

1: Reservoirs and entropy creation

$$m_i \ddot{\mathbf{x}}_i = -\partial_{\mathbf{x}_i} V(\mathbf{X}) + \mathbf{F}_i(\mathbf{X}; \Phi) - \vartheta_i, \quad i = 1, \dots, n$$

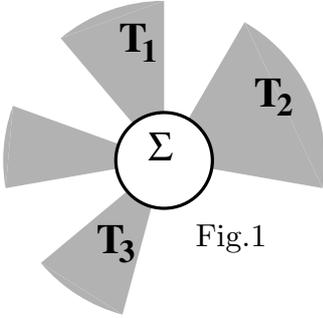


Fig.1

Reservoirs occupy infinite regions *e.g.* sectors $C_a \subset R^3$, $a = 1, 2, \dots$. Their particles are in a configuration typical of an equilibrium state at temperature T_a . The *empirical* probability of configurations in each C_a is Gibbsian with some temperature T_a .

$$\text{average}_{\mathbf{r}+\Lambda \subset C_a} (f_{\Lambda+\mathbf{r}}[(\dot{\mathbf{Y}}, \mathbf{Y} + \mathbf{r}); (\dot{\mathbf{W}}, \mathbf{W} + \mathbf{r})]) = \frac{e^{-\beta_a \left(\frac{1}{2m_a} |\dot{\mathbf{Y}}|^2 + V_a(\mathbf{Y}|\mathbf{W}) \right)}}{\text{normalization}}$$

In finite thermostats temperature is enforced by a constraint, *e.g.* Gaussian

$$K_a = \text{constant} = \frac{3}{2} N_a k_B T_a \equiv \frac{3}{2} N_a \beta_a^{-1}$$

Amount of heat \dot{Q} produced while in a stationary state identified with the work that the thermostat forces ϑ perform per unit time

$$\dot{Q} = \sum_i \vartheta_i \cdot \dot{\mathbf{x}}_i$$

Often $\vartheta = \sum_{a=1}^m \vartheta^{(a)}(\dot{\mathbf{X}}, \mathbf{X}) \Rightarrow \sigma^{(a)}(\dot{\mathbf{X}}, \mathbf{X}) \stackrel{\text{def}}{=} \sum_j \partial_{\dot{\mathbf{x}}_j} \cdot \vartheta_j^{(a)}(\dot{\mathbf{X}}, \mathbf{X})$ then

$$\sigma_+^{(a)} \stackrel{\text{def}}{=} \langle \sigma^{(a)}(\dot{\mathbf{X}}, \mathbf{X}) \rangle, \quad \dot{Q}_a \stackrel{\text{def}}{=} \sum_i \vartheta_i^{(a)} \cdot \dot{\mathbf{x}}_i$$

Temperature *defined* by $T_a = \frac{\langle \dot{Q}_a \rangle}{k_B \sigma_+^{(a)}}$. Is it > 0 ?

A class of thermostats with $T_a > 0$

N particles in C_0 interact via a potential $V_0 = \sum_{i < j} \varphi(\mathbf{q}_i - \mathbf{q}_j) + \sum_j V'(\mathbf{q}_j)$ (V' models external conservative forces like obstacles, walls, gravity, ...) and interact with M systems Σ_a , of N_a particles of mass m_a , in containers C_a contiguous to C_0 : “the M parts of the system in contact with thermostats at T_a , $a = 1, \dots, M$ ”.

$$m \ddot{\mathbf{q}}_j = -\partial_{\mathbf{q}_j} (V_0(\mathbf{Q}) + \sum_{a=1}^{N_a} W_a(\mathbf{Q}, \mathbf{x}^a)) \quad (\text{“conservative”})$$

$$m_a \ddot{\mathbf{x}}_j^a = -\partial_{\mathbf{x}_j^a} (V_a(\mathbf{x}^a) + W_a(\mathbf{Q}, \mathbf{x}^a)) - \boldsymbol{\vartheta}_j^a \quad (\text{“non conservative”})$$

