NONEQUILIBRIUM:

FROM HEAT TRANSPORT TO TURBULENCE (TO LIFE).

by David Ruelle†.

Abstract: *We review some problems in nonequilibrium physics from the point of view of statistical physics and differentiable dynamics. Specifically, we discuss the mathematical difficulties which inherently underlie applications to heat transport, to hydrodynamic turbulence, and to the study of life. The microscopic dynamics of transport phenomena (in particular heat transport) is necessarily non hyperbolic, which explains why it is a difficult problem. The 3D turbulent energy cascade can be analyzed formally as a heat flow, and experimental intermittency data indicate that this requires discussing a Hamiltonian system with* 10^4 *degrees of freedom. Life is a non-equilibrium statistical physics phenomenon which involves chemical reactions and not just transport. Considering life as a problem in nonequilibrium statistical mechanics at least shows how complex and difficult the study of nonequilibrium can be.*

1. Nonequilibrium and linear response theory.

The aim of nonequilibrium statistical mechanics is to understand the properties of matter outside of equilibrium, starting from microscopic dynamics. At this time nonequilibrium statistical mechanics of transport phenomena close to equilibrium is a well-developed physical theory (due to the work of Onsager, Green, Kubo, etc. in the 1950's, see for instance [5]). Away from this area, the theory of nonequilibrium is a program, or a variety of programs, rather than a theory. Here I shall make a choice, and describe an approach starting with classical Hamiltonian microscopic dynamics. From my point of view this approach has the interest that it uses nontrivial recent results in the theory of smooth dynamical systems, and that it sheds light on interesting physical phenomena: heat transport, hydrodynamic turbulence, and life.

A general study of nonequilibrium should begin with equilibrium statistical mechanics and nonequilibrium close to equilibrium, which are reasonably well understood physical

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theories, but for lack of time I shall skip those here. For my purposes I shall start with the microscopic evolution equations

$$\frac{d}{dt}\begin{pmatrix}\mathbf{p}\\ \mathbf{q}\end{pmatrix}=\begin{pmatrix}-\partial_{\mathbf{q}}U\\ \mathbf{p}/m\end{pmatrix}\qquad\text{or}\qquad\frac{d}{dt}\begin{pmatrix}\mathbf{p}\\ \mathbf{q}\end{pmatrix}=\begin{pmatrix}\xi(\mathbf{q})-\alpha\mathbf{p}\\ \mathbf{p}/m\end{pmatrix}\qquad(\text{with}\quad\alpha=\frac{\xi(\mathbf{q})\cdot\mathbf{p}}{\mathbf{p}\cdot\mathbf{p}})$$

On the left is the Hamiltonian evolution equation. To obtain nonequilibrium I have replaced on the right the gradient force by a more general force $\xi(q)$. But energy is then no longer conserved, so that $\mathbf{p}\cdot\mathbf{p}/2m$ would probably grow indefinitely with time for the modified system (the system heats up). An extra term $-\alpha\mathbf{p}$ (isokinetic or IK thermostat) has thus been introduced so that $\mathbf{p}\cdot\mathbf{p}/2m$ is constant in time. We have now a smooth time evolution (f^t) defined by

$$\frac{dx}{dt}=\mathcal{X}(x)\tag{1}$$

on a compact manifold $M=\{x=(p,q):\mathbf{p}\cdot\mathbf{p}/2m=\text{constant}\}$. To avoid unphysical behavior, it is necessary to assume that the time evolution (1) is sufficiently chaotic: this is the *chaotic hypothesis* of Gallavotti and Cohen [9]*. A *nonequilibrium steady state* (NESS) is now a probability measure ρ_0 on M invariant under (f^t). In fact we shall assume that, starting from an absolutely continuous probability measure m on M, time evolution will yield the NESS ρ_0 in the infinite time limit:

$$\rho_0=\lim_{t\to\infty}(f^t)^*m\ \text{in a suitable sense}\tag{2}$$

The limit ρ_0 is in general no longer absolutely continuous on M.

