THE KAC MODEL: VARIATIONS ON A THEME

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ABSTRACT

The Kac master equation provides a simple framework to understand systems of particles that interact through pairwise collisions. This article is a short review of results, chief among them is the approach to equilibrium for a gas of particles that undergo energy and momentum preserving collisions, as well as results on the entropy and information decay for a one-dimensional Kac system coupled to a reservoir. The principles underlying the Kac master equation can be extended to a Quantum Master Equation (QME) where the time evolution acts on density matrices and is a completely positive trace-preserving map. There is a rich set of equilibrium states and there is also a notion of propagation of chaos that leads to the Quantum Kac–Boltzmann equation. Likewise, the gap of the generator of the QME can be computed in certain special cases.

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1. INTRODUCTION

In 1956 Mark Kac published his influential paper "Foundations of kinetic theory" [14] in which he laid out a program to explain various issues about the interaction of a large number of particles. It is based on a model that, in its simplest form, describes a spatially homogenous gas of N particles undergoing pair collisions. Using this simple probabilistic model, he elucidated Boltzmann's chaos hypotheses and its propagation and gave a derivation of what is now known as the Kac–Boltzmann equation. He also formulated a quantitative version of approach to equilibrium known as Kac's conjecture.

The model can be described as follows: The states of the system are described by the velocities of N particles $\vec{v} = (v_1, \dots, v_N)$. If $T_{i,j}$ is the waiting time for the collision of the pair (i, j) then the first collision occurs at time $T = \min_{i,j}\{T_{i,j}\}$. If we assume that these variables are independent and that $\Pr\{T_{i,j} > t\} = e^{-2t/(N-1)}$ then T is exponentially distributed as well, with parameter N, i.e., $\Pr\{T > t\} = e^{-Nt}$. This simply reflects the fact that, on average, the collision time of a particular particle with any other particle is shortened by a factor of $1/(N-1)$. With this choice, the average number of collisions per unit time a given particle undergoes does not depend on N, as in the classical Grad–Boltzmann limit for the realistic Boltzmann equation. At time T, the pair furnishing the minimum collides and the velocity vector jumps

$$(v_1, \dots, v_i, \dots, v_j, \dots, v_N) \to (v_1, \dots, v_i^*, \dots, v_j^*, \dots, v_N).$$

The velocities v_i^* and v_j^* are then chosen according to the rule

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

where θ is picked randomly and uniformly in $[0, 2\pi)$. Obviously, the kinetic energy $\sum_{j=1}^N v_j^2$ is preserved during this process (we assume that all particles have the same mass 2 and the total energy is N) and hence we may describe this process as an evolution on the space of probability distributions $F(\vec{v}) \in L^1(\mathbb{S}^{N-1}(\sqrt{N}), d\sigma_N)$ (where σ_N is the uniform probability measure on the sphere), given by the Kac master equation

$$\partial_t F(\vec{v}, t) = -\mathcal{L}_N F(\vec{v}, t), \quad F(\vec{v}, 0) = F_0(\vec{v}), \quad \mathcal{L}_N = N(I - Q_N), \tag{1.1}$$

where

$$Q_N \phi(\vec{v}) = \frac{1}{\binom{N}{2}} \sum_{i<j} \frac{1}{2\pi} \int_0^{2\pi} \phi\big(\dots, v_i^*(\theta), \dots, v_j^*(\theta), \dots\big) d\theta.$$

The solution can be written as

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

We shall henceforth assume that the initial condition and hence the solution are symmetric, i.e., invariant under permutations of the particle labels.

On the sphere, the v_j variables are not independent, but any finite collection is asymptotically independent as the dimension $N \to \infty$. Such an "asymptotic" independence is known as "chaos" and this gets propagated by the Kac evolution. More precisely,

a sequence of distributions $\{F_N(v_1,\dots,v_N)\}_{N=1}^{\infty}$ is chaotic with marginal $f:\mathbb{R}\to\mathbb{R}_+$ if for any integer k and any bounded continuous function $\phi:\mathbb{R}^k\to\mathbb{R}$,

$$\lim_{N\to\infty}\int_{\mathbb{S}^{N-1}(\sqrt{N})} F_N(v_1,\dots,v_N)\phi(v_1,\dots,v_k)d\sigma_N = \int_{\mathbb{R}^k}\prod_{\ell=1}^{k} f(v_\ell)\phi(v_1,\dots,v_k)dv_1\cdots dv_k.$$

Kac's theorem states that if $F_{0N}(\cdot)$ is a chaotic sequence with marginal $f_0(\cdot)$ then the solution of the Kac master equation $F_N(\cdot,t)$ is chaotic with marginal $f(\cdot,t)$, which is a solution of the Kac–Boltzmann equation

$$\partial_t f(v,t) = \frac{1}{\pi}\int_{-\infty}^{\infty} dw \int_0^{2\pi} d\theta \times\left[f(v\cos\theta + w\sin\theta,t)f(-v\sin\theta + w\cos\theta,t) - f(v,t)f(w,t)\right]$$

with initial condition $f_0(v)$.