$\boldsymbol{\vartheta}^a$ via Gauss’ principle: $\Rightarrow \boldsymbol{\vartheta}_j^a = \frac{L_a - \dot{V}_a}{3N_a k_B T_a} \dot{\mathbf{x}}_j^a \stackrel{def}{=} \alpha^a \dot{\mathbf{x}}_j^a$ where L_a is the work per unit time done by the particles in C_0 on the particles of Σ_a and V_a is their potential. Partial divergence $\sigma^a = 3N_a \alpha^a = \frac{L_a}{k_B T_a} - \frac{\dot{V}_a}{k_B T_a} \Rightarrow T_a > 0$ because L_a can be naturally interpreted as *heat* Q_a ceded, per unit time, by the particles in C_0 to the subsystem Σ_a (hence to the a -th thermostat because the temperature of Σ_a is constant), while the derivative of V_a *will not contribute to the value of σ_+^a* . *Apart from the total derivative terms*, (“true” \longleftrightarrow “up to an additive total derivative”)

$$\sigma_{true}(\dot{\mathbf{X}}, \mathbf{X}) = \sum_{a=1}^{N_a} \frac{\dot{Q}_a}{k_B T_a}$$

\rightarrow interpretation of σ as *entropy creation rate*.

Another viewpoint: the system only consist of N particles in C_0 and the Σ_a are thermostats \Rightarrow model of system subject to thermostats.

This is a conservative system interacting with thermostats. *Instead of the divergence* interesting is $\sigma_{true} \Rightarrow$ general “entropy creation” in a subsystem \equiv amounts of work done on the external particles divided by the temperatures.

Note that σ_{true} **will satisfy FR**: the large deviations of $p \stackrel{def}{=} \frac{1}{T} \int_0^T \frac{\sigma_{true}(t)}{\langle \sigma_{true} \rangle_{SRB}}$ have rate function

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

2. How irreversible is an irreversible transformation?

Let $E(t)$ be a parameter varying from E_0 to $E_\infty = E_0 + \Delta E$.

System initially in SRB state μ_0 and equations of motion

$$\dot{\mathbf{X}} = \mathbf{F}_{E(t)}(\mathbf{X}, \dot{\mathbf{X}})$$

(thermostatted system under variable forcing).

Let μ_t be the distribution into which μ_0 evolves. Let $\mu_{E(t)}$ be the SRB distribution corresponding to a “frozen” value $E(t)$. The quantity (τ =time scale of $E(t)$)

$$I = \tau \int_0^\infty (\langle \sigma_t \rangle_{\mu_t} - \langle \sigma_t \rangle_{\mu_{E(t)}})^2 dt$$

can be regarded a quantitative indicator of irreversibility degree. If $E(t) = E_0 + (1 - e^{-\gamma \kappa t}) \Delta E$ then $I(\gamma) \xrightarrow{\gamma \rightarrow 0} 0$: *quasi static evolution* ($\tau = (\gamma \kappa)^{-1}$) does not create entropy and has 0 “irreversibility”.

3. Navier Stokes: equivalence and barometric formula

Application to **NS** (incompressible $\partial \cdot \mathbf{u} = 0$)

$$\dot{\mathbf{u}} + \underline{\mathbf{u}} \cdot \underline{\partial} \mathbf{u} = \nu \Delta \mathbf{u} - \partial p + f \mathbf{g}, \quad R = \frac{\sqrt{fL}}{\nu}$$

Actually think of: cut off at $|\mathbf{k}| \leq K_k = L^1 R^{\frac{3}{4}}$, $N \simeq R^{\frac{9}{4}}$, i.e. OK41 is assumed.

To apply the chaotic hyp. need

(1) *chaos* (yes, if R large).

