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A QUANTUM KAC MODEL

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Classical Kac master equation for colliding particles

Probabilistic model for 1-dim colliding particles (Kac 1956)

(i) For a collision randomly and uniformly pick a pair (i, j) of particles.

(ii) Randomly pick a 'scattering angle' θ with uniform probability .

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

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

(iv) Assume that the collision times are exponentially distributed, i.e, the probabiltity that the first collision time is larger than t is given by e^{-t}.

$$\vec{v} = (v_1, v_2, \cdots, v_N)$$

Given an initial symmetric distribution $F_0(\vec{v})$

$$F(\vec{v},t) = e^{-Nt(I-Q)}F_0$$

satisfies the linear

Kac Master equation

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

$$Q = \begin{pmatrix} N \\ 2 \end{pmatrix}^{-1} \sum_{i<j} R_{i,j}$$

$$R_{i,j}\Phi := \frac{1}{2\pi}\int_0^{2\pi} \Phi(v_1,\cdots,v_i^*(\theta),\cdots,v_j^*(\theta),\cdots,v_N)\mathrm{d}\theta$$

symmetric in i,j and self adjoint on $L^2(\mathbb{S}^{N-1}(R))$.

Quantum Kac master equation for 'colliding particles'

$\mathcal{H}$, Single particle Hilbert space $\dim \mathcal{H} = n$

$h : \mathcal{H} \to \mathcal{H}$, A single particle Hamiltonian

$\mathcal{H}^{\otimes N}$, $N-$ particle Hilbert space, (classical $\mathrm{L}^2(\mathbb{R}^{\mathrm{N}}, \mathrm{dv})$

$$H_N = \sum_{i=1}^{N} h_i \ , \quad \text{Multiparticle Hamiltonian,} \quad h_2 = I \otimes h \otimes I \cdots \otimes I$$

$$\text{(classical } E(\vec{v}) = \sum_{j=1}^{N} |v_j|^2 \text{)}$$

Binary collisions: Collision specification

Let $\mathcal{C}$ a compact metric space and a continuous one-to-one function

$U : \mathcal{C} \to \mathcal{U}(\mathcal{H}_2)$ and a Borel measure ν charging all open subsets of $\mathcal{C}$

$\mathcal{U}(\mathcal{H}_2)$, a set of unitary operators on $\mathcal{H} \otimes \mathcal{H}$

i) $U(\sigma)$ commutes with H_2

ii) For some $\sigma_0 \in \mathcal{C}$, $U(\sigma_0) = I_{\mathcal{H}_2}$

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

and $\sigma \to \sigma'$ with $U^*(\sigma) = U(\sigma')$ is measurable.

iv) Let $V : \mathcal{H}_2 \to \mathcal{H}_2$ be the swap transformation: $V\phi \otimes \psi = \psi \otimes \phi$. Then

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

and the map $\sigma \to \sigma'$ where $VU(\sigma)V^* = U(\sigma')$ is a measurable transformation that leaves ν invariant.

Collision operator

$$\mathcal{Q}(A) = \int_{\mathcal{C}} d\nu(\sigma)U(\sigma)AU^*(\sigma) \ , A \in \mathcal{B}(\mathcal{H}_2)$$

Specification of h,

$$\{e_1, \dots e_n\}\ , \quad \text{eigenvalues}$$

$$\{\varphi_1, \dots, \varphi_n\}\ , \quad \text{eigenvectors}$$

Eigenbasis for H_N , $\Psi_\alpha = \varphi_{\alpha_1} \otimes \cdots \otimes \varphi_{\alpha_N}$, $\alpha \in \{1, \dots, n\}^N$

$\mathcal{K}_E$ corresponding eigenspace , $E \in \mathrm{spec} H_N$, $\mathcal{H}_N = \bigoplus_{E \in \mathrm{spec} H_N} \mathcal{K}_E$

$\mathcal{K}_E$ corresponds to the level surfaces of the classical kinetic energy function

and we call them **energy shells**

A crucial feature of the classical Kac model is that for F defined on the velocity space we have that $F \circ R_{i,j}(\theta) = F$ for $\theta \in [-\pi, \pi]$ if and only if F is constant on level surfaces of the energy function $E_{i,j}(\vec{v}) = v_i^2 + v_j^2$.

