A Quantum Kac Walk and the Boltzmann Equation

Maria C. Carvalho

Rutgers University and C.M.A.F. Lisbon

Cambridge, May 13, 2016

Based in joint work with E. Carlen and M. Loss

The Kac Walk on the N-sphere

The Kac walk was introduced by Mark Kac in 1956 as a model for particles undergoing binary collisions. He was interested in the rate of equilibration.

In its simplest form, the model concerns N particles with one dimensional velocities

$$v_1, \ldots, v_N \ .$$

The state of the system will change due to a random process in which 2 of the velocities are changed at a time. This is intended to model binary collisions, and it is required that the total energy $E = \sum_{j=1}^{N} v_j^2$ is conserved.

Then for an N particle system with total energy N, the state space $\mathcal{S}_N$ is the set of all vectors

$$(v_1, v_2, \ldots, v_N)$$

on the sphere of radius $\sqrt{N}$.

In the *Kac walk* on $\mathcal{S}_N$, at each step one picks a pair i, j uniformly at random, and then an angle θ uniformly in $[0, 2\pi)$, and then moves from $\vec{v} = (v_1, v_2, \ldots, v_N)$ to

$$(v_1, \ldots, v_i', \ldots, v_j', \ldots, v_N) =: R_{i,j,\theta}\vec{v}$$

where

$$v_i' = \cos\theta v_i + \sin\theta v_j \quad \text{and} \quad v_j' = -\sin\theta v_i + \cos\theta v_j \ .$$

Let the jumps arrive in Poisson stream with an expected wait of time $1/N$ between jumps, so that the expected time between collisions of any one particle is 1.

Let $\mathcal{L}$ be the generator of this process, which is reversible, so that if the initial probability density for $\vec{v}$ is F, the density at time t is $e^{t\mathcal{L}}F$, where

$$\mathcal{L}F(\vec{v}) = N\binom{N}{2}^{-1}\sum_{i<j}(F^{i,j} - F)\ ,$$

$$F^{i,j}(\vec{v}) := \frac{1}{2\pi}\int_{-\pi}^{\pi} F(R_{i,j,\theta}\vec{v})\mathrm{d}\theta\ .$$

Chaos

$$\frac{\partial}{\partial t} F = \mathcal{L} F$$

is the *Kac Master equation*. Its connection with the Boltzmann equation comes through Kac's notion of *chaos*. The coordinate functions on $\mathcal{S}_N$ are never independent, but for large N, they are almost pairwise independent.

This is because the unit Gaussian probability measure on $\mathbb{R}^N$ is strongly concentrated on $\mathcal{S}_N$, the sphere of radius $\sqrt{N}$.

In particular, as $e^{t\mathcal{L}} f$ tends to 1, its single particle marginals tend to

$$\frac{1}{\sqrt{2\pi}} e^{-v^2/2} \ .$$

Moreover, the time evolution of the single particle marginal $g(v, t)$, for permutation symmetric f, depends on the two particle marginal distribution.

When this is well approximated by $g(v)g(w)$, the single particle marginal satisfies a closed form evolution equation with a quadratic non-linearity. Call this property “chaoticity”.

Moreover, Kac proved in his 1956 paper that the “chaotic property”, i.e., having the distribution of pairs to be the product of the single particle distribution in the large N limit, was propagated in time.

Let μ be a probability measure on $\mathbb{R}$. A sequence $\{\mu^{(N)}\}$ of probability measures on $\mathcal{S}^N$ is μ chaotic in case

$$\int \chi(v_1, \ldots, v_k) \mathrm{d}\mu^{(N)}(v_1, \ldots, v_N) \to \int \chi(v_1, \ldots, v_k) \mathrm{d}\mu(v_1) \cdots \mathrm{d}\mu(v_k)$$

