The Kac model with a thermostat.

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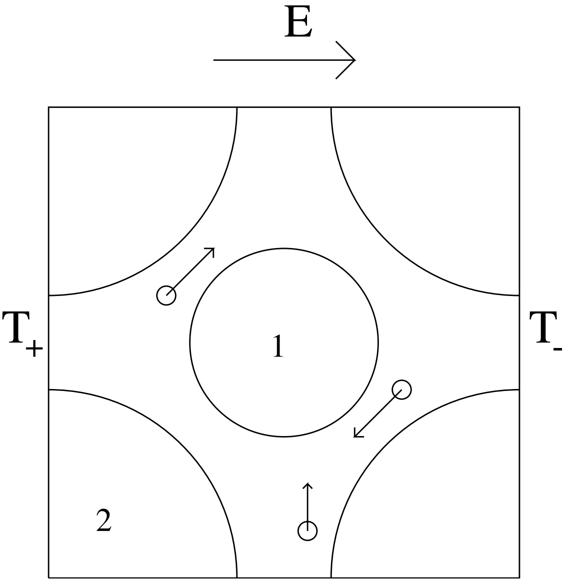
General Setting.

I have N particle in a box. They may interact with several different things to make the dynamics more interesting. Among others, we have considered:

1. Binary elastic collisions.
2. Elastic ollisions with scatterers.
3. Interaction with an external electric field **E** plus some mechanism to keep the energy finite. Normally this is given by a Gausssian thermostat.
4. Thermal reservoir at the boundary of the system. This can be modeled in different ways.


E
T+
T-
1
2

The questions.

The system is described by the collection of the positions q_i and velocity v_i of the particle. We set

$$V = (v_1, \ldots, v_N) \qquad\qquad Q = (q_1, \ldots, q_N)$$

The state of the system is a probability distribution $F_N(Q, V; t)$ and the evolution is in general given by a linear operator $\mathcal{L}_N$, that is

$$\dot{F}_N(t) = \mathcal{L} F_N(t)$$

Calling

$$\bar{F}_N = \lim_{t\to\infty} F_N(t)$$

the *Steady State* of the system, the typical question one can ask are:

- Existence of the limit for $N \to \infty$ of $\bar{F}_N$ and its behavior with respect to the parameters of the system.
- Rate of convergence to the steady state of a generic initial state.
- Call $f(v;t)$ the 1-particle marginal of $F_N(V;t)$ for N very large. Can we write a closed evolution equation for $f(v;t)$ in the style of the Boltzmann equation.

A rigorous answer to the above question in the original deterministic models is way too difficult for me. The deterministic collisionS make the problem extremely difficult.

One way out is to simplify the model by replacing the deterministic collisison with random collision. This idea was introduced first by Mark Kac in 1956.

The Kac model.

The particle are in 1 dimension and they are initially unifrmly distributed in space so that one can forget their positions.

The collision are described by a Poisson process whose intensity will be chosen later.

Every time a collision take place we select at random and uniformly two particles i and j with incoming velocities v_i and v_j.

The outgoing velocoties v_i^* and v_j^* of the two particle are chosen uniformly on the circle of radius $\sqrt{v_i^2 + v_j^2}$.

This rule is very similar to that used in the KMP model.

If the state of the system if $F_N(V)$ we can describe the effect of a collision by the operator $R_{i,j}$ given by

$$R_{1,2}F_N(V) = \frac{1}{2\pi}\int F_N(v_1\cos(\theta) - v_2\sin(\theta), v_1\sin(\theta) + v_2\cos(\theta), V^{(2)})$$

where $V^{(k)} = (v_{k+1}, \ldots, v_N)$.
The evolution is thus given by

$$\dot{F}_N = \mathcal{L}_N F_N$$

with

$$\mathcal{L}_N = \lambda \frac{N}{\binom{N}{2}} \sum_{i<j} (R_{i,j} - I)$$

The scaling factor in front of the sum assures that the average number of collision a particle suffers in a given time is independent of N.

This evolution preserve the total kinetic energy.

It is thus natural to look at $F(V)$ as defined of the sphere $S^{N-1}(\sqrt{N})$ of radius $\sqrt{N}$ in $\mathbb{R}^N$. In this way the evarage kinetic energy per particle is 1/2.

Let $d\sigma(V)$ the normalized volume measure on $S^{N-1}(\sqrt{N})$. It is easy to see that there is a unique steady state given by $F_N(V) = 1$.

Known facts.

The spectral gap of $\mathcal{L}_N$ can be computed exactly (Carlen-Carvalho-Loss (2000)):

$$\Lambda_N^{(1)} = -\frac{1}{2}\frac{N+1}{N-2}$$

It is clearly unifrom in N.