Define the 'Energy algebra $\mathcal{A}_N$' as the

commutative algebra generated by the spectral projections of H_N

$$\sum_{E \in \mathrm{spec} H_N} \lambda_E P_E$$

P_E projections onto $\mathcal{K}_E$

Functions of H_N

Obviously

$$\mathcal{A}_2 \subset \{U(\sigma) : \sigma \in \mathcal{C}\}' \text{ (commutant)}$$

Define an 'Ergodic Collision Specification' by requiring that

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

In what follows we use as the inner product on $\mathcal{B}(\mathcal{H}_N)$

$$(A, B) = \mathrm{Tr}[A^* B]$$

Examples

$$\mathcal{H} = \mathbb{C}^2 \, , \mathcal{H}_N = (\mathbb{C}^2)^{\otimes N}$$

$$h = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

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

has eigenvalues $\{0, \ldots, N\}$

For $E \in \{0, \ldots, N\}$,

$$\dim(\mathcal{K}_E) = \binom{N}{E} \, .$$

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

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

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

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

Basis of eigenvectors of H_N, $|\alpha_1, \ldots, \alpha_N\rangle$ in which each α_j is either 0 or 1.

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

In this basis,

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

$$\mathrm{Spec}(\mathcal{H}_2) = \{0, 1, 2\}$$

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

Example A: Define $\mathcal{C} = S^1 \times S^1 \times S^1 \times S^1$ identifying each copy of 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

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

Choosing ν to be the uniform probability measure (Haar 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 given above,

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

That

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

follows from Schur's lemma and hence $(\mathcal{C}, U, \nu)$ is ergodic.

Lemma

Let $(\mathcal{C}, U, \nu)$ be a collision specification.Let Φ be a convex function on $\mathcal{B}(\mathcal{H}_2)$ with the property that for all $U \in \mathcal{U}(\mathcal{H}_2)$ and all $A \in \mathcal{B}(\mathcal{H}_2)$, $\Phi(UAU^*) = \Phi(A)$. Then

$$\Phi(\mathcal{Q}A) \leq \Phi(A) \tag{2}$$

and if Φ is strictly convex, there is equality in (2) with $\Phi(A) < \infty$ if and only if $A \in \{U(\sigma)\ :\ \sigma \in \mathcal{C}\}'$. In particular, taking $\Phi(A) = \mathrm{Tr}[A^*A]$, the eigenspace of $\mathcal{Q}$ with eigenvalue 1 is $\{U(\sigma)\ :\ \sigma \in \mathcal{C}\}'$.

For the next simplest **example B**, we take $\mathcal{C}$ and U as in the previous example, but we take ν to be a non-uniform probability measure on $\mathcal{C}$. For example, take

$$\nu = (2\pi)^{-4}(1+\cos\varphi)(1+\cos\theta)(1+\cos\psi)(1+\cos\eta)\mathrm{d}\varphi\mathrm{d}\theta\mathrm{d}\psi\mathrm{d}\eta \ .$$

It is easy to check that conditions *(i)* through *(iv)* are satisfied. Then

$$\mathcal{Q}A = \begin{bmatrix} a_{1,1} & \frac{1}{8}a_{1,2} & \frac{1}{8}a_{1,3} & \frac{1}{2}a_{1,4} \\ \frac{1}{8}a_{2,1} & \frac{1}{2}(a_{2,2}+a_{3,3}) & 0 & \frac{1}{4}a_{2,4} \\ \frac{1}{8}a_{3,1} & 0 & \frac{1}{2}(a_{2,2}+a_{3,3}) & \frac{1}{4}a_{3,4} \\ \frac{1}{2}a_{4,1} & \frac{1}{4}a_{4,2} & \frac{1}{4}a_{3,4} & a_{4,4} \end{bmatrix} . \tag{3}$$

In this case, $\mathcal{Q}A \notin \mathcal{A}_2$. However, it is clear that $\lim_{n\to\infty} \mathcal{Q}^n A$ is in $\mathcal{A}_2$, and hence $(\mathcal{C}, U, \nu)$ is ergodic.

