Approach to equilibrium for the Kac model

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Abstract This is a review on the Kac Master Equation. Various issues will be presented such as the resolution of Kac's conjecture about the gap for the three dimensional hard sphere gas, entropic propagation of chaos and other topics such as systems coupled to reservoirs and thermostats. The discussion is informal with few proofs and those who are presented are only sketched.

Key words: Kinetic theory, Master equation, Kac Model, Decay of Entropy, Decay of Information, collision process, Boltzmann equation, Kac Master Equation, Kac-Boltzmann equation, Quantum Kac Model

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1 The one dimensional Kac model

It is the aim of this article to give an overview of a program to which Maria Carvalho contributed greatly and to show that her work has instigated further development in this area. In much of her career she worked on fundamental problems like to formulate the notion of equilibrium and to describe how systems that are out of equilibrium tend towards it. One particular fruitful avenue she pursued with collaborators is an approach to kinetic theory through master equations.

The standard description of a classical gas, going back to Boltzmann [2], is to replace the evolution equation of the interacting many body problem by an effective equation describing the evolution of marginals, known as the Boltzmann equation. Despite heroic efforts by Lanford and others [25], [19], there is no satisfactory derivation of this equation from microscopic dynamics. There was substantial progress by Bodineau, Gallagher and Saint Raimond [1] who gave a rigorous derivation of the linearized Boltzmann equation describing a hard sphere gas near equilibrium. This seems to be the first rigorous derivation of an effective equation from microscopic dynamics.

A less ambitious approach is to construct models that illuminate certain questions of interest. Many of the difficulties stemming from a fundamental description are ignored in such an approach. However it has brought some of the issues into a sharp focus and may lead to new ideas on how to proceed with the 'fundamentalist program'. The pedagogical aspect is an added bonus of this phenomenological approach. Maria Carvalho and Eric Carlen introduced one of the authors to these kind of questions, in particular to an approach based on the Kac model. This paper is a review of some of the work done over the years, but we also present some newer developments, albeit with a light touch.

The Kac Master Equation describing the evolutions of the probability density $F(\mathbf{v}_N,t)$ for the velocities of a one-dimensional spatially homogeneous gas of N particle is given by

$$\frac{\partial F(\mathbf{v}_N,t)}{\partial t} = \frac{N}{\binom{N}{2}} \sum_{i<j} \left[\frac{1}{2\pi} \int_0^{2\pi} F(\mathbf{v}_N(i,j;\theta),t) d\theta - F(\mathbf{v}_N,t) \right] \tag{1}$$

with initial condition $F(\mathbf{v}_N,0) = F_0(\mathbf{v}_N)$, where $\mathbf{v}_N = (v_1,\dots,v_N)$ is the velocity vector of the particles,

$$\mathbf{v}_N(i,j;\theta) = (v_1,\dots,v_i^*(\theta),\dots,v_j^*(\theta),\dots,v_N) \tag{2}$$

and

$$v_i^*(\theta) = v_i\cos\theta + v_j\sin\theta, \quad v_j^*(\theta) = -v_i\sin\theta + v_j\cos\theta \tag{3}$$

are the post-collisional velocities of the pair i,j undergoing this collision. Thus, the collisions are described by two dimensional random rotation. We assume that the density F is symmetric in the particle labels which is preserved by the time evolution. For a more detailed probabilistic explanation see [22],[7], [8] and especially [23]. It is useful to keep in mind that the rate at which a fixed particle collides with

any other particle is independent of $N$and equals 2 in our case. A good way of thinking about the evolution equation is to write it as

$$\partial_t F = -\mathcal{L}_N F\,, \text{where } \mathcal{L}_N = N(I-Q)\,, \tag{4}$$

where Q is the average over all rotations in the two dimensional coordinate hyperplanes. The solution of the master equation is then

$$F(\mathbf{v}_N,t) = e^{-\mathcal{L}_N t} F_0(\mathbf{v}_N)\,. \tag{5}$$

Since the collisions are modeled by two dimensional rotations, the kinetic energy

$$\sum_{j=1}^{N} v_j^2$$

is preserved and it suffices to consider the master equation (1) for densities $f \in L^1(\mathcal{S}_N, d\sigma_N)$ where $\mathcal{S}_N = \sqrt{N}\mathbb{S}^{N-1}$ and $d\sigma_N$ is the uniform probability measure on the sphere. We fix the total kinetic energy to be N, so that the average kinetic energy per particle is 1. If one requires for a one-dimensional collision that in addition the energy and the momentum are preserved, the only possible collisions would be that either the particles keep their velocities and pass through each other or exchange them. This would leave the symmetric density F invariant and hence not interesting.

It is fairly obvious that for product densities, i.e. densities of the form

$$F_N(\mathbf{v}_N) \coloneqq \frac{\prod_{j=1}^N f(v_j)}{\int_{\mathcal{S}_N} \prod_{j=1}^N f(v_j)\, d\sigma_N}\,, \tag{6}$$

the product structure is not strictly preserved under the evolution. It is, however, preserved asymptotically as the particle number tends to infinity, a fact known as propagation of chaos, a notion that goes back to Boltzmann [2]. Consider a sequence $\{F_N(\mathbf{v}_N)\}_{N=1}^{\infty}$. Assume that there exists a function $f : \mathbb{R} \to \mathbb{R}_+$ such that for any $k \in \mathbb{N}$ and any bounded continuous function $\phi_k : \mathbb{R}^k \to \mathbb{R}$ we have

$$\lim_{N\to\infty} \int_{\mathcal{S}_N} F_N(\mathbf{v}_N)\phi_k(v_1,\dots,v_k)\, d\sigma_N = \int_{\mathbb{R}^k} \prod_{j=1}^{k} f(v_j)\phi_k(v_1,\dots,v_k)\, dv_1 \cdots dv_k\,,$$

then we say that the sequence F_N is *chaotic with limiting marginal* f. The simplest example is the function 1 on the sphere $\mathcal{S}_N$ which is easily seen to be chaotic with limiting marginal

$$\gamma(v) \coloneqq (2\pi)^{-1/2} e^{-v^2/2}\,, \tag{7}$$

by a calculation that goes back to the 19th century to Mehler, Maxwell and Poincaré.

Kac's theorem states that chaos is propagated.

Theorem 1 (Kac Theorem). *Let $F_N(\mathbf{v}_N)$ be a chaotic sequence with limiting marginal $f_0(v)$ and $F_N(\mathbf{v}_N,t)$ be the solution of the Kac Master Equation with initial condition $F_N(\mathbf{v}_N)$. Then $F_N(\mathbf{v}_N,t)$ is chaotic with limiting marginal $f(v,t)$ and this*

function satisfies the Kac-Boltzmann Equation

$$\frac{\partial f(v,t)}{\partial t} = \frac{1}{\pi}\int_0^{2\pi}\int_{-\infty}^{\infty}[f(v^*(\theta),t)f(w^*(\theta),t) - f(v,t)f(w,t)]\,dw.. \tag{8}$$

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

This theorem is proved in [22] and is the antecedent of many results of similar type. It was shown in [12] that any distribution on $\mathbb{R}$ is the limit marginal of a chaotic sequence and hence this leads to an existence result for solutions of the Kac-Boltzmann equation.

It is not very difficult to see that the semi-group generated by the Kac Master Equation is ergodic in the sense that the only invariant distribution, i.e. *equilibrium*, is the function 1 on $\mathcal{S}_N$. Thus, 0 is a nondegenerate eigenvalue of $\mathcal{L}_N$. Moreover, one observes that the generator $\mathcal{L}_N$ of this semigroup is a selfadjoint non-negative operator on $L^2(\mathcal{S}_N, d\sigma_N)$ and according to what was said before, the function 1 spans the null space of this operator. Thus, 0 is a simple eigenvalue of $\mathcal{L}_N$. The next largest eigenvalue Δ_N is called the *gap*. A simple application of the spectral theorem shows that $F_N(\mathbf{v}_N,t)$ converges to 1 as $t\to\infty$ in $L^2(\mathcal{S}_N, d\sigma_N)$ with a rate that is given by the gap

$$\|F_N(\cdot,t) - 1(\cdot)\|_2 \le e^{-\Delta_N t}\|F_N(\cdot,0) - 1(\cdot)\|_2\,.$$

Kac [22] posed the conjecture that there exists a positive constant $c>0$ independent of N such that $\Delta_N \ge c$ for all N. This conjecture was eventually proved in [21]. In [7] it was further shown that

$$\Delta_N = \frac{1}{2}\frac{N+2}{N-1} > \frac{1}{2}\,.$$

The Kac Boltzmann equation has Gaussian functions such as (7) as equilibria and it is customary to linearize the Kac-Boltzmann equation about one of these equilibria. In this way one obtains some information about the speed of approach to equilibrium by computing the gap for the generator of this linear equation. Interestingly, this is furnished by the Kac master equation in the limit as $N\to\infty$. The linearized version of the Kac-Boltzmann equation has the gap eigenvalue $1/2$ which is the limit of Δ_N as $N\to\infty$. But more is true. The gap eigenvalue for the Kac master Equation is not degenerate and the eigenfunction (up to normalization) is given by

$$\sum_{j=1}^{N}\left[v_j^4 - \frac{3}{N(N+2)}\right].$$

As $N\to\infty$, the first marginal of this function converges to a fourth order hermitian polynomial which is the gap eigenfunction of the linearized Kac-Boltzmann equation. For details the reader may consult [8].