This model has several limitations. For one, it conserves only the energy since in one dimension particles that undergo energy and momentum preserving collisions either keep their velocities or exchange them. Moreover, in physical models, the likelihood of collision outcomes depends on momentum transfer and the scattering angles, while in this simplest version of the model, all energy conserving outcomes are equally likely.

The description of the Kac model for 3-dimensional momentum-preserving collisions is more involved. The velocities are now vectors in $\mathbb{R}^3$ and the evolution will take place on the space $L^1(\mathcal{S}_{N,E,p}, d\sigma_N)$ where $\mathcal{S}_{N,E,p}$ consists of all vectors in $\mathbb{R}^{3N}$ with total energy NE and total momentum Np, i.e.,

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

The measure σ_N is the normalized Euclidean measure induced from $\mathbb{R}^{3N}$ on $S_{N,E,p}$. The inverse collision time for the pair (i,j) depends now on the velocities v_i, v_j of the pair, and we set it to be

$$\lambda_{i,j} = \frac{N}{\binom{N}{2}}|v_i - v_j|^{\alpha}.$$

The momentum transfer for hard spheres is $|v_i - v_j|$, i.e., $\alpha = 1$. To specify the collision process, one must parametrize the collisions, and a convenient way is to set

$$\begin{aligned} v_i^*(\sigma) &= \frac{v_i + v_j}{2} + \frac{|v_i - v_j|}{2}\sigma, \\ v_j^*(\sigma) &= \frac{v_i + v_j}{2} - \frac{|v_i - v_j|}{2}\sigma, \end{aligned} \tag{1.2}$$

where $\sigma\in\mathbb{S}^2$. A particular kinematically possible collision is selected according to the following rule: in the specification of the process, there is a given nonnegative and even function

b on $[-1, 1]$ such that for any fixed $\sigma' \in S^2$, with $d\sigma$ denoting the uniform probability measure on $\mathbb{S}^2$,

$$\int_{\mathbb{S}^2} b(\sigma \cdot \sigma') d\sigma = 1 \quad \text{or, equivalently,} \quad \frac{1}{2}\int_{-1}^{1} b(t)dt = 1. \tag{1.3}$$

The most important case is

$$b(x) = 1. \tag{1.4}$$

When $\alpha = 1$ and b is given by (1.4), the Kac process models "hard sphere" or "billiard ball" collisions [15]. There are two standard parameterizations of the set of energy and momentum conserving collisions, the "σ parameterization" given by (1.2), and the "$\vec{n}$ parameterization". While the latter is often used in physics texts and in [15], the former, used here, has advantages: first, in this parameterization, b is constant, and second, it is not due to a nonconstant Jacobian relating the two parameterizations. See Appendix A.1 of [4] for more information; equation (A.18) of [4] is the formula relating the b functions for the two representations.

The generator of the Markov process is given by

$$L_{N,\alpha} F(\vec{v}) = -N \binom{N}{2}^{-1} \sum_{i<j} |v_i - v_j|^{\alpha} \left[F(\vec{v}) - [F]^{(i,j)}(\vec{v}) \right]$$

where

$$[F]^{(i,j)}(\vec{v}) = \int_{S^2} b\left(\sigma \cdot \frac{v_i - v_j}{|v_i - v_j|} \right) F(R_{i,j,\sigma}\vec{v}) d\sigma \tag{1.5}$$

and $(R_{i,j,\sigma}\vec{v})_k = \begin{cases} v_i^*(\sigma), & k = i, \\ v_j^*(\sigma), & k = j, \\ v_k, & k \neq i, j. \end{cases}$ The corresponding master equation then takes the form $\partial_t F = -L_{N,\alpha} F$ with the initial condition $F(\cdot, 0) = F_0(\cdot)$.