Quantum Kac generator

Let $\{U(\sigma) \ \ \sigma \in \mathcal{C}\}$ be an ergodic set of collision operators and let ν be a given Borel probability measure on $\mathcal{C}$. Define the operators $\mathcal{Q}_N$ and $\mathcal{L}_N$ on $\mathcal{B}(\mathcal{H}_N)$ by

$$\mathcal{Q}_N = \binom{N}{2}^{-1} \sum_{i<j} \mathcal{Q}_{i,j} \quad \text{and} \quad \mathcal{L}_N = N(\mathcal{Q}_N - I_{\mathcal{H}_N}) \ .$$

$$\mathcal{Q}_{i,j} A = \int_{\mathcal{C}} \mathrm{d}\nu(\sigma) U_{i,j}(\sigma) A U^*_{i,j}(\sigma) \ .$$

$\mathcal{Q}_{i,j}$ preserves positivity. $\mathrm{Tr}\mathcal{Q}_{i,j}A = \mathrm{Tr}A$, $\mathcal{Q}_{i,j}I = I$, $Q_{i,j}$ is a *Quantum Markov Operator* and restricted to density matrices a *Quantum Operation.*

The *Quantum Kac Master Equation* (QKME) is the evolution equation

on the set of density matrices given by

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

Since $\|\mathcal{L}_N\|_\infty \leq 2N$, the QKME is solved by exponentiation:

For each $t \geq 0$,we may define an operator $\mathcal{P}_{N,t}$ by

$$\mathcal{P}_{N,t} A = \sum_{k=1}^{\infty} e^{-Nt} \frac{(Nt)^k}{k!} \mathcal{Q}_N^k A = e^{t\mathcal{L}_N} A \ .$$

This map is *completely positive*, i.e., it induces a map in

$\mathcal{B}(\mathcal{H}_N) \otimes M_n(\mathbb{C})$ that is positive in $\oplus^n \mathcal{H}_N$

Spectrum of $\mathcal{L}_N$

Let $(\mathcal{C}, U, \nu)$ be a collision specification, and let $\mathcal{L}_N$ and $\mathcal{Q}_N$ be defined in terms of it as before. $\mathcal{Q}_N$ and $\mathcal{L}_N$ have discrete spectrum: There is a complete orthonormal basis consisting of eigenvectors of $\mathcal{Q}_N$ and $\mathcal{L}_N$. Moreover, $\mathrm{Spec}(\mathcal{Q}_N) \subset (0,1]$, and $\mathrm{Spec}(\mathcal{L}_N) \subset (-N, 0]$. The null space of $\mathcal{L}_N$, $\mathrm{Null}(\mathcal{L}_N)$, is given by

$$\mathrm{Null}(\mathcal{L}_N) = \{A \in \mathcal{B}(\mathcal{H}_N) :\ U_{i,j}(\sigma) A U^*_{i,j}(\sigma) = A \quad \text{all}\, 1 \le i < j \le N,\ \sigma \in \mathcal{C}\}\ .$$

For each N, let Co_N be the commutant

$$\mathrm{Co}_N = \{U_{i,j}(\sigma)\ : 1 \le i < j \le N, \sigma \in \mathcal{C}\}'\ .$$

Obviously, $\mathcal{A}_N \subset \mathrm{Co}_N = \mathrm{Null}(L_N)$ and $\mathcal{A}_2 = \mathrm{Co}_2$

Steady states

$$\lim_{t\to\infty} \mathcal{P}_{N,t}A = E_{\mathrm{Co_N}}A$$

Steady states are all the density matrices ρ with $\rho = E_{\mathrm{Co_N}}\rho$

If $(U, \mathcal{C}, \nu)$ is an ergodic collision specification, then

Co_N is a commutative algebra which is diagonal in the basis Ψ_α.

Co_N is in general not equal to $\mathcal{A}_N$, i.e., $A \in \mathrm{Co}_N$ is in general not a function of H_N.

How to describe Co_N?

Co_N is generated by its minimal projection.

A projection P is minimal if it is non-zero and there is no projection P' such that $P - P' > 0$.

If $P \in \mathrm{Co}_N$ is minimal, there exists a unique $E \in \mathrm{spec}H_N$ such that $P_E \geq P$.

It follows that $\mathrm{Co}_N = \mathcal{A}_N$ if and only if P_E is minimal for each $E \in \mathrm{spec}H_N$

Definition: $(U, \mathcal{C}, \nu)$ **is ergodic at** E **if** P_E **is minimal**

$(U, \mathcal{C}, \nu)$ **is fully ergodic if** P_E **is minimal for all** $E \in \mathrm{spec} H_N$

How to check full ergodicity?