This is only useful very close to the stedy state. Indeed if the initial state is of the form

$$F(V) = \prod_{i=1}^{N} f(v_i) \qquad \text{restriced on the sphere}$$

then

$$\|F-1\|_2 \simeq C^N$$

So that if we start far from the steady state, it takes a time of order N to get close.

We can define the entropy with respect to the steady state as

$$S(F|\bar{F}) = \int F(V) \log\left(\frac{F(V)}{\bar{F}(V)}\right) d\sigma(V)$$

where in this case $\bar{F} \equiv 1$.

It is easy to show that

$$S(F|\bar{F}) \geq 0 \qquad \dot{S}(F(t)|\bar{F}) \leq e^{-c_N t} S(F(0)|\bar{F})$$

The constant c_N is not uniform in N. Indeed for every δ there exists C_δ such that:

$$\frac{1}{N} \leq c_N \leq \frac{C_\delta}{N^{1-\delta}}$$

(Villani (2003), Einav (2011))

Boltzmann Property

Given a symmetric disfribution $F_N(V)$ we define the k particle marginal as

$$f_N^k(v_1, \ldots v_k) = \int F_N(V)\, dV^{(k)}$$

A sequence of distributions $F_N(V)$ has the *Boltzamnn Property* if

$$\lim_{N\to\infty} f_N^k(v_1, \ldots, v_k) = \prod_{i=1}^{k} f(v_i)$$

where

$$f(v) = \lim_{N\to\infty} f_N^1(v)$$

Propagation of Chaos

Let $F_N(t)$ be the state of the system at tine t with initial condition $F_N(0)$.

Kac (1956) (see also McKean (1966)) proved that if $F_N(0)$ has the Boltzman property that $F_N(t)$ also has the Boltzmann Property. His result is not uniform in t.

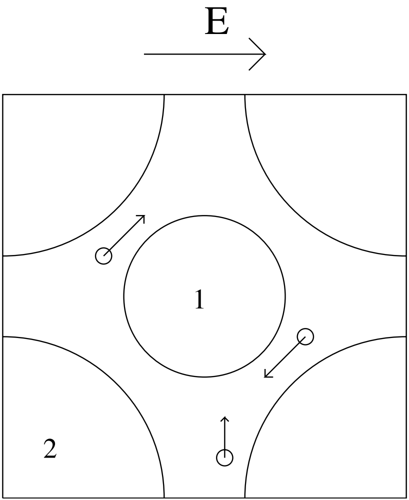
Form the above if follows, rather easily, that the limiting 1-particle marginal satisfy

$$\dot{f}(v;t) = 2\int dw \fint d\theta \, (f(v^*)f(w^*) - f(v)f(w))$$

where

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

Electric Conduction.



In B., Chernov, Korepanov, Lebowitz we studied a system of point like particles colliding with “virtual” obstacles under the influence of an electric field and a Gaussian thermostat.

In B., Carlen, Esposito, Lebowitz, Marra (2013) we proved validity of a self-consistent Boltzmann Equation with a technique completely different from that used by Kac or McKean.

This result is being extended to colliding particle by Carlen, Mustafa, Wennberg (2014).

We could also analize in detail the steady state for small electric field (B. Loss(2013)).

Thermostated Kac System.

We add to the system a second collision process. Again at Poisson distributed times a particle collides with a termostated wall. We can represent this wall in two ways.

A *strong* thermostat described by the operator:

$$T_1^s F(V) = \gamma_\beta(v_1) \int F(v_1, V^{(1)}) dv_1$$

where

$$\gamma_\beta(v) = \sqrt{\frac{\beta}{2\pi}} e^{-\beta \frac{v^2}{2}},$$

or a *weak* thermostat

$$T_1^w F(V) = \int \gamma_\beta(w^*) F(v_1^*, V^{(1)}) d\theta dw$$

The generator of the evolution becomes

$$\mathcal{L}_N = \mu \sum_i (T_i - I) + \frac{2\lambda}{N-1} \sum_{i<j} (R_{i,j} - I)$$

The evolution now take place on the full $\mathbb{R}^N$ since the energy is not conserved.

It is easy to see that there is a unique steady state given by the Maxwellian at inverse temperature β

$$\Gamma_\beta(V) = \prod_i \gamma_\beta(v_i).$$

We can ask the same question we asked for the original Kac model.

Spectral gaps.

Since $\mathcal{L}_N$ is not self adjoint in $L^2(\mathbb{R}^{\mathbb{N}})$ it is convenient to write

$$F(V) = \Gamma(V)H(V)$$

where now H satisfy the new evolution

$$\dot{H} = -L_N H$$

with

$$L_N = \mu \sum_i (\tilde{T}_i - I) + \frac{2\lambda}{N-1} \sum_{i<j} (R_{i,j} - I)$$

with

$$\tilde{T}_1 F(V) = \int \gamma_\beta(w) F(v_1^*, V^{(1)}) d\theta dw.$$

It is now easy to see that L_N is self adjoint on $L^2(\mathbb{R}^N, \Gamma(V))$.