It is of great physical interest to understand how ρ_0 is changed (to ρ^t) when when the time evolution (1) is perturbed to

$$\frac{dx}{dt}=\mathcal{X}(x)+\lambda X_t(x)\tag{3}$$

If we assume a time periodic force $X_\tau=Xe^{i\omega(t_0-\tau)}$, a formal first-order perturbation calculation yields the *linear response formula* for the expectation value of an observable A:

$$\rho^{t_0}(A)=\rho_0(A)+\lambda\hat\kappa(\omega)\quad\text{where}\quad\hat\kappa(\omega)=\int_0^\infty dt\,e^{i\omega t}\int_M\rho_0(dx)\,X(x)\cdot\partial_x(A\circ f^t)\tag{4}$$

Here A is a smooth function on M and $\hat\kappa$ is known as the *susceptibility*. If $X_t=X$ is independent of t, the perturbation λX replaces ρ_0 by $\rho_0+\hat\kappa(0)$.

Nonequilibrium close to equilibrium is obtained when ρ_0 is an equilibrium state, assumed to be absolutely continuous on M. As to a rigorous proof of (4), it can be obtained for "very chaotic" systems, namely Anosov with exponentially decaying correlations. This gives some useful examples (like the geodesic flow on a manifold of negative curvature, see

* technically, one assumes that the time evolution is *Anosov* or *hyperbolic* in some sense.

[14], [4], [12]) but the linear response formula us believed to hold much more generally. In fact we shall refer later to an application of a linear response formula proved by Dolgopyat [7] for time evolutions which are not Anosov but only *partially hyperbolic*.

2 A model of heat transport.*

Consider a chain of $N+1$ nodes:

$$\begin{array}{ccccccc} \bullet & — & \bullet & — \cdots — & \bullet \\ 0 & & 1 & & N \end{array}$$

At each node there is a Hamiltonian system with n degrees of freedom, and the systems at $j-1$ and j are weakly coupled to each other (with a coupling $\sim \lambda$) for $j = 1, \ldots, N$. Furthermore, the systems at 0 and N are coupled to external sources and one wants to study the heat flow (i.e., the energy flow) from 0 to N. A natural idea is to start with uncoupled systems at the nodes $0, 1, \ldots, N$ for $\lambda = 0$, and to use some sort of perturbation theory to study the coupled system for $\lambda \neq 0$. The dynamics of the uncoupled system at node j takes place at fixed energy, i.e., on an *energy shell* of dimension $2n-1$. After coupling, the phase space has dimension $\approx (N+1)2n$, so that we have a dimensional jump $\approx N$ between the uncoupled and the coupled situation: this prevents a straight use of perturbation theory, which should take place on a manifold of fixed dimension.

A natural physical idea is to determine somehow a temperature β_j^{-1} for the system at node j in the coupled situation. We may then hope to apply perturbation theory to obtain a NESS ρ in dimension $(N+1)(2n-1)$. Afterwards there remains the problem of studying the fluctuations in full-dimensional phase space. In what follows we shall see how to determine the NESS ρ in dimension $(N+1)(2n-1)$, leaving open the problem of fluctuations in full dimension, for which we know no rigorous approach**. In order to fix the temperature β_j^{-1} at the node j we use an isokinetic thermostat, i.e., a term in the evolution equation such that the kinetic energy at the node j remains constant, see Section 1. The temperature profile, i.e., the choice of the β_j is obtained by fixing β_0, β_N, and requiring that the net rate of energy transfer from the IK thermostat to the node j vanishes for $j = 1, \ldots, N-1$ (the IK thermostat removes thus the energy fluctuations which occur for the full Hamiltonian time evolution of the chain under study).

To make our model specific we take the uncoupled dynamics at the jth node to correspond to the geodesic flow at a velocity which is fixed at any value (not necessarily 1) on some compact manifold of negative curvature. This dynamics corresponds to a Hamiltonian $H_j(\mathbf{p}_j, \mathbf{q}_j)$ which is pure kinetic energy. The coupling between $j-1$ and j is given

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* In this Section we follow [15]. See the recent paper by Li and Young [11] for a number of references to other approaches (by Eckmann and coworkers, Young and coworkers, etc.)

