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Some Ill-Formulated Problems on Regular and Messy Behavior in Statistical Mechanics and Smooth Dynamics for Which I Would Like the Advice of Yasha Sinai

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At the occasion of the Rutgers Statistical Mechanics Meeting in December 2000, Joel Lebowitz organized a celebration for the end of the Millennium and the birthday of Yasha Sinai and myself. As part of the entertainment, Yasha Sinai and myself had each been asked to present a list of scientific questions for the other to solve in the next millennium. When I started to think about such a list a certain number of problems came to mind, which I had unsuccessfully tried to solve in the past. And I came to realize that I had thought about, and written about,[2] a cluster of questions concerning what I would call regular versus messy behavior both in statistical mechanics and in smooth dynamics. I must admit that my questions are rather imprecise: I would like to grasp the structure of certain physical or mathematical problems, but I think it is too early to propose very specific and precise mathematical conjectures. I shall thus not request that Yasha spend the new millennium proving some theorem or other for me. Rather, I would be very interested in having his informal opinion on some structural questions which I consider important, both in statistical mechanics

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[2] These are short papers, with more questions than answers: refs. 1–4.

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and in smooth dynamics. In fact, one way or the other Yasha Sinai probably has thought already quite a bit about these problems.

STATISTICAL MECHANICS AND SMOOTH DYNAMICS

Before I get started I should explain why I want to put together statistical mechanics and smooth dynamics. (Actually, this point has been already discussed in a joint paper by Yasha and myself[(5)]). The two areas have important connections: on one hand the ergodic hypothesis of statistical mechanics is a problem of smooth dynamics, in which Yasha Sinai did groundbreaking work (for a current update see the book, ref. 6). On the other hand, the invariant measures naturally associated with hyperbolic dynamical systems can be identified as Gibbs measures of equilibrium statistical mechanics. This follows from the existence of the Markov partitions and symbolic dynamics introduced by Sinai.[(7–9)] At a less technical level one might say that the fundamental problems of statistical mechanics and of smooth dynamics appear more and more to be related, and related to ergodic theory for which they provide natural and nontrivial examples.

REGULAR VERSUS MESSY BEHAVIOR

The scientific investigation of a problem naturally begins with the study of simple and regular behavior. For equilibrium statistical mechanics, simple behavior would be dilute gas, then liquids, etc. For smooth dynamics, simple behavior would be Morse–Smale, then Axiom A, etc. A natural attitude is to make a good guess at what simple (or regular) behavior is and then conjecture that messy (or nonregular) behavior is somehow exceptional. When the conjecture is disproved, after a while, one can say that science has progressed. Here I would like to take the opposite attitude: make myself the devil's advocate and propose that messy behavior is not exceptional. My (ill-formulated) questions to Yasha Sinai are thus of the following general nature: don't you believe that this or that kind of messy behavior is common rather than exceptional? Although the questions appear similar in statistical mechanics and smooth dynamics, the answers may be rather different (and depend critically on technical details of how the questions are asked).

THE LONG TIME BEHAVIOR SMOKE SCREEN

In order to get an idea of how prevalent messy behavior might be, one can think of using experiments (including numerical experiments). But note that we are interested in concepts of ergodic theory which involve a long time limit, and for statistical mechanics there is also a large volume limit. Experimentally then, possible messy behavior appears as "very long characteristic times," slow convergence or possibly no convergence at all: one doesn't know. You recognize here one of the favorite gimmicks of the Almighty when She is pulling a fast one: Her intentions remain hidden in the mists of the future. The best example is probably that of logically undecidable questions in mathematics: you put a Turing machine at work on a problem, and you don't know if the machine will halt after a very, very, very long time, or never at all. In statistical mechanics, very long relaxation times occur for instance in spin glasses, and that is one reason why these are such a difficult subject.

For definiteness we shall in what follows limit our considerations to *equilibrium* statistical mechanics. Let me however mention in passing that the complicated structures of many materials are of nonequilibrium origin, and due to the way the material is produced. To identify a messy equilibrium structure will thus be difficult.

SIMPLE EQUILIBRIUM STATISTICAL MECHANICS

For definiteness we consider a gas of classical particles in $\mathbf{R}^3$. If we assume short range interactions, the correlation functions of the gas are analytic with respect to the activity z in a neighborhood of 0. In fact let us denote by $z^m\phi^z(x_1,\dots, x_m)$ the *truncated* correlation functions (or *cluster functions* of the correlation functions) at activity z. We have then the formula

$$\phi^{z_0+z_1}(x_1,\dots, x_m) = \sum_{n=0}^{\infty} \frac{z_0^n}{n!} \int dy_1 \cdots dy_n \, \phi^{z_0}(x_1,\dots, x_m, y_1,\dots, y_n) \qquad (*)$$

which does not explicitly contain the interaction (the interaction is introduced via the Ursell functions $\phi_0(x_1,\dots, x_m)$). In the above miraculous formula the value $z=0$ plays no special role and the correlation functions at z_0+z_1 are obtained by a simple Taylor expansion from the correlation functions at z_0.

