Finite thermostats in nonequilibrium (classical and quantum)

Part of the recent progress has been due to

(a) Focus on stationary states out of equilibrium, [1].

(b) Modeling thermostats in terms of finite systems, [2, 3].

Finite thermostats have been essential to clarify that reversibility and dissipation are not to be identified.

Thermostats $\Rightarrow$ Equations of motion: NOT Hamiltonian $\Rightarrow$ phase space contraction

Rationale: properties should not depend on how thermostats are imagined to work.

Hence the question arises of which is the meaning of the phenomenological constants describing friction.

I consider first the paradigmatic case of the NS equations which generates a proposal for a general theory of equivalence between statistical descriptions of stationary states as an extension of the theory of equilibrium ensembles to nonequilibrium.

Then I shall discuss the possible further extension to quantum system in stationary nonequilibrium.

One idea behind the first equivalence studies is linked to the time reversal symmetry.

Time reversal is a fundamental symmetry while friction is phenomenological. Therefore one can investigate whether

Every (even if macroscopic) dissipative evolution can be equivalent to a reversible one, provided motions are sufficiently chaotic, (as they usually are under strong forcing or large N). [4, 5, 6, 7]

“In microscopically reversible (chaotic) systems time reversal symmetry cannot be spontaneously broken, but only phenomenologically so”,[8].

In the case of the NS2D:

$$\dot{\vec{u}} + (\vec{u} \cdot \boldsymbol{\partial})\vec{u} = -\boldsymbol{\partial} p + \vec{g} + \nu \Delta \vec{u}, \quad \boldsymbol{\partial} \cdot \vec{u} = 0 \qquad Eq$$

the proposal is (at fixed forcing $\vec{g}$) their equivalence to the equations

$$\dot{\vec{u}} + (\vec{u} \cdot \boldsymbol{\partial})\vec{u} = -\boldsymbol{\partial} p + \vec{g} + \alpha(\vec{u}) \Delta \vec{u}, \qquad \boldsymbol{\partial} \cdot \vec{u} = 0 \quad Eqnew$$

$$\alpha(\vec{u}) \stackrel{def}{=} \frac{\sum_{\vec{k}} \vec{k}^2 \, \vec{g}_{\vec{k}} \cdot \vec{u}_{-\vec{k}}}{\sum_{\vec{k}} \vec{k}^4 |\vec{u}_{\vec{k}}|^2}, \qquad D = 2$$

which have α so defined that the “dissipation” observable $\mathcal{E}(\vec{u}) = \int (\partial \vec{u}(x))^2 dx$ is an exact constant of motion.

Mechanism proposed: "same" as that for equilibrium ensembles, *i.e.* special collections of stationary states.

Consider two "ensembles", *i.e.* collections of stationary distributions

(1): Vary ν and let $\boldsymbol{\mu}_\nu^C$ stationary distrib. for (Eq). Let

$$\mathcal{E} = \boldsymbol{\mu}_\nu^C\Big(\int(\boldsymbol{\partial}\vec{u})^2\Big) = \boldsymbol{\mu}_\nu^C(\mathcal{E}(\mathbf{u}))$$

this is an "ensemble" (viscosity ensemble), [∼canonical].

Next consider the new equation (Eqnew): it has $\mathcal{E}(\mathbf{u}) = \int(\boldsymbol{\partial}\vec{u})^2$ as exact constant of motion

(2): Vary $\mathcal{E}$ and let $\boldsymbol{\mu}_{\mathcal{E}}^M$ station. distrib.: this is the (energy ensemble), [∼microcanonical].

