwanzig, we know tha the diffusion coefficient goes to zero when we close the opening between the disks, so tha the disk dimension will then go to 3.

HOOVER

That is the same dimension which goes to 1?

GASPARD

The small d_I will then be like $1 - D/\lambda$ x (geometric factor) and without the 2. But it wil be the same effect. So the small d_I, information dimension, will go to 1.

NICOLIS

One comment! All those microscopic simulations deal with Hamiltonian dynamics ir many cases but of course what Pierre has been discussing is, strictly speaking, valid fo billiards. So these are essentially very strongly unstable dynamical systems. The connectior between a real Hamiltonian system with smooth interactions remains still to be established. Maybe there is such a connection, but I think you will agree with me that all that has been done so far is valid only for billiards.

HOOVER

We did study a little bit the very steep Hooke's law potentials, just purely repulsive. and the hard disks results are recovered as limiting cases. You could look at the smooth Hamiltonian if you would like to. That would converge to these results.

GASPARD

Thank you for the suggestion.

EVANS

I have a couple of questions. One question comes to my mind with your first slide when you were talking about characteristic times for chaos and you said they were of the order of the reciprocal of the Lyapunov exponents. But as you go to thermodynamic limit, the Lyapunov spectrum fills in and produces a continuous line that actually usually goes through zero. So those times, as far as I can see, would actually be unbounded. So that is the first question.

GASPARD

Yes I agree there can be Lyapunov exponents which can be very small in a large system but the dynamical chaos, being given by the Kolmogorov-Sinai entropy is a sum of all the Lyapunov exponents, the positive Lyapunov exponents. In that sense, it is the order of magnitude of the maximum Lyapunov exponent which characterizes the instability in the system. I agree that there are interesting effects from the nearly zero Lyapunov exponents.

EVANS

The second question I had is not about the method in principle but in practice. You can see what is going to happen as the system becomes very large. The difference between the largest Lyapunov exponent, λ, and the Kolmogorov-Sinai entropy must go to zero like $1/R^2$ as R gets very large[3]...

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2 see Eq. (5.1)
3 see Eq. (1.7)

GASPARD

As it should to compensate this and give the diffusion coefficient when you take this (cf. Eq. (1.7)).

EVANS

It is just a comment that if you are trying to actually get numbers like Joel was talking about before, trying to get the microscopic numbers in the thermodynamic limit, that would appear from a practical, not from a theoretical point of view, extremely difficult.

GASPARD

I agree on this, I made some comments about the different time scales which, at the origin of this phenomenon, that these numbers are generally very large while the transport appears in the difference between them. If we have to measure numerically all these numbers, it could be difficult to see the slight difference between them.

LEVERMORE

First, just a short question! In the calculations, did you only do simulations with finite horizon for the balls? If not, did they have a well defined diffusion coefficient? How close to the streaming limit did you go? I did not see marked on the graphs, maybe it was there.

GASPARD

The limit where the billiards changed from finite horizon to infinite horizon is indicated by an arrow on figure 6 ($W=W_c$) and the last point is quite close to it. It would be interesting to see what happens at the transition.

FRISCH

When you say "large", do you mean there is a control parameter that allows you to become arbitrary large or just accidentally, let us say, one order of magnitude larger?

GASPARD

Excuse me, I did not understand the question.

FRISCH

You said that the transport coefficient is the difference of two large quantities. So the word "large" should not be used too loosely. Is there a control parameter that allows these things to become arbitrarily large? Is it just like having a situation where something which is 1.15 is a difference between two things that are about 15 or so? Is there some mathematics behind it or is it just accidental?

GASPARD

When I say "large" or "small" in this discussion, it is a comparison between, let us say, the Lyapunov exponent in its own unit, and the escape rate corresponding to the diffusion process so I mean the diffusion coefficient times the geometrical factor of the scatterers. And these quantities are given in units of the inverse of time.

COHEN

But the question is: when you say "large", those two numbers, how large are they to give a very small number over there, if I understood the question correctly.

GASPARD

In the example that I show, the Lyapunov exponent is around 1.14 and the diffusion coefficient itself- but I do not make the comparison with the diffusion coefficient- varies in the range 0.1 - 0.01... but the comparison is not made on the diffusion, it is done with the escape rate which is much smaller than the diffusion coefficient.

COHEN

It was not clear to me how you determine the difficult quantity in my opinion, the Kolmogorov-Sinai entropy, because the usual way to do it is using Pesin theorem but of course you cannot do it here by definition. So how did you determine the Kolmogorov-Sinai entropy?

GASPARD

This Eq. (1.6) is a generalization of the Pesin formula. It is recovered for finite and bounded systems because in that case the escape rate goes to zero and there is equality between them. So the Kolmogorov-Sinai entropy has its definition in terms of partition of phase space and measures how the probability of some cells goes to zero.

COHEN

Is that how you determine it?

GASPARD

No. We did not calculate numerically this quantity because it is very difficult to obtain and what we use is a comparison at the level of the fractal properties. So comparing the information dimension with the dimension of Hausdorff.

COHEN

And how did you get it then?

GASPARD

Because the Hausdorff dimension can be calculated independently and there are three quantities which are calculated independently and compared then. So here, there is a measurement of the escape rate and the Lyapunov exponent and there is the Kolmogorov-Sinai entropy which is not measured because it is the most difficult quantity but it is replaced by a measurement of the Hausdorff dimension.

COHEN

And how did you measure that?

GASPARD

By the algorithm of the Maryland Group and it is totally independent from the previous quantities.

COHEN

So I see.

Now Harald Posch would like to make some comments, I think, also on the work of Bill Hoover and him. I would like before he does that to thank you very much, Pierre.

As you may have gathered from the talk of Denis, the relationship which we are particularly interested in, namely this conjugated pairing, was anyway a later development of a more elementary connection which had been discussed before by Bill and by Harald, namely that there was a connection between the contraction of phase space and the transport coefficients and also, on the other hand, with the sum of all the Lyapunov exponents. So that preceded in a way our work and I think therefore it would be useful if Harald might want to comment a little bit more on that.

POSCH

Since our present chairman has threatened to cut me off after 5 minutes, I would like to comment shortly on some properties of the equilibrium Lyapunov spectra which might be of interest for the study of many-body systems or of the behavior of complex molecules. Secondly I would like to make a comment about the calculation of these properties. We have seen already in the talks by Bill and Denis how these algorithms work.