2 Momentum preserving collisions

As mentioned before, two particle collisions that preserve the kinetic energy and momentum are not very interesting in one dimension; particles either exchange the velocity or pass through each other without interaction. One can certainly write a Kac-type master equation for realistic collisional models such as hard spheres in three dimensions. Not only are the collisions energy and momentum preserving but there is the added complexity that the scattering cross section may depend on the momentum transfer $|v_i - v_j|$. There are multiple ways to parametrize the collision process and one convenient version used here is the swapping map

$$\begin{aligned} v_i^*(\sigma) &= \frac{v_i + v_j}{2} + \frac{|v_i - v_j|}{2}\sigma\,, \\ v_j^*(\sigma) &= \frac{v_i + v_j}{2} - \frac{|v_i - v_j|}{2}\sigma\,, \end{aligned} \tag{9}$$

where $\sigma \in \mathbb{S}^2$. To describe the collisions in the one dimensional case, we assumed that the angle θ was uniformly distributed. In the three dimensional case, we assume that there is given a function $b : [-1,1] \to \mathbb{R}_+$ with

$$\int_{\mathbb{S}^2} b(\sigma \cdot \sigma')\, d\sigma = \frac{1}{2}\int_{-1}^{1} b(t)\, dt = 1\,. \tag{10}$$

Here $d\sigma$ is the uniform probability measure on $\mathbb{S}^2$. For hard spheres, $b = 1$, see [11] for an explanation how the various parametrizations are connected. The model analogous to (1) is given by

$$\begin{aligned} \frac{\partial F}{\partial t}(\mathbf{v}_N, t) &= -L_{N,\alpha} F(\mathbf{v}_N, t)) \\ &= -\frac{N}{\binom{N}{2}} \sum_{i<j} |v_i - v_j|^\alpha \left[F(\mathbf{v}_N, t) - [F]^{(i,j)}(\mathbf{v}_N, t) \right] \end{aligned} \tag{11}$$

where

$$[F]^{(i,j)}(\mathbf{v}_N, t) = \int_{S^2} b\left(\sigma \cdot \frac{v_i - v_j}{|v_i - v_j|} \right) F(R_{i,j,\sigma}\mathbf{v}_N, t)\, d\sigma \tag{12}$$

and

$$(R_{i,j,\sigma}\mathbf{v})_k = \begin{cases} v_i^*(\sigma) & k = i, \\ v_j^*(\sigma) & k = j, \\ v_k & k \neq i, j. \end{cases}$$

The case of hard spheres is $\alpha = 1$ but it is of advantage to keep the power $0 \leq \alpha \leq 2$. Since the collisions preserve energy and momentum, it suffices to consider distributions on the surface given by the equation

$$\frac{1}{N}\sum_{j=1}^{N}|v_j|^2 = E\,, \quad \frac{1}{N}\sum_{j=1}^{N} v_j = p\,.$$

where E resp. p is the kinetic energy resp. momentum per particle. These equations determine a sphere in $\mathbb{R}^{3N}$ of co-dimension 4 and we denote this space by $\mathcal{S}_{N,E,p}$. As before, we denote the uniform probability measure on this space by $d\sigma_{N,E,p}$.

Propagation of chaos is much harder to prove for this model. The difficulty is that the factor $|v_i - v_j|^\alpha$ can grow with N. This problem, was first solved in a qualitative fashion in [27], and later in a quantitatively by Mischler and Mouhot in their seminal paper [26]. Likewise, to find a lower bound on the gap that is uniform in the number of particles is much harder. Ironically, one of the reasons for this difficulty is that the factor $|v_i - v_j|^\alpha$ can be small and suppress collisions. The gap is defined as

$$\Delta_{N,\alpha}(E,p) = \inf\left\{\mathcal{E}(F,F)\ :\ \langle F,1\rangle_{L^2(\mathcal{S}_{N,E,p})} = 0 \quad \text{and} \quad \|F\|^2_{L^2(\mathcal{S}_{N,E,p})} = 1\right\}, \tag{13}$$

where $\mathcal{E}(F,F) = \langle F, L_{N,\alpha}F\rangle_{L^2(\mathcal{S}_{N,E,p})}$, i.e.

$$\mathcal{E}(F,F) = \frac{N}{2}\binom{N}{2}^{-1}\sum_{i<j}\int_{\mathcal{S}_{N,E,p}}\int_{\mathbb{S}^2}|v_i - v_j|^\alpha b\left(\sigma\cdot\frac{v_i - v_j}{|v_i - v_j|}\right)\left[F(\mathbf{v}_N) - F(R_{i,j,\sigma}\mathbf{v}_N)\right]^2 d\sigma\, d\sigma_N\,. \tag{14}$$

By a unitary transformation mapping $L^2(\mathcal{S}_{N,1,0})$ to $L^2(\mathcal{S}_{N,E,p})$ (see [9]) one finds that

$$\Delta_{N,\alpha}(E,p) = (E - |p|^2)^{\alpha/2}\Delta_{N,\alpha}(1,0)\,, \tag{15}$$

and we call $\Delta_{N,\alpha}(1,0)$ the 'spectral gap for the Kac model'. The following theorem is proved in [9]:

Theorem 2 (Spectral gap for the Kac Model with $0 \le \alpha \le 2$). *For each continuous non-negative even function b on $[-1,1]$ satisfying* (10)*, and for each $\alpha \in [0,2]$, there is a strictly positive constant K depending only on b and α, and explicitly computable, such that*

$$\Delta_{N,\alpha} \ge K > 0 \tag{16}$$

for all N. In particular, this is true with b given by (10) *and $\alpha = 1$, the 3-dimensional hard sphere Kac model.*

3 Entropy

Unfortunately, the gap is not a very good notion to measure the rate of approach to equilibrium. It is generically the case that the L^2 norm of a probability distribution on $L^2(\sqrt{N}\mathbb{S}^{N-1})$ increases like c^N where $c > 1$. This is easy to see for chaotic se-

quences. The preferred notion is entropy which for the simple Kac model explained at the beginning is given by

$$H(F|1) = \int_{\mathcal{S}_N} F \log F \, d\sigma_N \, .$$

$H(F|1)$ is called 'entropy' which deviates from the usual notion in physics by a sign. The notation $H(F|1)$ also indicates that one is considering a relative entropy, in our case with respect to the 1 distribution. We note that in contrast to the L^2 norm, the entropy is extensive, i.e. for a state that is a product state $F = \prod_{j=1}^N f(v_j)$ we see that

$$H(F|1) = \sum_{j=1}^N \int_{\sqrt{N}\mathbb{S}^{N-1}} F \log f(v_i) \, d\sigma_N \approx N \int_{\sqrt{N}\mathbb{S}^{N-1}} f(v) \log f(v) \, d\sigma_N \, .$$

It is not very difficult to see that the entropy decreases to zero along the Kac flow, although little is known about the rate. Returning to the simplest version of the Kac model, it was shown in [28] that

$$H(F(t)|1) \leq e^{-\frac{2t}{N-1}} H(F_0|1) \, .$$

The proof consists of the analysis of entropy production. Taking the derivative

$$\frac{d}{dt}\Big|_{t=0} H(F(t)|1) = -N \int_{\sqrt{N}\mathbb{S}^{N-1}} (I-Q) F \log F \, d\sigma_N$$

one obtains the negative rate of dissipation and the entropy production is then defined by

$$\Gamma_N = \inf_F \frac{N \int_{\sqrt{N}\mathbb{S}^{N-1}} (I-Q) F \log F d\sigma_N}{H(F|1)} \, .$$

Villani [28] proved that

$$\Gamma_N \geq \frac{2}{N-1} \, .$$

That this estimate is almost optimal was shown by Einav [15]. Exponential decay of the entropy with a rate that is independent of N is known as Cercignani's conjecture. For details the reader may consult [28]. Although Einav's result does not preclude that the entropy might decrease eventually at an exponential rate, one could consider this as evidence against Cercignani's conjecture for the Kac model. The challenge is to show that the evolution of Einav's trial functions has small entropy decay for large times.

There are modifications of the Kac model with one dimensional collisions worked out by Villani [28] for which Cercignani's conjecture is true. These modifications accelerate the rate of collisions between the particles i and j by replacing the collision rate by $(1 + v_i^2 + v_j^2)$. Unfortunately nothing can be inferred from that about the original model. It is interesting that Villani's result is not known to hold when the collision rate is merely replaced by $v_i^2 + v_j^2$. The problem is that for small

velocities the collision rate is sharply depressed. Likewise, to our knowledge, similar results for the three dimensional 'hard sphere' collisions in which $\alpha = 2$ are not known.