State $\boldsymbol{\mu}_{\mathcal{E}}^{M}$ labeled by $\mathcal{E}$ corresponds to state $\boldsymbol{\mu}_{\nu}^{C}$ labeled by ν $\Rightarrow$ and are equivalent, denoted $\boldsymbol{\mu}_{\nu}^{C} \sim \boldsymbol{\mu}_{\mathcal{E}}^{M}$, if i) **OR** ii) hold

$$i)\ \mathcal{E} = \boldsymbol{\mu}_{\nu}^{C}(\mathcal{E}(\cdot))$$

$$ii)\ \nu = \boldsymbol{\mu}_{\mathcal{E}}^{M}(\alpha(\cdot))$$

in the sense that they give the same statistics in the limit of large $R = \frac{1}{\nu}$ to observables F which are "local observables": *i.e.* depend on finitely many Fourier comp. of $\vec{u}$.

Analogy: "canonical" $\boldsymbol{\mu}_{\beta}^{C}$ = "microcanonical" $\boldsymbol{\mu}_{E}^{M}$.

Why? Eg. chaoticity implies self averaging for the observable $\alpha(x)$ which replaces viscosity in (Eqnew):

$$\alpha(x(t)) = \frac{\sum_i F x_i}{\sum_i x_i^2} \qquad \text{“self} - \text{averaging}'' \text{ to } \ \nu$$

Problem: can reversibility be detected even in irreversible NS?

A theoretical basis can be searched in the "Chaotic hypothesis" (GC)

Chaotic hypothesis: "think of it as an Anosov system" (Cohen,G, if F is large), [9, 10, 11]

which is analogous to the periodicity≡ergodicity hypothesis of Boltzmann, Clausius, Maxwell, and possibly as unintuitive), [12, 13, 14].

Then in the reversible cases the phase space contraction rate $\sigma(\mathbf{u})$ averaged over a time τ

$$p \stackrel{def}{=} \frac{1}{\tau}\int_0^\tau \frac{\sigma(\mathbf{u}(t))}{\langle\,\sigma(\cdot)\,\rangle}dt \qquad (FT)$$

should have a PDF obeying a fluctuation relation, FR, [15].

This means that for large τ the probability distribution of p in $\boldsymbol{\mu}_{\mathcal{E}}^{M}$ (reversible viscossity ensemble) should fulfill

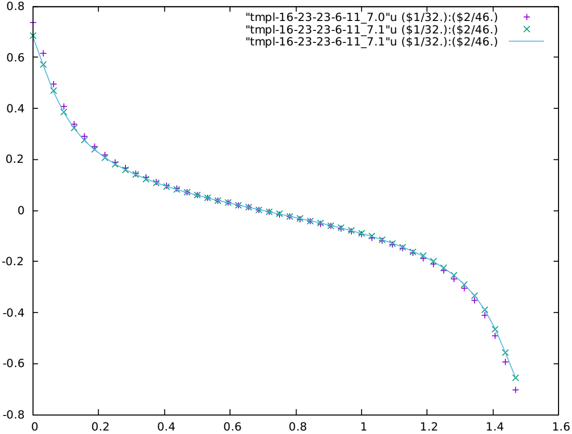
$$\frac{Prob_\tau(p)}{Prob_\tau(-p)} = e^{\tau\langle\,\sigma\,\rangle p + o(\tau)}, \qquad \tau \to \infty$$

Equivalence conjecture applied to the reversible viscosity ensemble $\boldsymbol{\mu}_{\mathcal{E}}^{M}$ and to the observable $\sigma(\mathbf{u})$ (which is not constant) would imply that $\sigma(\mathbf{u})$ fluctuates according to FR (the original one!) in the corresponding $\boldsymbol{\mu}_{\nu}^{C}$.