You look, in phase space, at trajectories originating from a (differential) hypersphere centered on the reference trajectory. In the figure 1, I have drawn a three-dimensional phase-space. Let us watch how this hypersphere evolves in time. It develops into an ellipse, and one determines the eigenvectors and the eigenvalues. The lengths of these vectors increase or decrease exponentially as a function of time.Now, Denis Evans has shown us that there is another way of calculating these exponents by adding a constraint force to keep these vectors orthogonal and of unit length. This algorithm was invented four years ago and the constraint force determined by Gauss' principle, is a measure of the Lyapunov exponent after averaging over the whole trajectory. I would like to show you that instead of invoking Gauss' principle, one can do the same thing with Nosé's ideas. Here are the equations of motion written down for the unit vectors evolving in tangent space.

Second Law of Thermodynamics in Real Systems

Follow the Liouville description for phase-space hypervolume deformation:

$-\dot{\otimes} = \zeta\otimes$; $\Leftrightarrow f(q,p) = f(t=0)\exp(\zeta t)$, giving a loss of dimensionality:

The Kaplan-Yorke Conjecture implies:

For Dilute Gas: $(\Delta D/N) = (\lambda\nabla u/c)^2$ or $(\lambda\nabla T/T)^2$; λ is the mean free path.

Liquid: $(\Delta D/N) = (\sigma\nabla u/c)^2$ or $(\sigma\nabla T/T)^2$; σ is the effective collision diameter.

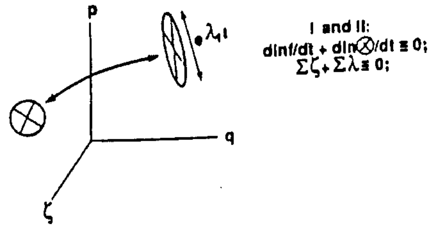


FIGURE 1. Definition of Lyapunov exponents.

The dynamical matrix which Denis was referring to comes from a linearized version of the original equations of motion.The calculation of the Lyapunov exponents proceeds such that a constraining force is added with a Lagrange multiplier determined from Gauss' principle of least constraint. But one can apply Nosé's idea to determine lambda from a differential equation which looks very similar to what you have seen from the Nosé thermostat. The length of the vector delta is contrained to unity and the vectors are kept orthogonal, not at every instant of time but on the average. One only has to make sure that the response time of the thermostat is small enough so that orthonormality does not deteriorate. This might be a different and even more efficient way of calculating Lyapunov exponents particularly in stiff cases where one is forced to use very tiny time steps for applying Gauss' principle of least constraint. So this is only an idea how to calculate the Lyapunov exponents invoking these principles.

Now let me turn to another important point. How do these Lyapunov spectra for many-body systems look like? In equilibrium, there is no external force. We have learned that the spectra are symmetrical. In the figure 3, Lyapunov spectra for a 32 particles system in three dimensions are shown. Only the positive branches are given.
As you may see, there is a quantitative change in shape if the density is changed from liquid to solid. I have got a number of these data here. Each of these curves, of course, consists of discrete points with the abcissa indicating the degree of freedom.They are only connected to guide the eye. The labels indicate the density of the system at constant temperature. This is an isothermal approach from the liquid to the solid. Here is the most dense solid, and if we reduce the density, the most positive Lyapunov exponent increases, goes through a maximum and becomes smaller again. This is interesting because you can study phase transitions by looking at the Lyapunov exponents . If you approach the phase transition, the Lyapunov exponent goes through a maximum.

EXTENDING NOSE'S IDEAS TO LYAPUNOV SPECTRA

In 1984 Shuishi Nosé discovered a new route to Gibbs'statistical mechanics. When the corresponding Nosé-Hoover equations of motion are generalized, applying then away from equilibrium, the dynamics of a single ["mixing"] system generates a NONEQUILIBRIUM ENSEMBLE in just the same way that a single equilibrium system generates Gibbs' equilibrium MICROCANONICAL ENSEMBLE.
The same idea can be applied to Lyapunov Spectra. Using δ to represent the offset between a reference trajectory and a satellite trajectory, feedback equations such as:

$$\dot{\delta} = D.\delta - \lambda\,\delta; \qquad \dot{\lambda} = [(\delta/\delta_0)^2 - 1]/\tau^2,$$

determine the Lyapunov exponents. For instance: $\lambda_1 = \langle\lambda\rangle$

FIGURE 2. H. Posch's second viewgraph.

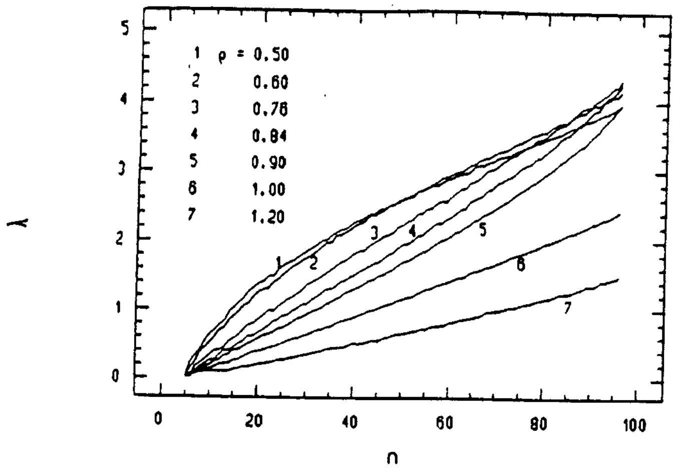


FIGURE 3. Third viewgraph: positive branch of Lyapunov spectra at various densities.

This tells us that, at the phase transition, the dynamics becomes most violent and chaotic. This would be also a way, for example, to study the dissipation of energy in a molecule. If you have a complex molecule and you would like to know how many modes of the molecule participate in the dissipation, you can calculate the Lyapunov spectrum and look how many positive Lyapunov exponents there are. We have done this, for example, for a polymeric chain and we have seen that violent chaotic dynamics takes place essentially in one or two degrees of freedom. All the other degrees of freedom are characterized by very small Lyapunov exponents. This would be another way of looking at phase transitions.

