Thermostats and thermodynamic limit in nonequilibrium

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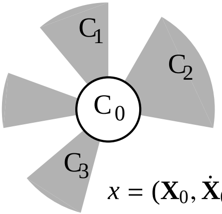
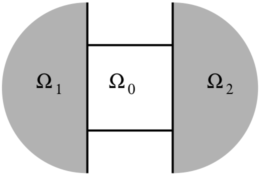
Thermostat models (Feynman-Vernon 1963): finite system in contact with infinite. Examples





$$x = (\mathbf{X}_0, \dot{\mathbf{X}}_0, \mathbf{X}_1, \dot{\mathbf{X}}_1, \ldots, \mathbf{X}_\nu, \dot{\mathbf{X}}_\nu)$$

Initial state: $\mu_0(dx) \stackrel{def}{=} C e^{-\sum_{j=0}^{\nu} \beta_j H_j(\mathbf{X}_j, \dot{\mathbf{X}}_j)} \prod_j \frac{d\mathbf{X}_j\, d\dot{\mathbf{X}}_j}{N_j!}$

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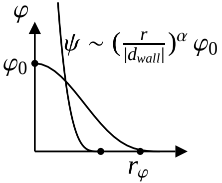
Equations of motion

$$m\ddot{\mathbf{X}}_{0i} = -\partial_i U_0(\mathbf{X}_0) - \sum_{j>0} \partial_i U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) + \partial_i \Psi(\mathbf{X}_j) + \Phi_i(\mathbf{X}_0)$$

$$m\ddot{\mathbf{X}}_{ji} = -\partial_i U_j(\mathbf{X}_j) - \partial_i U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) + \partial_i \Psi(\mathbf{X}_j)$$

$$U_j(\mathbf{X}_j) = \sum_{q,q' \in \mathbf{X}_j} \varphi(q - q'), \qquad U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) = \sum_{q \in \Omega_0, q' \in \Omega_j} \varphi(q - q')$$

$$\Psi(X) = \sum_{q \in X} \psi(q)$$



Initial state: infinite Gibbs at given density δ_j and temperatures β_j^{-1}

No phase transitions ⇒ kinetic-potential energy density, density and many observables are constant with μ_0 probability 1 at time $t = 0$: examples

$$\lim_{\Lambda\to\infty} \frac{1}{|\Lambda \cap \Omega_j|} K_{j,\Lambda}(x) = \frac{d}{2}\beta_j^{-1}\delta_j$$

$$\lim_{\Lambda\to\infty} \frac{1}{|\Lambda \cap \Omega_j|} N_{j,\Lambda}(x) = \delta_j$$

$$\lim_{\Lambda\to\infty} \frac{1}{|\Lambda \cap \Omega_j|} U_{j,\Lambda}(x) = u_j$$

Thermostats should admit evolution: defined by a limit

Regularize in a ball Λ_n (side $2^n r_\varphi$) $\Rightarrow$ Time evolution exists $x \to S_t^{(n,0)} x \Rightarrow$

it should be also $\lim_{n\to\infty} S_t^{(n,0)} x = S_t^{(0)} x$ **??**

Temperature, density, energy density **should** be fixed $\forall t, j > 0$

$$\lim_{\Lambda\to\infty} \frac{1}{|\Lambda \cap \Omega_j|} K_{j,\Lambda}(S_t^{(0)} x) = \frac{d}{2}\beta_j^{-1}\delta_j \equiv \frac{d}{2} k_B T_j \delta_j \qquad ??$$

Entropy: thermostats entropy increases by

$$\sigma_0(x) = \sum_{j>0} \frac{Q_j}{k_B T_j(x)}, \qquad Q_j \stackrel{def}{=} -\dot{\mathbf{X}}_j \cdot \partial_{\mathbf{X}_j} U_{0,j}(\mathbf{X}_0, \mathbf{X}_j))$$

Existence: Theorem by Caglioti, Marchioro, Pulvirenti (2000)

Remarkable conclusion of a series of works by

Lanford (1968) 1 dimension (a.e. for general states)

Sinai (1971) 1 dimension (a.e. for general states, proving cluster dynamics)

Marchioro, Pellegrinotti, Presutti (1974) (a.e. only for Gibbs states arbitrary dim.)

