Frictionless & Gaussian thermostats: equivalence and thermodynamics limit

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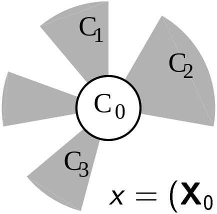
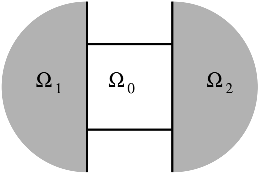
Thermostat models (Feynman-Vernon 1963): finite system in contact with infinite. Examples





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

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

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

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

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

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

Initial state: infinite Gibbs;
With given chemical potentials λ_j and temperatures β_j^{-1}

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

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

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

Thermostats should admit evolution: defined by "IR limit". Cut-off in a ball Λ_n (side size $2^n r_\varphi$). Time evolution exists $x \to S_t^{(n,0)} x$;

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

Thermostats should have fixed temperature, density, energy density at all times (actually all intensive observables). In part.

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

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)

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

Theorem: $\mathcal{E}(x) \stackrel{def}{=} \sup_\xi \sup_{R>(\log_+(\frac{\xi}{r_\varphi}))^{1/d}} \frac{W(x;\xi,R)}{R^d}$. Then *$\exists C(\mathcal{E}), c(\mathcal{E})^{-1}$, increasing functions of $\mathcal{E}$, such that the frictionless evolution satisfies the local dynamics property and if $q_i(0)\in\Lambda_k$ ($v_1=\sqrt{\frac{2\varphi(0)}{m}}$)*

$$
\begin{aligned}
&(1) \qquad |\dot q^{(n,0)}(t)| \le\ v_1\, C(\mathcal{E})\, k^{1/2},\\
&(2) \qquad \mathrm{distance}\big(q_i^{(n,0)}(t), \partial(\cup_j\Omega_j\cap\Lambda)\big) \ge\ c(\mathcal{E})\, k^{-3/2\alpha}\, r_\varphi\\
&(3) \qquad \mathcal{N}_i(t,n) \le\ C(\mathcal{E})\ k^{3/4}\\
&(4) \qquad |x_i^{(n,0)}(t) - x_i^{(0)}(t)| \le\ C(\mathcal{E})\, r_\varphi\, e^{-c(\mathcal{E})2^{nd/2}}
\end{aligned}
$$

$\forall\, n>k$. The $x^{(0)}(t)$ is the unique solution of the frictionless equations satisfying the first three items above.

Q1: is the temperature fixed for $t > 0$? are intensive quantities constants of motion?
Q2: Alternative models (Λ_n–regularized)

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

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

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

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

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

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 of the order $O(1)$ hence $\alpha_j = \frac{Q_j}{d\, N_j k_B T_{j,n}(x)}$ **tends to** 0 as $n \to \infty$.

But is $T_j(x) \ge c > 0$??

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

(a) $\frac{K_{j,\Lambda_n}(x)}{|\Lambda_n \cap \Omega_j|} \ge \frac{1}{4} d\, N_j \beta_j^{-1}$ *(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) $\frac{d\mu_0(dx)}{dt} = -\sigma(x)\mu_0(dx)$ and

$$\sigma(x) = \sum_{j>0} \frac{Q_j}{k_B T_j(x)} + \beta_0(\dot{K}_0 + \dot{U}_0 + \dot{\Psi}_0) \stackrel{def}{=} \sigma_0(x) + \dot{F}(x)$$

Entropy production differs by a time derivative of a bounded observable from the volume contraction:

$\Rightarrow$ average of $\sigma \equiv$ 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: *If* $G_{V_n}(x) \stackrel{def}{=} \frac{1}{|\Lambda_n \cap \Omega_j|} \sum_{Y \subset X \cap \Lambda_n} \Gamma(Y)$ *is superstable for* $|\varepsilon|$ *small and if there are no phase transitions in the thermostats* $(P(\varphi + \varepsilon\Gamma)$ *(twice) differentiable at* $\varepsilon = 0$*)*

$$\lim_{\Lambda_n \to \infty} \frac{1}{\Lambda_n \cap \Omega_j} G_{\Lambda_n \cap \Omega_j}(S_t x) = g$$

with μ_0*-probability* 1 *and for all* $t > 0$*.*

Same with "no conditions" 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 $\{y_1, \ldots, y_n\}$.

Method: "*Entropy estimates*" for thermostatted motions

(I) Proof that kinetic energy per particle (in the Λ_n–regularized motion) stays $> \frac{d}{4}\beta_j^{-1}$ 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 $(\log_+(|\xi|/r_\varphi)) \cdot (\log n)$

This is based on combining an idea of Sinai, and one of Fritz-Dobrushin, and Marchioro, Pellegrinotti, Presutti, Pulvirenti (1975,1976).

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

C_ξ= unit cube centered at ξ, $N_{C_\xi}(x)$= number of particles in C_ξ, $\varepsilon^2_{C_\xi} = \max_{q\in C_\xi}(\frac{1}{2}\dot{q}^2 + \psi(q))$.

1) Define for x s.t. $\mathcal{E}(x) \le E$, the **stopping time** $\tau(x)$

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

2) show that before reaching the stopping time the frictionless evolution and the 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

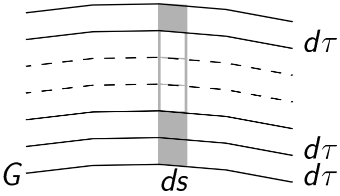
$$\mu_0(\mathcal{B}) \le \; C\, e^{-c(\log n)^{2\gamma}}.$$

Via large deviations estimates.

Estimate the probability of $\mathcal{X}_n \stackrel{def}{=} \{\mathcal{E}(x) \le E;\ T_n(x) < \Theta\}$. From (2) derive a bound on the *max entropy production within the stopping time* as $|\int_0^{\tau_n(x)} \sigma(S_t^{(n,1)}x)dt| \le C'$ with C' depending only on E.

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

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



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

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

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

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

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

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

$$\le \frac{1}{\varepsilon}\int \mu_0(dx)\,\chi(G-\eta \le K \le G)\,|\dot{K}|$$

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

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,
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http://ipparco.roma1.infn.it