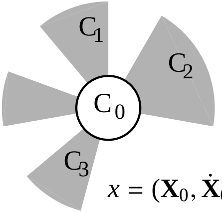
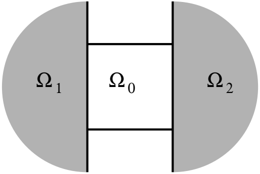
Thermostats and thermodynamic limit

by Errico Presutti, GG

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:

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

Equations of motion (thermostat force if $a = 1$)

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

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

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

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

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

If no phase transitions $\Rightarrow$ 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 of evolution in finite volume

Regularize in a ball Λ_n (side $2^n r_\varphi$)

i.e. enclose the system in a ball $\Omega \cap \mathcal{B}(R)$ of radius R

$\Rightarrow$ 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 $\forall t, j > 0$

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

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 (constructive, 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)

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

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

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

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Theorem: $\exists C(\mathcal{E}), c(\mathcal{E})^{-1} \uparrow \mathcal{E}$ *and if* $q_i(0) \in \Lambda_k$ $(v_1 = \sqrt{\frac{2\varphi(0)}{m}})$

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

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

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

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

$\forall\, n > k$. *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); OK?

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

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. $\Lambda_n \to \infty$)

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

But is $T_{j,n}(x) \geq c > 0$ **??** *not* $\forall x$*!*

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

(a) $\frac{\mathbf{K_{j,\Lambda_n}(x)}}{|\mathbf{\Lambda_n \cap \Omega_j}|} \geq \frac{1}{4}\, d\, \delta_j\, k_B T_j$ *(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

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

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 μ_0 "clusters"

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 $\gamma\in(\frac12,1)$ of $(\log_+(|\xi|/r_\varphi))^{\frac12}\cdot(\log n)^\gamma$

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(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,

$\varepsilon^2_{C_\xi} \stackrel{def}{=} \max_{q\in C_\xi}(\frac{1}{2}\dot{q}^2 + \psi(q))/\varphi_0.$ kinetic + wall energy

1) 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 $\mathcal{B} \stackrel{def}{=} \{x \,|\, x \in \mathcal{X}_E$ and $T_n(x) \le \Theta\}$ is

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

Via large deviations estimates $\Rightarrow$

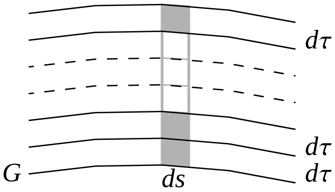
estimate the probability of $\mathcal{X}_n \stackrel{def}{=} \{\mathcal{E}(x) \le E;\ T_n(x) < \Theta\}$.

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

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



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.

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BBGKY hierarchy, Fourier's equation

(in progress)

by Guido Gentile, Alessandro Giuliani, GG

Key result in equilibrium has been virial expansion convergence → complete very detailed equilibrium rarefied gases at high temperature in Gibbs states.

It is highly desirable to achieve a similar understanding in systems in stationary states out of equilibrium.

Difficulty: 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: need infinite

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

Joel (1959): We try to find Γ-space ensembles that will represent systems not in equilibrium in the same way that microcanonical, canonical, g.c. ensembles represent systems in equilibrium ... And there is of course no *priori* assurance that such a parallel can be made

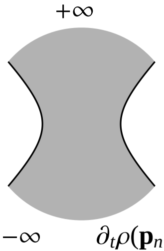


Fig.1: *A hyperboloid-like container* Ω. *Shape is symbolic (d=3)*

Stationary regular BBGKY hierarchy (hard core):

$$\partial_t \rho(\mathbf{p}_n, \mathbf{q}_n) = 0 = \sum_{i=1}^{n} \Big(-p_i \cdot \partial_i \rho(\mathbf{p}_n, \mathbf{q}_n) + \int_{\sigma(q_i, \mathbf{q}'_n)} \omega \cdot (\pi - p_i)\, \rho(\mathbf{p}_n, \mathbf{q}_n, \pi, q_i + r\omega) d\sigma_\omega \, d\pi \Big)$$

$\rho(\mathbf{q}_n, \mathbf{p}_n)$ differentiable in $|q_i - q_j| > r$ with continuous derivs in $|q_i - q_j| \geq r$.