(2) *reversibility* (no)

(3) *pairing* (mechanism to recover reversibility when the attractor is very small)

(1) Equivalence with reversible equations “Gaussian NS eq.”

$$\dot{\mathbf{u}} + \underline{\mathbf{u}} \cdot \underline{\partial} \mathbf{u} = \alpha(\mathbf{u}) \Delta \mathbf{u} - \partial p + f \mathbf{g}, \quad \alpha = \frac{\int \mathbf{u} \cdot f \mathbf{g}}{\int (\partial \mathbf{u})^2} \Rightarrow \int \mathbf{u}^2 = \mathcal{E} = \text{const}$$

Same statistics for “local observables”: F local $\Rightarrow F$ depends on finitely many Fourier components of \mathbf{u} . **Same statistics** as $R \rightarrow \infty$ if \mathcal{E} is chosen = $\langle \int \mathbf{u}^2 \rangle_{\mu_\nu}$ (equivalence)

Consequence $\langle \alpha \rangle / \nu \rightarrow 1$: **only numerical tests in strongly cut off equations and $d = 2$** (*Rondoni, Segre*).

Earlier *She, Jackson*: large numerical simulations (different reversible equation)

Other tests: are Lyapunov spectra also identical? (Rondoni, Segre, G.). Here are a few graphs in highly truncated equations ($d = 2$)

Also the linear FR relation comes out within the precision: the approximate pairing that can be observed leads to test the slope $(1 - \frac{2M}{2N})\sigma_+$ in the GNS equations: from the theory it is expected a slope $< \sigma_+$ by the ratio of the number of negative pairs to the number of total pairs.

Barometric formula:

Consider the equations (incompressible NS and ED)

$$\dot{\mathbf{u}} + \underline{\mathbf{u}} \cdot \underline{\partial} \mathbf{u} = \nu \Delta \mathbf{u} - \partial p + f \mathbf{g}, \quad \dot{\mathbf{u}} + \underline{\mathbf{u}} \cdot \underline{\partial} \mathbf{u} = -\chi \mathbf{u} - \partial p + f \mathbf{g},$$

here $\mathbf{u} = \sum_{\mathbf{k}} \gamma_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{x}}$, $\mathcal{E} = L^3 \sum_{\mathbf{k}} |\gamma_{\mathbf{k}}|^2$.

The equivalence idea leads to think that although the statistics of the two equations are certainly different *nevertheless they might coincide on an appropriate scale*. The friction in NS varies with the scale \mathbf{k} and at some scale it might match that of ED.

By OK41 $v_k^3 k = \text{constant} = \eta\nu$ in NS: OK41 does not hold for ED: to fix ideas assume that at fixed cut off k_χ there is *equipartition* between the modes. Then $\langle |\gamma_{\mathbf{k}}|^2 \rangle \equiv \gamma^2$

