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Decay of entropy and the Kac master equation

Part I

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KAC MASTER EQUATION

Simple **model describing collisions of** N **monoatomic gas particles**

Spatially homogeneous situation

Mean field description

Particles moving in one dimension

Energy should be conserved but not momentum

The state of the system at time t **is specified by a probability distribution** $F(v_1, \ldots, v_N, t)$

$$\vec{v} = (v_1, \ldots, v_N)$$

Probabilistic model for N colliding particles (Kac 1956)

(i) Randomly and pick a pair (i, j) of distinct indices in $\{1, \dots, N\}$ uniformly among all pairs. The particles with label i and j will collide.

(ii) Randomly pick a 'scattering angle' with probability $\rho(\theta)d\theta, -\pi \leq \theta \leq \pi$.

(iii) Update the velocities by a rotation, i.e.,

$$(v_i, v_j) \to (v_i^*(\theta), v_j^*(\theta)) := (\sin(\theta)v_i + \cos(\theta)v_j, \cos(\theta)v_i - \sin(\theta)v_j)$$

Energy is conserved.

$$\vec{v}^2 = \sum_{i=1}^{N} v_i^2 = E \ , \ \vec{v} = (v_1, \ldots, v_N)$$

Expectation values:

$$\Phi : \mathbb{S}^{N-1}(\sqrt{E}) \to \mathbb{R}$$

$$Q_N \Phi(\vec{v}) = \mathbb{E}\{\Phi(\vec{v}_{j+1}) | \vec{v}_j = \vec{v}\}$$

$$Q_N = \binom{N}{2}^{-1} \sum_{i<j} R_{i,j}$$

$$R_{i,j}\Phi := \int_{-\pi}^{\pi} \rho(\theta) \Phi(v_1, \cdots, v_i^*(\theta), \cdots, v_j^*(\theta), \cdots, v_N) \mathrm{d}\theta$$

Markov transition operator

Φ arbitrary real test function on $\mathbb{S}^{N-1}(\sqrt{E})$

$$\int_{\mathbb{S}^{N-1}(\sqrt{E})} \Phi(\vec{v}) F_1(\vec{v}) d\sigma^N(\vec{v}) = \int_{\mathbb{S}^{N-1}(\sqrt{E})} \mathbb{E}\{\Phi(\vec{v}_1) | \vec{v}_0 = \vec{v}\} F_0(\vec{v}) d\sigma^N(\vec{v})$$

$$= \int_{\mathbb{S}^{N-1}(\sqrt{E})} Q_N \Phi(\vec{v}) F_0(\vec{v}) d\sigma^N(\vec{v}) = \int_{\mathbb{S}^{N-1}(\sqrt{E})} \Phi(\vec{v}) Q_N^* F_0(\vec{v}) d\sigma^N(\vec{v})$$

$$F_1(\vec{v}) = Q_N^* F_0(\vec{v}) \; .$$

Microscopic reversibility: $\rho(-\theta) = \rho(\theta)$

$$Q_N^* = Q_N$$

Probability distribution after k collisions

$$F_k(\vec{v}) = Q_N^k F_0(\vec{v})$$

Let T_i be the first collision time for particle i with any other particle

Exponential waiting time for collision of particle i with any other particle

$$P\{T_i > t\} = e^{-\gamma t}$$

The waiting time for a collision among N independent particles

$$P\{min\{T_1, \cdots, T_N\} > t\} = \prod_i P\{T_i > t\} = e^{-\gamma N t} \ .$$

Probability distribution at time t after k collisions

$$e^{-\gamma N t}\frac{(\gamma N t)^k}{k!}Q_N^k F_0(\vec{v})$$

Probability distribution at time t after arbitrary many collisions

$$\sum_{k=0}^{\infty} e^{-\gamma N t}\frac{(\gamma N t)^k}{k!}Q_N^k F_0(\vec{v}) = e^{\gamma N (Q_N - I)t} F_0(\vec{v})$$