Representation (reference state activity=z_0, temperature $=\beta_0^{-1}$):

$$G_{\mathbf{q}_n}(\mathbf{p}_n) \stackrel{def}{=} \frac{e^{-\frac{1}{2}\beta(\mathbf{q}_n)\mathbf{p}_n\cdot\mathbf{p}_n}}{\sqrt{(2\pi)^{nd}\det\beta(\mathbf{q}_n)^{-1}}}, \qquad : x^k : \stackrel{def}{=} (2C)^{k/2} H_k\left(\frac{x}{\sqrt{2C}}\right)$$

Look for BBGKY solution expanded in Wick (Hermite) monomials:

$$\rho(\mathbf{p}_n, \mathbf{q}_n) = G_{\mathbf{q}_n}(\mathbf{p}_n) \sum_A \rho_A(\mathbf{q}_n) \; : {\mathbf{p}_n}^A :$$

$$: \mathbf{p}_n^A : \stackrel{def}{=} : \prod_{k=1}^{n} \prod_{\alpha=1}^{d} (\overline{p}_{k\,\alpha})^{a_\alpha^k} :, \qquad \overline{p}_k \stackrel{def}{=} -\sqrt{\beta(q_k)}p_k$$

Regular BBGKY $\Rightarrow$ hierarchy in the coefficients $\rho_A(\mathbf{q}_n)$.

Result 0: *For each $\rho_A(\mathbf{q}_n)$ the hierarchy involves $\rho_{A'}(\mathbf{q}_m)$ with $m = n + 1, |A'| = |A|$ or $\rho_{A'}(\mathbf{q}_n)$ with $|A'| = |A|, |A| + 2, |A| + 4$.*

Cancellation: $|A| + 6$ is missing

Up to boundary conditions: Even A and odd A are independent

BBGKY: Red = terms expected to yield all contributions of $O(\varepsilon_0)$:

$$\#1 \quad \sum_{i\alpha} \Big\{ \Big[\partial_{i\alpha} \rho_{B^{-1}_{i\alpha}} + \beta(q_i)^{-1} (b^i_\alpha + 1) \partial_{i\alpha} \rho_{B^{+1}_{i\alpha}} \Big]$$

$$\#2 \quad - \frac{1}{2} \partial_{i\alpha} \beta(q_i) \sum_{\alpha'} \Big[\rho_{(B^{-2}_{i\alpha'})^{-1}_{i\alpha}} (\mathbf{q}_n)$$

$$\#3 \quad + \beta(q_i)^{-1} \Big(2 \rho_{B^{-1}_{i\alpha'}} (\mathbf{q}_n) \delta_{\alpha\alpha'}$$

$$\#4 \quad + (b^i_\alpha + 1 - 2\delta_{\alpha\alpha'}) \rho_{(B^{-2}_{i\alpha'})^{+1}_{i\alpha}} (\mathbf{q}_n)$$

$$\#5 \quad + 2(b^i_{\alpha'} - \delta_{\alpha\alpha'}) \rho_{(B^{-1}_{i\alpha}{}^{-1}_{i\alpha'})^{+1}_{i\alpha'}} (\mathbf{q}_n) \Big)$$

$$\#6 \quad + \beta(q_i)^{-2} \Big(2\delta_{\alpha\alpha'} (b^i_{\alpha'} + 1) \rho_{B^{+1}_{i\alpha'}} (\mathbf{q}_n)$$

$$\#7 \quad + 2(b^i_\alpha + 1)\, b^i_{\alpha'} \rho_{(B^{-1}_{i\alpha'})^{+1+1}_{i\alpha i\alpha'}} (\mathbf{q}_n) \Big) \Big]$$

$$\#8 + \int_{s(q_i;\mathbf{q}_n)} \omega_\alpha \Big[-\beta(q_i + r\omega)^{-1} \rho_{(BA')^{+1}_{(n+1)\,\alpha}} (\mathbf{q}_n, q_i + r\omega)$$

$$+ \rho_{(BA')^{-1}_{i\alpha}} (\mathbf{q}_n, q_i + r\omega)$$

$$+ \beta(q_i)^{-1} (b^i_\alpha + 1) \rho_{(BA')^{+1}_{i\alpha}} (\mathbf{q}_n, q_i + r\omega) \Big]\, d\sigma_\omega \Big\} \Big] = 0$$

Ansatz: $\overline{p}_k \stackrel{def}{=} -\sqrt{\beta(q_i)}p_k$: then $\rho_A(\mathbf{q}_n) = 0$ if $|A| = 1, 2$ and

$$\Big(\rho_\emptyset(\mathbf{q}_n) + \sum_{a^1,\ldots,a^n} \rho_{a^1,\ldots,a^n}(\mathbf{q}_n) \prod_{i=1}^n \frac{:(\overline{p}_i^2)^{a^i}:}{(2a^i)!!}$$

$$+ \sum_{i,\alpha} \sum_{a^1,\ldots,a^n} \rho_{i,\alpha;a^1,\ldots,a^n}(\mathbf{q}_n)\partial_{\overline{p}_{i\alpha}} \prod_{i=1}^n \frac{:(\overline{p}_i^2)^{a^i}:}{(2a^i)!!}\Big)$$

i.e.

