Thermostats, large deviations and Fouriers law

by Errico Presutti, Guido Gentile, Alessandro Giuliani, GG

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



Initial state:

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

Equations of motion (thermostat force if a = 1)

$$\begin{split} m\ddot{\mathbf{X}}_{0i} &= -\partial_i U_0(\mathbf{X}_0) - \sum_{j>0} \partial_i U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) + \partial_i \Psi(\mathbf{X}_0) + \Phi_i(\mathbf{X}_0) \\ m\ddot{\mathbf{X}}_{ji} &= -\partial_i U_j(\mathbf{X}_j) - \partial_i U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) + \partial_i \Psi(\mathbf{X}_j) - \mathbf{a} \, \alpha_j \mathbf{\dot{X}}_{ji} \end{split}$$

$$U_{j}(\mathbf{X}_{j}) = \sum_{q,q' \in \mathbf{X}_{j}} \varphi(q - q'), \qquad j\text{-th thermostat energy}$$
$$U_{0,j}(\mathbf{X}_{0}, \mathbf{X}_{j}) = \sum_{q \in \Omega_{0}, q' \in \Omega_{j}} \varphi(q - q'), \quad j\text{-th thermostat-system interac.}$$

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

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

If no phase transitions \Rightarrow kinetic-potential energy density, density *etc* are constant with μ_0 -probability 1 at time t = 0: examples

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

- Thermostats evolution: should be limit of finite volume ???
- Macroscopic thermostats data: (T_j, δ_j, u_j) should be constant ???
- Equivalence of thermostats: a = 0 SAME a = 1, ????

More formally:

- Regularize: enclose system in ball $\Lambda_n = \Omega \cap \mathcal{B}(R)$ radius $R = 2^n r_{\varphi}$
- \Rightarrow Time evolutions $x \to S_t^{(n,a)}x$, a = 0, 1 have limits as $n \to \infty$??
- should also be also $\lim_{n\to\infty} S_t^{(n,a)} x = S_t^{(0)} x$ a = 0, 1??
- Temperature, density, energy density should be constant $\forall t, j > 0$, e.g.

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

Entropy: thermostats entropy "increases" by

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

History:

Existence: Theorem by Caglioti, Marchioro, Pulvirenti (2000), d = 3Remarkable conclusion of a series of works by Lanford (1968) 1 dimension (constructive, for "general" states) Sinai (1971) 1 dimension (a.e. general states, "cluster dynamics") Marchioro, Pellegrinotti, Presutti (1974) (a.e. only for Gibbs, $\forall d$) Dobrushin Fritz (1975) (a.e. for dim.=2 general states)

Control via specific energy in large balls: of radius $R \equiv R_n \stackrel{def}{=} 2^n r$

 $W(x;\xi,R) \stackrel{def}{=} \text{total } \frac{\text{energy}}{\varphi_0} + \text{number of particles in ball } \mathcal{B}(\xi,R)$

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



Large deviation for $\mu_0 \Rightarrow \mathcal{E}(x) < +\infty$.

Theorem: $\exists C(\mathcal{E}), c(\mathcal{E})^{-1} \uparrow \mathcal{E} \text{ and if } q_i(0) \in \Lambda_k \ (v_1 = \sqrt{\frac{2\varphi(0)}{m}})$ (1) $|\dot{q}^{(n,0)}(t)| \leq v_1 C(\mathcal{E}) k^{1/2},$

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

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

(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. (5) $\lim_{n\to\infty} S_t^{(n,1)}(x) \equiv S_t^{(0)}(x)$, with μ_0 -probability 1

 Λ_n -regularized Gaussian thermostats: thermostats force $\alpha_{j,n}$ so fixed that $U_{j,\Lambda_n} + K_{j,\Lambda_n} = E_{j,\Lambda_n}$ is exact constant of motion

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

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

Idea: Why to expect Equivalence? (in therm. lim. $\Lambda_n \to \infty$)

$$Q_j \stackrel{def}{=} - \dot{\mathbf{X}}_j \cdot \partial_j U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) = O(1)$$

(Williams, Searles, Evans 2004), hence

$$\alpha_{\mathbf{j}} = \frac{\mathbf{Q}_{\mathbf{j}}}{\mathbf{d} \, \mathbf{N}_{\mathbf{j}} \mathbf{k}_{\mathbf{B}} \mathbf{T}_{\mathbf{j},\mathbf{n}}(\mathbf{x})} \quad \xrightarrow[n \to \infty]{} \mathbf{0}.$$