Dobrushin Fritz (1975) (a.e. for dim.= 2 general states)

$$W(x;\xi,R) \stackrel{def}{=} \text{total energy} + \text{number of particles in ball } \mathcal{B}(\xi,R)$$

$$\mathcal{E}(x) \stackrel{def}{=} \sup_{\xi} \sup_{R>(\log_+(\frac{\xi}{r_\varphi}))^{1/d}} \frac{W(x;\xi,R)}{R^d}$$

Let $\mathcal{N}_i(t,n)$= number of particles within r of $q_i^{(n,0)}(t)$ and let $T > 0$, $v_1 = \sqrt{\frac{2\varphi_0}{m}}$

Theorem: $\exists\, C(\mathcal{E}), c(\mathcal{E})^{-1}, \uparrow \mathcal{E}$, *and if* $q_i(0) \in \Lambda_k$ $\forall t \le T$,

(1) $|\dot{q}^{(n,0)}(t)| \le v_1\, C(\mathcal{E})\, k^{1/2}$,

(2) $\text{distance}(q_i^{(n,0)}(t), \partial(\cup_j \Omega_j \cap \Lambda)) \ge c(\mathcal{E})\, k^{-3/2\alpha}\, r_\varphi$

(3) $\mathcal{N}_i(t,n) \le C(\mathcal{E})\, k^{3/4}$

(4) $|x_i^{(n,0)}(t) - x_i^{(0)}(t)| \le C(\mathcal{E})\, r_\varphi\, e^{-c(\mathcal{E}) 2^{nd/2}}$

$\forall\, n > k$. *The* $x^{(0)}(t)$ *is unique frictionless motion satisfying 1,2,3*

Q1: is the temperature fixed for $t > 0$? are intensive quantities constants of motion?

Q2: Alternative models (Λ_n–regularized Gaussian thermostats)

$$m\ddot{\mathbf{X}}_{0i} = -\partial_i U_0(\mathbf{X}_0) - \sum_{j>0} \partial_i U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) + \partial_i \Psi(\mathbf{X}_j) + \Phi_i(\mathbf{X}_0)$$

$$m\ddot{\mathbf{X}}_{ji} = -\partial_i U_j(\mathbf{X}_j) - \partial_i U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) + \partial_i \Psi(\mathbf{X}_j) - \alpha_{j,n}\dot{\mathbf{X}}_{ji}$$

With $\alpha_{j,n}$ so fixed that $U_{j,\Lambda_n} + K_{j,\Lambda_n} = E_{j,\Lambda_n}$ is exact constant

$$\alpha_{j,n} \stackrel{def}{=} \frac{Q_j}{d\,N_j k_B T_j(x)}, \qquad Q_j \stackrel{def}{=} -\dot{\mathbf{X}}_j \cdot \partial_j U_{0,j}(\mathbf{X}_0, \mathbf{X}_j)$$

with $m\dot{\mathbf{X}}_j^2 \stackrel{def}{=} 2K_{j,\Lambda_n}(x) \stackrel{def}{=} d\,N_j k_B T_j(x)$

Equivalence? (in therm. lim. $\Lambda_n \to \infty$)

Idea: $Q_j \stackrel{def}{=} -\dot{\mathbf{X}}_j \cdot \partial_j U_{0,j}(\mathbf{X}_0, \mathbf{X}_j)$ is $O(1)$ (Williams,Searles,Evans 2004)

hence $\alpha_j = \frac{Q_j}{d\, N_j k_B T_{j,n}(x)} \Rightarrow 0$ **as** $n \to \infty$.

But is $T_{j,n}(x) \ge c > 0$ **??**

Theorem (Presutti, G): *with* μ_0*–probability* 1

(a) $\frac{\mathbf{K_{j,\Lambda_n}(S^{(n,1)}x)}}{|\mathbf{\Lambda_n \cap \Omega_j}|} \ge \frac{1}{4}\, d\, \delta_j\, k_B T_j$ *for n large* *(hence* $\alpha \xrightarrow[n\to\infty]{} 0$*).*

(b) $\lim_{n\to\infty} S_t^{(n,1)} x = \lim_{n\to\infty} S_t^{(n,0)} x$ for all $t > 0$.

(c) $\frac{d\mu_t(dx)}{dt} = -\sigma(x)\,\mu_t(dx)$ and

$$\sigma(\mathbf{x}) = \sum_{\mathbf{j>0}} \frac{\mathbf{Q_j}}{\mathbf{k_B T_j(x)}} + \beta_0(\dot{\mathbf{K}}_\mathbf{0} + \dot{\mathbf{U}}_\mathbf{0} + \dot{\mathbf{\Psi}}_\mathbf{0}) \stackrel{\mathbf{def}}{=} \sigma_\mathbf{0}(\mathbf{x}) + \dot{\mathbf{F}}(\mathbf{x})$$

Entropy production = *volume contraction* + *a time derivative*:

$\Rightarrow$ (average of σ) $\equiv$ (average of σ_0)

provided $\beta_j(x)$ is a constant of motion as $n \to \infty$ and $\beta_j(S_t x) = \beta_j$

In other words: very generally phase space contraction can be identified with the physically defined entropy production.