Even correlations functions of the $\prod_i (p_i^2)^{a^i}$ only.
Odd correlations functions of first derivatives $\partial_{p_{j\alpha}} \prod_i (p_i^2)^{a^i}$ only.

Key remark: the equation for $\rho_\emptyset(\mathbf{q}_n)$ is, simply,

$$-\partial_{i\alpha}\rho_\emptyset(\mathbf{q}_n) + \frac{\partial_{i\alpha}\beta(q_i)}{\beta(q_i)}\rho_\emptyset(\mathbf{q}_n) - \int_{\sigma(q_i,\mathbf{q}'_n)} \omega_\alpha d\sigma_\omega\, \rho_\emptyset(\mathbf{q}_n q_i + r\omega) = 0$$

Eq. admits exact solution, close to the reference state z_0, β_0^{-1}: the equilibrium correlations of a hard spheres gas with activity $z(q) \stackrel{def}{=} z_0\, \frac{\beta(q)}{\beta_0}$

Even correlations: exact by recurrence, $\varepsilon(q) \stackrel{def}{=} \frac{\beta(q)}{\beta_0} - 1, \varepsilon_0 \stackrel{def}{=} \frac{\beta_-}{\beta_+} - 1,$

$$\rho_{even}(\mathbf{q}_n, \mathbf{p}_n) = \rho_\emptyset(\mathbf{q}_n) \prod_{i=1}^{n} \varphi(q_i, p_i) + \rho^{hom}(\mathbf{q}_n, \mathbf{p}_n) \quad \text{with}$$

$$\varphi(q,p) \stackrel{def}{=} G_{\beta(q)}(p) \frac{\beta_0}{\beta(q)} \Big(\sum_{k=0}^{\infty} \frac{(\varepsilon(q)^k + \varepsilon(q)\,(-1)^k)}{(2k)!!} : (\beta(q)p^2)^k : \Big)$$

$$\rho^{hom}(\mathbf{q}_n, \mathbf{p}_n) = z_0^n G_1(\overline{\mathbf{p}}_n) \sum_{i=1}^{n} \Big(\prod_{j \neq i} \widetilde{K}(\overline{p}_j) \Big) \varepsilon(q_i) \sum_{a=0}^{\infty} \frac{(-1)^a \ : (\overline{p}_i^2)^a :}{(2k)!!}$$

Odd correlations: exact

$$\rho_{odd}(\mathbf{q}_n, \mathbf{p}_n) G_1(\overline{\mathbf{p}}_n^{(i)}) = z_0^n \delta_{n>1} \sum_{i=1}^{n} G_1(\overline{\mathbf{p}}_n)$$

$$\cdot \Big(r\, \partial_i F(q_i) \cdot \partial_{\overline{p}_i} \sum_{k=0}^{\infty} \frac{(-1)^k : \overline{p}_i^{2k} :}{(2k)!!} \Big) \prod_{j \neq i} K(\overline{p}_j)$$

where $K(p) \stackrel{def}{=} \sum_{a=1}^{\infty} C(a) : \overline{p}^{2a} :$ & $\widetilde{K}(p) \stackrel{def}{=} \sum_{a=2}^{\infty} \widetilde{C}(a) : \overline{p}^{2a}$:with the $C(a)$'s arbitrary AND

$$-\Delta F(q) + \frac{1}{2}\frac{\partial\beta(q)\cdot\partial F(q)}{\beta(q)} = 0, \quad \text{in } \Omega,$$
$$\partial_n F(q) = 0, \quad \text{in } \partial\Omega$$

So far no approximation. But $\beta(q)$ arbitrary!

Given $\beta_\pm$ ($\beta_0 = \beta_+ < \beta_- \equiv \beta_0(1+\varepsilon_0)$): which B.C.?

Boundary conditions:

(1) **Equilibrium at** $\pm\infty$:

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

(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)

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

e.g. "weak form" for all 1-particle momentum observ. $Q(p)$ and $q \in \Omega$ this is

$$\sum_{\alpha=1}^{3} \partial_\alpha \int \rho(p,q) p_\alpha Q(p) d^3p =$$

$$\cdot \int_{\omega\cdot(p-\pi)>0} |\omega(\pi - p)| \cdot (Q(p') - Q(p))\, \rho(p,q,\pi,q+r\omega)\, d^3p\, d^3\pi\, d\sigma_\omega$$

if $p, \pi \Rightarrow p', \pi'$ after elastic scattering in the cone $d\omega$

Key question: is request correct? (warning: we get it only partially)

Continuity (strong) is generally demanded (Cercignani, Lanford) in the context of Boltzmann-Grad limit (not always, see Spohn).