Theorem 0.1 (Propagation of Chaos, Kac 1956). *Let* $\{F_0^{(N)}\sigma^{(N)}\}$ *be a* $f_0(v)\mathrm{d}v$*–chaotic sequence and denote by* $\{F_t^{(N)}\sigma^{(N)}\}$ *the sequence of measures where* $F_t^{(N)}$ *is the solution of the master equation, i.e.,* $F_t = e^{t\mathcal{L}}F_0$*. Then,* $\{F_t^{(N)}\sigma^{(N)}\}$ *is a* $f(v,t)\mathrm{d}v$*–chaotic sequence and* $f(v,t)$ *is a solution of the initial value problem*

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

with $f(v,0) = f_0(v)$*, i.e., it is a solution of the Kac equation where* $v^*(\theta)$ *and* $w^*(\theta)$ *are given by rotating* (v,w) *through an angle* θ*.*

Existence of Chaotic initial data

Theorem 0.2 (Carlen, C., La Roux, Loss, Villani)**.** *Let f be a probability density on $\mathbb{R}$ satisfying, for some $p > 1$,*

$$\int_{\mathbb{R}} f(v)v^2 \mathrm{d}v = 1 \, , \; \int_{\mathbb{R}} f(v)v^4 \mathrm{d}v < \infty \, , f \in L^p(\mathbb{R})$$

and let $\mu(\mathrm{d}v) = f(v)\mathrm{d}v$, and let $[\mu^{\otimes N}]_{S^{N-1}(\sqrt{N})}$ be the normalized restriction of $f^{\otimes N}$ to the sphere. Then $\{[\mu^{\otimes N}]_{S^{N-1}(\sqrt{N})}\}$ is μ –chaotic

In this case, $[\mu^{\otimes N}]_{S^{N-1}(\sqrt{N})}$ will have a density F^N with respect to the uniform measure on the sphere:

$$[\mu^{\otimes N}]_{S^{N-1}(\sqrt{N})} = F^N \mathrm{d}\sigma \, .$$

Approach to Equilibrium

It is easy to see that under the Kac walk, the density tends to become uniform:

$$\lim_{t\to\infty} e^{t\mathcal{L}} F = 1 \ .$$

Kac proposed to measure this in terms of the *spectral gap* of $\mathcal{L}$ which is

$$\Delta_N := \inf\{\langle F, -\mathcal{L}F\rangle_{L^2(\mathcal{S}_N)} \ : \ \|F\|_2 = 1 \ , \langle F, 1\rangle_{L^2(\mathcal{S}_N)} = 0 \ \} \ .$$

$$\|e^{t\mathcal{L}}F - 1\|_2 = \|e^{t\mathcal{L}}(F-1)\|_2 \le e^{-t\Delta_N}\|F-1\|_2 \ .$$

Kac conjectured that

$$\liminf_{N\to\infty} \Delta_N > 0 \ .$$

The Kac conjecture was proved by Janvresse with no estimate on the limiting gap. Carlen, C. and Loss gave the exact value:

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

In subsequent work, this was extended to three dimensional collisions and hard sphere collisions, going beyond the original Maxwellian setting considered by Kac.

We now discuss an extension to the quantum case.

The Quantum Kac Walk

Let $\mathcal{H}$ be a Hilbert space that will be called the *single particle state space*. Let h be a self-adjoint operator, the *single particle Hamiltonian*. The eigenvalues of h are the possible energy levels of a single particle in isolation.

In this talk, we focus on the case in which $\mathcal{H}$ is finite dimensional, but much of what we say applies when $\mathcal{H} = L^2(\Omega)$ and Ω is a box with periodic boundary conditions in $\mathbb{R}^3$, and $h = -\Delta_\Omega$.

For $N \in \mathbb{N}$, let $\mathcal{H}_N$ denote the N-fold tensor product $\mathcal{H}^{\otimes N}$. For $j \in (1, \ldots, N)$, let h_j denote the operator that acts with h on the jth factor, and it is the identity on the other factors, so that, e.g.,

$$h_2 = I \otimes h \otimes I \cdots \otimes I \ ,$$

where I is the identity on $\mathcal{H}$.