By looking at these orthonormal vectors, introduced above in connection with the computation of Lyapunov exponents, there is another property of interest. They do not only change their length in phase space as we go along the trajectory. These orthonormal vectors also rotate. Different information may be gained about the system if we look at the speed of rotation. We have introduced rotation numbers, and these rotation numbers are evaluated for the same system mentioned above with the density going from the liquid to the solid. These rotation spectra, as we could call them, go smoothly through the phase transition. We do not know what this really means because the relationship between the dynamical properties of the solid and of these spectra which were obtained numerically has not been worked out. But I am convinced that there are deep connections between these graphs and the dynamical properties of the solid, their frequency spectra. These were the only comments I wanted to make with respect to systems in equilibrium and I think that Bill is going to continue about what happens if the system is subjected to an external perturbation. Thank you.

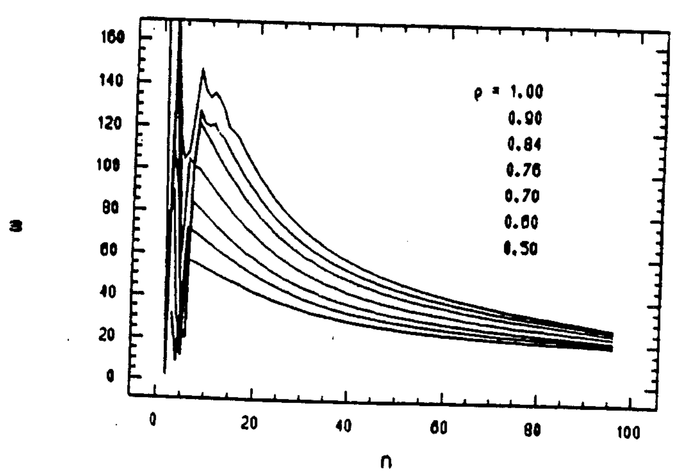


FIGURE 4. Fourth viewgraph: rotation spectra

FEIGENBAUM

Could you say a little bit better what this rotation numbers business is? I am just wondering if it is invariant under coordinate transformation.

POSCH

There is a well-known theorem for the Lyapunov exponents which guarantees their uniqueness and invariance A similar result is known to hold for rotation numbers introduced by Ruelle some time ago. These numbers are related -but not identical- to the rotation numbers evaluated by us. Whether there is a uniqueness theorem for our numbers, we do not know yet. The spectra shown in the figure are the only results we have for a larger system.

GASPARD

You showed the maximum Lyapunov exponent through the transition. What about the sum of the positive Lyapunov exponents ?

POSCH

The Kolmogorov entropy also goes through a maximum.

HOOVER

I just would like to continue along the lines that Harald was talking, to tell you a bit about what happens to the spectrum of the Lyapunov exponents as the system is driven away from equilibrium.

There are some reasonably interesting things which happen with respect to the dimensionality of the attractor in a non-equilibrium case. For the Galton board, the dimensionality is smaller than the dimensionality in the equilibrium case. Now I would like to show you the direct relationship between the dimensionality and the Lyapunov exponents. So I have shown that here for a particular special case. The reason for choosing this particular special case, which is planar Couette flow, is that we have done a considerable amount of work on it. So I would like to go through this one viewgraph relatively slowly, make sure that the notation is reasonably clear and also that the message is clear.

I am considering planar Couette flow with periodic boundary conditions. I have a cube, the side length of which is L, which contains all together N particles. It turns out to be

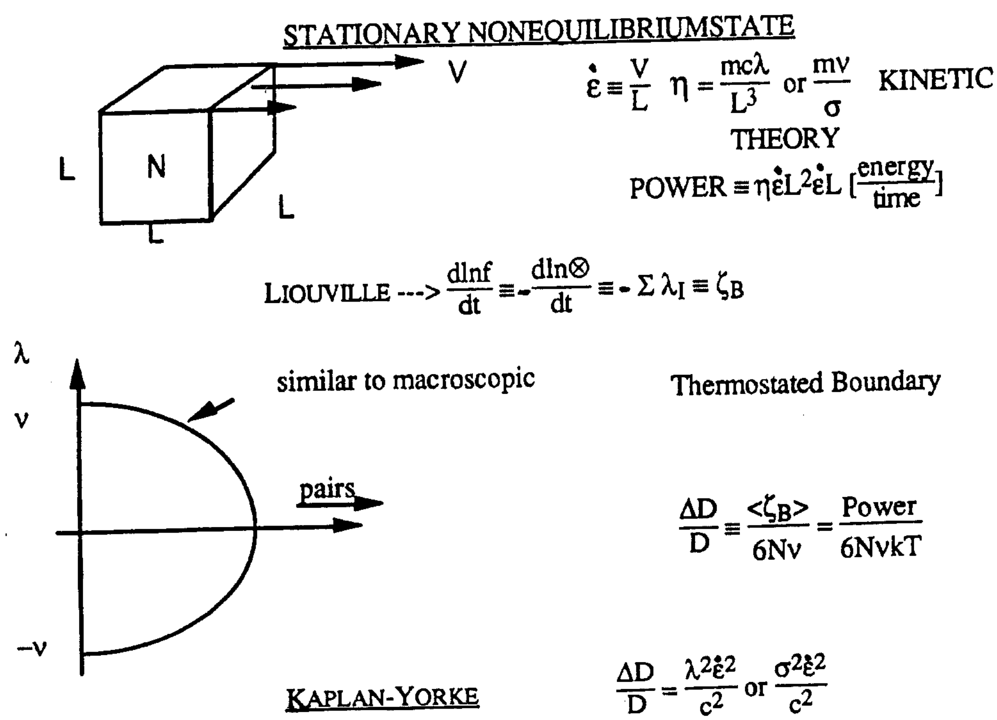


FIGURE 5. Bill Hoover's first viewgraph

unpractical to study at the present time more than about 100 particles in computing entirely the Lyapunov spectrum but we can do that with a fast computer. So if you pick the force low and the temperature of interest and the number of particles, the only remaining parameter is the strain rate. How fast is the top of the periodic cube moving with respect to the bottom? If you do that, you will observe a shift of the spectrum rather like that which Denis described in the diffusive case, that is, just a simple shift of the spectrum downwards from values which sum to zero to values which sum to the rate at which entropy has been dissipated divided by Boltzmann's constant.