But is $T_{j,n}(x) \ge c > 0$?? not $\forall x! \Rightarrow$ Large deviation

Theorem (Presutti, G): with
$$\mu_0$$
-probability 1
(a) $\frac{\mathbf{K}_{\mathbf{j},\mathbf{A}_{\mathbf{n}}}(\mathbf{x})}{|\mathbf{A}_{\mathbf{n}}\cap\mathbf{\Omega}_{\mathbf{j}}|} \geq \frac{1}{4} d \, \delta_j \, k_B T_j$ (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
 $\sigma(\mathbf{x}) = \sum_{\mathbf{j}>0} \frac{\mathbf{Q}_{\mathbf{j}}}{\mathbf{k}_B \mathbf{T}_{\mathbf{j}}(\mathbf{x})} + \beta_{\mathbf{0}}(\dot{\mathbf{K}}_{\mathbf{0}} + \dot{\mathbf{U}}_{\mathbf{0}} + \dot{\mathbf{\Psi}}_{\mathbf{0}}) \stackrel{\text{def}}{=} \sigma_{\mathbf{0}}(\mathbf{x}) + \dot{\mathbf{F}}(\mathbf{x})$

(1) Small kinetic energy is possible but large deviation

(2) Entropy production = volume contraction + a time derivative:

$$\Rightarrow (average of \sigma) \equiv (average of \sigma_0)$$

provided $\beta_j(x)$ is a constant of motion as $n \to \infty$ and $\beta_j(S_t x) = \beta_j$: very generally phase space contraction = physical entropy production. Marseille 7-2011 9 Method: "*Entropy estimates*" for thermostatted motions control large deviations

(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 $t \leq \Theta$: i.e stays $\geq \frac{1}{2}$ the equipartition value

(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 $(\log^{\frac{1}{d}}$ -growth of energy and energy density with distance to O):

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

 $C_{\xi} \stackrel{def}{=}$ unit cube centered at ξ , $N_{C_{\xi}}(x)$ = number of particles in C_{ξ} , $\varepsilon_{C_{\xi}}^2 \stackrel{def}{=} \max_{q \in C_{\xi}} (\frac{1}{2}\dot{q}^2 + \psi(q))/\varphi_0.$ kinetic + wall energy $r(\log \frac{|\xi|}{r})^{\frac{1}{d}}$ densities grow "log-distance" $|\xi|$

1) Define for x s.t. $\mathcal{E}(x) \leq E$, the stopping time $T_n(x)$

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

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

(Indeed within $T_n(x)$, α is very small of order $O(N_n^{-1})$).

Notice also $|\sigma| = O(1)$ depending only on E.

3) Check μ_0 -probability of $\mathcal{B} \stackrel{def}{=} \{x \mid x \in \mathcal{X}_E \text{ and } T_n(x) \leq \Theta\}$ is

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

because entropy bounds the μ_0 density of $\mu_0(S_{-t})$ before $T_n(x)$ allows us to bound via equilibrium large deviations \Rightarrow

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

For inst. estimate probab. that kinetic energy G becomes 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



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

Reference

G. Gallavotti and E. Presutti

Nonequilibrium, thermostats and thermodynamic Limit Journal of Mathematical Physics, 51, 015202 (+32), 2010 (arxiv: 0905.3150, doi: 10.1063/1.3257618)

G. Gallavotti and E. Presutti

Fritionless thermostats and intensive constants of motion Journal of Statistical Physics, 139, 618–629, 2010 (arxiv: 0907.1188, doi: 10.1007/s10955-010-9949-8)

G. Gallavotti and E. Presutti Thermodynamic limit for isokinetic thermostats Journal of Mathematical Physics, 51, 053303 (+9), 2010 (arxiv: 0908-3060, doi: 10.1007/s10955-010-9949-0)

Bonetto, Lebowitz, Rey-Bellet, In Mathematical Physics 2000,

Garrido, Gallavotti: J. Stat. Phys., 126, 1201-1207, 2007

BBGKY hierarchy, Fourier's equation (in progress)

by Guido Gentile, Alessandro Giuliani, GG

It is highly desirable to achieve a understanding similar to the one that can be obtained in systems in stationary states out of equilibrium.

In equilibrium systems enclosed in finite containers have a probability distribution with a density on phase space. This is no longer true for systems in steady non equilibrium.