Finally, define

$$H_N = \sum_{j=1}^{N} h_j \ .$$

This is the total Hamiltonian for N isolated particles.

Let us suppose that $\mathcal{H}$ is n dimensional and the eigenvalues of h are $\{e_1, \dots, e_n\}$. Let $\{\varphi_1, \dots, \varphi_n\}$ be an orthonormal basis of eigenvectors.

For $\alpha \in \{1, \dots, n\}^N$, let

$$|\alpha\rangle = \varphi_{\alpha_1} \otimes \cdots \otimes \varphi_{\alpha_n} \ .$$

The set of the $|\alpha\rangle$ are an eigenbasis of H_N

Let M_N be the number of distinct eigenvalues of H_N, and let

$$\{E_1, \ldots, E_{M_N}\}$$

be these distinct eigenvalues arranged in increasing order. For $E \in \{E_1, \ldots, E_{M_N}\}$, let $\mathcal{K}_E$ denote the eigenspace of H_N corresponding to eigenvalue E.

The $\mathcal{K}_E$ are the quantum analogs of the energy spheres in the classical case.

Uniform energy shell states

Definition 0.3 (Uniform energy shell states)**.** *For each $E \in \{E_1, \ldots, E_{M_N}\}$, let $\mathbf{p}_E$ be the normalized projection (normalized so that $\mathrm{Tr}[\mathbf{p}_E] = 1$) onto the energy eigenspace $\mathcal{K}_{E,N}$. We call $\mathbf{p}_E$ the* uniform energy shell state of energy E

Thus, $\mathbf{p}_E$ is a density matrix, and its Hilbert-Schmidt norm is

$$\|\mathbf{p}_{E,N}\|_2 = (\dim(\mathcal{K}_E))^{-1/2} \ .$$

Pair collisions

We now introduce pair collisions that preserve the energy of the pair of particles that collide. Let $\{U(\sigma) \ : \ \sigma \in \mathcal{S}\}$ be a set of unitary operators on $\mathcal{H} \otimes \mathcal{H}$ where $\mathcal{S}$ is some parameter space. We require that for each $\sigma \in \mathcal{S}$,

$$U(\sigma)H_2 = H_2U(\sigma) \ .$$

Think of the $U(\sigma)$ as representing S-*matrices* for various sorts of binary collisions.

For $1 \leq i < j \leq N$, decompose $\mathcal{H}_N$ as $\mathcal{H}_{(i,j)} \otimes \mathcal{H}^{(i,j)}$ where $\mathcal{H}_{(i,j)}$ is the product of ith and jth factors, and $\mathcal{H}^{(i,j)}$ is all the rest.

Let $U(\sigma)_{i,j}$ be the unitary that acts as $U(\sigma)$ on $\mathcal{H}_{(i,j)}$, and as the identitiy on $\mathcal{H}^{(i,j)}$.

Ergodicity

We require that the space of self-adjoint operators on $\mathcal{H}_N$ that commute with each $U(\sigma)_{i,j}$ is exactly the span of the $\{\mathbf{p}_E \ : \ E = E_1, \ldots E_{M_N}\}$. We refer to this requirement as the *ergodicity condition* in what follows.

We also assume that $\mathcal{S}$ is a compact metric space equipped with a Borel probability measure $\mathrm{d}\sigma$ that charges every open set with strictly positive probability. Finally, we suppose that $U(\sigma)$ depends continuously on σ.

Averaging over σ and the pair $i < j$, we define the operator $\mathcal{Q}^+$ on $\mathcal{B}(\mathcal{H}_N)$ by

$$Q_N^+(\varrho) = \binom{N}{2}^{-1} \sum_{i<j} \int_{\mathcal{S}} U_{i,j}(\sigma)\varrho U_{i,j}^*(\sigma)\mathrm{d}\sigma \ .$$

This is a *quantum operation*; i.e., a completely positive trace preserving linear transformation on $\mathcal{B}(\mathcal{H}_N)$.