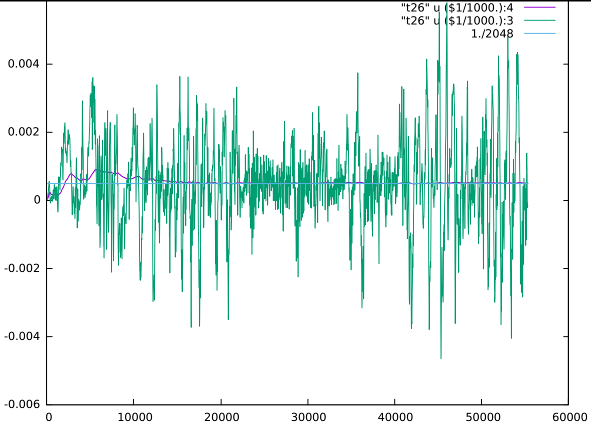
Of course consistency requires that the average $\mu_\nu^C(\alpha(\mathbf{u})) = \nu$.

The above "predictions" can be tested. And one can explore if the equivalence conjecture can be extended even to the Lyapunov spectrum (although the Lyapunov exponents, as well as $\sigma(\mathbf{u})$ are not local quantities).

It is interesting to present a few recent (mostly preliminary) results (encouraging but which need further confirmation as they are not yet very stable).



Local Lyapunov spectrum in a 48 modes truncation (7×7) of NS2D: $(+)=$ viscous, $(\times)=$ reversible and $R = 128$.



At 960 modes and $R = 2048$: the evolution of the observable "reversible viscosity": $\alpha(\mathbf{u}) = \dfrac{\sum |\mathbf{k}|^2 F_{\mathbf{k}} \overline{\mathbf{u}}_{\mathbf{k}}}{\sum |\mathbf{k}|^4 |\mathbf{u}_{\mathbf{k}}|^2}$

According to the equivalence the time average of α should be $\frac{\mathbf{1}}{\mathbf{R}}$. Represents the fluctuating values of α at intervals of 10^4 steps (see below); the middle line is the running average of α (at intervals of 100 steps) and it converges to $\frac{\mathbf{1}}{\mathbf{R}}$ (horiz. line).

The graph gives the values only every 1000 interaction steps (otherwise it would be just a black stain).

We see that once the attractor might be considered reached, for instance if the running average of the reversible viscosity is close to $\frac{1}{R}$ there are still wild fluctuations and the statistics can be sampled to check whether the FR applies.

For comparing the reversible and irreversible Lyapunov spectra it should be necessary to compute them over a time scale of 10^6 time steps. This is being attempted.

Quantum systems:

Temperature and heat are defined by the special apparata that measure them, [16].

However these are important physical obs. in *meso-physics* and *nano-physics*. [17, 18, 19].

Furthermore for simulations finite thermostat??, [20], are needed as well as a connection with dynamical systems formulation? ($\Rightarrow$ **CH & FT**)

A natural model is in Figure 1 where a quantum system C_0 is coupled to quantum thermostats $T_1, T2, \ldots$, proposed in [21] but studied only when the thermostats consisted of free gases.

Later considered in [17, 19, 18] with the thermostats interpreted as in the Ehrenfest therm. model or similar.

fig.1

H operator on $L_2(\mathcal{C}_0^{3N_0})$, (symm./antisy.) wave fnct.s Ψ,

$$H = -\frac{\hbar^2}{2}\Delta_{\vec{X}_0} + U_0(\vec{X}_0) + \sum_{j>0}\big(U_{0j}(\vec{X}_0,\vec{X}_j) + U_j(\vec{X}_j) + K_j\big)$$

Equations of motion

$$(1)\ \ -i\hbar\dot{\Psi}(\vec{X}_0) = \ (H(\{\vec{X}_j\}_{j>0})\Psi)(\vec{X}_0),$$

$$(2)\ \ \ddot{\vec{X}}_j = -\Big(\partial_j U_j(\vec{X}_j) + \langle\,\partial_j U_j(\vec{X}_0,\vec{X}_j)\,\rangle_\Psi\Big) - \alpha_j\dot{\vec{X}}_j, \qquad j>0$$