There is, however, another interesting link between the Kac-Boltzmann equation and the Kac master equation. In Section 1, we mentioned the close connection between the gap and the gap eigenfunction of the Kac model and the linearized Kac-Boltzmann equation. This can be carried further using the notion of entropic chaos. A sequence $\{F_N\}_{N=1}^{\infty}$ is entropically chaotic with limiting marginal f if it is chaotic and in addition satisfies

$$\lim_{N\to\infty} \frac{H(F_N|1)}{N} = H(f|\gamma)\,.$$

In [12] it was shown that for a given probability density f on the real line with

$$\int_{\mathbb{R}} f(v)v^2\,dv = 1\,, \quad H(f|\gamma) < \infty$$

there exists an entropically chaotic sequence with limiting marginal f. Using this connection one is able to transfer entropy decay of the Kac evolution to entropy decay for the Kac-Boltzmann equation. Unfortunately, the current entropy decay estimates are not strong enough to draw any quantitative conclusions.

From a practical point of view, one rarely considers systems that are very far from equilibrium. Usually one is in a situation in which only a part of the system is out of equilibrium. One way to model such a situation, is to couple a system of M particles to a larger one. The simplest possibility, pursued in [6], is to couple the finite system to a thermostat. By definition, a thermostat does not change during the interaction with the system, and this can be modeled by

$$\frac{\partial f}{\partial t} = -\lambda M(I-Q)f - \mu \sum_{j=1}^{M} (I-R_j)f =: -\mathcal{L}_T f\,. \tag{17}$$

where

$$R_j f := \int \frac{1}{2\pi}\int_0^{2\pi} e^{-\pi w_j^{*2}(\theta)} f(\mathbf{v}_M^j(\theta,w))\,d\theta\,dw$$

and

$$\begin{aligned}\mathbf{v}_M^j(\theta,w) &= (v_1,...,v_j\cos(\theta)+w\sin(\theta),\ldots,v_M),\\ w_j^*(\theta) &= -v_j\sin(\theta)+w\cos(\theta).\end{aligned}$$

The idea is that particle j interacts with a particle from the thermostat whose velocity distribution is given by a Gaussian of temperature $2/\pi$. Note, using these units has the advantage that the Gaussian function $e^{-\pi v^2}$ is normalized. It is easy to see that the Gaussian $\gamma_M = e^{-\pi|\mathbf{v}_M|^2}$ is the unique equilibrium state for the system. It was shown in [6] that for an initial condition f_0 with finite entropy

$$H(f_t|\gamma) \le e^{-\mu t/2} H(f_0|\gamma)\,.$$

Since the equilibrium state is a product function, one would hope to obtain a stronger version of propagation of chaos, namely one that is uniform in time. This was shown in [14] with an explicit error term proportional to $N^{-1/3}$.

It is natural to think that the evolution of the system is similar if one couples the system to a finite reservoir with a large number of particles. The system is then described by a probability distribution $F(\mathbf{v},\mathbf{w},t) = (v_1,\dots,v_M,w_{M+1},\dots,w_{M+N})$, where we label the particles from 1 to $M+N$. Thus, one considers the evolution equation

$$\partial_t F = -\left(\lambda_S \mathcal{L}_M F + \lambda_R \mathcal{L}_N + \mu \mathcal{I}_{M,N}\right) F =: -\mathcal{L}_R F \tag{18}$$

where

$$\begin{aligned}
\mathcal{L}_M F &:= \tfrac{2}{M-1} \textstyle\sum_{i<j=1}^{M} (I - R_{i,j}) F \\
\mathcal{L}_N F &:= \tfrac{2}{N-1} \textstyle\sum_{i<j=M+1}^{M+N} (I - R_{i,j}) F \\
\mathcal{I}_{M,N} F &:= \tfrac{1}{N} \textstyle\sum_{i=1}^{M} \sum_{j=M+1}^{M+N} (I - R_{i,j}) F
\end{aligned}$$

with the initial condition

$$F_0(\mathbf{v},\mathbf{w}) = f_0(\mathbf{v}) e^{-\pi|\mathbf{v}|^2}.$$

The kinetic energy is no longer preserved and therefore one has to consider distributions in $\mathbb{R}^{M+N}$. The collisions are here modeled in one dimension as follows

$$R_{i,j} F(\mathbf{u}) := \frac{1}{2\pi} \int_0^{2\pi} F(u_1,\dots,u_i^*(\theta),\dots,u_j^*(\theta),\dots,u_{M+N}), \quad \mathbf{u} \in \mathbb{R}^{M+N}, \tag{19}$$

where

$$u_i^*(\theta) := u_i \cos\theta + u_j \sin\theta, \quad u_j^*(\theta) := -u_i \sin\theta + u_j \cos\theta.$$

The generator $\mathcal{L}_M$ describes the collisions among the M particles in the considered system, $\mathcal{L}_N$ describes the collisions among the N particles in the reservoir and $I_{M,N}$ the collisions between the particles in the system and the reservoir. Note that the collision rate of a particle in the system with any particle in the reservoir is μ. The interesting point about this evolution is that although initially the reservoir is in an equilibrium it does not stay that way in the course of the evolution. This is in contrast to the thermostat. One would, however, expect that the solution $F(\mathbf{v},\mathbf{w},t)$ is well approximated by the solution of the thermostat problem for large N. That this is the case was shown in [4] using the Gabetta-Toscani-Wennberg metric [17]

$$d_2(f,g) := \sup_{\xi\neq 0,\eta\neq 0} \frac{|\widehat{f}(\xi,\eta) - \widehat{g}(\xi,\eta)|}{|\xi|^2 + |\eta|^2}. \tag{20}$$

where $\widehat{f}$ is the Fourier transform of f and one has to impose that the first moments of f and g vanish and the second moments of f and g are finite.

Theorem 3. *Let $F(\mathbf{v},\mathbf{w})$ be the initial distribution for the system plus reservoir of the form*

$$F_0(\mathbf{v},\mathbf{w}) = f_0(\mathbf{v})\gamma_N(\mathbf{w}).$$

with f_0 symmetric and satisfying the moment conditions mentioned above. Assume moreover that

$$\int v_i^4 f_0(\mathbf{v})\, d\mathbf{v} = E_4 < \infty, \tag{21}$$

then for every $t > 0$ we have

$$d_2\left(e^{\mathcal{L}_R t}F_0, e^{\mathcal{L}_T t}F_0\right) \leq \frac{KM}{N}\left(1 - e^{-\frac{\mu}{4}t}\right)\sqrt{d_2(f_0,\gamma_N)(F_4 + d_2(f_0,\gamma_N))}\,. \tag{22}$$

with $F_4 = 3\pi^4\left(E_4 + \frac{\pi+2}{\pi^2}\right)$ and $K = 16\sqrt{3}$ and where $\gamma_N(\mathbf{w}) = e^{-\pi|\mathbf{w}|^2}$.

This theorem shows, that if one starts with an initial condition in which the reservoir is in equilibrium, then the two evolutions, the one with the thermostat and the one with the finite reservoir, stay close uniformly in time at least for the case where $N >> M$. The reservoir does never move far from its equilibrium.

Unfortunately, the above result does not allow to draw any conclusions about the decay of entropy for the finite reservoir problem. A reasonable proposal, which is in some ways closer to Boltzmann's ideas [2], is to find good rates for entropy decay for the marginals of the distributions. Returning to (18) one focuses on the marginal

$$f(\mathbf{v},t) = \int_{\mathbb{R}^N} e^{-\mathcal{L}_R t}F_0(\mathbf{v},\mathbf{w})\, d\mathbf{w}$$

and considers the relative entropy

$$H(f(\cdot,t)|\gamma_M)\,.$$

Note that γ_M is the equilibrium state for the system coupled to the thermostat. However, it is not the equilibrium state for the system coupled to the reservoir. The following theorem is proved in [5]

Theorem 4. *For any positive integers N, M we have that*

$$H(f(\cdot,t)|\gamma_M) \leq \left(\frac{M}{N+M} + e^{-\frac{\mu(N+M)}{2N}t}\frac{N}{N+M}\right)H(f_0(\cdot)|\gamma_M)\,. \tag{23}$$

The entropy relative to the Gaussian cannot converge to zero, because the Gaussian is not the equilibrium state. The theorem, however, states that if the reservoir is large compared to the system, then the entropy relative to the Gaussian decreases at an exponential rate which is uniform in N. In fact, as $N \to \infty$ this converges to the rate of the thermostat.

4 Information

The proof of Theorem 4 in [5] is rather cumbersome and required the sharp form of the Brascamp-Lieb inequalities. In this section, we indicate a relatively simple proof using the notion of information which was published in [3] for a one-dimensional model. In [18], this was generalized to multidimensional models with a different collision mechanism. We explain the ideas for the case of a three dimensional system undergoing momentum preserving collisions. The law governing the collision between particles i and j is given by

$$v_i^*(\sigma) = v_i - (\sigma \cdot (v_i - v_j))\sigma\,, \quad v_j^*(\sigma) = v_j + (\sigma \cdot (v_j - v_i))\sigma\,, \quad \sigma \in \mathbb{S}^2\,, \tag{24}$$

while the velocities of the other particles are fixed. We set

$$R_{i,j}F(\mathbf{u}) = \int_{\mathbb{S}^2} F(u_1, \ldots, u_i^*(\sigma), \ldots, u_j^*(\sigma), \ldots, u_{M+N})\,\rho(d\sigma) \tag{25}$$

where $\rho(d\sigma)$ is a probability measure on $\mathbb{S}^2$. Note that this is a much simpler model than the three dimensional hard sphere model. The collision cross section is independent of the momentum transfer.