For this model, propagation of chaos was proved by Mischler and Mouhot in [16]. This is much more complicated than for the previous model since, due to the dependence on the velocities, the operator $L_{N,\alpha}$ is not uniformly bounded. For a general view on propagation of chaos, see [17].

2. KAC'S CONJECTURE

It is easy to see that the only equilibrium for the evolution given in (1.1) is the constant function. The operator $\mathcal{L}_N$ given in (1.1), as an operator in $L^2(\mathbb{S}^{N-1}(\sqrt{N}), d\sigma_N)$, is self-adjoint. The eigenvalue 0 is nondegenerate and the gap, i.e, the first nonzero eigenvalue Δ_N, is a measure for the approach to equilibrium since

$$\left\| F(t) - 1 \right\|_2 \leq e^{-\Delta_N t} \| F_0 - 1 \|_2.$$

Kac conjectured that there exists a constant $C > 0$ independent of N such that $\Delta_N \geq C$ for all N. This conjecture was proved in [13] and shortly thereafter in [6] the gap was explicitly computed to be

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

The argument is an induction procedure and can be adapted to many other situations. It is maybe useful to explain it in this simple case. It is easy to see that $\mathscr{L}_N$ is self-adjoint. Then the gap is defined to be

$$\inf_{F\perp 1, \|F\|_2=1} \langle F, \mathscr{L} F\rangle,$$

where $\langle\cdot,\cdot\rangle$ is the inner product in $L^2(\mathbb{S}^{N-1}(\sqrt{N}), d\sigma_N)$. An elementary argument shows that

$$\mathscr{L}_N = \frac{N}{N-1}\sum_{k=1}^{N} \mathscr{L}_{N-1}^{(k)},$$

where $\mathscr{L}_{N-1}^{(k)}$ is the generator for the $N-1$ particle Kac operator with particle k removed. Denote by P_k the orthogonal projection onto the space of functions on the sphere that depend only on the variable v_k. One can think of $P_k f$ as taking the average of the function f over all rotations that fix the k-axis. Then

$$\langle F, \mathscr{L}_N F\rangle = \frac{N}{N-1}\frac{1}{N}\sum_{k=1}^{N}\big\langle F, \mathscr{L}_{N-1}^{(k)} F\big\rangle = \frac{N}{N-1}\frac{1}{N}\sum_{k=1}^{N}\big\langle (F-P_k F), \mathscr{L}_{N-1}^{(k)}(F-P_k F)\big\rangle$$

since $\mathscr{L}_{N-1}^{(k)}$ does not act on functions that depend only on the variable v_k. By the induction assumption,

$$\big\langle (F-P_k F), \mathscr{L}_{N-1}^{(k)}(F-P_k F)\big\rangle \geq \Delta_{N-1}\|F-P_k F\|_2^2$$

because $F - P_k F \perp 1$ on the sphere with the variable v_k fixed. Hence we have the lower bound

$$\langle F, \mathscr{L}_N F\rangle \geq \frac{N}{N-1}\Delta_{N-1}\frac{1}{N}\sum_{k=1}^{N}\|F-P_k F\|_2^2 = \frac{N}{N-1}\Delta_{N-1}\big[\big\langle F, (I-P)F\big\rangle\big],$$

where

$$P = \frac{1}{N}\sum_{k=1}^{N} P_k.$$

In other words, the gap Δ_N is the product of the gap Δ_{N-1} multiplied by the gap of $I-P$. Now one observes that the eigenfunction of P that belong to a nonzero eigenvalue must be sums of functions of one variable. Using this, it is not very difficult to compute Λ_N, the gap of $I-P$ being

$$\Lambda_N = \frac{N-1}{N}\left(1-\frac{3}{N^2-1}\right),$$

(see, e.g., [6] and [7] for details), and hence

$$\Delta_N \geq \Delta_{N-1}\left(1-\frac{3}{N^2-1}\right)$$

and, iterating this bound using the fact that $\Delta_2 = 2$, one obtains

$$\Delta_N \geq \prod_{j=3}^{N}\left(1-\frac{3}{j^2-1}\right)\Delta_2 = \frac{1}{2}\frac{N+2}{N-1}.$$

