NONEQUILIBRIUM: FROM HEAT TRANSPORT TO TURBULENCE (TO LIFE)

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(Classical) statistical mechanics

Equilibrium statistical mechanics:

an emergent theory from Hamiltonian mechanics

no dynamics, but

energy function,

phase space volume (entropy),

statistical description of *equilibrium state*

= probability measure with density in phase space

Nonequilibrium (a program rather than a theory):

entropy creation (but entropy not defined in general)

non gradient forces + thermostat

$\Rightarrow$ NESS $= \lim_{t\to+\infty} f^t$ Lebesgue measure in phase space

(singular but smooth along unstable directions)

Nonequilibrium close to equilibrium:

linear response formula (Green-Kubo)

uses time correlation function

Linear response formula from smooth dynamics (formal theory)

NESS $\rho + \delta_t \rho$ for the evolution equation

$$\frac{dx}{dt} = \mathcal{X}(x) + \delta_t \mathcal{X}(x) \quad , \quad \delta_t \mathcal{X} = X_t$$

Formal first order perturbation calculation gives for observable A

$$\delta_t \rho(A) = \int_{-\infty}^{t} d\tau \int \rho(dy)\, X_\tau(y) \cdot \partial_y A(f^{t-\tau} y)$$

For periodic perturbation, we get the *susceptibility*:

$$\omega \mapsto \int_0^\infty e^{i\omega t} dt \int \rho(dx)\, X(x) \cdot \partial_x (A \circ f^t)$$

Linear response close to equilibrium (formal theory)

Equilibrium: $\rho(dx) =$ has a density w.r.t. Lebesgue
Integration by part then gives the susceptibility

$$\omega \mapsto -\int_0^\infty e^{i\omega t} dt \int \rho(dx)\,(\mathrm{div}_x X)(A(f^t x))$$

(Green-Kubo)
$\Rightarrow$ fluctuation-dissipation
 and dispersion relation ("causality")

Linear response away from equilibrium (formal theory)

Write $X = X^s + X^{u0}$ (*stable* and *unstable* components)
The susceptibility is formally:

$$\omega \mapsto \int_0^\infty e^{i\omega t} dt \int \rho(dx)\, X^s(x) \cdot \partial_x (A \circ f^t)$$

$$- \int_0^\infty e^{i\omega t} dt \int \rho(dx)\, (\mathrm{div}_x^{u0} X)(A(f^t x))$$

(s): *relaxation to attractor*
(u0): "half" *fluctuation-dissipation*"

dispersion relation?

Linear response (rigorous results)

Hyperbolic diffeomorphisms and flows

NESS: SRB states

the formal results can be made rigorous

Example: geodesic flow on manifold of negative curvature

Unimodal maps of the interval

breakdown of dispersion relations

Partially hyperbolic systems

NESS: u-Gibbs states

References: Sinai, Bowen, Ruelle,

Pollicott, Baladi, Katok, Young, Liverani, Dolgopyat, ...

Eckmann, Gallavotti,...

Heat transport (1)

Chain of $N+1$ nodes

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

Hamiltonian

$$H = \sum_j H_j(\mathbf{p}_j, \mathbf{q}_j) + \lambda \sum_{j=1}^{N} W(\mathbf{q}_{j-1}, \mathbf{q}_j)$$

H_j corresponds to Anosov Hamiltonian flow. Define

$$\alpha_j = \frac{1}{\langle \mathbf{p}_j, \mathbf{p}_j \rangle} \langle -\partial_{\mathbf{q}_j} (W(\mathbf{q}_{j-1}, \mathbf{q}_j) + W(\mathbf{q}_j, \mathbf{q}_{j+1}), \mathbf{p}_j \rangle$$

Thermostatted time evolution (f^t):

$$\frac{d\mathbf{p}_j}{dt} = -\partial_{\mathbf{q}_j} H_j + \lambda X_j - \lambda \alpha_j \mathbf{p}_j \qquad , \qquad \frac{d\mathbf{q}_j}{dt} = \partial_{\mathbf{p}_j} H_j$$

Heat transport (2)

Fix $H_j = K_j$ and define temperatures $\beta_j^{-1} = 2K/(n-1)$

Perturbation theorem:

product state $\rho_\times$ at $\lambda = 0 \quad \Rightarrow \quad u$-Gibbs state ρ

$$\rho(A) - \rho_\times(A) = \lambda(n-1)\int_0^\infty d\tau\, \rho_\times((\sum_{j=0}^{N} \alpha_j)(A \circ f_\times^\tau)) + o(\lambda)$$