The model under consideration is the same as in equation (18) except that we replace all the collision operators $R_{i,j}$ of (19) by (25). As before one starts with the initial condition

$$F_0(\mathbf{v}, \mathbf{w}) = f_0(\mathbf{v}) e^{-\pi|\mathbf{w}|^2}$$

and we label the variables as

$$F(\mathbf{v}, \mathbf{w}, t) = F(v_1, \ldots, v_M, w_{M+1}, \ldots, w_{M+N}, t)$$

where $F(\mathbf{v}, \mathbf{w}, t)$ is the probability distribution on $\mathbb{R}^{3M+3N}$ given by $e^{-\mathcal{L}_R t} F_0$. As before we consider the marginal

$$f(\mathbf{v}, t) = \int_{\mathbb{R}^{3N}} F(\mathbf{v}, \mathbf{w}, t)\, d\mathbf{w}$$

and the relative entropy

$$H(f(\cdot, t)|\gamma_M) = \int_{\mathbb{R}^{3M}} f(\mathbf{v}, t) \log \frac{f(\mathbf{v}, t)}{\gamma_M(\mathbf{v})}\, d\mathbf{v}$$

where $\gamma_M(\mathbf{v}) = e^{-\pi|\mathbf{v}|^2}$. The following theorem is proved in [18].

Theorem 5. *Assume that the initial distribution $f_0 \in L^1(\mathbb{R}^M)$ has finite second moment and $\sqrt{f_0} \in H^1\left(\mathbb{R}^M\right)$. Assume further that*

$$\int_{\mathbb{S}^2} \sigma_i \sigma_j\, \rho(d\sigma) = C \cdot \delta_{ij}\,, \tag{26}$$

for some constant $C \in \mathbb{R}$. Then

$$H(f(\cdot,t)|\gamma_M) \leq \left(\frac{M}{M+N} + \frac{N}{M+N}e^{-\frac{\mu}{3}\frac{M+N}{N}t}\right) H(f_0|\gamma_M)\,. \tag{27}$$

The time evolution keeps the Gaussian $e^{-\pi[|\mathbf{v}|^2+|\mathbf{w}|^2]}$ fixed and it will be convenient to set

$$F(\mathbf{v},\mathbf{w},t) = G(\mathbf{v},\mathbf{w},t)e^{-\pi[|\mathbf{v}|^2+|\mathbf{w}|^2]}\,,$$

where

$$G(\mathbf{v},\mathbf{w},t) = [e^{-\mathcal{L}_R t}g_0](\mathbf{v},\mathbf{w})\,.$$

With

$$f_0(\mathbf{v}) = g_0(\mathbf{v})e^{-\pi|\mathbf{v}|^2}\,, \quad f(\mathbf{v},t) = g(\mathbf{v},t)e^{-\pi|\mathbf{v}|^2}$$

we find that

$$g(\mathbf{v},t) = \int_{\mathbb{R}^{3N}} G(\mathbf{v},\mathbf{w},t)e^{-\pi|\mathbf{w}|^2}d\mathbf{w}$$

and

$$H(f(\cdot,t)|\gamma_M) = \int_{\mathbb{R}^{3M}} g(\mathbf{v},t)\log g(\mathbf{v},t)e^{-\pi|\mathbf{v}|^2}d\mathbf{v}\,.$$

We also note that the time evolution for G is essentially the same as the one for F. In this new representation, we define the *information*

$$I(g) = \int_{\mathbb{R}^{3M}} \frac{|\nabla g(\mathbf{v})|^2}{g(\mathbf{v})}e^{-\pi|\mathbf{v}|^2}d\mathbf{v}\,.$$

The following theorem about the decay of information is proven in [18]. A sketch of the proof is given at the end of the section.

Theorem 6. *Assume that the initial distribution $f_0 \in L^1(\mathbb{R}^M)$ has finite second moment and $\sqrt{f_0} \in H^1(\mathbb{R}^M)$. Assume further that*

$$\int_{\mathbb{S}^2} \sigma_i\sigma_j\,\rho(d\sigma) = C\cdot\delta_{ij}\,, \tag{28}$$

for some constant $C \in \mathbb{R}$. Then

$$I(g(\cdot,t)) \leq \left(\frac{M}{M+N} + \frac{N}{M+N}e^{-\frac{\mu}{3}\frac{M+N}{N}t}\right) I(g_0)\,. \tag{29}$$

Theorem 5 can be derived from Theorem 6. To see this, consider the Ornstein-Uhlenbeck semigroup on $\mathbb{R}^{3M+3N}$ defined as

$$P_s G(\mathbf{v},\mathbf{w}) = \int_{\mathbb{R}^{3M+3N}} G(e^{-s}(\mathbf{v},\mathbf{w}) + \sqrt{1-e^{-2s}}(\mathbf{x},\mathbf{y}))e^{-\pi[|\mathbf{x}|^2+|\mathbf{y}|^2]}\,d\mathbf{x}\,d\mathbf{y}\,.$$

It is well known and easy to check that

$$H(g) = \int_0^\infty I(P_{M,s}g)\,ds,$$

where we denoted by $P_{M,s}$ the Ornstein-Uhlenbeck semigroup on $\mathbb{R}^{3M}$. To use this connection between entropy and information, we first claim that for all $s,t \geq 0$

$$P_s e^{-\mathcal{L}_R t} = e^{-\mathcal{L}_R t} P_s .$$

The collision law is given by a reflection in $\mathbb{R}^{3M+3N}$ which commutes with P_s, i.e. the operators $R_{i,j}$ representing the reflections of a single collision process commute with P_s. Since the time evolution operator is an average over reflections, the claim follows.

Further, we observe that

$$\begin{aligned}
&\int_{\mathbb{R}^{3N}} P_s G(\mathbf{v},\mathbf{w}) e^{-\pi|\mathbf{w}|^2}\, d\mathbf{w} \\
&\quad = \int G(e^{-s}v + \sqrt{1-e^{-2s}}x, e^{-s}w + \sqrt{1-e^{-2s}}y) e^{-\pi[|\mathbf{x}|^2+|\mathbf{y}|^2]} e^{-\pi|\mathbf{w}|^2}\, d\mathbf{x}\, d\mathbf{y}\, d\mathbf{w}
\end{aligned}$$

which by choosing variables $p = e^{-s}w + \sqrt{1-e^{-2s}}y$ and $q = -\sqrt{1-e^{-2s}}w + e^{-s}y$ equals

$$\begin{aligned}
&\int G(e^{-s}v + \sqrt{1-e^{-2s}}x, p) e^{-\pi[|\mathbf{x}|^2+|\mathbf{p}|^2+|\mathbf{q}|^2]}\, d\mathbf{x}\, d\mathbf{p}\, d\mathbf{q} \\
&\qquad = \int G(e^{-s}v + \sqrt{1-e^{-2s}}x, p) e^{-\pi[|\mathbf{x}|^2+|\mathbf{p}|^2]}\, d\mathbf{x}\, d\mathbf{p} \\
&\qquad = P_{M,s} g(\mathbf{v}) .
\end{aligned}$$

This enables us to compute

$$\begin{aligned}
H(g(\cdot,t)|\gamma_M) &= \int_0^\infty I(P_{M,s} g(\mathbf{v},t))\, ds = \int_0^\infty I\left(\int_{\mathbb{R}^{3N}} P_s G(\mathbf{v},\mathbf{w})\, e^{-\pi|\mathbf{w}|^2}\, d\mathbf{w} \right) ds \\
&= \int_0^\infty I\left(\int_{\mathbb{R}^{3N}} \left[P_s e^{-\mathcal{L}_R t} g_0 \right](\mathbf{v},\mathbf{w})\, e^{-\pi|\mathbf{w}|^2}\, d\mathbf{w} \right) ds .
\end{aligned}$$

Using that $P_s e^{-\mathcal{L}_R t} = e^{-\mathcal{L}_R t} P_s$, we get

$$\begin{aligned}
H(g(\cdot,t)|\gamma_M) &= \int_0^\infty I\left(\int_{\mathbb{R}^{3N}} \left[e^{-\mathcal{L}_R t} P_s g_0 \right](\mathbf{v},\mathbf{w})\, e^{-\pi|\mathbf{w}|^2}\, d\mathbf{w} \right) ds \\
&= \int_0^\infty I\left(\int_{\mathbb{R}^{3N}} \left[e^{-\mathcal{L}_R t} P_{M,s} g_0 \right](\mathbf{v},\mathbf{w})\, e^{-\pi|\mathbf{w}|^2} d\mathbf{w} \right) ds .
\end{aligned}$$

Applying theorem 6 to the function $[P_{M,s} g](\mathbf{v},t)$ yields the desired bound

$$\begin{aligned}
H(g(\cdot,t)|\gamma_M) &\leq \left(\frac{M}{M+N} + \frac{N}{M+N} e^{-\mu \frac{M+N}{3N} t} \right) \int_0^\infty I(P_{M,s} g_0(\mathbf{v}))\, ds \\
&= \left(\frac{M}{M+N} + \frac{N}{M+N} e^{-\mu \frac{M+N}{3N} t} \right) H(g_0|\gamma_M).
\end{aligned}$$