Dynamical sys. on phase space: $\big(\Psi,(\{\vec{X}_j\},\ \{\dot{\vec{X}}_j\})_{j>0}\big)$
if $\langle\,\cdot\,\rangle_\Psi \stackrel{def}{=} \langle\Psi|\cdot|\Psi\rangle$ and α_i= (rev./irr.) thermostat.

$$\alpha_j \stackrel{def}{=} \frac{\langle W_j \rangle_\Psi - \dot U_j}{2K_j}, \qquad W_j \stackrel{def}{=} -\dot{\vec X}_j \cdot \vec\partial_j U_{0j}(\vec X_0, \vec X_j)$$

Evolution: $K_j \equiv \frac12 \dot{\vec X}_j^2 \stackrel{def}{=} \frac32 k_B T_j N_j$ exact constants, (as classical).

NOT a time dep. Schrödinger eq.: *essential interaction syst-thermos*; Ehrenfest dynamics, [17],

Divergence (dissipation): $\sigma(x) = \sum_j \big(\frac{Q_j}{k_B T_j} + \frac{\dot U_j}{k_B T_j}\big)$ (*same as in the corresponding classical case*).

Equations are reversible and (expected) chaotic: Chaotic hypothesis ⇒ SRB + FT (original one)..

Consistency: *system with a single thermostat* $\rightarrow$ SRB distrib. should be equivalent to a canonical distribution. (*True in classical case*).

Candidate for μ: probability proportional to $d\Psi\, d\vec{X}_1\, d\dot{\vec{X}}_1$ times

$$\sum_{n=1}^{\infty} e^{-\beta E_n(\vec{X}_1)} \delta(\Psi - \Psi_n(\vec{X}_1)\, e^{i\varphi_n})\, d\varphi_n\, \delta(\dot{\vec{X}}_1^2 - 2K_1)$$

maybe $\Rightarrow$ expectation of O is a Gibbs state of therm. equil. with a special kind (random $\vec{X}_1, \dot{\vec{X}}_1$) of boundary condition and temperature T_1.

$$\langle\, O\,\rangle_\mu = Z^{-1} \int \sum_{n=1}^{\infty} e^{-\beta E_n(\vec{X}_1)} \langle \Psi_n(\vec{X}_1)|O|\Psi_n(\vec{X}_1)\rangle \delta(\dot{\vec{X}}_1^2 - 2K_1) d\vec{X}_1 \dot{\vec{X}}_1$$

$$\langle\, O \,\rangle = Z_0^{-1} \int \left(\mathrm{Tr}\, e^{-\beta H(\vec{X}_1)}\, O \right) d\vec{X}_1$$

However is not invariant under evolution: difficult to exhibit explicitly an invariant distribution (why should it be easy? *Aesopus*, [22]), [17].

Nevertheless if *adiabatic approximation* (*i.e.* classical motion in thermostat on a time scale much slower than quantum evolution), [17].

Eigenstates at time 0 follow variations of Hamiltonian $H(\vec{X}_1(t))$ due to thermostats motion, without changing quantum numbers.

Conjecture: true SRB is *also* equivalent to Gibbs at temp. $(k_B\beta)^{-1}$: instance of equivalence.

$\Rightarrow$ possibility of checking FR and of defining temperature via FR if Q is measurable absolute measurement of T, (originally suggested, [23], as a possible appl of FT to spin glasses)

In presence of forcing and a single thermostat measure $\langle\, Q\,\rangle$ and *if*

$$\zeta(-p)-\zeta(p)=-p\sigma_+$$

use slope σ_+ (in the simplest cases) to set

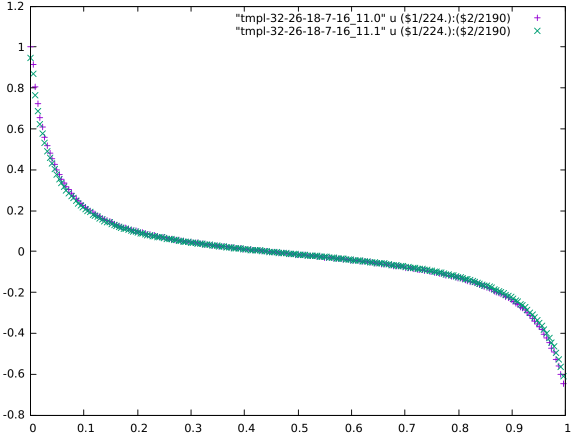
$$k_BT=\frac{\langle\, Q\,\rangle}{\sigma_+}$$