Can define (to first order in λ) stable temperature profile:

$$\beta_o^{-1} > \beta_1^{-1} > \cdots > \beta_{N-1}^{-1} > \beta_N^{-1}$$

(no net energy flux from thermostats)

$\Rightarrow$ Fourier's law (cf Dolgopyat-Liverani)

3D turbulent fluid as a physical system

Hamiltonian dynamics of incompressible fluid
$+$ viscous dissipation

Physical description
localized structures (eddies)
direct energy cascade $+$ small scale dissipation
folding and stretching of vorticity tubes

Kolmogorov theory
If turbulence is assumed isotropic and homogeneous, the features of the energy cascade in inertial range are determined by a dimensional argument.

But experimentally, turbulence is intermittent
(i.e., not homogeneous) $\Rightarrow$ multifractal approach:
Mandelbrot, Frisch, Parisi, Sreenivasan, Yakhot, ...

$$\langle |\Delta_r v|^p \rangle \sim r^{\zeta_p} \qquad , \qquad \zeta_p = \frac{p}{3} - \frac{1}{\ln \kappa} \ln \Gamma(\frac{p}{3} + 1)$$

Mechanics of energy cascade and intermittency (1)

Formulation of mechanical problem:

cubes C_{ni} ($n = 0, 1, \ldots$ and $i = 1, \ldots, \kappa^{3n}$)

side $\ell_n = \ell_0 \kappa^{-n}$

homothecy $\phi_{ni} : C_0 \to C_{ni}$

$2(\kappa^3 - 1)$ divergence-free real vector fields U_α with

$$\int_{\mathbf{R}^3} U_\alpha = 0$$

velocity field v with $\int v = 0$ has wavelet decomposition

$$v = \sum_{n=0}^{\infty} \sum_{i=1}^{\kappa^{3n}} \sum_{\alpha=1}^{2(\kappa^3-1)} c_{ni\alpha} U_\alpha \circ \phi_{ni}^{-1}$$

Mechanics of energy cascade and intermittency (2)

Claim:

The equations of fluid mechanics can be rewritten as

Hamiltonian evolution equations for coupled systems
(n, i) with $\kappa^3 - 1$ degrees of freedom

$+$ external forces at small n (large scales)

$+$ dissipation at large n (small scales)

with small coupling between systems (n, i)
for different n

Mechanics of energy cascade and intermittency (3)

Problem of non-equilibrium statistical mechanics:

heat transport between the systems (n, i)

$\Rightarrow$ explains direction of energy cascade

Boltzmann, Kolmogorov $\Rightarrow$ temperature

$$T_n = \frac{1}{k} \frac{\epsilon^{2/3} \ell_n^{11/3}}{2(\kappa^3 - 1)}$$

very small $k \Rightarrow$ huge T_n and heat resistance (small coupling)

general problem of looking for *SRB* measure replaced by study of heat transport close to equilibrium

- Macroscopic approximation: Kolmogorov
- Microscopic fluctuations: intermittency.

Stat Mech fluctuations and turbulent intermittency

Warning: a rigorous microscopic theory of heat transport is still missing, what follows is "theoretical physics"

We assume that, given the energy V_{ni} in (n,i),the velocity $v = v_{(n+1)j}$ is fluctuating with Boltzmannian distribution:

$$\sim \exp\big(-\frac{|v|^3}{V_{ni}\kappa^{-1}}\big)d^3v$$

- Because of the large temperature gradient, the flow of energy is overwhelmingly from (n,i) to the systems $(n+1,j)$
- The energy V is proportional to the kinetic energy $\frac{1}{2}|v|^2$ with a weight 1/time spent in a given spatial energy range, hence we take $V = |v|^3$
- $$|v_{ni}|^3/\ell_n = |v_{(n+1)j}|^3/\ell_{n+1} \quad \text{or} \quad |v|^3 = V_{ni}\kappa^{-1}$$
- Choice of κ discussed below.