Study existence of stationary states of a hard spheres gas with temperatures at $\pm \infty$ different: $\rho_{\pm\infty}(\mathbf{q}_n)$ correspond to ρ_{\pm} and $\frac{3}{2}\beta_{\pm}^{-1} = \langle p_i^2 \rangle$.

+∞
Fig.1: A hyperboloid-like container Ω.
Shape is symbolic (d=3)
Stationary regular BBGKY hierarchy (hard core)
-∞
$$\partial_t \rho(\mathbf{p}_n, \mathbf{q}_n; t) = \mathbf{0} = \sum_{i=1}^n \left(-p_i \cdot \partial_i \rho(\mathbf{p}_n, \mathbf{q}_n; t) + \int_{\sigma(q_i, \mathbf{q}'_n)} \omega \cdot (\pi - p_i) \rho(\mathbf{p}_n, \mathbf{q}_n, \pi, q_i + r\omega; t) d\sigma_\omega d\pi \right)$$

 $\stackrel{\text{def}}{=} BBGKY_n(\rho(t))$

 $\rho(\mathbf{q}_n, \mathbf{p}_n)$ diff.ble in $|q_i - q_j| > r$ with continuous derives in $|q_i - q_j| \ge r$. Has this anything to do with Physics???

• Equation holds (Cercignani) at t = 0 in finite volume, smooth initial

$$D_N(\mathbf{p}_N,\mathbf{q}_N) = D_N(\mathbf{p}'_N,\mathbf{q}_N)$$

pair collision continuity $((\mathbf{p}_N, \mathbf{q}_N)$ before) and $((\mathbf{p}'_N, \mathbf{q}_N)$ after). Marseille 7-2011 16



• BUT smoothness lost at t > 0 and singularities become dense with t although kept on a set of volume 1 in phase space, and continuity too.

• Nevertheless Lanford has shewn how to derive, by simple iteration,

$$\rho(\mathbf{p}_n, \mathbf{q}_n; t) = \rho(\mathbf{p}_n, \mathbf{q}_n; 0) + \int_0^t BBGKY_n(\rho(t')) dt'$$

the B.E. in the Grad limit and Spohn has proved iteration correct in spite of singularities acquired by correlations, densely on phase space

• Thus if a stationary state is studied the equation looks precarious "workig hypothesis".

Heuristic approach: look for solutions of the regular BBGKY equation

Boundary conditions:

(1) **Equilibrium at** $\pm \infty$ at given $T_+ > T_-$:

 $\rho_{\emptyset}(\mathbf{q}_n) \xrightarrow[\mathbf{q}_n \to \pm \infty]{}$ equilibrium with suitable activity z_{\pm}

The condition is **not** "Gibbs at infinity" but **only** Gibbsian positional correlations \Rightarrow more freedom but possible interpretation problems.

(2) Collision continuity: Inspired from original Maxwell's form of the Boltzmann's equation if suitable factorization of ρ is added 1866.

(2) Collision continuity: if $p_1, p_2 \Rightarrow p'_1, p'_2$ is a collision btwn q_1 and $q_1 + r\omega$ (with $\omega \cdot (p_2 - p_1) < 0$) in the direction ω then (strong form) of continuity (strong) is generally demanded (not Spohn).

$$\rho(\mathbf{q}_n, \mathbf{p}_n) = \rho(\mathbf{q}_n, \mathbf{p}'_n)$$

too strong. It admits a "weak form": for all 1-particle observ. Q(p)

$$\begin{split} &\sum_{\alpha=1}^{3} \partial_{\alpha} \int \rho(p,q) p_{\alpha} Q(p) d^{3}p = \\ &\cdot \int_{\omega \cdot (p-\pi) > 0} \lvert \omega(\pi-p) \rvert \, \cdot \, (Q(p') - Q(p)) \, \rho(p,q,\pi,q+r\omega) \, d^{3}p \, d^{3}\pi \, d\sigma_{\omega} \end{split}$$

and $\forall q \in \Omega$ if $p, \pi \Rightarrow p', \pi'$ after elastic scattering in the cone $d\omega$. If true $\forall Q$'s equivalent to collision continuity for pair correlations only.

Even this weak continuity might be too strong:

no continuity proof is available: (and it will not be available for long).

Problems

(1) at volume $< \infty$ and out of eq. correl. not even defined in SRB

(2) if the initial state has the property it keeps it forever (Spohn): however discontinuity might develop at $t = +\infty$

as they do in the other limit of Grad.

Questions:

(a) Are there exact solutions of the BBGKY?