The Quantum Kac Master Equation

Define a quantum Markov semigroup P_t, $t > 0$, on $\mathcal{B}(\mathcal{H}_N)$ by

$$P_t = \sum_{k=0}^{N} e^{-tN} \frac{(tN)^k}{k!} (Q_N^+)^k = e^{tN(Q_N^+ - I)} \ .$$

The generator is

$$\mathcal{L} = N(Q_N^+ - I) \ .$$

Evidently, each P_t is a quantum operation; i.e., a completely positive trace preserving linear map.

A time dependent density matrix $\varrho(t)$ on $\mathcal{H}_N$ satisfies the *quantum Kac master equation* in case

$$\frac{\mathrm{d}}{\mathrm{d}t} \varrho(t) = \mathcal{L} \varrho(t) \ .$$

Steady state solutions

Let $F[\varrho]$ be any unitarily invariant, strictly convex function on the set of density matrices on $\mathcal{H}_N$. For example, consider

$$F[\rho] = \mathrm{Tr}[\varrho \log \varrho] \quad \text{or} \quad F[\rho] = \mathrm{Tr}[\rho^2] \; .$$

$$F[Q_N^+ \varrho] \le \binom{N}{2}^{-1} \sum_{i<j} \int_{\mathcal{S}} F[U_{i,j}(\sigma) \varrho U_{i,j}^*(\sigma)] \mathrm{d}\sigma = F[\varrho] \; .$$

By the strict convexity, there is equality if and only if

$$U_{i,j}(\sigma) \varrho U_{i,j}^*(\sigma) = \varrho$$

for all pairs i, j, and all $\sigma \in S$. By the ergodicity condition, this means that ϱ is a positive linear combination of the orthonormal projectors onto the $\mathcal{K}_E$.

It is clear that if ϱ is a steady state solution of the quantum Kac master equation, then is must be the case that $F[P_t\varrho] = F[\varrho]$ for all t, and hence that

$$F[Q_N^+\varrho] = F[\varrho] \ .$$

As we have just seen, this is the case if and only if ϱ is a positive linear combination of the orthonormal projectors onto the $\mathcal{K}_E$.

Convergence to equilibrium

Recall that $\mathcal{L}$ denotes the generator of our semigroup;

$$\mathcal{L} = N(Q_N^+ - I)\ .$$

We have seen that for each eigenvalue E of $\mathcal{H}_N$, $\mathcal{L}\mathbf{p}_E = 0$. Then since $\mathcal{L}$ is self adjoint, for all states ϱ_0,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \mathbf{p}_E\ ,\ e^{t\mathcal{L}}\varrho_0\rangle = 0\ .$$

If $\lim_{t\to\infty} e^{t\mathcal{L}}\varrho_0$ exists and equals some equilibrium density, ϱ_∞, then necessarily

$$\langle \mathbf{p}_E\ , \varrho_\infty\rangle = \langle \mathbf{p}_E\ , \varrho_0\rangle$$

for all E.

Let $\lambda_0, \dots, \lambda_{M_N}$ be M_N non-negative numbers that sum to 1 Consider the equilibrium density

$$\varrho_{\{\lambda_0,\dots,\lambda_{M_N}\}} = \sum_E \lambda_E \mathbf{p}_E \ .$$

The general equilibrium density has this form for some choice of the $\lambda_0, \dots, \lambda_N$. Note that

$$\langle \mathbf{p}_{E,N} \ , \varrho_{\{\lambda_0,\dots,\lambda_N\}} \rangle = \lambda_E (\dim(\mathcal{K}_E))^{-1} \ .$$

As a consequence of convexity, we know that

$$\|e^{t\mathcal{L}_N}\varrho\|_2^2 := \mathrm{Tr}[(e^{t\mathcal{L}_N}\varrho)^2]$$

is strictly decreasing in t, unless ϱ is an equilibrium state. Moreover, by the same reasoning, if ϱ_∞ is the equilibrium state having the same conservation properties as ϱ, then

$$\|e^{t\mathcal{L}_N}\varrho - \varrho_\infty\|_2^2$$

is strictly decreasing in t, unless ϱ is an equilibrium state.