We set $\gamma = 1$

Microscopic reversibility, $\rho(-\theta) = \rho(\theta)$ **implies that**

$$\langle f, Q_N g\rangle_{\mathcal{H}} = \langle Q_N f, g\rangle_{\mathcal{H}} \ .$$

$$\mathcal{H} = L^2(S^{N-1}(\sqrt{E}), \sigma^N)$$

with normalized uniform surface measure σ^N

Fix $E = N$

$$N(Q_N - I) = \frac{2}{N-1}\sum_{i<j}(R_{i,j} - I)$$

1) The probability of a particular particle colliding with any other within a time interval dt is $2dt$, i.e., independent of N. (Grad limit)

2) The evolution is linear

3) Can be generalized to momentum preserving collisions in $\mathbb{R}^3$

$$\begin{aligned} v_i^* &= v_i + \omega(v_j - v_i) \cdot \omega \\ v_j^* &= v_j - \omega(v_j - v_i) \cdot \omega \end{aligned}$$

$$\omega \in \mathbb{S}^2$$

$$R_{i,j}\Phi = \int_{\mathbb{S}^2} B(|v_i - v_j|, |\frac{v_i - v_j}{|v_i - v_j|} \cdot \omega|) \Phi(v_1, \ldots, v_i^*(\omega), \ldots, v_j^*(\omega), \ldots, v_N)$$

Given a symmetric initial distribution $F_0(\vec{v}) \in L^1(\mathbb{S}^{N-1}(\sqrt{N}); \sigma^N)$

$$F(\vec{v},t) = e^{-Nt(I-Q_N)}F_0 = \sum_{k=0}^{\infty} \frac{e^{-Nt}(Nt)^k}{k!} Q_N^k F_0$$

stays symmetric and satisfies the LINEAR Kac master equation

$$\frac{\mathrm{d}}{\mathrm{d}t} F(\vec{v},t) = -N(I - Q_N)F(\vec{v},t) \ , \ F(\vec{v},0) = F_0(\vec{v})$$

$$R_{i,j}\Phi := \int_0^{2\pi} \rho(\theta)\Phi(v_1, \cdots, v_i^*(\theta), \cdots, v_j^*(\theta), \cdots, v_N)\mathrm{d}\theta \ , \ Q_N^* = Q_N$$

$$(v_i^*(\theta), v_j^*(\theta)) := (\sin(\theta)v_i + \cos(\theta)v_j, \cos(\theta)v_i - \sin(\theta)v_j)$$

Why consider such a simple LINEAR model?

Derivation of an effective equation for N large.

It should be an equation for the marginal of the N particle density

Important will be the notion of Propagation of Chaos

Approach to equilibrium

Find quantitative rates

Using the notion of gap

Using the notion of entropy

$$\phi : \mathbb{R} \to \mathbb{R}$$

$$\int_{\mathbb{S}^{N-1}(\sqrt{N})} F_N(\vec{v}, t)\phi(v_1) d\sigma^N = \int_{-\sqrt{N}}^{\sqrt{N}} f_N^{(1)}(v, t)\phi(v) dv$$

$$\psi : \mathbb{R}^2 \to \mathbb{R}$$

$$\int_{\mathbb{S}^{N-1}(\sqrt{N})} F_N(\vec{v}, t)\psi(v_1, v_2) d\sigma^N = \int_{v^2+w^2 \leq N} f_N^{(2)}(v, w, t)\psi(v, w) dv dw$$

$$\frac{\partial f_N^{(1)}}{\partial t}(v,t) =$$

$$2\int_{-\sqrt{N-v^2}}^{\sqrt{N-v^2}} dw \int_{-\pi}^{\pi} \rho(\theta)d\theta[f_N^{(2)}(\cos\theta v - \sin\theta w, \sin\theta v + \cos\theta w, t) - f_N^{(2)}(v,w,t)]$$

If it is true that

$$f_N^{(2)}(v,w,t) \approx f_N^{(1)}(v,t) f_N^{(1)}(w,t)$$

then $f_N^{(1)}(v,t)$ satisfies the **Kac-Boltzmann** equation

$$\frac{\partial f}{\partial t}(v,t) =$$

$$2\int_{-\sqrt{N-v^2}}^{\sqrt{N-v^2}} dw \int_{-\pi}^{\pi} \rho(\theta)d\theta[f(\cos\theta v - \sin\theta w, t) f(\sin\theta v + \cos\theta w, t) - f(v,t)f(w,t)]$$