** An approximate description of fluctuations is provided by equilibrium fluctuation theory at temperature β_j^{-1} for the node j, but this ignores the long range correlations known to be present (see [3] and [6]). Note that an approach to the problem of heat transport by Dolgopyat and Liverani [8] uses a macroscopic limit in which the fluctuations vanish. We shall however want to discuss fluctuations in the problem of turbulence, see Section 3.

by a potential energy term $\lambda W(\mathbf{q}_{j-1}, \mathbf{q}_j)$. Introducing IK thermostats gives the final dynamics, for which $dH_j/dt = 0$: the kinetic energy at j is fixed at a value K_j corresponding to a temperature* $\beta_j^{-1} = 2K_j/(n-1)$. Dolgopyat's perturbation result [7] referred to in Section 1 may be applied here to obtain the NESS ρ for the coupled thermostatted dynamics from the uncoupled state ρ_0 to first order in λ, see formula (4). Since $\hat{\kappa}(0)$ in (4) is explicitly known, one can determine to first order in λ the temperature profile β_j^{-1} so that there is no net flux of energy from the thermostats to our system. As discussed above, this gives a description of heat transport along a coupled chain when energy fluctuations at each node are removed. We must refer to [15] for a detailed discussion**. In any case, our presentation shows the difficulty of a rigorous approach to the problem of heat transport: even choosing the unperturbed dynamics at the nodes to be Anosov, even removing energy fluctuations by IK thermostats, we face a difficult perturbation problem for a non-hyperbolic system. The non-hyperbolicity of the unperturbed system is because a product of Anosov dynamical systems (with continuous time) at each of our $N+1$ nodes is no longer hyperbolic. This has a physical basis since it reflects the near translation invariance of the chain of small systems which transport heat.

3. Hydrodynamic turbulence.

We discuss now a physical system formed by a finite volume of incompressible fluid, as described by the 3-dimensional Navier-Stokes equation (or an analogous equation: the precise form of the dissipation term will not be important in what follows). A traditional view of developed hydrodynamic turbulence is that energy is supplied to the fluid at large spatial wavelengths, cascades down to small wavelengths, and is dissipated there by viscosity: this is the turbulent *energy cascade*. The fluid motion is assumed to have a spatially *homogeneous and isotropic* probability distribution, and as a consequence many features of the fluid motion can be determined by *dimensional arguments* (i.e., the scaling properties of the hydrodynamic equation imply that physical quantities scale in a definite manner with space and time). This is the heart of *Kolmogorov theory* [10], a very successful theory which fails however to predict correctly some velocity correlations. The reason of the failure is *intermittency*: turbulence is actually not homogeneous.

The following is an attempt at a physical understanding of the energy cascade and intermittency, as proposed in [16]. The degrees of freedom of our fluid which correspond to sufficiently large spatial wavelengths constitute the *inertial range*, where viscous dissipation is deemed unimportant. The degrees of freedom in the inertial range constitute in principle a finite Hamiltonian system*** coupled on one side to a source of energy (at large wavelength) and on the other side to dissipation (at small wavelength). An explicit Hamiltonian using a wavelet description of the degrees of freedom of the fluid and respecting the

* One can argue that in the presence of the IK thermostat, a denominator $n-1$ should occur in the following formula rather than n as expected.

** In particular, choosing the β_j such that the energy flux from the thermostats vanishes exactly and not just to first order requires a uniformity result for $o(\lambda)$ which has not been proved at this time.

*** A Hamiltonian description of fluid motion without dissipation has been given by Arnold [2] (the Hamiltonian is the total kinetic energy of the fluid).

inviscid scaling should be possible to construct, but the construction will not be attempted here. Our point is that in this description the turbulent energy cascade is equivalent to a heat flow though a collection of coupled Hamiltonian systems.

The heat flow obtained here to describe turbulence differs from the heat flow model discussed in Section 2 in two main respects: geometric structure and dynamical assumptions. As to geometric structure, instead of coupled nodes forming a chain, we have now a hierarchy of nodes with a scaling such that the dimensional arguments of Kolmogorov should be applicable (in particular we want the same number of degrees of freedom at each node). The nearest neighbor interaction postulated between nodes in Section 2 would be reflected in our hierarchy by *locality* (like the locality of the interaction of Fourier modes usually assumed by turbulence theorists). The possibility to describe our system as a scaling hierarchical collection of Hamiltonian subsystems with weak local interactions remains to be assessed, but we shall assume it in the following discussion. As to dynamical assumptions, we cannot realistically suppose that the Hamiltonian subsystems in our hierarchical collection are Anosov. We cannot therefore hope at this time for a rigorous dynamical analysis of our system.