Proof (Sketch of a proof of Theorem 6). We write the master equation as

$$\partial_t F = \Lambda[Q - I]F$$

where $\Lambda = \mu M + \lambda_S M + \lambda_R N$ and

$$Q = \frac{2\lambda_S}{(M-1)\Lambda} \sum_{i<j=1}^{M} R_{i,j} + \frac{2\lambda_R}{(N-1)\Lambda} \sum_{i<j=M+1}^{M+N} R_{i,j} + \frac{\mu}{N\Lambda} \sum_{i=1}^{M} \sum_{j=M+1}^{M+N} R_{i,j}$$

which is a convex combination of the $R_{i,j}$. Thus we may abbreviate this as

$$Q = \sum_{\text{pairs}} \lambda^{\alpha} R_{\alpha}\,.$$

with $\sum_\alpha \lambda^\alpha = 1$. The time evolution can then be written as a sum over collision histories

$$e^{\mathcal{L}t} = e^{-\Lambda t} \sum_{k=0}^{\infty} \frac{(\Lambda t)^k}{k!} Q^k = e^{-\Lambda t} \sum_{k=0}^{\infty} \frac{(\Lambda t)^k}{k!} \sum_{\underline{\alpha}_k} \lambda^{\underline{\alpha}_k} R_{\underline{\alpha}_k}\,,$$

where we used multi index notation. Each operator $R_{\underline{\alpha}_k} = R_{\alpha_k} \cdots R_{\alpha_1}$ is now a product of pair collision operators $R_\alpha = R_{i,j}$. The action on the initial condition g_0 of k-collisions is given by

$$[R_{\underline{\alpha}_k} g_0](\mathbf{v},\mathbf{w}) = \int d\rho(\sigma_1)\cdots d\rho(\sigma_k)\, g_0(M_{\underline{\alpha}_k}(\underline{\sigma}_k)(\mathbf{v},\mathbf{w}))$$

where the $3(M+N)\times 3(M+N)$ orthogonal matrix $M_{\underline{\alpha}_k}(\underline{\sigma}_k)$ is a product of collision matrices.[1] We use the notation $\underline{\sigma}_k = (\sigma_k,\ldots,\sigma_1)$. Writing

$$M_{\underline{\alpha}_k}(\underline{\sigma}_k) = \begin{bmatrix} A_{\underline{\alpha}_k}(\underline{\sigma}_k) & B_{\underline{\alpha}_k}(\underline{\sigma}_k) \\ C_{\underline{\alpha}_k}(\underline{\sigma}_k) & D_{\underline{\alpha}_k}(\underline{\sigma}_k) \end{bmatrix},$$

we find, since g_0 is only a function of the variable $\mathbf{v}$, that

$$[R_{\underline{\alpha}_k} g_0](\mathbf{v},\mathbf{w}) = \int d\rho(\sigma_1)\cdots d\rho(\sigma_k)\, g_0(A_{\underline{\alpha}_k}(\underline{\sigma}_k)\mathbf{v} + B_{\underline{\alpha}_k}(\underline{\sigma}_k)\mathbf{w}))\,.$$

Note that the last expression does not depend on $C_{\underline{\alpha}_k}(\underline{\sigma}_k)$ and $D_{\underline{\alpha}_k}(\underline{\sigma}_k)$. With the notation

$$g_{0,\underline{\alpha}_k}(\mathbf{v}) = \int_{\mathbb{R}^N} [R_{\underline{\alpha}_k} g_0](\mathbf{v},\mathbf{w})\gamma_N(\mathbf{w})\, d\mathbf{w}\,,$$

[1] Note that the collision mechanism (24) is linear, i.e it can be represented by a matrix

$$\begin{pmatrix} v_i^*(\sigma) \\ v_j^*(\sigma) \end{pmatrix} = M^{\sigma}_{(i,j)} \begin{pmatrix} v_i \\ v_j \end{pmatrix}, \quad M^{\sigma}_{(i,j)} := \begin{pmatrix} I - \sigma\oplus\sigma & \sigma\oplus\sigma \\ \sigma\oplus\sigma & I - \sigma\oplus\sigma \end{pmatrix}. \tag{30}$$

Extending $M^{\sigma}_{(i,j)}$ such that it leaves all other particles invariant, we obtain a collision matrix $\underline{M}^{\sigma}_{(i,j)}$ acting on $\mathbb{R}^{3M+3N}$ that satisfies $F(u_1,\ldots,u_i^*(\sigma),\ldots,u_j^*(\sigma),\ldots,u_{M+N}) = F(\underline{M}^{\sigma}_{(i,j)}\mathbf{u})$.

we find using the convexity of information that

$$I(g(\cdot,t)) \leq e^{-\Lambda t} \sum_{k=0}^{\infty} \frac{(\Lambda t)^k}{k!} \sum_{\underline{\alpha}_k} \lambda^{\underline{\alpha}_k} I(g_{0,\underline{\alpha}_k}(\cdot)) .$$

This reduces the problem to showing the decay of information caused by a sequence of collisions. Note that this is now separated from the evolution in time.

A straightforward computation using convexity and the fact that $M_{\underline{\alpha}_k}(\underline{\sigma}_k)$ is an orthogonal matrix, shows that

$$I(g_{\underline{\alpha}_k}(\cdot)) \leq \int \rho(d\sigma_1)\cdots\rho(d\sigma_k) \int_{\mathbb{R}^{3M}} \frac{(\nabla g_0)^T(\mathbf{v}) A_{\underline{\alpha}_k}(\underline{\sigma}_k)^T A_{\underline{\alpha}_k}(\underline{\sigma}_k)(\nabla g_0)(\mathbf{v})}{g_0(\mathbf{v})} \gamma_M(\mathbf{v})\, d\mathbf{v} .$$

After a somewhat more difficult calculation using the symmetry assumption on the probability measure ρ, one can see that

$$e^{-\Lambda t} \sum_{k=0}^{\infty} \frac{(\Lambda t)^k}{k!} \sum_{\underline{\alpha}_k} \lambda^{\underline{\alpha}_k} \int \rho(d\sigma_1)\cdots\rho(d\sigma_k) A_{\underline{\alpha}_k}(\underline{\sigma}_k)^T A_{\underline{\alpha}_k}(\underline{\sigma}_k) = \left[\frac{M}{M+N} + \frac{N}{M+N} e^{-\frac{\mu}{3}\frac{M+N}{N}t} \right] I_{3M} .$$

The last three (in-)equalities prove theorem 6. For the details we refer the reader to [18]. □

5 A quantum Kac model

Pair collisions of molecules, and more generally, pair interactions of microscopic particles, are properly described by quantum mechanics. It is natural to ask how quantum mechanics can be incorporated in Kac type models. Towards this end, let us return to (1) and write it another way, which, while a little more complex, opens an interesting door. It is well known since the work of Koopman [24] and von Neumann [29] that the classical mechanical time evolution can be written in terms of unitary flows on the Hilbert space consisting of the phase space equipped with Liouville measure (which is preserved by the classical flow). This perspective brings the classical and quantum dynamics close together, and is our point of departure.

Introduce the Hilbert space $L^2(\mathbb{R}^n)$, and define for $1 \leq i < j \leq N$, $\theta \in [0, 2\pi)$, the unitary operator $U_{i,j,\theta}$ by

$$U_{i,j,\theta}\psi(\mathbf{v}_N) = \psi(\mathbf{v}_N(i,j;\theta))$$

where $\mathbf{v}_N(i,j;\theta)$ is the pair rotation of $\mathbf{v}_N$ specified in (2) and (3). To any probability density F on $\mathbb{R}^N$, associate the multiplication operator ρ_F on $L^2(\mathbb{R}^n)$ by

$$\rho_F \psi(\mathbf{v}_N) := F(\mathbf{v}_N)\psi(\mathbf{v}_N).$$

Note that ρ_F is in general an unbounded positive operator. It is then easy to check that

$$U_{i,j,\theta}\rho_F U_{i,j,\theta}^* = \rho_G \quad \text{where} \quad G(\mathbf{v}_N) = F(\mathbf{v}_N(i,j;\theta)) \ .$$

In particular, for each i, j and θ, $U_{i,j,\theta}\rho_F U_{i,j,\theta}^*(\mathbf{v}_N)$ has the form ρ_G where G is another probability density on $\mathbb{R}^N$

$$\begin{aligned}\binom{N}{2}^{-1} &\sum_{i<j}\left(\frac{1}{2\pi}\int_0^{2\pi}\rho_F(\mathbf{v}_N(i,j;\theta))d\theta\right)\\ &= \binom{N}{2}^{-1}\sum_{i<j}\left(\frac{1}{2\pi}\int_0^{2\pi}\left[U_{i,j,\theta}\psi(\mathbf{v}_N)\rho_F U_{i,j,\theta}\psi(\mathbf{v}_N)^*(\mathbf{v}_N)\right]d\theta\right)\\ &=: \mathcal{Q}(\rho_F) \ . \end{aligned} \tag{31}$$

We can then rewrite (1) as

$$\frac{\partial}{\partial t}\rho_{F(t)} = N\left[\mathcal{Q}(\rho_{F(t)}) - \rho_{F(t)}\right]. \tag{32}$$

In kinetic theory, the collisions take place on a much more rapid time scale than in Kac Master Equation, and thus are instantaneous. Each unitary transformation $U_{i,j,\theta}$ in this Koopman-von Neumann picture represents the final phase space transformation associated to one type of a completed collision between particles i and j. The operator $\mathcal{Q}$ represents an average over the output densities for all kinematically possible collisions.