Propagation of Chaos

A sequence of probability distributions $\{F_N(\vec{v})\}_{N=1}^{\infty}$ on $\mathbb{S}^{N-1}(\sqrt{N})$ is said to be **chaotic** if, $\forall k \geq 1$,

$$\lim_{N\to\infty} \int_{\mathbb{S}^{N-1}(\sqrt{N})} \Pi_{j=1}^{k} \phi(v_j) F_N(\vec{v}) d\sigma^N(\vec{v})$$
$$= \lim_{N\to\infty} \left(\int_{\mathbb{S}^{N-1}(\sqrt{N})} \phi(v_1) F_N(\vec{v}) d\sigma^N(\vec{v}) \right)^k ,$$

$\phi : \mathbb{R} \to \mathbb{R}$ any bounded continuous function

Asymptotic independence

We denote the limiting one particle marginal by f

Example: Poincaré limit

$$
\begin{aligned}
&\lim_{N\to\infty} \int_{\mathbb{S}^{N-1}(\sqrt{N})} \Pi_{j=1}^{k} \phi(v_j)\, 1 \, d\sigma^N(\vec{v}) \\
= &\int_{\mathbb{R}^k} \Pi_{j=1}^{k} \phi(v_j)(2\pi)^{-k/2} e^{-\frac{\sum_{j=1}^{k} |v_j|^2}{2}} dv_1 \cdots dv_k \\
= &\left(\int_{\mathbb{R}} \phi(v) \frac{e^{-\frac{|v|^2}{2}}}{\sqrt{2\pi}} dv \right)^k
\end{aligned}
$$

Propagation of chaos, Kac (1956), McKean (1965)

Suppose that $F_N^{(0)}(\vec{v})$ is chaotic with limiting one particle marginal $f_0(v)$.

Then $F_N(\vec{v},t)$ is also chaotic and its limiting one particle marginal $f(v,t)$ satifies

the Kac-Boltzmann equation

$$\frac{\partial f}{\partial t}(v,t) = 2\int_{\mathbb{R}}\int_{-\pi}^{\pi}\rho(\theta)[f(v^*(\theta),t)f(w^*(\theta),t) - f(v,t)f(w,t)]d\theta dw$$

$$f(v,0) = f_0(v)\ .$$

$$v^*(\theta) = \cos(\theta)v - \sin(\theta)w\ ,\ \ w^*(\theta) = \sin(\theta)v + \cos(\theta)w$$

Sketch of a proof. We follow Mc Kean (1965)

$$\int_{\mathbb{S}^{N-1}(\sqrt{N})} F_N(\vec{v},t)\phi(v_1,\ldots,v_k)d\sigma^N$$

$$\sum_{\ell=0}^{\infty}\frac{t^\ell}{\ell!}\int_{\mathbb{S}^{N-1}(\sqrt{N})} F_N^{(0)}(\vec{v})(N(Q_N-I))^\ell\phi(\vec{v})d\sigma^N$$

Define

$$\Gamma\phi(v_1,\ldots,v_{k+1}) =$$

$$2\sum_{j\le k}\int_{-\pi}^{\pi} d\theta\rho(\theta)[\phi(v_1,\ldots,\cos\theta v_j-\sin\theta v_{k+1},\ldots,v_k)-\phi(v_1,\ldots,v_k)]$$

Γ adds a variable!

Because $F_N^{(0)}$ and ϕ are symmetric

$$\int_{\mathbb{S}^{N-1}(\sqrt{N})} F_N^{(0)}(\vec{v})(N(Q_N - I))^\ell \phi(\vec{v}) d\sigma^N = \int_{\mathbb{S}^{N-1}(\sqrt{N})} F_N^{(0)}(\vec{v}) G^\ell \phi(\vec{v}) d\sigma^N$$