Normalized distribution of the energy $V = V_{(n+1)j}$:

$$\frac{1}{V_n \kappa^{-1}} \exp\big(-\frac{V}{V_n \kappa^{-1}}\big)\, dV$$

Let $\tilde{V}_n = \kappa^n V_n$, then $\tilde{V} = \tilde{V}_{n+1}$ is distributed according to

$$\frac{1}{\tilde{V}_n} \exp\big(-\frac{\tilde{V}}{\tilde{V}_n}\big)\, d\tilde{V}$$

Structure functions, and exponents ζ_p

$$\langle |v_n|^p \rangle = \ell_n^{\zeta_p}$$

Estimating ζ_p

$$\zeta_p \ln \ell_n \sim \ln\langle V_n^{p/3}\rangle = -\frac{p}{3}\ln\kappa + \ln\langle \tilde{V}_n^{\frac{p}{3}}\rangle$$

where $\langle \tilde{V}_n^{\frac{p}{3}}\rangle$

$$= \int d\tilde{V}_1 \frac{e^{\tilde{V}_1/\tilde{V}_0}}{\tilde{V}_0}\int \cdots \int d\tilde{V}_{n-1}\frac{e^{-\tilde{V}_{n-1}/\tilde{V}_{n-2}}}{\tilde{V}_{n-2}}\int d\tilde{V}_n \frac{e^{-\tilde{V}_n/\tilde{V}_{n-1}}}{\tilde{V}_{n-1}}\cdot \tilde{V}_n^{p/3}$$

and

$$\int d\tilde{V}_n \frac{e^{-\tilde{V}_n/\tilde{V}_{n-1}}}{\tilde{V}_{n-1}}\cdot \tilde{V}_n^{p/3} = \tilde{V}_{n-1}^{p/3}\int_0^\infty d\xi\, e^{-\xi}\xi^{p/3} = \tilde{V}_{n-1}^{p/3}\Gamma(\frac{p}{3}+1)$$

hence by induction

$$\langle \tilde{V}_n^{\frac{p}{3}}\rangle = \Gamma(\frac{p}{3}+1)^n \tilde{V}_0^{p/3}$$

and

$$\zeta_p = \frac{p}{3} - \frac{1}{\ln\kappa}\ln\Gamma(\frac{p}{3}+1) \qquad (*)$$

Turbulence: discussion

- $(*)$ is approximate: cannot hold for large p ($p \geq 50$: Yakhot)
- Experimentally $(\ln \kappa)^{-1} = .32 \pm .01$ (i.e. κ between 20 and 25)
- It is assumed that a single value of the energy V at a certain spatial scale ℓ_n thermalizes to a Boltzmann distribution at scale $\ell_{n+1} = \ell_n/\kappa$
- Attempted physical interpretation:

  change of behavior as one passes to small spatial scales analogous to onset of turbulence, namely:

  fast transport $\rightarrow$ thermalization

- Critical Reynolds number R_c corresponding to κ

$$R_c = \kappa^{4/3} \approx 60$$

Turbulence: conclusion

Nonequilibrium statistical mechanics locally close to equilibrium provides a physically coherent picture of turbulence.

In this picture there is a natural scaling factor $\kappa^3 \sim 10^4$ which gives an idea of the complexity underlying turbulent dynamics.

We have estimated κ from experimental data, but it should be eventually accessible from computations of turbulent dynamics.

Life: what is it?

Consider a thermostatted system formed of impure water maintained outside of equilibrium.

Observation suggests that under certain conditions this system may develop nonequilibrium states described as "containing life".

These states have the following characteristics:
(1) they are not locally close to equilibrium
(2) they are (in some sense) very complex
(3) they are slowly changing (increasing complexity in some idealizations)

(1) corresponds to the fact that chemical reactions take place, and not only transport phenomena

(2) is not unexpected for nonequilibrium (cf turbulence)

(3) in our best-known example corresponds to the persistence of genetic information

Life: discussion

What does the existence of life tells us about non equilibrium statistical mechanics in general?

The only general principle of non equilibrium stat mech that seem to apply are:

> the conservation laws (atomic composition, energy)
> and the increase of entropy

Schrödinger puts the problem of life in the framework of stat mech and concentrates on the question of the persistence of genetic information in the presence of thermal noise

Contrary to the case of hydrodynamics, the energy here is injected (as well as dissipated) at microscopic scales.

Information of microscopic origin percolates to (more) macroscopic structures (this also occurs in crystal growth, but "living structures" have persistent "metabolic activity" for which it is however not easy to give an abstract definition).