This strategy can be used to estimate the gap for the three-dimensional momentum-preserving collisions [9]. Associated with the generator $L_{N,\alpha}$ is the quadratic form $\mathcal{E}(f,f) = -\langle f, L_{N,\alpha} f\rangle_{L^2(\mathcal{S}_{N,E,p})}$, i.e.,

$$\mathcal{E}(f,f) = \frac{N}{2}\binom{N}{2}^{-1} \sum_{i<j} \int_{\mathcal{S}_{N,E,p}} \int_{\mathbb{S}^2} |v_i - v_j|^\alpha b\left(\sigma \cdot \frac{v_i - v_j}{|v_i - v_j|}\right)\left[f(\vec{v}) - f(R_{i,j,\sigma}\vec{v})\right]^2 d\sigma d\sigma_N. \tag{2.1}$$

It is easy to see that for $L_{N,\alpha}$ the constant function 1 is the only equilibrium. It is straightforward to see that $L_{N,\alpha}$ is self-adjoint on $L^2(\mathcal{S}_{N,E,p})$. The gap is the distance between the lowest and the next lowest eigenvalue of $L_{N,\alpha}$, i.e.,

$$\Delta_{N,\alpha}(E,p) = \inf\left\{\mathcal{E}(f,f) : \langle f, 1\rangle_{L^2(S_{N,E,p})} = 0 \text{ and } \|f\|^2_{L^2(S_{N,E,p})} = 1\right\}. \tag{2.2}$$

Using a unitary transformation mapping $L^2(S_{N,1,0})$ to $L^2(S_{N,E,p})$ (see [9]), one writes

$$\Delta_{N,\alpha}(E,p) = \left(E - |p|^2\right)^{\alpha/2} \Delta_{N,\alpha}(1,0), \tag{2.3}$$

and we call $\Delta_{N,\alpha}(1,0)$ the "spectral gap for the Kac model."

Theorem 2.1 (Spectral gap for the Kac model with $0 \le \alpha \le 2$). *For each continuous non-negative even function b on $[-1,1]$ satisfying (1.3) 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*

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

for all N. In particular, this is true with b given by (1.4) and $\alpha = 1$, the 3-dimensional hard sphere Kac model.

This theorem was conjectured by Kac [15]. The proof is considerably more involved than that for the one-dimensional gas, and we refer the reader to [9] for the details. The fundamental idea is to find a replacement for the operator $(I - P)$. On the space $L^2(S_{N,1,0})$ consider the operator

$$\hat{L}_{N,\alpha} f = -\frac{1}{N}\sum_{k=1}^{N}\left[\frac{N^2 - (1+|v_k|^2)N}{(N-1)^2}\right]^{\alpha/2}[f - P_k f], \tag{2.4}$$

where P_k is the orthogonal projection defined by the map $\phi(\vec{v}) \to f(v_k)$ given defined by the relation

$$\int_{S_{N,1,0}} \phi(\vec{v}) g(v_k) d\sigma_N = \int_{S_{N,1,0}} f(v_k) g(v_k) d\sigma_N.$$

This operator is again self-adjoint on $L^2(S_{N,1,0})$, has 0 as its lowest eigenvalue, and we denote its gap by $\widehat{\Delta}_{N,\alpha}$. The reason for this operator is that it provides again an inductive approach to the whole problem. We have

Theorem 2.2. *For all $N \ge 3$,*

$$\Delta_{N,\alpha} \ge \frac{N}{N-1}\Delta_{N-1,\alpha}\widehat{\Delta}_{N,\alpha}. \tag{2.5}$$

In a further step, one proves, and this is the main work,

Theorem 2.3. *For all $N \geq 3$ and all $\alpha \in [0,2]$, $\widehat{\Delta}_{N,\alpha} > 0$. Moreover, there is a constant C independent of N such that*

$$\widehat{\Delta}_{N,\alpha} \geq 1 - \frac{1}{N} - \frac{C}{N^{3/2}}. \tag{2.6}$$

As a corollary, one obtains for any N large,

$$\Delta_{N,\alpha} \geq \prod_{j=N_0+1}^{N} \left(1 - \frac{C}{j^{1/2}(j-1)}\right) \Delta_{N_0,\alpha},$$

where N_0 is chosen such that $1 - \frac{C}{N_0^{1/2}(N_0-1)} > 0$. One now observes that

$$\lim_{N\to\infty} \prod_{j=N_0+1}^{N} \left(1 - \frac{C}{j^{1/2}(j-1)}\right) =: D > 0.$$

3. APPROACH TO EQUILIBRIUM IN ENTROPY

For simplicity we restrict ourselves to the one-dimensional case. To measure the approach to equilibrium in terms of the gap is unsatisfactory because the square norm of a probability distribution in general grows exponentially with the dimension. The right quantity is the entropy, relative to the uniform measure on the sphere,

$$S_N(F) = \int_{\mathbb{S}^{N-1}(\sqrt{n})} F(\vec{v}) \log F(\vec{v}) d\sigma_N,$$

which is proportional to the number of particles for the case of approximate independence. For the connection between the entropy and a strengthened notion of chaos know as entropic chaos, we refer to [5].