But no proof available:

(1) at finite volume and out of equilibrium correlations not even defined in SRB states

(2) if the initial state has the property (not easy to impose) it keeps it forever (Spohn): however discontinuity might develop at $t = +\infty$

Boundary cond. imposed on the exact solutions at first order in ε_0 (temperature difference) by requiring it only on "isolated" collisions: *i.e.*

$$0 = \int_{\omega(p-\widetilde{p})>0} Q(p) dp d\widetilde{p} d\sigma_\omega$$

$$(\rho(x_n, q, p, q + r\omega, \widetilde{p}) - \rho(\mathbf{x}_n, q, p', q + r\omega, \widetilde{p}'))\omega \cdot (p - \pi)$$

(where $x_n = (\mathbf{p}_n, \mathbf{q}_n)$) demanded (up to $O(\varepsilon_0^2, \frac{r}{L},))$ for

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

and only up to $O((z_0 r^3)^{\ell/r}, \varepsilon_0^2)$ if ℓ = distance of $q,\ q + r\omega$ from $\mathbf{q}_n$ and $\partial\Omega$.

Begin with $\rho(q, p, q', p')$: then ℓ = distance to $\partial\Omega$. Let $Q(p) = p^2$ and require

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

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 Kirkwood-Salsburg theory of the Mayer expansion.

True if $\beta(q)$ is harmonic (Fourier).

BUT there are infinitely many other conditions ($\forall x_n$):
"all even" $Q(p) = p_x^{2s_x} p_y^{2s_y} p_z^{2s_z}$ with $s_x + s_y + s_z > 2$ &
"all odd" $p_\alpha p_x^{2s_x} p_y^{2s_y} p_z^{2s_z}$ $s_x + s_y + s_z > 1$: remarkably the free constants $C(a)$ are determined by the condition and for all **s**.

Let $\overline{I}_s \overset{def}{=} \frac{(2s+3)!!}{3(s+3)2^s s!}$ and $\overline{C}(k) \overset{def}{=} \frac{(-1)^k}{\sqrt{2\pi}} k! 2^k C(k)$ then to lowest order in z_0 (for simplicity):

$$\overline{I}_s = \sum_{k=1}^{\infty} \overline{\gamma}_{s,k} \overline{C}(k), \quad \overline{\gamma}_{s,k} \overset{def}{=} \binom{k - (s + \frac{3}{2})}{-(s + \frac{3}{2})}$$

is the condition for all odd $Q(p)$ coupled with

$$\frac{\beta(q)}{\beta_0} - 1 = F(q)$$

which is also compatible to $O(\varepsilon_0^2)$ with the condition of F.

Still there are infinitely many other conditions: however the even and odd correlations have cluster properties (from KS):

$$\rho_{even}(\mathbf{q}_n, \mathbf{p}_n) = \rho_{\emptyset}(\mathbf{q}_n) \prod_{i=1}^{n} \varphi(q_i, p_i) + \rho^{hom}(\mathbf{q}_n, \mathbf{p}_n)$$

$$\rho_{odd}(\mathbf{q}_n, \mathbf{p}_n) G_1(\overline{\mathbf{p}}_n^{(i)}) = z_0^n \delta_{n>1} \sum_{i=1}^{n} G_1(\overline{\mathbf{p}}_n)$$

$$\cdot \Big(r\, \partial_i F(q_i) \cdot \partial_{\overline{p}_i} \sum_{k=0}^{\infty} \frac{(-1)^k : \overline{p}_i^{2k} :}{(2k)!!} \Big) \prod_{j \neq i} K(\overline{p}_j)$$

this allows to reduce the case to the pair correlations continuity if the colliding pair is far enough from the remaining $\mathbf{q}_n$.

In other words the problem is reduced to two infinite linear systems like

$$\overline{I}_s = \sum_{k=1}^{\infty} \overline{\gamma}_{s,k} \overline{C}(k), \quad \overline{\gamma}_{s,k} \stackrel{def}{=} \binom{k - (s + \frac{3}{2})}{-(s + \frac{3}{2})}, \quad s, k = 1, \ldots,$$

The latter linear system is soluble.

Also: the equation is of Toeplitz type and its coefficients are integer fractions therefore if the linear system is truncated to a $N \times N$ system it can be studied with arithmetic precision up to exhaustion of computer power.

