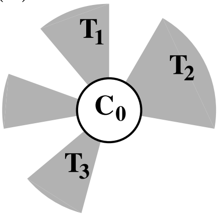
Process irreversibility and stationary states in small (and large) systems

Process: Evolution starting at a stationary state $\to$ ending in stationary state. Equations of motion are $t-dependent$

$$\dot{x} = f(x,t) = J\partial V(x) + g(x,t)$$

(1) Gas in contact with reservoirs with varying temperature



$U_i = \sum_{jk} v(q_k - q_j)$: internal energy of T_i

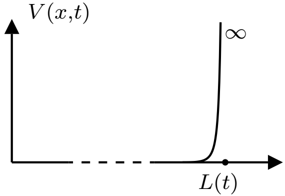
$W_{0i} = \sum_{j\in C_0, k\in T_i} v(q_k - q_j)$: interact. $T_i - -C_0$

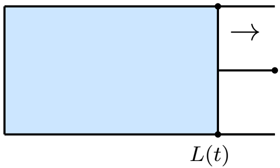
$\ddot{\vec{X}}_0 = -\partial_{\vec{X}_0}(U_0(\vec{X}_0) + \sum_{i>0} W_{0i}(\vec{X}_0, \vec{X}_i)) + \vec{E}(\vec{X}_0)$

$\ddot{\vec{X}}_i = -\partial_{\vec{X}_i}(U_i(\vec{X}_i) + W_{0i}(\vec{X}_0, \vec{X}_i)) - \alpha_i \dot{\vec{X}}_i$

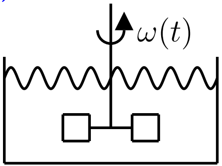
α_i s.t. $\frac{\dot{\vec{X}}_i^2}{2} = \frac{3}{2} N_i k_B T_i(\overline{t}) = \mathrm{const}$ if $t \equiv \overline{t}$: $\alpha_i = \frac{Q_i - \dot{U}_i}{3 N_i k_B T_i(t)}$

(2) Gas in a container with moving wall





(3) Paddle wheels stirring a liquid



2: Joule-Thompson expansion

3: Joule paddle wheels to measure heat-work conversion

t dependence of $g(x,t)$ vanishes as t becomes large: then
1: stationary $\rightarrow$ stationary; 2,3: equilibrium $\rightarrow$ equilibrium
Irreversible processes: how irreversible?
Natural time scale is associated with the process.

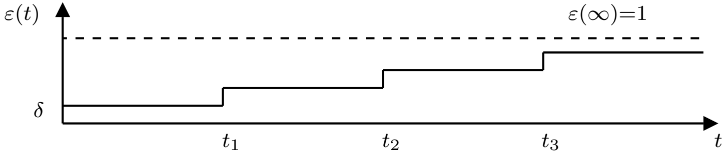
(a) Initial state: distribution μ_0,
(b) μ_0 evolves into μ_t in time t
(c) $\mu_t \xrightarrow[t\to\infty]{} \mu_\infty$

A natural time scale (GG 2006) to be interpreted as time scale over which irreversibility becomes manifest is

$$\frac{1}{\tau_{proc}} \stackrel{def}{=} \int_0^\infty (\langle\, \sigma_t \,\rangle_{\mu_t} - \langle\, \sigma_t \,\rangle_{\mu_{srb}(t)})^2 dt$$

$\sigma_t(x)$ = entropy production≡phase space contr. rate at t
$\mu_{srb}(t)$ is the SRB distribution eventually reached if the t-dependence of $g(x,t)$ were "frozen".

Example $g(x,t) = \varepsilon(t)g(x)$: under the chaotic hypothesis τ_{proc} is finite



If $\varepsilon(t)$ is frozen to $\varepsilon(t_i)$ in the interval t_i, t_{i+1}:

$$\left(\langle\, \sigma_{t_i}\,\rangle_{\mu_t} - \langle\, \sigma_{t_i}\,\rangle_{\mu_{srb}(t_i)}\right)^2 \sim O(\delta^2\, e^{-\kappa(t-t_i)})$$

$$\Rightarrow \tau_{proc}^{-1} \sim const\,\delta^2 \textstyle\sum_i^n \int_{t_i}^{t_{i+1}} dt e^{-\kappa t} = const\,\delta^2\, n = const\,\delta$$

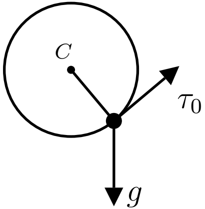
Intepretation: "quasi static processes" from equil. to equil. manifest irreversibility after arbitrarily long time τ_{proc}.

τ_{proc} is larger the slower is the process. vacuum expansion of free gas $\tau_{proc} = 0$ (as $\sigma(x) = \frac{\dot V}{V} = \delta(t), \int \delta(t)^2 = \infty$).

Monotonic: if slow $\Rightarrow \tau_{proc} = t =$ duration,
if fast $\to \tau_{proc} \simeq \tau_{relax}^{-1} \sigma_+^2$.