I would like to consider here the possibility of something that would perhaps make Joel and Eddie a little more happy, namely a system which has been driven from the boundary. So let us consider the top of the system to be a rough plate, like sand paper, moving along, and to have inside a set of Newtonian particles. So it is basically Newton mechanics plus a single boundary degree of freedom which is attached to a Nosé oscillator in order to maintain the desired temperature. If you do that, then the rest of it, to an order of magnitude, is a back-of-the-envelope calculation which can be corroborated by machine calculations. What I have done here is to calculate the viscosity from kinetic theory, both the low density gas version written in terms of the mean free path, indicated by a green lambda, so it is not confused with the red lambda, that is the Lyapunov exponent, and also the high density version based on a solid-like theory which gives the viscosity coefficient in terms of the vibration frequency and the interparticle diameter. If you have the viscosity coefficient, then you can calculate the frictional force on the upper plate, just the shear stress, $\eta.\varepsilon$, times the area of the plate multiplied by the velocity, εL, at which that plate is moving ($\eta\varepsilon L^2\varepsilon L$) gives the power dissipation .That can be measured in watts for instance. And that power dissipation, thanks to the Nosé equations of motion, can be expressed exactly in terms of the single friction coefficient which applies to the boundary degree of freedom and also to the sum of all Lyapunov exponents. The reason for that is the conservation relation in the phase space, namely that the volume in the phase space multiplied by the probability density must be a constant of the motion. It is just conservation and probability. So when the probability density is increasing, then the volume must be decreasing in a corresponding way. And by using a chain rule, essentially the Liouville theorem, it is quite easy to calculate the rate at which the probability density changes in the phase space. In this particular system, with only a single friction coefficient, it is exactly the friction coefficient characteristic of the boundary particle. So it gives the relationship between Nosé friction coefficient (ζ) and the Lyapunov spectrum which we just have been discussing, because of course the sum of the total Lyapunov spectrum gives the rate at which the volume element in the phase space is changing with time.

Now, in the steady state, it should be obvious that the volume, if it is changing, can only get smaller. The possibility that it gets larger is contrary to the existence of a steady state. It cannot get larger forever. And so of course, it turns out in our simulations, that the sum of the Lyapunov exponents is a negative number and gives the rate at which the phase space volume is contracting in the strange attractor corresponding to a transport process. So typically the friction coefficient for the boundary degree of freedom is positive and the sum of the Lyapunov exponents is negative. I have indicated a shift here for the situation that Denis was talking about in which all of the pairs undergo equal negative shifts. The situation is maybe a little bit more complicated in a flow that is driven by the boundary. I can show you some spectra here, just a bunch of discrete dots for a system which is ranging up to 25 particles in 2 dimensions. 25 particles have basically a 100 dimensional phase space and it is already a rather discouraging job to keep track of the motion of the 100 basis vectors rotating in that space. If you look very carefully at the zero line, you will notice that it is above the mean value of all of the spectra, they have been shifted downwards.If you add the spectra up, you get a negative number which describes the rate at which the phase space volume is contracting and if you ask yourself the question: "how many of the Lyapunov exponents would have to be left out of this negative sum in order to get zero instead?", where zero would correspond to an object in the phase space that has a constant volume rather than a shrinking volume, the answer to that gives you the information dimension of the strange attractor characterizing the non-equilibrium motion. If you calculate that, simply using the collision frequency as an estimate of the largest Lyapunov exponent, which is qualitatively correct, and divide the shrinkage in the phase space dimensionality by the total dimensionality, that would be 6 N in the case of a N particle problem in 3 dimensions. Then the result is rather simple, namely the relative loss of dimensionality in the phase space: it was the result at the bottom, I think, of Harald's first viewgraph, that is the square of the

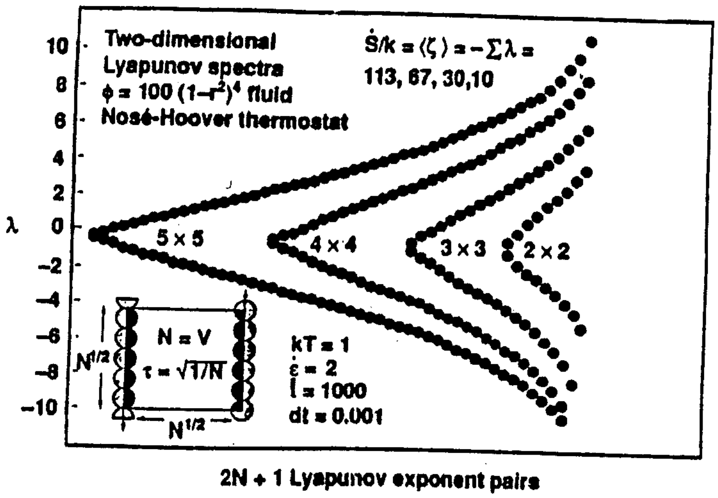


FIGURE 6. Bill. Hoover's second viewgraph

gradient, the square of the strain rate in this case. It would be the square of the temperature gradient in the case of heat transfer for instance, multiplied by the particle diameter squared and divided by the square of the speed of sound in a high density case, the mean free path replacing the particle diameter in a low density case. Now in the cases which we have investigated numerically, the phase space shrinkage has typically been no more than a few. I think the maximum may be 5 or 6 for these boundary driven problems in 2 dimensions. However, not having thought out the problem too carefully in advance, we have done almost all of our shear boundary driven calculations at relatively high density. And it is clear from this analysis, I think, that the phase space shrinkage would be much more dramatic in the case of a lower density system. So I think Harald and I, as soon as we are forced to leave this beautiful place, are going to hot foot it to our computers and see if we can verify that indeed the phase space shrinkage is gravely accelerated by using a low density rather than a high density simulation. So that is all I wanted to say.

GASPARD

I would like to make a comment on the way the boundary conditions are imposed on the system. You use a dissipative assumption about the dynamics at the boundary but there is another way which would be a stochastic model of sticking to the boundary and then reemission of the particles. In this kind of stochastic models, the concept of Lyapunov exponents should be replaced by another type of concept which is closer to the Kolmogorov-Sinai entropy or the epsilon entropy because if we make a stochastic assumption at the boundaries then we know that the complete Kolmogorov-Sinai entropy of the system will be infinite like in ideal gases. So if we use an epsilon entropy, then we can separate different contributions, the epsilon entropy will go to the Kolmogorov-Sinai infinite entropy as epsilon goes to zero, but then there are different terms, some of which are divergent, some are not, and these terms which are not divergent could be then related to the sum of the Lyapunov exponents. So I think that there are some possibilities to relate stochastic models to the assumption that you are doing, which is more deterministic.