Between collisions, when the particles are not interacting, the energy is simply given by $H := \sum_{j=1}^N v_j^2$, but this does not encode the part of the dynamics that drives the collisions. However, the absolutely crucial point is that with H regarded as a multiplication operator, for each i, j and θ, $U_{i,j,\theta}HU_{i,j,\theta}^* = H$. Thus H commutes with the unitary describing each collision, which is the analytical expression of the fact that the collisions conserve the energy in this Koopman-von Neumann picture.

In [13] this point of view was developed to define a Quantum Markov Semigroup that describes pair collisions of quantum particles. The energy of a single particle is given by a Hamiltonian h on a Hilbert space $\mathcal{H}$ which we take to be finite dimensional for simplicity. A state of the system of N particles is described by a density matrix ρ on $\otimes^N\mathcal{H} = \mathcal{H}_N$, i.e. a self adjoint positive trace class operator with unit trace. The role of the kinetic energy in the classical Kac model is now taken by the N-particle Hamiltonian

$$H_N = \sum_{j=1}^N I\otimes\cdots I\otimes h_i\otimes I\cdots\otimes I \ .$$

One specifies the binary collisions by a family of unitary operators $U(\sigma)$ on the two particle Hilbert space $\mathcal{H}_2 = \mathcal{H}\otimes\mathcal{H}$ that commute with $H_2 = h\otimes I + I\otimes h$. Here σ

lives in a measure space $(\mathcal{C}, \nu)$. The precise conditions will be given below. Note that if we extend $U(\sigma)$ to the other factors of the tensor product by the identity, then $U(\sigma)$ also commutes with H_N. The collision operator $\mathcal{Q} : \mathcal{B}(\mathcal{H}_2) \to \mathcal{B}(\mathcal{H}_2)$ is given by

$$\mathcal{Q}(A) = \int_{\mathcal{C}} U(\sigma) A U^*(\sigma)\, d\nu(\sigma)$$

where $\mathcal{B}(\mathcal{H}_2)$ denotes the space of bounded operators on $\mathcal{H}_2$. Note the parallel with (31).

The measure ν is a probability measure and it is easily seen that $\mathcal{Q}$ is a trace preserving map that is positivity preserving, in fact completely positive. Since $U(\sigma)$ commutes with H_2 this collision process preserves energy, i.e. if all the eigenstates of A have the same energy so does $\mathcal{Q}(A)$. Naturally, one wants that the collision of particle 1 with particle 2 and the collision of particle 2 with particle 1 leads to the same result. If V denotes the swap operation

$$V(\phi \otimes \psi) = \psi \otimes \phi$$

then one imposes the condition that

$$\{U(\sigma) : \sigma \in \mathcal{C}\} = \{VU(\sigma)V^* : \sigma \in \mathcal{C}\}$$

and the map $\sigma \to \sigma'$ where $VU(\sigma)V^* = U(\sigma')$ is a measurable transformation that leaves ν invariant. It is also desirable that the collision satisfies local reversibility, i.e. that

$$\{U(\sigma) : \sigma \in \mathcal{C}\} = \{U^*(\sigma) : \sigma \in \mathcal{C}\},$$

and the map $\sigma \to \sigma'$ where $U^*(\sigma) = U(\sigma')$ is a measurable transformation that leaves ν invariant. One easily sees that for any two operators A, B on $\mathcal{H}_2$ one has

$$Tr(A^* \mathcal{Q}(B)) = Tr(\mathcal{Q}(A)^* B)$$

i.e. the operation is self adjoint on the Hilbert space $\mathcal{B}(\mathcal{H}_2)$ with inner product $(A,B) = Tr(A^*B)$. We call $(\mathcal{C}, U, \nu)$ satisfying these conditions a collision specification.

The Quantum Kac Master Equation is then

$$\frac{\partial}{\partial t}\rho(t) = N[\mathcal{Q}(\rho)(t) - \rho(t)]\,, \tag{33}$$

which is formally very similar to (32). We shall be interested in the same sort of questions that we asked about solutions of (32). In particular, we shall be concerned with the long time behavior, and in this context, the question of ergodicity is crucial. Denote by $\mathcal{A}_2$ the commutative subalgebra of $\mathcal{B}(\mathcal{H}_2)$ consisting of all operators that are of the form $f(H_2)$ where $f : \sigma(H_2) \to \mathbb{C}$ is a continuous bounded function. Obviously $\mathcal{A}_2$ is a subset of $\{U(\sigma) : \sigma \in \mathcal{C}\}'$, the commutant of $\{U(\sigma) : \sigma \in \mathcal{C}\}$. We shall require that the two particle collisions are ergodic, that is

$$\mathcal{A}_2 = \{U(\sigma) : \sigma \in \mathcal{C}\}'.$$

In this case, *at least for* $N = 2$, the steady state solutions of (33) are exactly the density matrices ρ of the form $\rho = f(H_2)$ for some f. A natural question then is when ergodicity at the level of 2 particles implies ergodicity at the level of N particles.

5.1 Example

The following example taken from [13] is useful for understanding these concepts. For the simplest possible example, take $\mathbb{H} = \mathbb{C}^2$, so that $\mathcal{H}_2 = (\mathbb{C}^2)^{\otimes 2}$. Define the single particle Hamiltonian h by $h = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$. Identify $\mathbb{C}^2 \otimes \mathbb{C}^2$ with $\mathbb{C}^4$ using the basis

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

The standard physics notation for this basis is simply

$$|00\rangle, \quad |10\rangle, \quad |01\rangle, \quad |11\rangle, \tag{34}$$

which will be useful. With this identification of $\mathbb{C}^2 \otimes \mathbb{C}^2$ with $\mathbb{C}^4$,

$$\begin{bmatrix} a_{1,1} & a_{1,2} \\ a_{2,1} & a_{2,2} \end{bmatrix} \otimes \begin{bmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{bmatrix} =: A \otimes B \quad \text{is represented by} \quad \begin{bmatrix} b_{1,1}A & b_{1,2}A \\ b_{2,1}A & b_{2,2}A \end{bmatrix}.$$

(Switching the order of the second and third basis elements swaps the roles of A and B in the block matrix representation of the tensor product $A \otimes B$.)

In this basis,

$$H_2 = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \otimes I + I \otimes \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix}.$$

Therefore, the spectrum of H_2 is $\{0,1,2\}$ and

$$P_0 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad P_1 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad \textit{and} \quad P_2 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

Now define $\mathcal{C} = \mathbb{S}^1 \times \mathbb{S}^1 \times \mathbb{S}^1 \times \mathbb{S}^1$ identifying each copy of $\mathbb{S}^1$ with the unit circle in $\mathbb{C}$ so that the general point in $\sigma \in \mathcal{C}$ has the form $\sigma = (e^{i\varphi}, e^{i\theta}, e^{i\psi}, e^{i\eta})$. Then

define

$$U(\sigma) := \begin{bmatrix} e^{i\theta} & 0 & 0 & 0 \\ 0 & e^{i\psi}\cos\theta & -e^{i\varphi}\sin\theta & 0 \\ 0 & e^{-i\varphi}\sin\theta & e^{-i\psi}\cos\theta & 0 \\ 0 & 0 & 0 & e^{i\eta} \end{bmatrix}$$

Choosing ν to be the uniform probability measure on $\mathcal{C}$ gives us a collision specification $(\mathcal{C}, U, \nu)$.

A simple computation shows that for every operator A on $\mathcal{H}_2 = \mathbb{C}^2 \otimes \mathbb{C}^2$ identified as the 4×4 matrix with entries $a_{i,j}$ using the basis (34),

$$\mathcal{Q}(A) = \int_{\mathcal{C}} d\nu(\sigma) U(\sigma) A U^*(\sigma) = \begin{bmatrix} a_{1,1} & 0 & 0 & 0 \\ 0 & \frac{1}{2}(a_{2,2}+a_{3,3}) & 0 & 0 \\ 0 & 0 & \frac{1}{2}(a_{2,2}+a_{3,3}) & 0 \\ 0 & 0 & 0 & a_{4,4} \end{bmatrix}$$
$$= a_{1,1}P_0 + \frac{a_{2,2}+a_{3,3}}{2} P_1 + a_{4,4}P_2 \in \mathcal{A}_2 \,. \quad (35)$$

Therefore,

$$\{U(\sigma) \,:\, \sigma \in \mathcal{C}\}' \subset \mathrm{ran}(\mathcal{Q}) \subset \mathcal{A}_2 \subset \{U(\sigma) \,:\, \sigma \in \mathcal{C}\}' ,$$

showing that $(\mathcal{C}, U, \nu)$ is ergodic.