Theorem: *Let* Γ *be a pair potential and* $\varphi + \varepsilon\Gamma$ *be superstable for* $|\varepsilon|$ *small and* $P(\varphi + \varepsilon\Gamma)$ *(twice) differentiable at* $\varepsilon = 0$ *(i.e. "no phase trans."))*

$$g(S_t x) \stackrel{def}{=} \lim_{\Lambda_n \to \infty} \frac{1}{\Lambda_n \cap \Omega_j} \sum_{q,q' \in x} \Gamma(q(t) - q'(t)) = g$$

with μ_0*-probability* 1 *and for all* $t > 0$*: i.e.* $g(x)$ *constant of motion*.

Same with "no conditions" (of differentiability nor superstability) (including many body potentials Γ)" if, for each fixed m, n, the correlation functions of μ_0 cluster

$$\rho(q_1, \ldots, q_n, y_1 + \xi, \ldots, y_m + \xi) - \rho(q_1, \ldots, q_n)\rho(y_1 + \xi, \ldots, y_m + \xi) \xrightarrow[\xi \to \infty]{} 0$$

uniformly in the diameters of the sets $\{q_1, \ldots, q_n\}$ and $\{y_1, \ldots, y_n\}$.

$\Rightarrow$ Infinitely many constants of motion.

Method: "*Entropy estimates*" for thermostatted motions

(I) Proof that kinetic energy per particle (in the Λ_n–regularized motion) stays $> \frac{d}{4}\delta_j \beta_j^{-1}$ with μ_0-probability 1 for $t \le \Theta$.

(II) Proof that the number of particles and their (kinetic+wall) energy in a unit box grows at most with a power $\gamma \in (\frac{1}{2}, 1)$ of $(\log_+(|\xi|/r_\varphi))^{\frac{1}{2}} \cdot (\log n)^\gamma$

Combining ideas of Sinai, Fritz-Dobrushin, and Marchioro, Pellegrinotti, Presutti, Pulvirenti (1975,1976).

Let $||x|| \stackrel{def}{=} \max_{\xi\in\Lambda_n} \frac{\max(N_{C_\xi}(x),\varepsilon_{C_\xi}(x))}{(\log_+(\xi/r_\varphi))^{1/2}}$ where

$C_\xi \stackrel{def}{=}$ unit cube centered at ξ, $N_{C_\xi}(x)$= number of particles in C_ξ,

$\varepsilon^2_{C_\xi} \stackrel{def}{=} \max_{q\in C_\xi}(\frac{1}{2}\dot{q}^2 + \psi(q))$. kinetic+wall energy

1) Given $1 > \gamma > \frac{1}{2}$, define for x s.t. $\mathcal{E}(x) \le E$, the **stopping time** $\tau(x)$

$$T_n(x) \stackrel{def}{=} \max\{t : \ t \le \Theta : \ \forall\, \tau < t, \\ \frac{K_{j,n}(S^{(n,1)}_\tau x)}{\varphi_0} > \kappa 2^{nd}, \quad \|S^{(n,1)}_t x\|_n < (\log n)^\gamma\}.$$

2) show that before the stopping time frictionless evolution and thermostatted evolution are very close for particles starting within Λ_k provided the cut-off $n \gg k$.

3) Check that the μ_0-probability of $\mathcal{B} \stackrel{def}{=} \{x \,|\, x \in \mathcal{X}_E \text{ and } T_n(x) \le \Theta\}$ is

$$\mu_0(\mathcal{B}) \le \ C\, e^{-c(\log n)^{2\gamma}}.$$

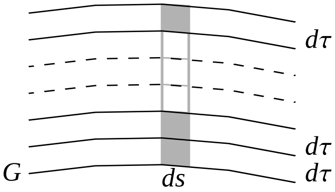
Via large deviations estimates.

Estimate the probability of $\mathcal{X}_n \stackrel{def}{=} \{\mathcal{E}(x) \le E;\ T_n(x) < \Theta\}$.

(2) $\Rightarrow$ bound on the *max entropy production within the stopping time*:
$|\int_0^{\tau_n(x)} \sigma(S_t^{(n,1)}x)dt| \le C'$ with C' depending only on E.

For inst. estimate probab. that kinetic energy becomes $G = 1/2$ of its μ_0-almost sure asympt. value. $G = \frac{1}{4}N_j d\beta_j^{-1}$. IF μ_0 were invariant

$$dsd\tau \stackrel{def}{=} (\int \mu_0(dx)|\dot K|\delta(K-G))d\tau$$



Remark: *all shaded volumes would have the same* μ_0 *volume* !