HOOVER

I just wanted to say that I agree completely with what you had to say. It is true that if you use the stochastic boundary then the Lyapunov exponent for that degree of freedom will become infinite. So to us, it seems that it would be a simpler thing to use a boundary condition for which there are no singularities in the Lyapunov spectrum.

COHEN

So we have talked quite a while about the Lyapunov exponents. I would like to make one final remark unless there is objection or comment from the audience. I want to come back to what Pierre has been saying and what Denis has been saying. In the case of Denis, one is interested in the stationary state and even in the non linear regime where the viscosity is dependent on the field, in this case the shear rate. The work of Pierre refers of course to the linear regime. So if you look at the overlapping regime, then there are two different expressions if you replace for a moment our viscosity by his diffusion coefficient, and what seems interesting to me, Denis, is that while Pierre would have the Kolmogorov-Sinai entropy as part of his formula, which is also an entropy rate or entropy production, in our case, it would be what you could call the Gibbs-Boltzmann entropy production of the "chemical physicist". And therefore, in that overlapping regime, there should be a relationship between the two. I think that maybe true but I have no idea of what that would mean and what that would imply. Now if nobody has any comment on that which...

LEVERMORE

I just wanted to make one comment pertaining to the connection of this to the discussion I made about going to incompressible fluid dynamics, at least for the Boltzmann case. The entropy dissipation rate which, if you linearize about one of these equilibrium, more or less, involves the symmetric part of the linearized flow, which is related to the Lyapunov exponents of the Boltzmann flow. The entropy dissipation rate goes exactly to the viscosity times the square of the gradient of the velocity, which is formally consistent with so many of these observations. I did not consider driven systems, but I think the discussion here makes it interesting to go back and look at these rigorous limits and maybe confirm some of these things. In any event, those dissipation terms you get from the fluid equations are exactly the limit of the dissipation terms in the entropy relations.

HOOVER

You mentioned the Gibbs entropy. I just wanted to say that one of the characteristics of the attractors is that the Gibbs entropy always diverges in the non-equilibrium case, always minus infinity.

COHEN

Well I do not think so but I would rather not answer this question because Joel has been waiting patiently before he leaves tomorrow morning at six, to make his contribution to this discussion. There are many more questions, I will not forget the questions but I think it is fair that Joel can make his remarks now unless somebody feels he cannot exist any longer unless he has made a remark. Is that the case with you Pierre?

GASPARD

It is a comment on what you have said....

COHEN

So Joel, if it is so personal, I cannot refuse.

GASPARD

The entropy production is a different quantity than the Kolmogorov-Sinai entropy. An example is that the Kolmogorov-Sinai entropy is positive at equilibrium while the entropy production goes to zero. So if there is a connection between them, it is not a direct connection.

COHEN

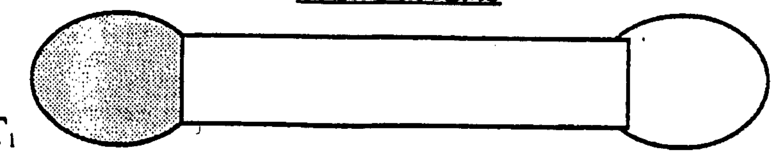
Yes, I agree. I meant it in another way. I did not want to imply they were equal or proportional but only that there is a connection between the two. That is all I ever said. It may not be simple. I agree completely. Now it is irresistible to give Joel the microphone.

LEBOWITZ

Thank you, Eddie.

I have never in my life, so far, studied really the Lyapunov exponents. But I find it very interesting. It reminded me that there is some relationship perhaps with one system we had studied in particular, a system in which you have heat conduction. So you take some material, gas in a tube, liquid in a tube or a crystal and put it between two different temperatures. This is an old slide with some additions to it, in fact in the discussion with Bill or with Denis, it does not really matter in some ways what the reservoirs are for the properties of the system. So you could make this with iced water or better iced champagne or in fact you could make this with boiling water or if you want boiling oil. Basically we believe, and I think that everybody agrees, that if you take a bulk system, and if you drive a

OPEN SYSTEMS



T_1 T_2

boiling water or oil Ice water or champagne

Take diffuse reflections at the walls: Maxwellian.

For suitable Interactions $H(x)$; $x \in \Gamma$; 6Nd, N fixed

Uniform temperature case $T_2=T_1$

$$\int \nu(x,dx)\, P_t(x,dy) \longrightarrow \mu_{can}(dx), \text{ strongly } = \frac{1}{Z}\exp\{-\beta H\}dx$$

Non-uniform case, $T_1 \neq T_2$

we still have

$$\int \nu(x) P_t(x,dy) \longrightarrow \mu_{st}(x)$$

NON FRACTAL

FIGURE 7. Joel Lebowitz' first viewgraph

current through it, in this case a heat current, the boundary conditions will only be effective at the boundary.

There will be basically a state in the bulk where all the properties will be. Now we have studied a particular context together with S. Goldstein and E. Presutti and then there was another work on this by S. Goldstein, N. Ianero and C. Kepnes (Joel, check the names spelling, please), particular boundary conditions, just the kind of things Pierre Gaspard just mentioned, so called diffuse reflection. Namely you imagine that you have here in fact a wall and whenever a molecule comes and hits the wall, it comes out with a Maxwellian distribution of velocities at the temperature of the wall. So you make that reservoir, that was a particular model that we studied but we also studied some other models. But this one is particular, I can remember, I do not have my papers here but I confirm that at least by three minutes telephone conversations with Enrico Presutti, before the telephone went dead, that I remember it correctly. If the temperature is the same, you know that the Gibbs probability distribution is $\exp(-\beta H)$, at the reciprocal temperature β, let H be the Hamiltonian of the system...So I am talking about the finite system not like what I was talking this morning, I am not going to go to any infinite volume limits, I have a system of N particles and d dimensions, let say d bigger than or equal to 2, I do not worry about one dimension pathologies, so the phase space has exactly 2 N d and N can be, as far as the result I want to state, anywhere from 1 to 10^{17}. Starting from some initial state or some initial distribution, will the system be driven by the boundaries to a final steady state? That steady state would have to be the equilibrium state if the temperature is the same and clearly would not be the equilibrium state if the temperature is not the same. Now in order....

COHEN

Joel, for my sake, tell me, what are you after ?