The dissipation is defined as

$$D_N(F) := -\frac{d}{dt} S_N\big(F(t)\big)\Big|_{t=0} = \int_{\mathbb{S}^{N-1}(\sqrt{N})} \mathcal{L}_N F \log F d\sigma_N.$$

It is not hard to see that the dissipation is positive. The entropy production is then defined by

$$\Gamma_N = \inf_F \frac{D_N(F)}{S_N(F)}.$$

It was shown by Villani [18] that

$$\Gamma_N \geq \frac{2}{N-1}, \tag{3.1}$$

which leads to exponential decay of the entropy

$$S_N\big(F(t)\big) \leq e^{-\frac{2}{N-1}t} S(F_0).$$

Obviously, the rate vanishes as the particle number tends to infinity. It was shown by Einav [11] that the entropy production estimate (3.1) is essentially correct by producing a trial function that yields an upper bound very close to Villani's estimate. While such considerations do not preclude the possibility that the entropy stays essentially constant for a time of order 1

and then decays exponentially with a rate independent of N, this seems somewhat unlikely. If one imagines a gas where few particles contain most of the energy, it will presumably take a long time until these particles have imparted their energy to the others and the system is near some equilibrium. This intuition was used in [11] to produce a state with very small entropy production.

A reasonable approach is to consider a system of M particles that interact with a reservoir of N particles that are initially at equilibrium. One envisions that N is large when compared to M. The Kac evolution for this situation can be written as

$$\partial_t F = -(\lambda_S \mathcal{L}_M F + \lambda_R \mathcal{L}_N + \mu \mathcal{I}_{M,N}) F,$$

where $F = F(\vec{v}, \vec{w})$ and $\vec{v} = (v_1, \dots, v_M)$ are the velocities of the particles in the system and $\vec{w} = (w_1, \dots, w_N)$ are the velocities of the particles in the reservoir; λ_S, λ_R are constants and the term $\mu \mathcal{I}_{M,N}$, describing the interaction between the system and the reservoir, is given by

$$\mu \mathcal{I}_{M,N} F = \frac{\mu}{N} \sum_{i=1}^{M} \sum_{j=1}^{N} R_{i,j} F,$$

where

$$R_{i,j} F(\vec{v}, \vec{w}) = \frac{1}{2\pi} \int_0^{2\pi} F\big(\dots, v_i^*(\theta), \dots, w_j^*(\theta), \dots\big) d\theta.$$

The factors μ/N are chosen in such a way that the average collision time between a fixed particle in the system with any particle in the reservoir is of order μ. To keep the problem simple, we consider distributions on $\mathbb{R}^{M+N}$ and assume that the initial condition is of the form

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

where f_0 is normalized. The quantity of interest is the relative entropy of the system at time t which is defined by

$$S\big(f(t)|\gamma\big) = \int_{\mathbb{R}^M} f(\vec{v}, t) \log \frac{f(\vec{v}, t)}{\gamma} d\vec{v},$$

where

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

and $\gamma = e^{-\pi |\vec{v}|^2}$. The following theorem is proved in [1]

Theorem 3.1. *For any positive integers N, M, we have that*

$$S\big(f(t)|\gamma\big) \le \left(\frac{M}{N+M} + e^{-\frac{\mu(N+M)}{2N} t} \frac{N}{N+M} \right) S(f_0|\gamma).$$

This theorem states that for $N \gg M$ the entropy decays with a rate approximately $\mu/2$ to a very small fraction of the original entropy. The original proof in [1] is rather cumbersome using Brascamp–Lieb inequalities. Another, simpler, proof based on the concept of information can be found in [2]. One should emphasize that the reservoir does not stay in

equilibrium in this process, and it is interesting to compare the process with a system interacting with a thermostat, i.e., a system interacting with an "infinite reservoir." Such a model can be described by the following master equation:

$$\partial_t f = -\lambda \mathcal{L}_M f - \mu \sum_{j=1}^{M} (I - R_j) f,$$

where

$$R_j f(\vec{v}) = \int_{\mathbb{R}} dw \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-\pi(-v_j \sin(\theta) + w \cos(\theta))^2} \times f\big(v_1, \ldots, v_j \cos(\theta) + w \sin(\theta), \ldots, v_M\big).$$

This describes the collision between the particle with label j and a particle randomly picked from the Gaussian ensemble with temperature $\frac{1}{2\pi}$. It is easy to see that $e^{-\pi|\vec{v}|^2}$ is the equilibrium for this process.