The convergence to the steady state is dominated by the thermostat.

The spectral gap of $\mathcal{L}_N$ is given by

$$\Lambda_N^{(1)} = -\frac{\mu}{2}$$

with eigenfunction

$$H^{(1)}(V) = \sum_i v_i^2 - \frac{1}{\beta} = \sum_i h_2(v_i)$$

where h_2 is the Hermite polynomial of degree 2.
To see the effect of the particle-particle collision we compute the second eigenvalue of L_N and find, when $N \to \infty$,

$$\Lambda_\infty^{(2)} = -\frac{\lambda}{2} - \frac{5}{8}\mu$$

with eigenfunction

$$H^{(2)}(V) = \sum_i h_4(v_i).$$

Convergence in entropy

One can also study the convergence in entropy.

In this case one finds, thanks to the thermostat, that

$$S(F(t)|\Gamma) \leq e^{\frac{\mu}{2}} S(F(0)|\Gamma)$$

To obtain this one can reduce the problem to a one particle system using a Loomis-Whitney style inequality and then map the evolution of the one particle system into a Ornstein-Uhlembeck process.

Propagation of Chaos.

It is quite straight forward to extend Kac prove of validity of Propagation of Chaos to this system.

We get the validity of a Boltzmann-type equation with a thermostat added:

$$\begin{aligned}\dot{f}(v;t) =& 2\int\!\!\!\!\!\!\;\int d\theta\,(f(v^*)f(w^*) - f(v)f(w))\,dw + \\ &+ \int\!\!\!\!\!\!\;\int d\theta\,(\gamma(v^*)f(w^*) - \gamma(v)f(w))\,dw\end{aligned}$$

Our result is not uniform in time. We think we can get a unifrom Propagation of Chaos by using the thermostat.

Origin of the thermostat.

We want to understand a little better the nature of the thermostat.

We take a system of N particles evolving with the original Kac evolution with no thermostat ($mu = 0$). We look at the evolution in $L^2(\mathbb{R}^N, \Gamma(V))$.

We assume that the initial state is of the form

$$F(V) = \Gamma_\beta(V) h(v_1)$$

that is all particle but one are in equilibrium at temperature β.

We expect that for N large the out of equilibrium particle will converge to equilibrium at temperature β with the same evolution as if it was in contact with a thermostat.

If we keep t fixed and let $N \to \infty$ the result would betrivial. Thus we want this to be unifrom in time.

We can show that for every t,

$$\|e^{t(L_N-I)}h - e^{t(\tilde{T}_1-I)}h\|_2 \leq \frac{C\|h\|_2}{\sqrt{N}}$$

Moreover if we have M particle initialy out of equilibrium we get a similar estimates with $\frac{M}{\sqrt{N-M}}$ instead of $\frac{1}{\sqrt{N}}$.

You cannot do better since we can compute that

$$\lim_{t\to\infty} \|e^{t(L_N-I)}h - e^{t(\tilde{T}_1-I)}h\|_2 = O\left(\frac{1}{\sqrt{N}}\right)$$

Newton Law of Cooling.

We now go back to our Kac model with a thermostat of strenght μ.

We can define the average kinetic energy as

$$E(V) = \frac{1}{2} \sum_i \frac{v_i^2}{2}$$

and call

$$\tau(t) = \frac{1}{2} \int E(V) F_N(V) dV$$

A straighforward computation show that

$$\dot{\tau}(t) = -\frac{\mu}{2} \left(\tau(t) - \frac{1}{\beta} \right)$$

that looks very much like Newton Law of Cooling.

But it is not!

It is easy to see that even starting the system in a initial state at inverse temperature $\beta' \neq \beta$, that is

$$F_N(V, 0) = \Gamma_{\beta'}(V)$$

we have

$$F(V, t) \neq \Gamma_{\beta(t)}(V)$$

where $\beta(t) = 1/\tau(t)$.

To obtain Newton Law of Cooling we need a Thermodynamic Trasformation, that is an infinitely slow trasformation so that the system is always infinitesimaly close to equilibrium.

To do this we can take μ very small and look at it on a time scale of the form $t = s/\mu$.

More precesely we can define

$$G_N(V, s) = \lim_{\mu \to 0} F_N\left(V, \frac{s}{\mu}\right)$$

Again we get

$$G_N(V, s) \neq \Gamma_{\beta(t)}(V)$$

but we expect that

$$\lim_{N \to \infty} g_N^{(1)}(v, t) = \gamma_{\beta(t)}(v)$$

Moreover, $G_N(V, s)$ has the Boltzmann Property.

In this situation, we can call $\tau(t) = T(t)$ and speak of Newton Law of Cooling.

We have some initial result for the case in which only some of the particle are thermostated. They are still unclear to me so I'll close here.

Thank You