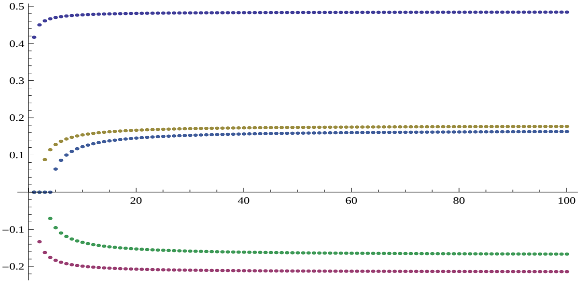


Fig.2: *The value of the first five coefficients* $\overline{C}(k)$, $k = 1, \ldots, 5$ *as functions of the truncation of the matrix* γ*: they decrease in absolute value and alternate in sign: a trend that persists for all the truncations sizes* N *and all the* $C(k)$*'s that have been checked, exactly, up to* $N = 100$*. The small discontinuities are due to the plotter reaction to a* 4 *decimals expression of the exact results (which requires hundreds of digits in their rational expressions, for* N *large).*

Let $\mathcal{Q}$ be the observables polynomial in p and let $\frac{r}{L} < \varepsilon_0^2$.

Result: There are solutions up to $O(\varepsilon_0^2)$ which satisfy the boundary conditions up to $O(\varepsilon_0^2, (z_0 r^3)^{\ell/r})$ $\forall Q \in \mathcal{Q}$ and

$$\Delta T(q) = 0 \quad \text{in } \Omega, \qquad \partial_n T(q) = 0 \quad \text{in } \partial\Omega$$

$T(\pm\infty) = T_{\pm\infty}$.

Question: is collision continuity to be requested?

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

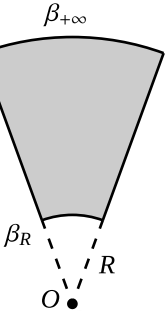


Fig.2: *Ω is a cone with vertex at O truncated at a distance R from its vertex; $T(q) = T_0 + \tau(q)$ solves $\Delta T = 0$ with $\partial_n T = 0$ on $\partial\Omega$ and value τ_- at bottom of Ω and $\tau_+ = 0$ at ∞: i.e. $\tau_- = \frac{\delta}{R}$, $\tau_+ = 0$*

special case

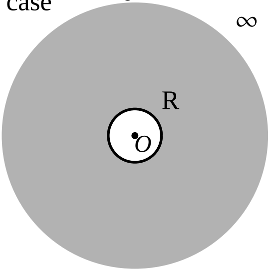


Fig.3: *A special case of Fig.2 the "exterior problem", i.e. the heat conduction outside a ball: a "hot potato" problem. It has an exact solution $T(q)$.*

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

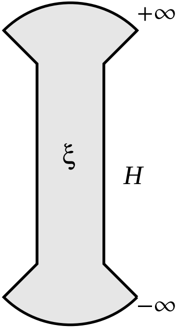


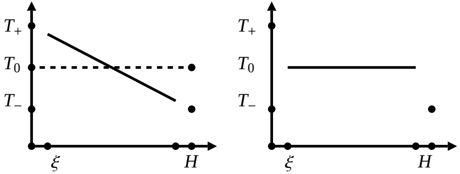
Fig. 4
The container Ω is a cylinder of diameter ξ and height $Hgg\xi \gg r$ continued into two cones extending to ∞.

The interpolating inverse temperature $\beta(q)$ will be close to β_+ at the upper end of the cylinder and close to β_- at the bottom.

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. ($\partial_n \beta = 0$ on $\partial\Omega$)

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



respectively.

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

Summary

(0) Investigation of Formal series solutions (in powers of momentum)

(1) Exact solutions of the hierarchy without B.C. (no closure approx.)

(2) Boundary conditions of "continuity at collisions" are imposed to determine uniquely the free constants: this is done up $O(\varepsilon_0^2, \varepsilon_0 \frac{r}{L}, (z_0 r^3)^{\ell/r})$

$$\varepsilon_0 \stackrel{def}{=} \frac{\beta_-}{\beta_+} - 1, \qquad L \stackrel{def}{=} \text{container width}, \qquad z_0 r^3 \stackrel{def}{=} \text{Boltzmann-Grad const}$$