Using these preliminaries it is now straightforward to write the corresponding Quantum Master Equation (QME) as

$$\partial_t \rho = -\mathfrak{L}_N(\rho)$$

with

$$\mathfrak{L}_N(A) = N \binom{N}{2}^{-1} \sum_{i<j} [A - \mathcal{Q}_{i,j}(A)] \quad (36)$$

and where the unitaries in the definition of $\mathcal{Q}_{i,j}$ act nontrivially only on the i-th and j-th factors in the tensor product $\otimes^N \mathcal{H}$. This is a trace preserving completely positive map, i.e. a Quantum Evolution.

5.2 Propagation of chaos

A density matrix is symmetric if it is invariant under the swap operation between any two factors in the tensor product $\otimes^N \mathcal{H}$. A sequence of symmetric density matrices $\{\rho_N\}_{N=1}^{\infty}$ is chaotic with marginal ρ, or in short ρ-chaotic, if

$$\lim_{N\to\infty} \mathrm{Tr}_{2,\ldots,N}\, \rho_N = \rho \text{ and } \lim_{N\to\infty} \mathrm{Tr}_{k+1,\ldots,N}\, \rho_N = \otimes^k \rho$$

where $\mathrm{Tr}_{k+1,\dots,N}$ is the trace taken in the factors $k+1,\dots,N$. A trivial example of a chaotic sequence is $\otimes^N \rho$, but one can also construct chaotic sequences that have a sharply defined energy for large N.

We have (see [13])

Theorem 7. *Let $\{U(\sigma)\ \sigma \in \mathcal{C}\}$ be a set of collision operators and let ν be a given Borel probability measure on $\mathcal{C}$. Let $\mathfrak{L}_N$ be defined in terms of these as in (36). Then the semigroup $\mathcal{P}_{N,t} = e^{t\mathfrak{L}_N}$ propagates chaos for all t meaning that if $\{\rho_N\}_{N\in\mathbb{N}}$ is a ρ-chaotic sequence, then for each t, $\{\mathcal{P}_{N,t}\rho_N\}_{N\in\mathbb{N}}$ is a $\rho(t)$-chaotic sequence for some $\rho(t) = \lim_{N\to\infty}(\mathcal{P}_{N,t}\rho_N)^{(1)}$, where in particular this limit of the one-particle marginal exists and is a density matrix.*

As expected the marginal density matrix $\rho(t)$ satisfies a Quantum Kac-Boltzmann equation

$$\frac{d}{dt}\rho(t) = 2(\rho(t)\star\rho(t) - \rho(t))$$

where quite generally for operators in $\mathcal{B}(\mathcal{H})$

$$A\star B = \mathrm{Tr}_2\left[d\nu(\sigma)\,U(\sigma)[A\otimes B]U^*(\sigma)\right] = \mathrm{Tr}_2[\mathcal{Q}(A\otimes B)]$$

is the Quantum Wild Convolution.

5.3 Equilibrium states

An equilibrium density matrix for the evolution (36) is given by all those density matrices ρ_N that satisfy

$$\mathfrak{L}_N(\rho_N) = 0\,.$$

Recall that the N-particle Hamiltonian is $H_N = \sum_{j=1}^N h_j$ where h_j is the single particle Hamiltonian acting on the jth factor. List the eigenvalues of h as $e_1,\dots,e_K$ counting their multiplicities and denote the corresponding eigenvectors by $\phi_1,\dots,\phi_K$. Using the multi-index notation $\alpha = (\alpha_1,\dots,\alpha_N)$ where $\alpha_j \in \{1,\dots,K\}, j = 1,\dots,N$ the eigenvalues of H_N are given by $E_\alpha = \sum_{j=1}^N e_{\alpha_j}$ and $\Psi_\alpha = \phi_{\alpha_1}\otimes\cdots\otimes\phi_{\alpha_N}$ are the eigenvectors.

It is not very difficult to show that the set $\mathfrak{C}_N$ of equilibrium states forms a commutative von Neumann algebra, and hence it is generated by the minimal projections. The algebra $\mathcal{A}_N$ consisting of all operators of the form $f(H_N)$, where f is a bounded continuous function, is a sub-algebra of $\mathfrak{C}_N$ and it is generated by the spectral projections of the Hamiltonian H_N. Define two multi-indices α,α' to be adjacent if for some pair (i,j), $e_{\alpha_i} + e_{\alpha_j} = e_{\alpha'_i} + e_{\alpha'_j}$ and $\alpha_k = \alpha'_k, k \neq i,j$. With this notion of adjacency the multi-indices α form a graph, the adjacency graph $\mathcal{G}_N$. We denote by $\gamma_1,\dots,\gamma_n$ the connected components of $\mathcal{G}_N$. In [13] the following theorem is proved.

Theorem 8. *The minimal projections of $\mathfrak{C}_N$ are in one to one correspondence with the connected components of the adjacency graph $\mathcal{G}_N$ and are given by*

$$\mathcal{P}_k = \sum_{\alpha\in\gamma_k} |\Psi_\alpha\rangle\langle\Psi_\alpha| .$$

Ergodicity in our context is the notion that the only equilibrium states of the Quantum Kac Model are given by the algebra $\mathcal{A}_N$. By the above theorem this is the case if the connected components of the adjacency graph are determined by the energies of the Hamiltonian H_N. The occupation number representation is useful in this context. We write $E_\alpha = \sum_{j=1}^K k_j(\alpha)e_j$ where $k_j(\alpha)$ denotes the number of times the index j occurs in α. Thus, if the energies of h, $\{e_1,\dots,e_K\}$ are rationally independent then any eigenvalue of H_N is uniquely determined by the occupation numbers $k_1(\alpha),\dots,k_K(\alpha)$ (see below). Hence, in this case we have that the minimal projections of $\mathfrak{C}_N$ are eigenprojections of H_N and hence $\mathfrak{C}_N = \mathcal{A}_N$.

Here is an example where $\mathfrak{C}_N \neq \mathcal{A}_N$. Assume the single particle Hamiltonian has the eigenvalues $1,2,4$ with the corresponding eigenvectors ψ_1,ψ_2,ψ_3. Then pick n_1 to be even integers and set

$$n_2 = N - \frac{3}{2}n_1 , \quad n_3 = \frac{1}{2}n_1 .$$

Then

$$n_1 + 2n_2 + 4n_3 = 2N , n_1 + n_2 + n_3 = N .$$

The number $e = 2N$ is an eigenvalue of the Hamiltonian H_N and it is degenerate. The eigenvectors are of the form $\psi_{\alpha_1}\otimes\cdots\otimes\psi_{\alpha_N}$ where $\alpha_j \in \{1,2,3\}$. We set $\alpha = (\alpha_1,\dots,\alpha_N)$ and $n_1(\alpha)$ the number of ψ_1 factors, $n_2(\alpha)$ the number of ψ_2 factors and $n_3(\alpha)$ the number of ψ_3 factors. If α and β are adjacent, then the condition $e_{\alpha_k} + e_{\alpha_\ell} = e_{\beta_k} + e_{\beta_\ell}$ implies that either $e_{\alpha_k} = e_{\beta_k}$ and $e_{\alpha_\ell} = e_{\beta_\ell}$ or $e_{\alpha_k} = e_{\beta_\ell}$ and $e_{\alpha_\ell} = e_{\beta_k}$; anything else is not possible. Hence for any of the indices α and β to be adjacent, we must have that $n_1(\alpha) = n_1(\beta)$, $n_2(\alpha) = n_2(\beta)$, $n_3(\alpha) = n_3(\beta)$. Thus, if these triples are different, but with the same N and e, the two states are not adjacent and hence $\mathcal{G}_{e,N}$, the adjacency graph for a fixed energy e is not a connected graph. The number of elements in a connected component of $\mathcal{G}_{e,N}$ is given by

$$\frac{N!}{n_1!n_2!n_3!}$$

where $N = n_1 + n_2 + n_3$.