The following theorem is proved in [3]

Theorem 3.2. *The relative entropy with respect to γ satisfies the estimate*

$$S\big(f(t)|\gamma\big) \leq e^{-\frac{\mu}{2}t} S(f_0|\gamma).$$

It is satisfying to see that the result in Theorem 3.1 takes the form of Theorem 3.2 as $N \to \infty$.

4. A QUANTUM KAC MODEL

In [8], the list of Kac models was extended by 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 $\otimes^N \mathcal{H}$, i.e., a self-adjoint positive trace class operator with unit trace. 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. The collision operators $\mathcal{Q} : \mathcal{B}(\mathcal{H}_2) \to \mathcal{B}(\mathcal{H}_2)$ is given by

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

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

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 ρ have the same energy so does $\mathcal{Q}(\rho)$. 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 $\sigma \to \sigma'$ is such that $VU(\sigma)V^* = U(\sigma')$ 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 $\sigma \to \sigma'$ is measurable and leaves ν invariant. One easily sees that for any two operators A, B on $\mathcal{H}_2$ one has

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

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

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,

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

4.1. Example

The following example taken from [8] is useful for understanding these concepts. For the simplest possible example, take $\mathcal{H} = \mathbb{C}^2$, so that $\mathcal{H}_2 = (\mathbb{C}^2)^{\otimes 2}$. Define the single particle Hamiltonian h by $h = \left[\begin{smallmatrix} 0 & 0 \\ 0 & 1 \end{smallmatrix}\right]$. 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

$$|00\rangle, \quad |10\rangle, \quad |01\rangle, \quad |11\rangle, \tag{4.1}$$

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

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

(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 $H_2 = \{0, 1, 2\}$ and

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

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 (4.1),

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

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

$$\mathfrak{L}_N(A) = N \binom{N}{2}^{-1} \sum_{i<j} [A - \mathcal{Q}_{i,j}(A)] \tag{4.2}$$

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

4.2. 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

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

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 $\otimes^N \varrho$, but one can also construct chaotic sequences that have a sharply defined energy for large N.

We have (see [8])

Theorem 4.1. *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 (4.2). 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, $\{\mathcal{P}_{N,t}\varrho_N\}_{N\in\mathbb{N}}$ is a $\varrho(t)$-chaotic sequence for some $\varrho(t) = \lim_{N\to\infty}(\mathcal{P}_{N,t}\varrho_N)^{(1)}$, where in particular this limit of the one-particle marginal exists and is a density matrix.*

As expected, the marginal density matrix $\varrho(t)$ satisfies a Quantum Kac–Boltzmann equation

$$\frac{d}{dt}\varrho(t) = 2\big(\varrho(t) \star \varrho(t) - \varrho(t)\big),$$

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

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

is the Quantum Wild Convolution.

4.3. Equilibrium states

An equilibrium density matrix for the evolution (4.2) 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 form 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 subalgebra of $\mathfrak{C}_N$ and it is generated by the spectral projections of the Hamiltonian H_N. Define two multiindices 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 multiindices 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 [8] the following theorem is proved.

Theorem 4.2. *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

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

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 let $n_1(\alpha)$ be 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 connected. 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, 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 the 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 4.1, is the following Lindblad equation $\partial_t \rho = L_N(\rho)$, where

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

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 4.1 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_js are rationally independent, the eigenvalues of H_N are in a one-to-one correspondence with the "occupation numbers" $\mathbf{k}(\alpha) = (k_1(\alpha), \ldots, k_K(\alpha))$. 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 4.1. 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 multiindices of length N consisting of 1s and 0s and if two indices are connected then one can be transformed into the other by a series of transpositions. Thus, in this case multiindices 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 [12]. The following theorem is a special case of a result that will appear in [10].

Theorem 4.3. *Assume that the eigenalues of h are rationally independent and $N > 2$. Then the gap of $\mathcal{L}_N$ is*

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

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