Equation (*) truly represents simple analytic behavior and one might conjecture that it extends outside of the small activity region. A natural idea is that the correlation functions are piecewise analytic functions of thermodynamic parameters (like the activity z), with singularities corresponding to phase transitions. Naively, the variational principle of thermodynamics would select a branch of analytic function to be the physical branch, and assumed generic behavior would yield the Gibbs phase rule.

The van der Waals theory fits such naive ideas, but it has now been abundantly demonstrated that this theory does not correctly describe critical behavior and gas-liquid coexistence for short range interactions.

At this point we have some general understanding of some kinds of phase transitions, due to Pirogov and Sinai,[10] but we do not understand the Gibbs phase rule (see the analysis in ref. 1, the negative examples in ref. 11, and on a more positive side[12]).

In conclusion we may say that there is some simple behavior in equilibrium statistical mechanics. But our understanding of this simple behavior is limited to certain situations (like dilute gases), and it may well be that simple behavior is not general.

MESSY EQUILIBRIUM STATISTICAL MECHANICS

In a crystal, the truncated correlation functions invariant under the Euclidean group do not have the necessary decay at infinity for (*) to make sense. But one might hope that after fixing the crystal orientation and position one has restored sufficient decay at infinity of the $\phi(x_1,..., x_m)$ for (*) to hold. This would entail analyticity with repect to z in the crystal phase. But if (*) holds this implies that the lattice constants of the crystal are the same at activity $z_0 + z_1$ as at activity z_0, contradicting the known compressibility of crystals. We are thus left without a proof of analyticity in z for the crystal phase, and the very definite possibility that analyticity does not hold.[2] Clearly, attempting to prove the existence of a crystal phase for continuous systems in $\mathbf{R}^3$ with short range forces will be a formidable problem: we don't even know what the correct concept of phase is. Here is obviously a good "problem for Yasha Sinai" but, to repeat, I would be satisfied with his informal opinion on what is going on, I don't demand a general rigorous analysis!

As far as we know, it may be that equilibrium statistical mechanics with short range forces in $\mathbf{R}^3$ conforms with a simple vision: piecewise analyticity and Gibbs phase rule. Reality may however deviate from this prescription, with messy regions in the space of thermodynamic parameters: no piecewise analyticity and no clear definition of phases.

Among other examples of possibly messy behavior one may mention here glasses, and *turbulent crystals*.[3] What is a turbulent crystal? An equilibrium state is taken to be invariant under the translation group $\mathbf{R}^3$ (we assume that the symmetry under rotations has been broken). The equilibrium state can then be decomposed into extremal Gibbs states: $\rho = \int \rho_\lambda \, \mu(d\lambda)$, and $\mathbf{R}^3$ preserves the probability measure $\mu(d\lambda)$. The action on λ-space may be periodic (crystal), quasiperiodic (quasicrystal), or might be "messy" (say with entropy >0 with respect to a subgroup $\mathbf{R}$ of $\mathbf{R}^3$).

This would be a turbulent crystal. At this point one can only say that demonstrating experimentally the existence of turbulent crystals appears extremely difficult. And the theoretical proof or disproof of their existence seems a formidable problem.

SIMPLE AND MESSY BEHAVIOR IN SMOOTH DYNAMICS

Smooth dynamics is a very wide subject and I want to restrict myself to a few remarks.

The distinction between simple and messy behavior was at the heart of the approch to differentiable dynamical systems by Steve Smale and his collaborators. Smale defined and studied (relatively) simple "hyperbolic" behavior asssociated with "Axiom A" and structural stability, and conjectured that systems not conforming to such simple behavior would be rare. The conjecture was wrong, but the point of view was enormously fruitful. Smale's approach resulted in a structured theory of uniformly hyperbolic systems, not just a collection of theorems, and at the same time a theory of nonuniform hyperbolicity was started.

After Smale (and a lot of new work, in particular by Pesin, Ledrappier, Young) there is now a new unifying conjecture by Jacob Palis.[13] Roughly speaking it says that a smooth dynamical system on a manifold M typically has a few ergodic measures (called SRB, or Sinai-Ruelle-Bowen measures) such that the asymptotic measure of most points on M (for Lebesgue measure) is given by one of the SRB measures. This conjecture may be wrong, but it is proving very fruitful, driving a lot of research which establishes, in one case after another that certain classes of systems conform to the simple behavior proposed by Palis.

Let me now make myself the devil's advocate, and suggest that something opposite to the vision of Palis is actually taking place (see ref. 4). Perhaps there exists a nonempty open set of diffeomorphisms on M and a set $S \subset M$ with Lebesgue measure > 0 such that if $x \in S$ the time averages

$$\frac{1}{n} \sum_{k=0}^{n-1} \delta_{f^k x}$$

do not converge when $n \to \infty$. In one of the last conversations I had with Michel Herman, he confirmed that nothing is known which would prevent this from happening. What I suggest is that, in a persistent way, a system may exhibit *historical behavior*: instead of recurrence, the point $f^k x$ keeps having new ideas about its future. Historical behavior does happen for random walks in random environments (as rigorously studied by Sinai[14]). Could it be that persistent historical behavior also occurs in smooth dynamics? Here is again a good question for Yasha Sinai. But again I would be satisfied if he just gives me his opinion as to what is going on. The proof may be very hard, and I prefer not to wait for another millennium.

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