One of our goals is to quantify the rate of approach to equilibrium in this metric.

Chaos and the quantum K-B equation

The permutation group acts unitarily on $\mathcal{H}_N$ by permuting the indices of each $|\alpha_1, \ldots, \alpha_N\rangle$. A density matrix ϱ on $\mathcal{H}_N$ is *symmetric under permutations* in case it is invariant under this action. The adjective *symmetric* indicates this condition. For example, each $\mathbf{p}_E$ is symmetric.

Given a state ϱ, let

$$\varrho^{(1)} = \mathrm{Tr}_{2\ldots N}\, \varrho \qquad \text{and} \qquad \varrho^{(2)} = \mathrm{Tr}_{3\ldots N}\, \varrho$$

where we take the partial trace of the last $N-1$, respectively $N-2$, factors in $\mathcal{H}_N$. As usual, $\varrho^{(1)}$ is called the *single particle reduced density matrix* and $\varrho^{(2)}$ is called the *two particle reduced density matrix*.

Definition 0.4 (Chaoticity)**.** *Let* ρ *be a density matrix on* $\mathcal{H}$*. A sequence* $\{\varrho_N\}_{N\in\mathbb{N}}$ *of symmetric density matrices on* $\mathcal{H}_N$ *is* ρ*-chaotic in case*

$$\lim_{N\to\infty} \varrho^{(1)} = \rho \qquad \text{and} \qquad \lim_{N\to\infty} \varrho^{(2)} = \rho \otimes \rho \,.$$

Of course, the sequences of states $\{\rho^{\otimes N}\}_{N\in\mathbb{N}}$ on $\mathcal{H}_N$ is ρ-chaotic in a trivial sort of way.

It is natural to ask: Do there exist ρ-chaotic sequences $\{\varrho_N\}_{N\in\mathbb{N}}$ with more sharply defined values of the energy? The answer is “yes”, but we cannot take the ϱ_N to be supported on a single energy shell.

The point of the definition is that, as in the clasical case, chaos is propagated, and propagation of chaos leads to a non-linear Boltzmann type equation.

Propagation of Chaos

Definition 0.5. *For k an integer in $[1, \ldots, N-1]$, let $\mathcal{B}(k)$ denote the set of operators A on $\mathcal{H}_k$ that act non-trivially on at most the first k factors of $\mathcal{H}$ in $\mathcal{H}_N$.*

Theorem 0.6. *Let $A \in \mathcal{B}(k)$. Then the power series*

$$\sum_{j=0}^{\infty} \frac{t^j}{j!} \mathcal{L}^j A$$

converges in the operator norm uniformly on $[0, T]$ for any $0 < T < 1/4$.

The proof is essentially combinatoric, and follows the corresponding proof of Kac. Again, following Kac, this leads to propagation of chaos.

A key bound in the proof is:

$$\|\mathcal{L}A\|_\infty \leq 2N\|A\|_\infty$$

for A on $\bigotimes^N \mathcal{H}$, but depending only on one particle.

Since *chaos is propagated*, if $\{\varrho_N\}_{N\in\mathbb{N}}$ is ρ-chaotic, then $\{\exp(t\mathcal{L})\varrho_N\}_{N\in\mathbb{N}}$ is $\rho(t)$ chaotic for a time-dependent density matrix $\rho(t)$ on $\mathbb{C}^2$.

Let ϱ be a symmetric density matrix on $\mathcal{H}_N$, and define

$$\varrho(t) = \exp(t\mathcal{L})\varrho\ .$$

The evolution of the one particle density matrix depends also on the two particle density matrix:

Lemma 0.7. *Let* $\varrho(t) = e^{t\mathcal{L}}\varrho$ *for a symmetric density matrix* ϱ *on* $\mathcal{H}_N$*. Then the one and two particle reduced density matrices are related by*

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho^{(1)}(t) = 2\,\mathrm{Tr}_2\left[\int_{\mathcal{S}} U(\sigma)[\varrho^{(2)}(t)]U^*(\sigma)\mathrm{d}\sigma - \varrho^{(2)}(t)\right]\;.$$

However, when chaos is propagated, the equation closes, and we obtain the *quantum Kac-Boltzmann equation*.