Then $\mu_0(\mathcal{X}_n)$ is bounded, if $C \geq |\int_0^{\tau_n(x)} \sigma(S_{-t}x)dt|$, by:

$$e^{C'}\Theta \int ds|\dot{K}| \equiv e^{C'}\Theta \int \mu_0(dx)\delta(K-G)|\dot{K}|$$

Hence $\leq e^{C'}\Theta \int \mu_0(dx)\delta(K-(G+\eta))|\dot{K}|$, for $\varepsilon \geq \eta \geq 0 \Rightarrow$ (any $\varepsilon > \eta > 0$!)

$$\leq C\frac{1}{\varepsilon}\int_0^{\varepsilon} d\eta \int \mu_0(dx)\,\delta(K-(G+\eta))\,|\dot{K}|$$

thus, *by a large (kinetic energy) deviation estimate*

$$\leq \frac{1}{\varepsilon}\int \mu_0(dx)\,\chi(G+\varepsilon \leq K \leq G)\,|\dot{K}|$$

$$\leq \frac{1}{\varepsilon}\sqrt{\mu_0(\chi(G+\varepsilon \leq K \leq G))}\,\sqrt{\mu_0(\dot{K}^2)} \leq e^{-\gamma|\Lambda_n|}$$

with $\gamma > 0$: *summable* $\Rightarrow$ "Borel-Cantelli" (after a similar bound on the second item appearing in definition of stopping time) yields that the stopping time must be Θ with μ_0-prob 1.

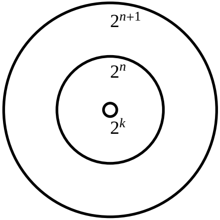
Reference

G. Gallavotti, E. Presutti:
Nonequilibrium, thermostats and thermodynamic limit,
Journal of Mathematical Physics, **51**, 015202, 2010
Archivi: arxiv.org 0905.3150
http://ipparco.roma1.infn.it

Some Details

Convergence $x_i^{(n,0)}(t) \to \overline{x}_i^{(0)}(t), \qquad q_i(0) \in \Lambda_k$

$$u_k^n(t) \stackrel{def}{=} \max_{q_i(0)\in\Lambda_k} |q_i^{(n,0)}(t) - q_i^{(n+1,0)}(t)|$$



Relation: $q_i^{(n,0)}(t) = q_i^{(n,0)}(0) + \dot{q}_i^{(n,0)}(0)\, t + \int_0^t f_i(x^{(n,0)}(\tau) d\tau \to$ comparison

subtract: n and $n+1$ relations $(\eta = \frac{3}{2} + \frac{3}{\alpha}) \;\Rightarrow$

$$u_k^n(t) \leq C n^\eta \int_0^t u_{k_1}^n(\tau) d\tau \qquad k_1 = k + C\sqrt{n}$$

#iteration steps $\gg \ell = 2^{n/2} \;\Rightarrow\; |u_k^n(t)| \leq C \frac{(n^\eta \Theta)^\ell}{\ell!}$

Why not “same” for thermostatted dynamics ?

$$u_k^n(t) \le Cn^\eta \int_0^\Theta u_{k_1}^n(\tau)d\tau + C2^{-nd} \qquad k_1 = k + C\sqrt{n}$$

#iteration steps is same $\gg \ell = 2^{n/2}$ BUT error $Ce^{C n^\eta \Theta} 2^{-n d} \to \infty$

Up to Stopping time properties

$$|\dot{q}_i^{(n,1)}(t)| \le C v_1 (k \log n)^\gamma, \qquad |q_i^{(n,1)}(t)| \le r_\varphi (2^k + C(k \log n)^\gamma)$$

$$\Rightarrow \mathcal{N} \le C(k \log n)^{d\gamma}, \quad \rho \ge c(k \log n)^{-2(d\gamma+1)/\alpha}$$

Only $(k \log n)^\eta$ particles interact with $q_i \in \Lambda_k$

Compare $x^{(n,1)}(t)$ and $x^{(n,0)}(t)$ ℓ times $2^{k_\ell} = 2^k + \ell C(k \log n)^\gamma$

Compare $x^{(n,1)}(t)$ and $x^{(n,0)}(t)$ ℓ times $2^{k_\ell} = 2^k + \ell\, C\,(k \log n)^\gamma$ with $\ell = \ell^* \sim 2^n/(\log n)^\gamma$ (ℓ^* is largest s.t. $2^{k_\ell} < 2^{k+1}$)

$$\frac{u_{k_\ell}(t,n)}{r_\varphi} \leq C\,(k \log n)^\eta \,(2^{-nd} + \int_0^t \frac{u_{k_{\ell+1}}(s,n)ds}{r_\varphi \Theta})$$

Iterate. This time the Lyapunov exponent is small

$$\frac{u_k(t,n)}{r_\varphi} \leq e^{C\,(k\ \log n)^\eta} C(k \log n)^\eta 2^{-dn} + \frac{(C\,(k\ \log n)^\eta)^{\ell^*}}{\ell^*!}\, C\,(2^k + k(\log n)^\gamma + k^{1/2})$$