The Quantum Kac Master Equation (QKME), being a completely positive map can be written in terms of Kraus operators (see [10]). The collision specifications yield that the Kraus operators are self-adjoint and hence the QKME can be brought into a Lindblad form $\partial_t\rho = \sum_k [V_k,[V_k,\rho]]$. An example, closely related to Example 5.1, is the following Lindblad equation $\partial_t\rho = L_N(\rho)$, where

$$L_N(\rho) = \frac{1}{N-1} \sum_{[\alpha,\beta]\in\mathcal{E}_N} [L_{\alpha,\beta}, [L_{\alpha,\beta}, \rho]] \,.$$

Here, $\mathcal{E}_N$ is the edge set of the graph $\mathcal{G}_N$. With $F_{\alpha,\beta} = |\Psi_\alpha\rangle\langle\Psi_\beta|$, the 'angular' momentum operators $L_{\alpha,\beta}$ are given by

$$L_{\alpha,\beta} = F_{\alpha,\beta} - F_{\beta,\alpha} \,.$$

Note that in Example 5.1 the operator given by the collision specifications is L_N up to a factor that commutes with the angular momenta $L_{\alpha,\beta}$. The interesting point is that the gap of the generator L_N is given by the gap of the combinatorial or graph Laplacian on $\mathcal{G}_N$. To describe this we shall assume that the eigenvalues of h are rationally independent. The energies of the Hamiltonian H_N are given by

$$E(\alpha) = \sum_{j=1}^{K} k_j(\alpha) e_j$$

where the $k_j(\alpha)$ are integers and $\sum_{j=1}^K k_j(\alpha) = N$. Since the e_j's are rationally independent, the eigenvalues of H_N are in one to one correspondence with the 'occupation numbers' $\mathbf{k}(\alpha) = (k_1(\alpha), \dots, k_K(\alpha))$. Next, note that $\mathbf{k}(\alpha) = \mathbf{k}(\beta)$ if and only if α and β are related by a finite sequence of pair transpositions. Thus, $H\Psi_\alpha = E\Psi_\alpha$ and $H_N\Psi_\beta = E\Psi_\beta$ if and only if α and β are adjacent in $\mathcal{G}_N$. In other words, there is a one to one correspondence between the eigenspaces of H_N and the connected components of $\mathcal{G}_N$. This is precisely the case in Example 5.1. Indeed the energies of $\mathcal{H}_N$ are given by

$$E(\alpha) = k_1(\alpha) \times 0 + k_2(\alpha) \times 1$$

and with $k_1(\alpha) + k_2(\alpha) = N$ the occupation numbers determine $E(\alpha)$ uniquely. The vertices of the graph $\mathcal{G}_N$ are given by multi indices of length N consisting of 1s and 0s and two indices are connected if one can be transformed into the other by a series of transpositions. Thus, in this case multi indices are adjacent if and only if they have the same number of 0s and hence 1s and clearly the occupation numbers determine the connected components of $\mathcal{G}_N$ uniquely. The subgraphs given by the connected components are well known under the name Johnson Graphs or Johnson Association Schemes. In particular the eigenvalues of the graph Laplacian of these graphs are all known as are the eigenvectors [16]. The following theorem is a special case of a result that will appear in [10].

Theorem 9. *Assume that the eigenalues of h are rationally independent and $N > 2$. Then the gap of $\mathcal{L}_N$ is*

$$\frac{2N}{N-1} \,.$$

Much remains to be understood concerning the Quantum Kac Master Equation. At present, little is known about sharp entropy production inequalities. Beyond this, there are very interesting questions that have no classical analog – these questions concern *entanglement* which Schrödinger singled out as the fundamental feature

setting quantum mechanics apart from classical mechanics. The equilibrium states of the Quantum Kac Master Equations studied here are *separable*; that is, free of entanglement. The rate at which entanglement is "broken" along the flow is of physical interest, and has been investigated in related models [20].

We hope this account of various aspects of the Kac model, classical and quantum, inspires further progress in this favorite field of research of Maria Carvalho.

References

1. Thierry Bodineau, Isabelle Gallagher, and Laure Saint-Raymond. The Brownian motion as the limit of a deterministic system of hard-spheres. *Invent. Math.*, 203(2):493–553, 2016.
2. Ludwig Boltzmann. *Lectures on gas theory*. University of California Press, Berkeley-Los Angeles, Calif., 1964. Translated by Stephen G. Brush.
3. F. Bonetto, R. Han, and M. Loss. Decay of information for the Kac evolution. *Ann. Henri Poincaré*, 22(9):2975–2993, 2021.
4. F. Bonetto, M. Loss, H. Tossounian, and R. Vaidyanathan. Uniform approximation of a Maxwellian thermostat by finite reservoirs. *Comm. Math. Phys.*, 351(1):311–339, 2017.
5. Federico Bonetto, Alissa Geisinger, Michael Loss, and Tobias Ried. Entropy decay for the Kac evolution. *Comm. Math. Phys.*, 363(3):847–875, 2018.
6. Federico Bonetto, Michael Loss, and Ranjini Vaidyanathan. The Kac model coupled to a thermostat. *J. Stat. Phys.*, 156(4):647–667, 2014.
7. E. Carlen, M. C. Carvalho, and M. Loss. Many-body aspects of approach to equilibrium. In *Séminaire: Équations aux Dérivées Partielles, 2000–2001*, Sémin. Équ. Dériv. Partielles, pages Exp. No. XIX, 12. École Polytech., Palaiseau, 2001.
8. E. A. Carlen, M. C. Carvalho, and M. Loss. Determination of the spectral gap for Kac's master equation and related stochastic evolution. *Acta Math.*, 191(1):1–54, 2003.
9. Eric Carlen, Maria Carvalho, and Michael Loss. Spectral gaps for reversible Markov processes with chaotic invariant measures: the Kac process with hard sphere collisions in three dimensions. *Ann. Probab.*, 48(6):2807–2844, 2020.
10. Eric Carlen and Michael Loss. *in preparation*, 2023.
11. Eric A. Carlen, José A. Carrillo, and Maria C. Carvalho. Strong convergence towards homogeneous cooling states for dissipative Maxwell models. *Ann. Inst. H. Poincaré C Anal. Non Linéaire*, 26(5):1675–1700, 2009.
12. Eric A. Carlen, Maria C. Carvalho, Jonathan Le Roux, Michael Loss, and Cédric Villani. Entropy and chaos in the Kac model. *Kinet. Relat. Models*, 3(1):85–122, 2010.
13. Eric A. Carlen, Maria C. Carvalho, and Michael P. Loss. Chaos, ergodicity, and equilibria in a quantum Kac model. *Adv. Math.*, 358:106827, 50, 2019.
14. Roberto Cortez and Hagop Tossounian. Uniform propagation of chaos for the thermostated Kac model. *J. Stat. Phys.*, 183(2):Paper No. 28, 17, 2021.
15. Amit Einav. On Villani's conjecture concerning entropy production for the Kac master equation. *Kinet. Relat. Models*, 4(2):479–497, 2011.
16. Yuval Filmus. An orthogonal basis for functions over a slice of the Boolean hypercube. *Electron. J. Combin.*, 23(1):Paper 1.23, 27, 2016.
17. Ester Gabetta, Guiseppe Toscani, and Bernt Wennberg. Metrics for probability distributions and the trend to equilibrium for solutions of the boltzmann equation. *Journal of statistical physics*, 81:901–934, 1995.
18. Lukas Hauger. Decay of entropy and information for multidimensional kac models. *arXiv preprint arXiv:2301.09592*, 2023.
19. R. Illner and M. Pulvirenti. Global validity of the Boltzmann equation for two- and three-dimensional rare gas in vacuum. Erratum and improved result: "Global validity of the Boltzmann equation for a two-dimensional rare gas in vacuum" [Comm. Math. Phys. **105** (1986),

no. 2, 189–203; MR0849204 (88d:82061)] and "Global validity of the Boltzmann equation for a three-dimensional rare gas in vacuum" [ibid. **113** (1987), no. 1, 79–85; MR0918406 (89b:82052)] by Pulvirenti. *Comm. Math. Phys.*, 121(1):143–146, 1989.

20. Matteo Ippoliti, Michael J. Gullans, Sarang Gopalakrishnan, David A. Huse, and Vedika Khemani. Entanglement phase transitions in measurement-only dynamics. *Phys. Rev. X*, 11:011030, Feb 2021.
21. Elise Janvresse. Spectral gap for Kac's model of Boltzmann equation. *Ann. Probab.*, 29(1):288–304, 2001.
22. M. Kac. Foundations of kinetic theory. In *Proceedings of the Third Berkeley Symposium on Mathematical Statistics and Probability, 1954–1955, vol. III*, pages 171–197. University of California Press, Berkeley-Los Angeles, Calif., 1956.
23. M. Kac. *Probability and related topics in physical sciences*, volume 1957 of *Lectures in Applied Mathematics (Proceedings of the Summer Seminar, Boulder, Colorado*. Interscience Publishers, London-New York, 1959. With special lectures by G. E. Uhlenbeck, A. R. Hibbs, and B. van der Pol.
24. Bernard O. Koopman. Hamiltonian systems and transformations in Hilbert space. *Proceedings of the National Academy of Sciences*, 17(5):315–318, 1931.
25. Oscar E. Lanford, III. A derivation of the Boltzmann equation from classical mechanics. In *Probability (Proc. Sympos. Pure Math., Vol. XXXI, Univ. Illinois, Urbana, Ill., 1976)*, pages 87–89. Amer. Math. Soc., Providence, R.I., 1977.
26. Stéphane Mischler and Clément Mouhot. Kac's program in kinetic theory. *Invent. Math.*, 193(1):1–147, 2013.
27. Alain-Sol Sznitman. Équations de type de Boltzmann, spatialement homogènes. *Z. Wahrsch. Verw. Gebiete*, 66(4):559–592, 1984.
28. Cédric Villani. Cercignani's conjecture is sometimes true and always almost true. *Comm. Math. Phys.*, 234(3):455–490, 2003.
29. John von Neumann. Zur Operatorenmethode in der klassischen Mechanik. *Annals of Mathematics (in German)*, 33(3):587–642, 1932.