Proof.

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\rho^{(1)}(t) &= \mathrm{Tr}_{2,\ldots,N}\left[\mathcal{L}\varrho(t)\right] \\
&= \mathrm{Tr}_{2,\ldots,N}\left[\frac{2}{N-1}\sum_{j=2}^{N}\int_{\mathcal{S}}\left[U_{1,j}(\sigma)\varrho(t)U^*_{1,j}(\sigma)-\varrho(t)\right]\mathrm{d}\sigma\right] \\
&= \mathrm{Tr}_{2,\ldots,N}\left[2\int_{\mathcal{S}}\left[U_{1,2}(\sigma)\varrho(t)U^*_{1,2}(\sigma)-\varrho(t)\right]\mathrm{d}\sigma\right]
\end{aligned}$$

where we have used the symmetry in the last step. Now taking $\mathrm{Tr}_{3,\ldots,N}$ we obtain the result. □

Definition 0.8 (Gain term). *Given density matrices ρ_1, ρ_2 on $\mathbb{C}^2$, we define*

$$\mathcal{Q}_+[\rho_1, \rho_2] = \mathrm{Tr}_2 \left[\int_{\mathcal{S}} U(\sigma)[\rho_1 \otimes \rho_2] U^*(\sigma) \mathrm{d}\sigma \right] .$$

The Quantum Kac-Boltzmann Equation *is*

$$\frac{\partial}{\partial t}\rho(t) = 2[\mathcal{Q}_+[\rho(t), \rho(t)] - \rho(t)] .$$

Theorem 0.9. *Suppose that $\{\varrho_N(0)\}_{N\in\mathbb{N}}$ is $\rho(0)$-chaotic, and that for each N, $\varrho_N(t) = \exp(t\mathcal{L})\varrho_N(0)$ for all $t > 0$. Then $\rho(t)$ satisfies the Quantum Kac-Boltzmann Equation.*

The simplest concrete model

We now turn to one general question in the context of the simplest concrete model – that in which $\mathcal{H}$ is two dimensional. The question we focus on is:

Does the solution of the Quantum Kac master equation relax to equilibrium at an exponential rate that is bounded away from zero uniformly in N?

The 2 dimensional Quantum Kac Walk

For $N \in \mathbb{N}$, let $\mathcal{H}_N$ denote the N-fold tensor product $(\mathbb{C}^2)^{\otimes N}$. For $j \in (1, \dots, N)$, let h_j denote the operator that acts with $\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$ on the jth factor, and it is the identity on the other factors, so that, e.g.,

$$h_2 = I \otimes \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \otimes I \cdots \otimes I \ ,$$

where I is the 2×2 identity matrix.

Some notation

We identify $\mathbb{C}^2 \otimes \mathbb{C}^2$ with $\mathbb{C}^4$ using the basis

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |11\rangle \quad , \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |10\rangle \ , etc.$$

The full basis is simply

$$|11\rangle \ , \quad |10\rangle \ , \quad |01\rangle \ , \quad |00\rangle \ ,$$

An orthonormal basis of $\mathcal{H}_N$ consisting of eigenvectors of H_N is provided by the set of vectors $|\alpha_1, \ldots, \alpha_N\rangle$ in which each α_j is either zero or 1. Then

$$H_N|\alpha_1, \ldots, \alpha_N\rangle = \left(\sum_{j=1}^{N} \alpha_j \right) |\alpha_1, \ldots, \alpha_N\rangle \ .$$

In this basis $H_2 = h_1 \otimes I + I \otimes h_2$ is given by

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

The unitary matrices of the form

$$U := \begin{bmatrix} e^{i\varphi_1} & 0 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta & 0 \\ 0 & \sin\theta & \cos\theta & 0 \\ 0 & 0 & 0 & e^{i\varphi_2} \end{bmatrix}$$

all commute with $h_1 \otimes I + I \otimes h_2$.