(Free gas) Carnot's cycle: $\tau_{proc} \sim t\ e^{-\frac{Q}{nRT}}$

Problem: Construct examples of nonequilibrium states



$$\dot q = \frac{p}{J}$$

$$\dot p = -2gV\sin q + \tau_0 - \frac{\xi}{J}p + \sqrt{\frac{2\xi}{\beta}}\,\dot w$$

Pendulum with inertia J, gravity $2Vg$
torque τ_0, white noise w, damping ξ

$\dot w$ white noise with $\langle\, dw^2 \,\rangle = \langle\, (w(t+dt) - w(t))^2 \,\rangle = dt$

β^{-1} noise temperature.

Problem: find the stationary state, Simulations exist
Stationary $F(p,q)dpdq$: $\Rightarrow$ the PDE $\mathcal{L}^*F = 0$

$$\mathcal{L}^*F = -\Big\{ \Big(\frac{p}{J}\partial_q F(q,p) + (2gV\sin q - \tau_0)\partial_p F(q,p) \Big) - \xi\, \Big(\beta_0^{-1}\partial_p^2 F(q,p) + \frac{1}{J}\partial_p (p\, F(q,p)) \Big) \Big\}$$

Gen. results: simulations and theory, [1]: $\exists$ smooth F

$$0 < F(q,p) = \frac{e^{-\frac{\beta}{2J}p^2}}{\sqrt{2J\beta^{-1}}}\rho(p,q) = G(p)\rho(p,q),$$

$$\rho(p,q) \in L_2(G(p)dpdq) \cap L_1(G(p)dpdq)$$

Hence $\rho(p,q) = \sum_{n=0}^{\infty} \rho_n(q) \; :p^n:$ with

$:p^n: \stackrel{def}{=} \left(\frac{J\beta^{-1}}{2}\right)^{\frac{n}{2}} H_n\left(\frac{p}{\sqrt{2J\beta^{-1}}}\right)$ (Wick,Hermite polynomials)

In dimensionless form

$$\sigma_n(q) \stackrel{def}{=} \rho_n(q)\xi^n n!, \qquad \eta \stackrel{def}{=} \beta\xi^2/J, \qquad \beta\tau_0, \qquad \beta V,$$

Problem: "Construct $\rho_n(q)$" so that $\mathcal{L}^* F = 0$

Let $\sigma_n(q) = \overline{\sigma}_n + \widetilde{\sigma}_n(q)$: average + average-less

Hermite polyn. rules yield

$$
\begin{aligned}
\partial\widetilde{\sigma}_n =& -\eta(n-1)\Big(\partial\widetilde{\sigma}_{n-2} + \beta\widetilde{\partial U\widetilde{\sigma}_{n-2}} + \beta\partial U\overline{\sigma}_{n-2} \\
& + \beta\tau_0\widetilde{\sigma}_{n-2} + \widetilde{\sigma}_{n-1}\Big) \\
\overline{\sigma}_n =& -\Big(\overline{\beta\partial U\widetilde{\sigma}_{n-1}} + \beta\tau_0\,\overline{\sigma}_{n-1}\Big)
\end{aligned}
$$

Identity: $\widetilde{\sigma}_1 = 0$ (from $n = 1$), $\overline{\sigma}_0 = 1$. But **two regimes**:

$gV \ll \tau_0$	"Rotational regime"
$gV \gg \tau_0$	"Oscillation regime"

If $\tau_0 = g\tau$ distinguish the two as $V \ll \tau$ and $V \gg \tau$

Idea: possibly σ_n analytic in g ??. Only in a given regime.

$$\widetilde{\sigma}_n(q) = g\widetilde{\sigma}_n^{[1]}(q) + g^2\widetilde{\sigma}_n^{[2]}(q) + \dots, \qquad F.T.\ \widetilde{\sigma}_{n,k}^{[r]}$$
$$\overline{\sigma}_n = \overline{\sigma}_n^{[0]} + g\overline{\sigma}_n^{[1]} + g^2\overline{\sigma}_n^{[2]} + \dots$$

$\Rightarrow$ convergence problems expected: "phase transitions"?

Algebraic steps $\Rightarrow$ recursion for $\vec{S}_{n,k}^{[r]} = \binom{\sigma_{n,k}^{[r]}}{\sigma_{n-1,k}^{[r]}}\overline{\sigma}_n^{[r]}$

$\Rightarrow$ link $\vec{S}_{n,k}^{[r]}$ to $\vec{S}_{n-1,k'}^{[r]}$, $\qquad k' = k, k \pm 1$

$$M^{-1}_{n+1,k} \stackrel{def}{=} \begin{pmatrix} 0 & 1 \\ -\frac{1}{n\,\eta} & -\frac{1}{i\,k} \end{pmatrix}$$

$$\vec{S}^{[r]}_{n,k} = M^{-1}_{n+1,k}\vec{S}^{[r]}_{n+1,k} - \vec{X}^{[r]}_{n+1,k}, \qquad \vec{S}^{[r]}_{2,k} = \widetilde{\sigma}^{[r]}_{2,k}\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\overline{\sigma}^{[r]}_{n} = v^{[r]}_{n}, \qquad \overline{\sigma}^{[r]}_{0} = 0, \qquad \widetilde{\sigma}_1, \widetilde{\sigma}^{[0]}_{n} \equiv 0, \qquad \overline{\sigma}_0 \equiv 1$$

with $\vec{X}^{[r]}, v^{[r]}$ depend on $r' < r$ and $\widetilde{\sigma}^{[r]}_{0,k}$ depends on $\widetilde{\sigma}^{[r]}_{2,k}$.