LEBOWITZ

There is a surprise at the bottom of the transparency. At least it is irrelevant in this particular discussion. As I said this transparency dates back, I believe, to 1984, at least part of it up to the top, but the bottom part is new. So I am saying: We consider potentials which are smooth and soft and in fact, do not have any cut-off. But you could take them like Lennard-Jones but smooth on the top over there. Well, you do not want to make some infinite, I believe, in the whole work at any point. But something which could represent physical systems. Is it clear what the model is? You have a model where you have a Hamiltonian H(x), particles interacting with Newtonian dynamics and you have boundary conditions just of the kind that Pierre Gaspard was saying, when a particle hits the boundary, it comes out with a Maxwellian distribution of velocities appropriate to the temperature at the boundary. So neither champagne, nor oil, just plain idealized boundary conditions representing the temperature of the reservoirs. The question is what is the stationary probability distribution of this system. Is it clear, the dynamics, the model and the question? OK. The theorem says that in fact whether the temperatures are the same or not, under these conditions on the Hamiltonian I said, you do get a stationary distribution and it is non fractal. It lives on the whole phase space and has a smooth density, it has a perfectly well defined Gibbs entropy μ. That is a theorem for these particular types of systems. I mean I never thought of the connection with fractal but the point is we had to prove that the boundary can penetrate the system. The reason we need soft potentials is that we are worried always that maybe some particles never get to the boundary and never see effects of the boundary in which case we would not have a unique stationary distribution. That is the whole point if you have particles with soft potentials, then if a particle gets a large velocity at the boundary, which is always possible in a Maxwellian, it can kick that region or the particle which is standing still in the way and makes it move. That is the reason why we need the soft potential, technically. And of course, we do not want to have a situation where you have hard spheres jammed together, that is nothing that can happen. I believe that anything which is reasonable, that there is free motion, that the particles hit the boundary, can influence the system,.. we will have exactly the same result, at least I believe. I mean the theorem is proven for the case of soft potentials, but quite general soft potentials, no cut-off also in those potentials. So I do not know whether these conflict with anything,... surely it does not conflict with anything that Pierre Gaspard said and I do not know if it conflicts with anything that Bill Hoover said, however, I do believe that the same result should apply if you have a quiet flow in a box and you put the same kind of boundary conditions on it, so the heat gets dissipated at the boundary, a stationary state is established, I believe but you will have to make of course,.. when a particle hits the boundary, it comes out with a Maxwellian distribution, with a mean velocity corresponding to the boundary, that you would also get for a finite system, linear and non linear stationary state which would have a density which would not be fractal at all. But I say the theorem is established for temperature boundary conditions for soft potentials. I can pause here or I can talk about other things. Let me pause here for some questions.

COHEN

Let me abuse my chairmanship and ask immediately a question: "To what extent does this result depend on the stochasticity of the boundary conditions?"

LEBOWITZ

Completely! This transition rate involves both the Hamiltonian dynamics and the boundary. You do not have a unique stationary state for a finite isolated system. This depends on the boundaries because for a finite isolated system, any function of the energy is clearly a constant of the motion and would be a stationary state, that could not be any possibility of having unique stationary state wherever you start. In fact, wherever you start I guess for these systems, it is quite right because you can try to start them all sitting still but in fact all potentials, I say, are smooth and repulsive and go therefore..., even if you try to start all the particles sitting still, they will push the particles to a.... and they do not have any cut-off. Otherwise, you could just start all the particles sitting in the middle and they never feel the boundaries. So to make the statement completely precise, we need to have that condition.

NICOLIS

I also believe that if we evoke stochastic boundary conditions, we are indeed going to have non fractal measures filling the whole phase space. What about, of course, deterministic boundary conditions? and can we formulate properly without logical gaps, deterministic boundary conditions? I believe personally that we can along the lines perhaps Pierre has been talking about for instance, one can have dynamical systems which are described by the laws of hard disks or whatever, but different densities, let us say, on the two sides of a central system which is interacting with them and therefore, which is subjected to deterministic boundary conditions. One can also simulate a non-equilibrium state through an initial condition, like Pierre has been insisting on. May I make one comment concerning entropy ?

LEBOWITZ

May I answer your question first ? If you believe that you are going to get a different physics for the system, you can do all kinds of different things. But at least, the conventional wisdom, I believe, if you look at the system conducting heat or what, in fact you do not want to worry about the boundary conditions. You should get the same physics independently. It just happens to be an accident that I was talking to Bill Hoover at lunch, that I remember this work we had done in the late seventies, which happens to have an implication, we did not look at it in the question of fractals but the way we could prove that you get a stationary state, was in fact to prove you have a density, to prove that the stochasticity of the walls gets put in. Now, if you want to have a different system, is it going to be a different physics? For this physics, I believe, that is what the answer is.

NICOLIS

I think, one should distinguish between a Gibbs entropy which, as Joel said, should remain perfectly well defined, and perhaps information entropy. I wonder whether Doctor Hoover does not have in mind information entropy when he thinks about something getting infinite. In other words, if I divide my phase space into boxes and I compute p log p, I get something finite. Now, if the resolution goes to zero, for a stupid reason, I get something infinite, and simply when we compute a Gibbs entropy, we do not think about this infinite which is nothing but log epsilon, as epsilon goes to zero. This deficiency, this peculiarity of information entropy is well known and people have learned to live with it. Now are you thinking of this kind of infinity when you say that entropy should go to infinity ?

HOOVER

I would say that I do not think so.

COHEN

After this revealing answer, who has another question?

EVANS

I just have a comment for Joel. I do not think that there is any contradiction between this and the conjugate pairing rule. The conjugate pairing rule that Eddie and I proved is for dynamical systems, not for stochastic systems and in fact it is a comment I made when Matthieu Ernst was giving us an excellent review on cellular automatons. I made the comment, I believe, that I was surprized that there was not more distinction made between the stochastic models and the completely deterministic models. We deal with Liouville equations. It is not clear, as Bill mentioned in his comment, how you actually characterize the Lyapunov exponents for stochastic systems. I guess they are infinite.

LEBOWITZ

For Lyapunov exponents, it is certainly not clear how to define. This evolution is stochastic at the boundaries. However, the phase space density is well defined in both cases. And my statement has nothing to do with the Lyapunov exponents, it has to do with the phase space density. And I am claiming that at least for this model system, these phase space densities live on the whole phase space, they do not live on anything fractal. That is all I am claiming. I do not say anything about the Lyapunov exponents.

