Universal large fluctuations and time reversal

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Equilibrium states as special stationary states.

Basic: is extension of classical thermodynamics possible?

Aim: Thermodyn. $\Rightarrow$ general principles independent of microscopic properties

Major understanding of Therm. through Stat. Mech. and the assumption of Gibbs distribution

Isolated system (in equil.) $\Rightarrow$ probability on $(\mathbf{p},\mathbf{q}) \in R^{3N} \times V^N$

$$\mu_0(d\mathbf{p}d\mathbf{q}) = \frac{1}{Z} e^{-\beta H(\mathbf{p},\mathbf{q})}$$

$H(\mathbf{p},\mathbf{q}) = \sum_i p_i^2 + \sum_{i,j} V(q_1 - q_j) + walls$

If $V(\mathbf{q})$ subject to physical cond. short range and $V(\mathbf{q}) \geq -B_N$ therm. follows

$$U = (int.energy) = H, \qquad S = (entropy) = -k_B \frac{\partial}{\partial \beta^{-1}} (\beta^{-1} \log Z)$$

equivalent to

$$dU = dQ + dL, \qquad \frac{dQ}{T} = dS \longleftrightarrow \frac{\partial p}{\partial T} = \frac{\partial S}{\partial V}$$

Why ? : Ergodic Hypothesis implies Gibbs Distr. **But**

(1) EH is not a theorem (in any generality)
(2) even if true: long way to apply (how long wait until..? FPU!

Alexandrinian way out: proceed "as if". Rationalize as
(1) stationarity is attained locally (few degrees of freedom)
(2) motion is chaotic (short time scale to stionarity)

Can this be done in NEQ??? where eq. motion not Hamiltonian

Nonconservative forces act: energy must be dissipated by **thermostats** i.e. environment

Idea: stationary states are attained locally $\Rightarrow$ study small systems $\Rightarrow$ since '980's simulations $\Rightarrow$ built to understand NESS

Problem: *no Gibbs formula*
(a) equation of motion non Hamiltonian,
(b) phase space volume not conserved.
(c) (too) many models of thermostats.
Simplest example (electric resistance D̃rude, 1̃890's)

$$\dot{q} = p, \qquad \dot{p} = E - \alpha(p)\dot{p} - \partial V(q), \qquad \alpha(p) = \frac{E \cdot p}{p^2}$$

α s.t. p^2=const. or $\frac{1}{2}p^2 + V$=const
α not constant but same friction effect in the average
BUT reversible

More elaborated example in fluids (NS)

$$\dot{\mathbf{u}}+\underset{\sim}{u}\cdot\underset{\sim}{\partial}\mathbf{u}=\alpha(\mathbf{u})\Delta\mathbf{u}-\partial p+\mathbf{f}$$

incompressible and $\int\mathbf{u}^2 = const$ if

$$\alpha(\mathbf{u})=\frac{\int\mathbf{f}\cdot\mathbf{u}}{\int(\underset{\sim}{\partial}\mathbf{u})^2}$$

equivalent to NS if $\langle\,\alpha\,\rangle=\nu$ (??). **But reversible !!**.

Many thermostats, typically with unphysical forces: problem "their equivalence". I.e. ensembles equiv.

Idea: reversibility important even in presence of dissipation: Onsager Recip., Green-Kubo formulae, Fluct.-Dissip. theorem (at infinitesimal forcing!!).

Chaotic hypothesis (Cohen-GG): "it can be assumed that motion is chaotic in the math. sense", i.e. it is "Anosov" (by Ruelle this implies a natural formula for stationary states)

Key observation: in all NE thermostat models the phase space contraction rate can be interpreted as **entropy production rate** of the thermostats

$$\varepsilon = \frac{\dot{Q}}{k_B T}$$

(a) $\langle\varepsilon\rangle \geq \mathbf{0}$ ("friction" $\Rightarrow$ as entropy increase of thermostats)
(b) $\mathbf{p} \stackrel{\mathbf{def}}{=} \frac{\mathbf{1}}{\mathbf{t}} \int_{\mathbf{0}}^{\mathbf{t}} \frac{\varepsilon(\tau)}{\langle\varepsilon\rangle} \mathbf{d}\tau$ fluctuates in NESS with average $\langle p\rangle = 1$
(c) (Sinai's theorem): $Prob(p \in \Delta) = e^{tf(p)}$ for some "large deviation $f(p)$

Fluctuation theorem (Cohen,GG): reversible & chaotic $\Rightarrow$

$$f(p) - f(-p) = \langle\varepsilon\rangle p, \quad \longleftrightarrow \quad \frac{Prob(p \in dp)}{Prob(-p \in dp)} = e^{t\langle\varepsilon\rangle p}$$

no free parameters. If $\langle\varepsilon\rangle \to 0$ this reduces to Gree-Kubo, Onsager Rec., and FD-theorem

What about NS? and its **constant friction?** $\longleftrightarrow$ irreversible??

Reversible NS should be equivalent to the irreversible one: however on a macroscopic scale the fluctuations are not observable. Philosophy is that reversibility can be observed on small scale

In NS where can one look for reversibility?

OK theory: friction appears on the Kolmogorov scale

$$\lambda_k = LR^{-\frac{3}{4}}$$

where L = scale over which forcing occurs.

$$\text{Average of } \alpha(\mathbf{u}) = \frac{\int \mathbf{f}\dot{\mathbf{u}}}{\int (\partial \mathbf{u})^2}$$

if $\mathbf{u}$ is the velocity field without the viscosity components should be equal to ν and its fluctations should obey the FR

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