(b) If yes which weak continuity conditon can be imposed?

Answer to (a) **yes**

Answer to (b) $\mathbf{Q}(\mathbf{p}) = \mathbf{1}, \frac{1}{2}\mathbf{p}^2$ and others, but **not** $\mathbf{Q}(\mathbf{p}) = \mathbf{p}$!!!

Exact solution:

$$\rho_{even}(\mathbf{q}_n, \mathbf{p}_n) = \rho_{\emptyset}(\mathbf{q}_n) \prod_{i=1}^n \varphi(q_i, p_i)$$
$$\varepsilon(q) \stackrel{def}{=} \frac{\beta(q)}{\beta_0} - 1, \ \varepsilon_0 \stackrel{def}{=} \frac{\beta_-}{\beta_+} - 1, \ \varphi(q, p) \stackrel{def}{=} \frac{\beta_0}{\beta(q)} \Big(G_{\beta_0}(p) + \varepsilon(q)\delta(p) \Big)$$

Boundary c. imposed at 1-th order in ε_0 (temperature difference) by

$$0 = \int_{\omega(p-\tilde{p})>0} Q(p)dpd\tilde{p}d\sigma_{\omega}$$
$$(\rho(q, p, q + r\omega, \tilde{p}) - \rho(q, p', q + r\omega, \tilde{p}'))\omega \cdot (p - \pi)$$

demanded for $Q(p) = p^2$ for elastic collisions

$$p' = p - \omega \cdot (p - \widetilde{p}) \omega, \qquad \widetilde{p}' = \widetilde{p} + \omega \cdot (p - \widetilde{p}) \omega$$

and only up to $O((z_0r^3)^{\ell/r}, \varepsilon_0^2)$ if $\ell = \text{distance of } q \text{ from } \mathbf{q}_n \text{ and } \partial\Omega$. Marseille 7-2011 21 A brief computation shews that this is equivalent to

$$0 = \int_{s(q)\cap\Omega} \rho_{eq}(q, q + r\omega) \left(\beta(q) - \beta(q + r\omega)\right) d\omega$$

At distance ℓ from $\partial\Omega$ the $\rho_{eq}(q, q + r\omega)$ is rotation and translation invariant (up to $O((z_0 r^3)^{\ell/r})$) by K.S. theory of the Mayer expansion.

Hence up to an exp. small error on microscopic scale, $O((z_0 r^3)^{\ell/r})$:

$$\int_{s(q)} (\beta(q+r\omega) - \beta(q)) \, d\omega = 0$$

True if $\beta(q)$ is harmonic (*i.e.* if Fourier Law holds).

Don't shoot at the pianist

Also Dirichlet b.c. on $\partial\Omega$ can be considered as well as other geometries can be considered. For instance conic geometry $\beta_{+\infty}$



A geometry with a long cylinder which opens up in two reservoirs



An essentially 1-dimensional geometry; temperature values at the top and the bottom (dictated by the b.c. at $\pm \infty$ via the heat equation) will be interpolated essentially linearly ("Saint-Venant's principle"), but $\delta T = O(H^{-1})$.

Very different for Dirichlet $(\beta(q) - \beta_0 = const$ on $\partial\Omega)$ and Neumann b.c. $(\partial_n \beta = 0 \text{ on } \partial\Omega)$

Consider both Neumann b.c. $(\partial_n \beta = 0 \text{ on } \partial\Omega)$ and Dirichlet $(\beta(q) - \beta_0 = const \text{ on } \partial\Omega)$



The transients at the extremes decay exponentially on scale ξ of the cylinder diameter.

References

Bonetto, Lebowitz, Rey-Bellet, In Mathematical Physics 2000, Garrido, Gallavotti: J. Stat. Phys., 126, 1201-1207, 2007

Some Details

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

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

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

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

Why not "same" for thermostatted dynamics ?

$$u_k^n(t) \le C n^\eta \int_0^\Theta u_{k_1}^n(\tau) d\tau + C 2^{-nd} \qquad k_1 = k + C \sqrt{n}$$

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

Up to Stopping time properties

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

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

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 $2^{k_\ell} = 2^k + \ell C (k \log n)^{\gamma}$ Marseille 7-2011 27 Compare $x^{(n,1)}(t)$ and $x^{(n,0)}(t)$ ℓ times $2^{k_\ell}=2^k+\ell\,C\,(k\log n)^\gamma$ with $\ell\sim 2^n/(\log n)^\gamma$

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

This time the Lyapunov exponent is small

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