HOLIAN

The phase space that you have here, is 6N dimensional. It is only the sample in the middle. In the case that we have been doing with the deterministic boundaries, you have at least one extra degree of freedom, 6N+1 degrees of freedom, it seems a bit miraculous that the fractal dimensionality can in fact be so strongly governed by one out of the 6N+1 dimensions, but I think it is true that if you make the boundary intimate with the distribution function, that is in fact what leads to a fractal, that is just the way the things are.

LEBOWITZ

I keep on saying again. I mean, the question is "Are the different boundary conditions going to affect the system?" and if they are going to affect it, then you have to justify and do different boundary conditions. I believe to study a system conducting heat, these are perfectly reasonable boundary conditions. And for these, just accidently it happens to be a theorem. If we had not done the work in the late seventies, I would not have had anything to comment on that and I am personally, well I do not know about deterministic, I do not know what it would mean in this context. But given my system conducting heat, does the density live on a fractal dimension or not..I am willing to bet a quarter or a little bit more that it does not.

POSCH

Maybe there is a possibility that both ideas are compatible. Suppose you have, as Brad has mentioned, in the dynamical case a phase space with, let us say, 6N+5 dimensions, depending on the number of dimensions you are driving the system with (5 in this case). And let us assume that you could separate the system into the Newtonian part (between these two plates) and the boundary. Then you could project down a fractal with, say, 6N+1.5 dimensions onto a 6N dimensional Newtonian subspace and obtain a continuous distribution. So conceptually, it is always possible that a 6N+5 dimensional driven system projected down to a 6N dimensional phase space corresponding to the Newtonian particles is totally homogeneous and is not fractal. But I do not see at the moment theoretically how this projection can be done. We have only one piece of evidence which, maybe, is not in correspondence with that. We have done a driven system where the reduction in dimension just about exceeds the dimension of the driving particles. So this would not be in agreement with what I have said just now. We have certainly to check this particular separation but I think there is at least a possibility that these points of view are quite compatible.

LEVERMORE

I want to make two comments. One is about stochastic boundary conditions. If Pierre would have had stochastic boundary conditions, even a little bit on his scatterers, it is quite clear that things would be ergodic and the structure that he discusses would not be there. Clearly, there is a big difference between stochastic and deterministic boundary conditions.

I also want to make the distinction between the stochastic and the deterministic cellular automaton. I was thinking about some of these issues very early on in the business, and I wanted to play a little game. What I did was consider a 2 by 2 periodic FHP lattice and begin computing orbits for this lattice. I did this for two cases. First, I did it for the deterministic case, and of course to no one's surprise, the orbits were periodic and sometimes with a surprisingly long period. It is quite clear that the discrete phase space had an enormous amount of structure. It is very easy to prove for such a small system that if you add a little stochasticity (essentially you make the collisions outcomes stochastic) that every orbit is ergodic. The distinction is an important one between the deterministic and the stochastic systems. Systems which are stochastic, where we add any kind of dissipation as a way to smooth things are much easier to analyze.

The answer to the question about the role of micro-structure in macroscopic dynamics will, in some sense, depend upon the interpretation as to the proper way to set up the system. I think the holy Grail is the route Pierre is examining and other people should be thinking about: to find a simple deterministic dynamical system through which we can truly understand microscopic behavior. Stochasticity or fuzziness is a good way to practice, but it is not the answer.

COHEN

After these remarks, I must ask you all to come to my Monday lecture. It will be completely devoted to the difference between probabilistic and deterministic cellular automata. I must say I cannot resist mentioning this.

LEBOWITZ

Before going back, let me just say again that the stochasticity here is only at the boundary and it is only a method of how to drive the system. I do not accept as physically meaning for them. If you can create the same system, but with other boundary conditions, and you get something fractal, that it has anything relevant to the physics of the problem. At least that is my opinion at the present time. I am ready and will be happy to be proven wrong.

GASPARD

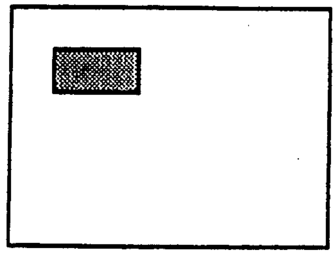
There is another argument against the existence of the fractal, going to a quantum mechanical description of the system, then the concept of fractal disappears. I rather think it is an intermediate mathematical tool in order to obtain numerical results and relationship between quantities like Lyapunov exponent or Kolmogorov-Sinai entropy on one side, and diffusion on the other side, which I think are the most important.

LEBOWITZ

I think your system was really a mechanical system. You were talking about the diffusion of a single particle, a kind of pseudo-diffusion, not pseudo I mean, but it is not a thermal diffusion, not with many particles, just one particle in a fixed array of scatterers. Were you not? It is a purely mechanical thing and I have absolutely no reason to doubt anything about what you have said, it is perfectly correct and quite interesting but it is a real mechanical system you were dealing with. Here I am talking about a thermal, also mechanical. I am talking about different types of behaviors. I do not think there is any contradiction and I do not want, in any way, to discourage, it is quite the opposite. I found it very interesting, I had not seen it before.

LEVERMORE

I want to make a picture to clarify my remark just a little bit. I did not want to sound so negative about stochasticity. I think the problem, perhaps first posed by Gibbs in the equilibrium setting, is the following one.



The big box represents a large deterministic system (no stochasticity). The small shaded box represents a subsystem. While the whole system is deterministic, when we model the subsystem we think of it as being somehow driven by stochasticity that represents the influence of the remainder of the large system. What we want to understand is whether this is a good model or in what sense it is a good model. This being a deterministic system, if it is classical, we will have pattern structures. If it is quantum mechanical, the structures become fuzzy, but then we get into the whole theology of quantum chaos which I think we should avoid at this level. The question I think we want to understand is how stochasticity can be used to describe the dynamics of the subsystem when it is driven by avery large deterministic system. That is to justify the Gibbs picture in a non-equilibrium setting. That is what the focus should be.

COHEN

Now, we have 10 more minutes. I wonder if anybody wants to make a statement, a remark, maybe even a confession. Does anybody want to comment on the role of the Lyapunov exponents in fluid instabilities or things like that in different contexts? And I am looking either at Uriel or at you. It does not have to be a theorem just a thought provoking remark.