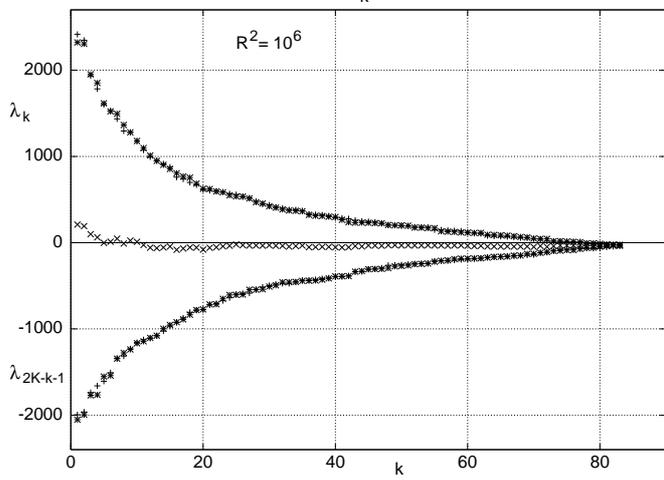
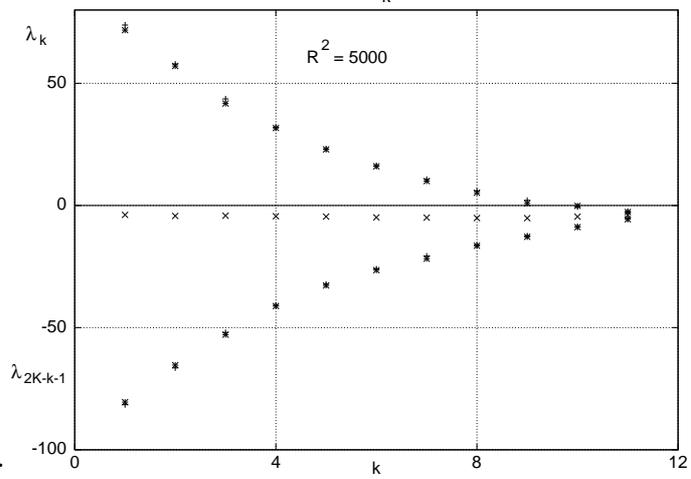
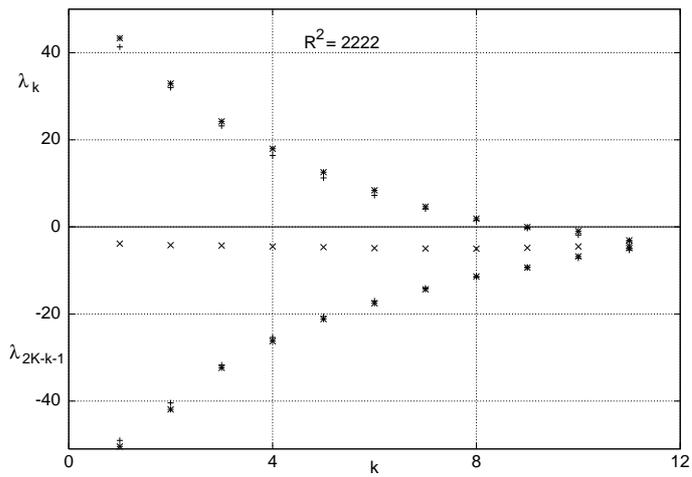
$$\frac{4\pi}{3} \gamma^2 (k_\chi \frac{L}{2\pi})^3 = \varepsilon, \quad \text{energy density at equipartition}$$

$$K_E(k) = \frac{3\varepsilon}{4\pi} \frac{k^2}{k_\chi^3}, \quad \text{energy density between } k \text{ and } k + dk$$

$$v_k^3 k = ((kL)^3 \gamma^2)^{\frac{3}{2}} k = \varepsilon^{\frac{3}{2}} k_\chi \left(\frac{k}{k_\chi}\right)^{\frac{11}{2}}, \quad \text{dimensionless dissipation on scale } k$$

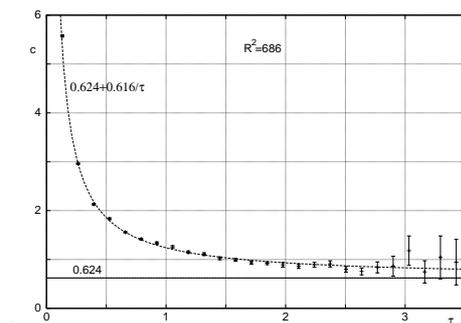
If $\varepsilon^{\frac{3}{2}} k_\chi \left(\frac{k}{k_\chi}\right)^{\frac{11}{2}} = \eta\nu$ then NS equation and ED equations have the same statistics on scale k : doubling the dissipation in NS the statistics of the two equations agree on scale 1.3 higher.

The k , or better $\log \frac{k}{k_\chi}$, is the analog of the height and the dim.less dissipation is the analogue of the pressure.



R^2	$\delta Q_0 / \langle Q_0 \rangle_{NS}$	$\Delta\alpha$	ΔQ_1	$o(M)/M$
800	0.005	0.030	0.053	0.068
1250	0.020	0.018	0.062	0.057
2222	0.002	0.039	0.058	0.077
4444	0.050	0.021	0.093	0.059
5000	0.010	0.008	0.058	0.033

Equivalence NS-GNS dynamics at different Reynolds numbers, column $\Delta\alpha$ to be compared with 1, cfr. [RS99]).



Evolution towards limiting slope as τ increases