[Under time evolution a time $t > 0$ infinitesimal:

$$\begin{aligned}
\vec{X}_1 &\to \vec{X}_1 + t\dot{\vec{X}}_1 + O(t^2) \\
E_n(\vec{X}_1) &\to E_n + t\,e_n + O(t^2) \qquad \text{with} \\
e_n &\stackrel{def}{=} \langle\, \dot{\vec{X}}_1 \cdot \vec{\partial}_{\vec{X}_1} U_{01} \,\rangle_{\Psi_n} + t\dot{\vec{X}}_1 \cdot \vec{\partial}_{\vec{X}_1} U_1 = -t\,(Q_1 + \dot{U}_1) \\
e^{-\beta E_n(\vec{X}_1)} &\to e^{-\beta t e_n}
\end{aligned}$$

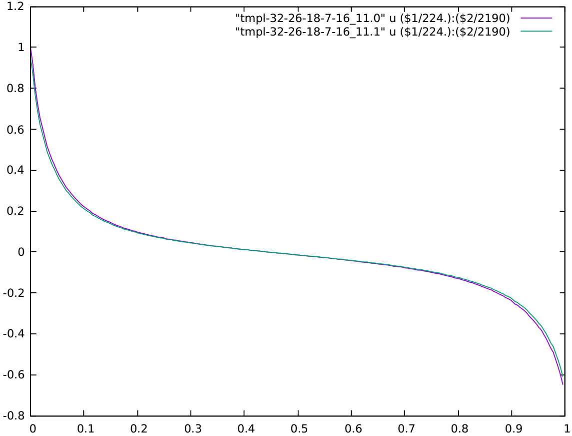
thermostat phase space contracts by $e^{t\sigma} \equiv e^{t\frac{3N_1 e_n}{2K_1}}$

Therefore if β is chosen such that $\beta = \frac{3N_1}{2K_1} \equiv (k_B T_1)^{-1}$ the distribution $\langle \cdot \rangle_\mu$ is stationary.]



Graph of the Lyapunov spectra in a 15×15 truncation for the NS2D with viscosity and reversible viscosity (captions ending respectively in 0 or 1). Preliminary

Supplement



Graph of the Lyapunov spectra in a 15×15 truncation for the NS2D with viscosity and reversible viscosity (captions ending respectively in 0 or 1) with points interpolated by lines. Preliminary

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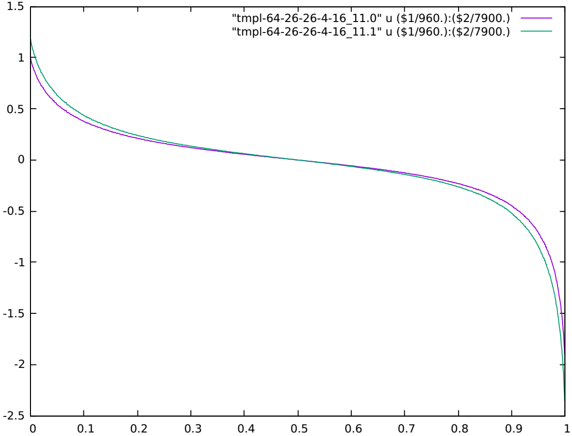

Graph of the Lyapunov spectra in a 31×31 truncation for the NS2D with viscosity and reversible viscosity (captions ending respectively in 0 or 1) with points interpolated by lines. Preliminary

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