FRISCH

I wish to comment on the relation between microscopic and macroscopic Lyapunov exponents. In order to get hydrodynamics, you need a separation of scales in space and time controlled by the Knudsen number. One the one hand, if you work in microscopic units, say with the mean free path, the collision times, etc, then of course the Lyapunov exponents characteristic of molecular motion will be of order one in those microscopic units. On the other hand, as you go to the hydrodynamic limit, you have very long time scales, order epsilon to the -2, and the Lyapunov exponents characteristic of the behavior of the Navier-Stokes equations will be of the order of epsilon squared, that is much much smaller than the Lyapunov exponent characteristic of the microscopic motion. Thus there is no simple relation. Actually considering the case of lattice gases, we can see that there cannot be much of a relation because for lattice gases, the hydrodynamic limit still emerges just the same way as in molecular dynamics but microscopically we do not have really a concept of Lyapunov exponent because things can change only in a discrete way. Of course if we consider a very large lattice, and we change one bit, then in some sense the perturbation will grow. But the exact concept of microscopic Lyapunov exponents certainly has no parallel in lattice gases, even purely deterministic ones.

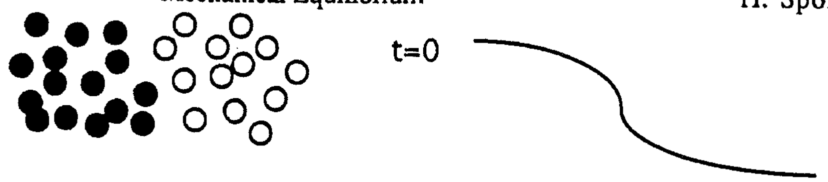
LEBOWITZ

I do not know if anybody wants to listen as these are the last five minutes but the question has been raised about irreversibility of macroscopic phenomena and the reversibility of the microscopic equation. The models I discussed today were stochastic and even for the theorems I quoted about, you had to have some stochasticity and you do not really get dissipative things from the deterministic system. However, there is at least one model system which we have studied with Herbert Spohn some years ago, which at least illustrates the things. Namely, it is a system which consists of 2 kinds of particles but they only differ from each other by their color. The dynamics is exactly the same, mechanically. So we simply think of hard spheres but we just color some of them differently.

COLOR DIFFUSION

Mechanical Equilibrium

H. Spohn, J.L.



$\rho_1(x,t)+\rho_0(x,t)=\rho$ constant

one particle (average) density

$\rho_1(x,0)=\rho g_0(\varepsilon x)$ $\quad x\in R^d$

$\rho_0(x,0)=\rho[1-g_0(\varepsilon x)]$

$0< g_0(\varepsilon x) <1$ No color correlation

If tagged fluid particle $\longrightarrow$ B. M. then

$$\lim_{\varepsilon\to 0} \varepsilon^3 \int_{\Delta\varepsilon} 1/2\, [\rho_1(x,t/\varepsilon^2)-\rho_0(x,t/\varepsilon^2)]dx = \rho \int_{\Delta\varepsilon} g(q',t)\, dq' \text{ average color density}$$

where $g(q',t)$ satisfies the equation

$$\frac{\partial g(q',t)}{\partial t} = D\, \nabla^2 g(q',t) \qquad \text{with } D=D_{\text{self}}, \text{ and } g(q',0)=g(q')$$

Further, if two or more test particles go to independent Brownian Motion then let

$n^{\varepsilon}(\Delta,t/\varepsilon^2)$=(signed)#of particles in $\Delta\varepsilon$, i.e. $\varepsilon x_1(t) \in \Delta$

$$\varepsilon^3\, n^{\varepsilon}(\Delta,t/\varepsilon^2) \longrightarrow \rho \int_{\Delta} g(q,t)dq \quad \text{almost surely}$$

This corresponds to local equilibrium with respect to color $\mu_\varepsilon(\varepsilon^{-2}t)\longrightarrow\mu_q(q,t)$

FIGURE 8. Joel Lebowitz' second viewgraph

Physically you can actually realize such a thing if you take Helium 3, spin polarized up and spin polarized down, that is very little effect on the dynamics. But conceptually we just think classical systems. That system, you can drive on the basis of one assumption which I want to state : A diffusion equation, exactly the same way I discussed today, a diffusion equation for the bulk density of non mechanical systems. Here I am going to talk about the diffusion of the color density, so I start with red on the left and black on the right. I think in fact that was the system first studied in Los Alamos by Bill Wood and Jerry Erpenbeck, I think I got the idea of considering that system from talking to them. There is the following theorem in that system : Let us forget, now, about the color. Just consider the system in equilibrium, and look at the trajectory of one marked particle, so called test particle, which again is only colored. This is a mechanical system in equilibrium and we look at one particle which is marked down, everything is mechanical except that we are taking it in equilibrium. So we look at the trajectory of that particle, purely mechanical thing, which of course will depend on the positions and velocities of all the particles in the system. Having a probability distribution on positions and velocities of these other particles, its own position and velocity translates to a probability distribution on trajectories. Let us assume that in fact this trajectory properly scaled, I have to have infinite systems, I look at times of order $1/\varepsilon^2$, and multiply by ε, converges to Brownian motion. One can prove this, at present time, only in one system which is not very interesting, a mechanical system of hard scatterers has that property. Assume that that is true, assume first that if you start several particles nearby they are able eventually on this very long time scale, to converge to independent brownian motion. It certainly does not violate any mechanical law. Under those conditions, one can prove that starting with a non uniform color density, you get, under hydrodynamical scaling, you get to the diffusion equation for the color density, which is certainly an irreversible equation. Simply this was an illustration that there is absolutely no contradiction between reversible microscopic laws and going to a macroscopic, non reversible, for almost all initial configurations of the system.

COHEN

One minute left.

EVANS

Just a comment about this. I do not want really to go into the entropy, it might be not the time. But even in a deterministic system, I do not think there is necessarily a great problem with the divergence of the entropy. It goes back to Harald's and also David's comments that in these deterministic non equilibrium steady states, the dimensional reduction in the full phase space is not very large. Obviously in the real world, there are external perturbations which, no matter how small, must wash out the fractal structure at some length scale, and they are not going to change the macroscopic properties of the system. You can view your stochastic boundaries as just another version of that. This must mean that if you calculate the Gibbs entropy, f log f, by integrating in some suitable fashion, over a sub-space of the full phase space, that has dimension less than the fractal dimension of the space, you will get a finite answer for that Gibbs entropy.

COHEN

After this confession, I would like to thank all the speakers, the superb technician[4] who made it all possible, and to have a drink before dinner.

LEBOWITZ

Thanks for the chairman !

[4] Dr. Brigitte Herpigny