where

$$G\phi(v_1, \ldots, v_{k+1}) =$$

$$\frac{2}{N-1} \sum_{1 \le i < j \le k} \int_{-\pi}^{\pi} d\theta \rho(\theta) [\phi(v_1, \ldots, v_i^*(\theta), \ldots, v_j^*(\theta), \ldots, v_k) - \phi(v_1, \ldots, v_k)]$$

$$+ \frac{N-k}{N-1} \Gamma\phi \ , \ k \le N$$

Lemma 1

Assume that ϕ is a bounded function of $1 \leq k < N$ variables. Then

$$\|G\phi\|_\infty \leq 4k\|\phi\|_\infty$$

$$\|\Gamma\phi\|_\infty \leq 4k\|\phi\|_\infty$$

$$\|(G-\Gamma)\phi\|_\infty \leq \frac{6k^2}{N-1}\|\phi\|_\infty$$

Proof:

The second statement is obvious

The first statement follows from

$$\|G\phi\|_\infty \le \frac{2}{N-1}\binom{k}{2}2\|\phi\|_\infty$$

$$+\frac{N-k}{N-1}4k\|\phi\|_\infty$$

$$=\frac{2}{N-1}[2Nk-k^2-k]\|\phi\|_\infty \le 4k\|\phi\|_\infty$$

The last estimate follows from

$$\|(G-\Gamma)\phi\|_\infty \le \frac{2}{N-1}\binom{k}{2}2\|\phi\|_\infty + (1-\frac{N-k}{N-1})\|\Gamma\phi\|_\infty$$

$$\le \frac{2}{N-1}\binom{k}{2}2\|\phi\|_\infty + (1-\frac{N-k}{N-1})4k\|\phi\|_\infty$$

$$=\frac{2}{N-1}[k^2-k+2k(k-1)]\|\phi\|_\infty \le \frac{6k^2}{N-1}\|\phi\|_\infty$$

Lemma 2

Let ϕ be a function of $1 \leq k < N$ variables. Then for any $\ell \in \mathbb{N}$

$$\|G^\ell \phi\|_\infty \leq 4^\ell k(k+1)(k+2)\cdots(k+\ell-1)\|\phi\|_\infty$$

$$\|\Gamma^\ell \phi\|_\infty \leq 4^\ell k(k+1)(k+2)\cdots(k+\ell-1)\|\phi\|_\infty$$

There exists a constant C such that

$$\|(G^\ell - \Gamma^\ell)\phi\|_\infty \leq \frac{C}{N-1} 4^\ell \ell^{k+1} \ell!$$

Proof

We only have to prove the last statement, the others are obvious.

$$(G^\ell - \Gamma^\ell)\phi = \sum_{j=1}^{\ell} G^{\ell-j}(G-\Gamma)\Gamma^{j-1}\phi$$

$$\|\sum_{j=1}^{\ell} G^{\ell-j}(G-\Gamma)\Gamma^{j-1}\phi\|_\infty \leq \sum_{j=1}^{\ell} \|G^{\ell-j}(G-\Gamma)\Gamma^{j-1}\phi\|_\infty$$

$$\leq \sum_{j=1}^{\ell} 4^{j-1}k(k+1)\cdots(k+j-2)\frac{6(k+j-1)^2}{N-1}(k+j)\cdots(k+\ell-1)4^{\ell-j}\|\phi\|_\infty$$

$$= 4^{\ell-1}\frac{6}{N-1}\frac{(k+\ell-1)!}{(k-1)!}\sum_{j=1}^{\ell}(k+j-1)$$

The result follows from Sterling's formula

$$\frac{(k+\ell-1)!}{\ell!} \approx \frac{(k+\ell-1)^{k+\ell-1+1/2}e^{-k-\ell-1}}{\ell^{\ell+1/2}e^{-\ell}} = \ell^{k-1}(1+\frac{k-1}{\ell})^{k+\ell-1/2}e^{-k-1}$$

$$\leq C\ell^{k-1}$$

Since

$$\sum_{j=1}^{\ell}(k+j-1) \leq C\ell^2$$

the result follows

Corollary 3

For $t < \frac{1}{4}$ we have that

$$\sum_{\ell=0}^{\infty} \frac{t^\ell}{\ell!} \|(G^\ell - \Gamma^\ell)\phi\|_\infty \leq \frac{C}{(1-4t)^{k+1}} \frac{\|\phi\|_\infty}{N-1}$$