Solution: $\rho(\mathbf{q}_n, \mathbf{p}_n) = \rho_e(\mathbf{q}_n, \mathbf{p}_n) + \rho^{hom}(\mathbf{P}_n, \mathbf{q}_n) + \rho_{odd}(\mathbf{q}_n, \mathbf{p}_n)$

$$\rho_e(\mathbf{q}_n, \mathbf{p}_n) = G_1(\overline{p}_n)\rho_\emptyset(\mathbf{q}_n) \prod_{i=1}^{n} \frac{\beta_0}{\beta(q_i)} \Big(\sum_{k=0}^{\infty} \frac{(-1)^k \Big(\varepsilon(q_i)^k + \varepsilon(q_i)\Big)}{(2k)!!} : (\overline{p}_i^2)^k : \Big)$$

$$\rho^{hom}(\mathbf{q}_n, \mathbf{p}_n) = z_0^n G_1(\overline{\mathbf{p}}_n) \sum_{i=1}^{n} \Big(\prod_{j \neq i} \widetilde{K}(\overline{p}_j) \Big) \varepsilon(q_i) \sum_{a=0}^{\infty} \frac{(-1)^a \; : (\overline{p}_i^2)^a :}{(2k)!!}$$

$$\rho_{odd}(\mathbf{q}_n, \mathbf{p}_n) = z_0^n \delta_{n>1} G_1(\overline{\mathbf{p}}_n) \sum_{i=1}^{n} \Big[\prod_{j \neq i} K(\overline{p}_j) \Big] r \partial_{q_i} F(q_i) \partial_{\overline{p}_i} \sum_{k=1}^{\infty} \frac{(-1)^k}{(2k)!!} : (\overline{p}_i^2)^k :$$

$$K(p) \stackrel{def}{=} \sum_{a=1}^{\infty} C(a) : \overline{p}^{2a} :, \qquad \widetilde{K}(p) \stackrel{def}{=} \sum_{a=2}^{\infty} \widetilde{C}(a) : \overline{p}^{2a} :$$

Critiques (somewhat negative)

(1) even correlations (exact solutions) can be exactly summed

$$\rho_{even}(\mathbf{q}_n,\mathbf{p}_n) = \rho_\emptyset(\mathbf{q}_n)\prod_{i=1}^n\Big(\frac{\beta_0}{\beta(q_i)}\frac{e^{-\frac12\beta_0 p_i^2}}{(2\pi\beta_0^{-1})^{3/2}} - (\frac{\beta_0}{\beta(q_i)}-1)\delta(\overline{p}_i)\Big)$$
$$+ z_0^n\sum_{i=1}^n \varepsilon(q_i)\delta(\overline{p}_i)\prod_{j\neq i}\widetilde{K}(\overline{p}_j)G(\overline{p}_j)$$
$$\rho_{odd}(\mathbf{q}_n,\mathbf{p}_n) = z_0^n\delta_{n>1}\sum_{i=1}^n\Big[\prod_{j\neq i}K(\overline{p}_j)G_1(\overline{p}_j)\Big]r\partial_{q_i}F(q_i)\partial_{\overline{p}_i}\delta(\overline{p}_j)$$

Nevertheless $\langle\,\frac12 p^2\,\rangle = \frac32\beta(q)^{-1}$.

(2) The odd correlations can also be resummed and lead to terms proportional to delta function derivatives: not positive?

(3) Also $\rho_{odd}(q,p)\equiv 0$.

Possibly the above phenomena are due to the lowest order in $T_+ - T_-$ studied and to a nonuniform convergence of the series considered.

Solution is *only a first order* approximation constructed by series whose convergence is not discussed.

Deltas arise from exact formula for "Wick's Gaussians" for $\lambda < 1$:

$$G_\beta(p) \sum_{k=0}^{\infty} \frac{(-\beta)^k}{(2k)!!} : p^{2k} : \stackrel{def}{=} G_\beta(p) \; : e^{-\frac{1}{2}\beta\lambda p^2} := G_\mu(p), \qquad \mu = \frac{\beta}{1-\lambda}$$

This is used to keep order by order track of $\varepsilon(q)\, G_\beta(p)\, \frac{-\beta(q)^{2k}}{k!} : p^{2k} :$ which, summed over k, yield formally delta.

Hence the meaning that so far can be attributed to the solutions is that of allowing computation of expectation of polynomials in the momenta.

The resulting quantities should be asymptotic to the exact values as $\varepsilon_0 \to 0$ and $\frac{\log \varepsilon_0^2}{\log(z_0 r^3)} \to 0$. The errors however will depend on the particular observables and will not be uniform for all observables.

(a) The analysis cannot be applied to dimension $1, 2$ because the heat equation has no solution asymptotically equal to $\beta_{\pm}$

(c) Looking for higher order corrections a diagonal ansatz on $\beta(q)$ should be (likely) abandoned and a non diagonal quadratic form should be considered.