For each order $\widetilde{\sigma}^{[r]}_{2,k}$ has to be determined. Is it Arbitrary?

$\widetilde{\sigma}^{[r]}_{2,k}$ has to be determined. Not Arbitrary

e.g. $\widetilde{\sigma}^{[r]}_{n,k}$ must be s.t. $\sum_{n,k} \rho^{[r]}_{n,k} : p^n :$ is convergent

(1) As $\rho^{[r]}_{n,k} = \frac{\sigma^{[r]}_{n,k}}{\xi^n\, n!}$ it must be $\widetilde{\sigma}^{[r]}_{n,k} \ll O(A_r e^{-\kappa|k|}\sqrt{n!})$, $\kappa > 0$.

(2) Special sol. $\boldsymbol{\xi}_n \stackrel{def}{=} -\sum_{h=n}^{\infty} (M^{-1}_{n+1})^{*(h-n)} \vec{X}_{h+1},\ n > 2$?
(3) Solution

$$\lambda\ (M^{-1}_{n+1})^{*(h-n)} \begin{pmatrix} 0 \\ 1 \end{pmatrix} - \sum_{h=n}^{\infty} (M^{-1}_{n+1})^{*(h-n)} \vec{X}_{h+1}$$

Homogeneous equation (i.e. $\vec{X} = 0$) solution $\boldsymbol{\zeta}_n$ with the sequence $\Lambda(3,n)\, M_{3,k}^{-1} M_{4,k}^{-1} \ldots M_{n,k}^{-1} \binom{0}{1} \xrightarrow[n\to\infty]{} \boldsymbol{\zeta}_2$.

Product of 2×2 matrices $\Rightarrow$ continued fractions

$$\varphi(n,h) = \frac{1}{1 + \frac{z}{n}\frac{1}{1+\frac{z}{n+1}} \cdots \frac{}{\frac{1}{1+\frac{z}{h-2}}}}, \qquad z \stackrel{def}{=} \frac{k^2}{\eta} > 0$$

$$\boldsymbol{\zeta}_2 = -ik\binom{\varphi(2,\infty)}{1}$$

Complete solution is expressed in closed form in terms of $\varphi(n,h)$;

Bounds follow from the continued fractions theory.

Result (Iacobucci, Olla, G, 2013, [2, 3]: $\forall J, \beta, \xi, V, \tau$

(1) the order $r \ge 0$ coeff. $\rho_n^{[r]}(q)$ of formal Taylor expansion for $\rho_n(q)$ in powers of g can be constructed for all r.

(2) Fourier's coefficients $\rho_{n,k}^{[r]}$ vanish for $|k| > r$ and satisfy

$$\xi^n |\rho_{n,k}^{[r]}| \le A_r \frac{r^{\,n}}{n!} e^{-c|k|}, \qquad \forall r \le R,\, \forall k$$

for A_r, c suitably chosen.

Thus: Formal solution to all orders in g for the Taylor expansion of $\rho(p,q) = \sum_{k=0}^{\infty} g^r \, \rho^{[r]}(q,p)$.

However: the coefficients can be estimated uniformly in V, τ in any bounded set $\Rightarrow$ convergence is not expected.

At best an asymptotic solution in one of the two regimes.

Questions: (1) find a constructive solution;

(2) is there a phase transition between the two regimes?

References

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Carnot cycle $V_0 \to V_1 \to V_2 \to V_3 \to V_0$

$$\sigma_{01}dt = -\sigma_{23}dt = -\left(3N\frac{dV}{V} - \frac{dQ}{NRT_+}\right) = -4N\frac{dV}{V}$$

$$\sigma_{12}dt = \sigma_{30}dt = -\left(3N\frac{dV}{V}\right)$$

$$\int \Big(\frac{(V_{i+1} - V_i)}{V_i + \frac{t}{t_{i,i+1}}(V_{i+1} - V_i)}\Big)^2 dt = \frac{1}{t_{i,i+1}}\frac{1}{\lambda_i(1 - \lambda_i^{-1})^2}$$

$$\lambda_0 = \frac{V_1}{V_0} = e^{\frac{Q}{nRT}}$$

$$\tau_{proc} \sim const\ t\ e^{-\frac{Q}{nRT}}$$