Lemma 4

Γ is a derivation, i.e.,

$$\Gamma(\phi(v_1, \ldots, v_k)\psi(v_{k+1}, \ldots, v_m)) = (\Gamma g)\psi + \phi(\Gamma\psi)$$

Fix $t < \frac{1}{4}$

$$\lim_{N\to\infty} \int_{\mathbb{S}^{N-1}(\sqrt{N})} F_N(\vec{v}, t)\phi^{\otimes k} d\sigma^N$$

$$= \sum_{\ell=0}^{\infty} \frac{t^\ell}{\ell!} \lim_{N\to\infty} \int_{\mathbb{S}^{N-1}(\sqrt{N})} F_N^{(0)}(\vec{v}) G^\ell \phi^{\otimes k} d\sigma^N$$

$$= \sum_{\ell=0}^{\infty} \frac{t^\ell}{\ell!} \lim_{N\to\infty} \int_{\mathbb{S}^{N-1}(\sqrt{N})} F_N^{(0)}(\vec{v}) \Gamma^\ell \phi^{\otimes k} d\sigma^N$$

$$= \sum_{\ell=0}^{\infty} \frac{t^\ell}{\ell!} \int_{\mathbb{R}^{k+\ell}} f^{\otimes(k+\ell)} \Gamma^\ell \phi^{\otimes k} d^{k+\ell} v$$

Because $F_N^{(0)}$ is chaotic

$$\sum_{\ell=0}^{\infty} \frac{t^{\ell}}{\ell!} \int_{\mathbb{R}^{k+\ell}} f^{\otimes(k+\ell)} \Gamma^{\ell} \phi^{\otimes k} d^{k+\ell} v$$

Because Γ is a derivation

$$= \sum_{\ell=0}^{\infty} \frac{t^{\ell}}{\ell!} \sum_{\ell_1+\cdots+\ell_k=\ell} \frac{\ell!}{\ell_1! \cdots \ell_k!} \int_{\mathbb{R}^{k+\ell}} f^{\otimes(k+\ell)} \Gamma^{\ell_1} \phi \otimes \cdots \otimes \Gamma^{\ell_k} \phi d^{k+\ell} v$$

$$= \sum_{\ell=0}^{\infty} \sum_{\ell_1+\cdots+\ell_k=\ell} \frac{t^{\ell_1}}{\ell_1!} \int_{\mathbb{R}^{1+\ell_1}} f^{\otimes(1+\ell_1)} \Gamma^{\ell_1} \phi d^{1+\ell_1} v \cdots \frac{t^{\ell_k}}{\ell_k!} \int_{\mathbb{R}^{1+\ell_k}} f^{\otimes(1+\ell_k)} \Gamma^{\ell_k} \phi d^{1+\ell_k} v$$

which equals

$$= \left(\sum_{\ell=0}^{\infty} \frac{t^{\ell}}{\ell!} \int_{\mathbb{R}^{1+\ell}} f^{\otimes(1+\ell)} \Gamma^{\ell} \phi d^{1+\ell} v \right)^{k}$$

$$= \lim_{N \to \infty} \left(\int_{\mathbb{S}^{N-1}(\sqrt{N})} F_N(\vec{v}, t) \phi d\sigma^{N} \right)^{k}$$

Note that this argument shows that the limits exist

This theorem leads to an existence theorem for the Kac-Boltzmann equation

For a given $f \in L^1(\mathbb{R})$ find a chaotic sequence $F_N^{(0)}$ with f as limiting marginal

$$\frac{\Pi_{j=1}^N f(v_j)}{\int_{\mathbb{S}^{N-1}(\sqrt{N})} \Pi_{j=1}^N f(v_j) d\sigma^N} \delta(\sum_{j=1}^N v_j^2 - N)$$

Solve the Kac master equation with initial condition $F_N^{(0)}$

The resulting solution $F_N(\cdot, t)$ is chaotic with limiting marginal $f(\cdot, t)$

which satisfies the Kac Boltzmann equation with initial condition f