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Continuity? It is not clear why the correlation functions of a stationary state shoud be continuous at collisions, *e.g.* why

$$\rho(q_1, p_1, q_1 + r\omega, p_2) = \rho(q_1, p_1', q_1 + r\omega, p_2')$$

if $p_1, p_2 \longleftrightarrow p_1', p_2'$ is a collision at q_1 and $q_1 + r\omega$.
True: conserved by dynamics; but no contradiction with initial states in which does not hold. And even if holding at any finite time might fail to hold in the stationary state. Scenario:

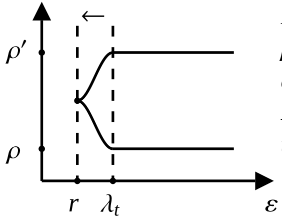


Fig.6: a pair correlations $\rho(\varepsilon)$, $\rho'(\varepsilon)$ discontinuity developing at t large: $\lambda_t \xrightarrow[t\to\infty]{} r$. For $t = +\infty$ $\lambda_t = r$ and discontinuity is sharp.

Which should be appropriate collision b.c. is therefore open: is continuity a required property? are the multiple collisions relevant (notice that they occurr in the hierarchy).

Odd Hierarchy: For $B=(A_1,\dots,A_n)$ it is

$C_n(A)z_0^n(\prod_{i=1}^n \frac{(-\beta_i)^{a^i}}{(2\mathbf{a}^i)!!})(\prod_{i=2}^n \widetilde{F}(q_i))$ times

$$1\#\beta_1^{-\frac{1}{2}}\Big\{\lambda(A,\alpha)\Big[\partial_\alpha^2\widetilde{F}_{2a^1}+(a^1-\frac{1}{2})\cdot\partial_{1\alpha}\widetilde{F}_{2a^1}\frac{\partial_\alpha\beta_1}{\beta_1}\Big]$$

$$\#-\lambda(A_\alpha^{+2},\alpha)\frac{2a_\alpha+1}{2(a_\alpha+1)}\Big[\partial_\alpha^2\widetilde{F}_{2(a^1+1)}+(a^1+\frac{1}{2})\,\partial_\alpha\widetilde{F}_{2(a^1+1)}\frac{\partial_\alpha\beta_1}{\beta_1}\Big]$$

$$23\#+\frac{\partial_\alpha\beta_1}{\beta_1}\Big[\sum_{\alpha'}\lambda(A_{\alpha'}^{-2},\alpha)\,a_{\alpha'}\partial_\alpha\widetilde{F}_{2(a^1-1)}+\partial_\alpha\widetilde{F}_{2a^1}\Big(-\lambda(A,\alpha)$$

$$4\#-\sum_{\alpha'}\lambda(A^{+2}_{\alpha}{}^{-2}_{\alpha'},\alpha)(a_\alpha+\frac{1}{2}-\delta_{\alpha\alpha'})\frac{2(a_{\alpha'}+\delta_{\alpha\alpha'})}{2(a_\alpha+1)}$$

$$5\#-\sum_{\alpha'}\lambda(A,\alpha)(2a^1_{\alpha'}-\delta_{\alpha\alpha'})\Big)$$

$$67\#+\partial_\alpha\widetilde{F}_{2(a^1+1),2a^2}\lambda(A_\alpha^{+2},\alpha)\cdot(1+2a^1)\Big]\Big\}\frac{2a_\alpha+1}{2(a_\alpha+1)}\Big\}$$

$$+C_{n+1}(A')I_{1\alpha}+\ldots=0$$

$I_{1,\alpha}$ is $(\prod_{i=1}^n \frac{(-\beta_i)^{a^i}}{(2\mathbf{a}^i)!})(\prod_{i=1}^n \widetilde{F}(q_i))$ times

$$-\, z_0^{n+1} \int_{s(q_i;\mathbf{q}_n)} d\sigma_\omega\, \omega_\alpha\, \beta_{n+1}^{-\frac{1}{2}}\, \partial_{q_{n+1,\alpha}} \widetilde{F}(\mathbf{q}_n, q_1 + r\omega)$$

with $\beta_{n+1} = \beta(q_{n+1})$, $q_{n+1} \equiv q_1 + r\omega$, $A' = \emptyset$ and the proportionality constant is i, α-independent. Other equations: by symmetry over the selection of the particles positions.

cancellations?