This set of matrices is a group, which may be identified with

$$\mathcal{S} = S^1 \times S^1 \times S^1 \ .$$

and each unitary in the group commutes with $h_1 \otimes I + I \otimes h_2$. This group is not the full group of all unitary operators that commute with $h_1 \otimes I + I \otimes h_2$, but is large enough for ergodicity.
We denote the uniform Haar measure on $\mathcal{S}$ by $\mathrm{d}\sigma$ and write $U(\sigma)$ to denote the unitary operator at $\sigma \in \mathcal{S}$.

Lemma 0.10. *Let A be any operator on $\mathcal{H}_2$ that commutes with $U(\sigma)$ for all σ. Then A is a polynomial (of degree 2 at most) in H_2. More generally, for any operator A on $\mathcal{H}_2$,*

$$\int_{\mathcal{S}} U(\sigma) A U^*(\sigma) \mathrm{d}\sigma$$

is the orthogonal projection in the Hilbert-Schmidt inner product onto polynomials in H_2.

Proof. For any operator A on $\mathcal{H}_2$,

$$\int_{\mathcal{S}} U(\sigma) A U^*(\sigma) \mathrm{d}\sigma = \begin{bmatrix} a & 0 & 0 & 0 \\ 0 & b & 0 & 0 \\ 0 & 0 & b & 0 \\ 0 & 0 & 0 & c \end{bmatrix}$$

Relaxation for N particles

The null space of $\mathcal{L}_N$ is spanned by $\{\mathbf{p}_{E_1}, \ldots, \mathbf{p}_{E_{M_N}}\}$ Since $\mathcal{L}_N$ is evidently self-adjoint with respect to the Hilbert-Schmidt inner product on self-adjoint operators on $\mathcal{H}_N$, the spectral gap of $\mathcal{L}_N$ is the quantity

$$\Delta_N = \inf \left\{ -N \frac{\mathrm{Tr}[A(Q_N^+ - I)A]}{\mathrm{Tr}[A^2]} \ : \ \mathrm{Tr}[A\mathbf{p}_{E,N}] = 0 \ \forall \ E \in \mathrm{spec}(H_N) \right\} .$$

We also define

$$\lambda_N = \sup \left\{ \frac{\mathrm{Tr}[AQ_N^+(A)]}{\mathrm{Tr}[A^2]} \ : \ \mathrm{Tr}[A\mathbf{p}_{E,N}] = 0 \ \forall \ E \in \mathrm{spec}(H_N) \right\} .$$

That is, λ_N is the largest eigenvalue of Q_N^+ apart from 1.

The case $N = 2$

It is trivial to analyze the case $N = 2$. It is clear by the definition of Q_2^+ that its range on $\mathcal{H}_2$ is spanned by matrices of the form

$$\begin{bmatrix} a & 0 & 0 & 0 \\ 0 & b & 0 & 0 \\ 0 & 0 & b & 0 \\ 0 & 0 & 0 & c \end{bmatrix} = a\mathbf{p}_{2,2} + b\mathbf{p}_{1,2} + c\mathbf{p}_{0,2} \ .$$

Therefore, when A is orthogonal to $\mathbf{p}_{2,2}$, $\mathbf{p}_{1,2}$ and $\mathbf{p}_{0,2}$

$$-2\,\mathrm{Tr}[A(Q_2^+ - I)A] = 2\,\mathrm{Tr}[A^2] \ ,$$

and so

$$\Delta_2 = 2 \ .$$

The induction on N

Our goal is to compute Δ_N through an induction on N starting from the previous lemma. We shall prove:

Theorem 0.11 (Gap for $N \geq 2$)**.** *For all $N \geq 2$,*

$$\Delta_N = 2 \, .$$

The method of proof is based on the classical induction. It is possible to write:

$$Q_N^+(A) = \frac{1}{N} \sum_{k=1}^{N} (I_{\mathcal{B}(\mathcal{H}_{(k)})} \otimes Q_{N-1,k}^+)(A) \, .$$

We next relate the gap eigenvalue of Q_N^+ to that of Q_{N-1}^+.