Although a rigorous analysis escapes us, we have sufficient physical understanding of heat transport to draw some useful conclusions. The input of energy at large wavelength gives a macroscopic kinetic energy to a system with a relatively small number of degrees of freedom. In view of the smallness of the Boltzmann constant this corresponds to a huge temperature. We expect thus the energy cascade to go from large to small spatial wavelengths because this corresponds to heat going from large to small temperature (ultimately this is because entropy must increase with time). Our argument about heat flows requires some chaoticity assumption. Indeed it is known that heat transport can be pathological in completely integrable Hamiltonian systems [17]. The difference between 2- and 3-dimensional hydrodynamics with respect to the energy cascade can thus be understood because 2-dimensional inviscid flows have many conserved quantities (contrary to 3-dimensional flows).

Identifying the turbulent energy cascade with a heat flow gives the correct direction of the cascade, but if we ignore microscopic fluctuations we cannot expect a description of this cascade other than that given by Kolmogorov theory, and dictated by dimensional arguments. Taking into account the microscopic fluctuations, we can however hope to understand intermittency. Since there is no good microscopic theory of nonequilibrium fluctuations, we shall use equilibrium fluctuation theory in the following manner. We assume that the ratio κ of sizes of subsystems in our hierarchy of nodes is such that a fluctuating temperature β_j^{-1} can be attributed to each node j (temperature imposed mostly by the node of the next larger size) in such a way that the degrees of freedom at j have a Boltzmannian energy distribution corresponding to the temperature β_j^{-1}. Such an assumption is clearly approximate, but physically not unreasonable. The assumed local equilibrium fluctuations lead to fluctuating velocity differences over finite distances, which correspond to intermittency and deviate from the predictions of Kolmogorov theory. We have called κ the ratio of the linear size associated with one node in the hierarchy, and the size of the next smaller node. Our predictions for intermittency* depend on κ, and comparison with experimental results [1] yield $\kappa \approx 20$ or 25.

The above estimate for κ , which corresponds to $\kappa^3 \approx 10^4$, may appear very large. It does however make sense if we realize that the intermittency effects we are trying to understand have a complicated physical basis consisting of vorticity tubes being formed, stretched, folded, etc. In conclusion we have a physically reasonable understanding of turbulence based on nonequilibrium statistical mechanics.

Apparently simple problems often lead to very complicated developments. Gödel's incompleteness theorem says something of that sort. Dynamical systems (for example $z \mapsto \lambda z(1-z)$ in the complex plane) give many examples of this situation. The evidence is that turbulence, if one goes beyond Kolmogorov theory, is a very complicated phenomenon, although based on simple equations. This is probably a warning that nonequilibrium problems must often lead to intrinsic and unavoidable complications.

4. Life.

One can readily argue that the phenomena of life belong to nonequilibrium. Here we propose a definition of life based on nonequilibrium statistical mechanics:

a slowly evolving nonequilibrium state contains life if, using a source of negentropy at atomic level, it steadily maintains structures containing a large amount of information.

Living structures belong thus to the class of dissipative structures**: their existence depends on entropy production, i.e., on a source of negentropy (or a source of Gibbs free energy in the isothermal isobaric situation appropriate to the life forms that we know). Structures containing a large amount of information are necessarily of relatively large scale. In the case familiar to us, the large scale structures are the living structures necessary to maintain and propagate genetic information, and this information is slowly evolving. A slow evolution appears necessary for the creation of life (of any kind) because it takes time to invent self-sustaining structures with a large amount of information. Eventually, the appearance of intelligence changes the nature of the problem: think of the evermore efficient creation and transmission of information that humans have achieved.

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* Let $|\Delta_r(v)|$ be the velocity change $|v(x')-v(x)|$ over a distance $|x'-x|=r$ and write $\langle|\Delta_r(v)|^p\rangle \sim r^{\zeta_p}$. For the exponent ζ_p we predict $\zeta_p = p/3 - (\ln\kappa)^{-1}\ln\Gamma(p/3+1)$ while Kolmogorov theory gives $\zeta_p = p/3$. Note that our prediction is based on approximate assumptions, and V. Yakhot has pointed out that our formula for ζ_p must fail for $p \geq 50$. But the formula works well for the moderate values of p for which measurements are available (and is exact for $p=3$). We must refer to [16] for further details.

** While not enthusiastic about Prigogine's later work, I like his early presentation of dissipative structures [13].

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