Odd hierarchy: For $B = (A^{+\,+1}_{\eta\,\eta'}, A_2, \ldots, A_n)$ it is

$C_n(A) z_0^n \beta_1^{-\frac{1}{2}} \prod_i \frac{(-\beta_i)^{a^i+\delta_{1i}}}{(2\mathbf{a}^i)!!} \frac{\prod_{i=2}^n \widetilde{F}(q_i)}{2(a_{\eta'}+1)2(a_\eta+1)}$ times

$$
\begin{aligned}
1\#\ &\Big\{\lambda(A^{+2}_{\eta'}, \eta')2(a_\eta + 1)\partial_{\eta\eta'}\widetilde{F}_{2(a^1+1)} - \lambda(A^{+2\,+2}_{\eta\ \ \eta'}, \eta')2(a_\eta + 1)\partial_{\eta\eta'}\widetilde{F}_{2(a^1+2)} \\
&\quad + \frac{\partial_\eta \beta}{\beta}\Big(\lambda(A^{+2}_{\eta'}, \eta')(a^1 + \frac{1}{2})\, 2(a_\eta + 1)\partial_{\eta'}\widetilde{F}_{2(a^1+1)} \\
&\quad - \lambda(A^{+2\,+2}_{\eta\ \ \eta'}, \eta')(a^1 + \frac{3}{2})2(a_\eta + 1)\partial_{\eta'}\widetilde{F}_{2(a^1+2)} \\
2\#\ &+ \frac{1}{2}\sum_{\alpha'} \lambda(A^{-2\,+2}_{\alpha'\ \ \eta'}, \eta')2(a_\eta + 1)2(a_{\alpha'} + \delta_{\alpha'\eta'})\partial_{\eta'}\widetilde{F}_{2a} \\
345\#\ &+ \partial_{\eta'}\widetilde{F}_{2(a+1)}\Big[- \lambda(A^{+2}_{\eta'}, \eta')2(a_\eta + 1) \\
&\quad - \frac{1}{2}\sum_{\alpha'} \lambda(A^{+2\,+2\,-2}_{\eta\ \ \eta'\ \ \alpha'}, \eta')(2a_\eta + 2 - 2\delta_{a'\eta}) \cdot (2a_{\alpha'} + 2\delta_{\alpha'\eta} + 2\delta_{\alpha'\eta'}) \\
&\quad - \lambda(A^{+2}_{\eta'}, \eta')2(a_\eta + 1)\sum_{\alpha'}(2a_{\alpha'} + \delta_{\alpha'\eta'})\Big]
\end{aligned}
$$

$$7\# + \Big[\lambda(A^{+2}_{\eta}{}^{+2}_{\eta'}, \eta')2(a_\eta + 1)\sum_{\alpha'}(2a_{\alpha'} + \delta_{\alpha'\eta} + \delta_{\alpha'\eta'})$$

$$6\# + \lambda(A^{+2}_{\eta}{}^{+2}_{\eta'}, \eta')2(a_\eta + 1)\Big]\partial_{\eta'}\widetilde{F}_{2(a+2)}\Big)\Big\} + (\eta\longleftrightarrow\eta')$$

which must be 0 after adding similar term with $(\eta\longleftrightarrow\eta')$.

For $B = (A_1{}^{+1}_{\eta}, A_2{}^{+1}_{\eta'}, \ldots, A_n)$ it is

$C_n(A_2)z_0^n\beta_2^{\frac{1}{2}} \prod_i \frac{(-\beta_i)^{a^i}}{(2\mathbf{a}^i)!!} \frac{1}{2(a^2_{\eta'}+1)2(a^1_\eta+1)}(\prod_{i>2}^n \widetilde{F}(q_i))$ times an analogous sum

Cancellation

Why do the integrals $\sum_{i,\alpha} I_{i,\alpha}$ vanish?

Realize that sum over i *is an integration over a closed surface* with ω as normal. Then

$$\sum_{\alpha} \int_{\partial} \omega_\alpha \partial_\alpha \beta(q_1 + r\omega)^{-\frac{1}{2}} \partial_\alpha \widetilde{F}(q_{n+1}) d\sigma_\omega$$

$$= \int_{D(\mathbf{q}_n)} \beta(q)^{-\frac{1}{2}} \left(\Delta \widetilde{F}(q) - \frac{1}{2} \frac{\partial \beta(q) \cdot \partial \widetilde{F}(q)}{\beta(q)} \right) dq$$

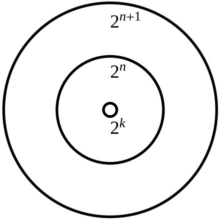
by Green's formula; here Neumann's or Dirichlet b.c. on $\partial\Omega$ is relevant if ∂ contains a part on $\partial\Omega$.

Hence the problem is purely algebraic.

Some Details

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

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



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 ($\eta = \frac{3}{2} + \frac{3}{\alpha}$) $\Rightarrow$

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

#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 $Ce^{Cn^\eta\Theta}\, 2^{-nd} \to \infty$

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 $\ell \sim 2^n/(\log n)^\gamma$

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

This time the Lyapunov exponent is small

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