The projection operators

We cannot immediately apply the induction with $A = \varrho - \varrho_\infty$ since it is not necessarily the case that

$$\mathrm{Tr}[A(X \otimes \mathbf{p}_{E,N-1})] = 0$$

for all $E \in \mathrm{spec}(H_{N-1})$ and all $X \in \mathcal{B}(\mathcal{H}_{(k)})$.
The classical analog of this would be

$$\int_{\mathcal{S}_N} F(v_1, \ldots, v_N)\chi(v_k)\mathrm{d}\sigma = 0 \ .$$

As in the classical case, we need to add and subtract the projection onto the space spanned by $\{\mathbf{p}_{0,N-1}, \ldots, \mathbf{p}_{N-1,N-1}\}$.

Let $\mathcal{H}_{(k)}$ denote the kth factor of $\mathcal{H}$ in $\mathcal{H}_N = \bigotimes^N \mathcal{H}$. Let $\widehat{H}_{(k)}$ denote the other $N-1$ factors. Then $\mathcal{H}_N$ can be identified with $\mathcal{H}_{(k)} \otimes \widehat{H}_{(k)}$ Let $\mathcal{U}_{k,N}$ be the group unitaries on $\widehat{H}_{(k)}$ that commute with $\sum_{j \neq k} h_j$ regarded as an operator on $\widehat{H}_{(k)}$.

Then with $\mathrm{d}U$ denoting normalized Haar measure, define

$$P_k(A) = \int_{\mathcal{U}_{k,N}} (I_{\mathcal{H}_{(k)}} \otimes U) A (I_{\mathcal{H}_{(k)}} \otimes U)^* \mathrm{d}U$$

P_k is the orthogonal projection, with respect to the Hilbert-Schmidt inner product, of $\mathcal{B}(\mathcal{H}_N)$ onto the sub algebra of operators that commute with each $U \in \mathcal{U}_{k,N}$.

We also define

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

It is easy to show that:

Lemma 0.12. *For all k and E and N,*

$$P_k(\mathbf{p}_{E,N}) = \mathbf{p}_{E,N} \ ,$$

and in fact the $\mathbf{p}_{E,N}$ span the eigenspace of P with eigenvalue 1.

The spectral gap for P

Definition 0.13 (Spectral gap for P). *Let μ_N denote the eigenvalue of P given by*

$$\mu_N = \sup\left\{\mathrm{Tr}[APA] \ : \ \|A\| = 1 \quad \text{and} \quad \mathrm{Tr}[A\mathbf{p}_{E,N}] = 0 \quad \text{for all } E\right\} \ .$$

Lemma 0.14. *For all $N \geq 3$,*

$$\lambda_N \leq \left[\lambda_{N-1} + (1-\lambda_{N-1})\mu_N\right] \ ,$$

and consequently,

$$\Delta_N \geq \frac{N}{N-1}(1-\mu_N)\Delta_{N-1} \ .$$

Determination of the Spectral Gap

Theorem 0.15. *The spectrum of P on the symmetric sector consists of*

$$\left\{1, \frac{1}{N}, 0\right\} \ .$$

The eigenspace corresponding to eigenvalue 1 is spanned by $\{\mathbf{p}_{N,E}\}_{E=0,\dots,N}$, and consequently, for all N, $\mu_N = 1/N$ and hence

$$\Delta_N = 2 \, .$$

This result would be obvious if all of the projections P_k commuted with one another, but this is not the case because when the energy is fixed, and we know some components are, say, “up”, we have information about how likely it is that the others are “up” or “down”.