Observation: If a collision specification $(\mathcal{C}, U, \nu)$ is ergodic,

there is a finite sequence $\{\sigma_1, \ldots, \sigma_s\}$ in $\mathcal{C}$ such that

$$\langle \psi_{e_k} \otimes \psi_{e_\ell}, U(\sigma_s) \cdots U(\sigma_2) U(\sigma_1) \psi_{e_m} \otimes \psi_{e_n} \rangle_{\mathcal{H}_2} \neq 0 \quad \iff \quad e_k + e_\ell = e_m + e_n \,.$$

$\alpha, \alpha' \in \{1, \ldots, n\}^N$ are *adjacent* iff for some pair i, j we have that $e_{\alpha_i} + e_{\alpha_j} = e_{\alpha'_i} + e_{\alpha'_j}$,

and for each $k \neq i, j$, $e_{\alpha_k} = e_{\alpha'_k}$.

$\alpha, \alpha' \in \{1, \ldots, n\}^N$ are *equivalent* iff there exists a path of adjacent pairs connecting α and α'.

Fact: The minimal projections $P \in \mathrm{Co}_N$ are precisely those that are given by

$$P = \sum_{\alpha \sim \alpha_0} |\Psi_\alpha\rangle\langle\Psi_\alpha|$$

for some α_0 with $H_N \Psi_{\alpha_0} = E\Psi_{\alpha_0}$

A collision specification is fully ergodic if and only if whenever

$\alpha, \alpha' \in \{1, \ldots, n\}^N$ satisfiy $E_\alpha = E_{\alpha'}$ then $\alpha \sim \alpha'$.

Example 1: Assume that $\{e_1, \ldots, e_n\}$ are rationally independent. Then $\alpha \sim \alpha'$

if and only if α' is a permutation of α

As a consequence $\mathrm{Co}_N = \mathcal{A}_N$ and the system is fully ergodic.

Example 2: Three single particle states: $e_1 = 1$, $e_2 = 2$, and $e_3 = 3$, 10 particles.

$$\alpha_1, \alpha_2, \alpha_3 \in \{1, 2, 3\}^{10}$$

Occupation number representation: $\alpha_1 : (4, 4, 3); \alpha_2 : (5, 2, 4); \alpha_3 : (3, 3, 4)$

Total energy 21.

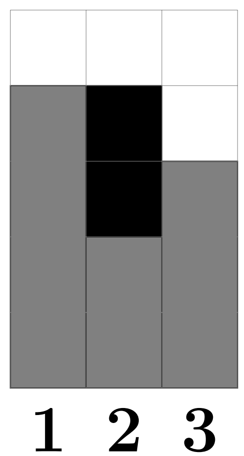

Fig. 1

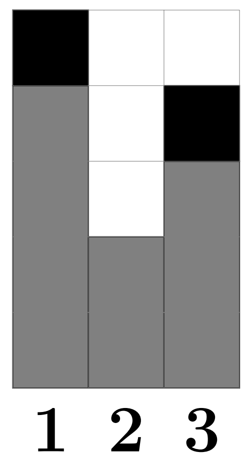

Fig. 2

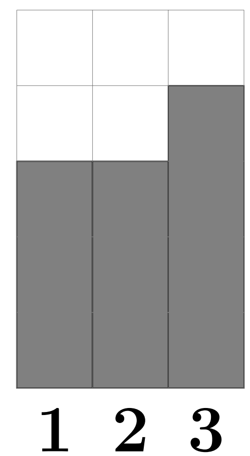

Fig. 3

Theorem

Let $(\mathcal{C}, U, \nu)$ be an ergodic collision specification, and let $\mathcal{L}_N$ be defined as before. A density matrix ϱ on $\mathcal{H}_N$ satisfies $\mathcal{L}_N\varrho = 0$ if and only if it is a convex combination of normalized minimal projections in Co_N.

A density matrix ϱ on $\mathcal{H}_N$ is a *product state* if $\varrho = \rho_1 \otimes \cdots \otimes \rho_N$ where each ρ_j is a density matrix on $\mathcal{H}$.

A density matrix ϱ on $\mathcal{H}_N$ is *separable* in case ϱ is a closed convex hull of the product states.

A density matrix ϱ on $\mathcal{H}_N$ is *entangled* in case is is not separable,

Corollary: Separability of steady states

Let $(\mathcal{C}, U, \nu)$ be an ergodic collision specification, and let $\mathcal{L}_N$ be defined as before. All density matrices ϱ on $\mathcal{H}_N$ that satisfy $\mathcal{L}_N\varrho = 0$ are separable. In other words, the Quantum Kac evolution destroys entanglement.

Propagation of chaos, the Quantum Kac Boltzmann equation

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

$$\lim_{N\to\infty} \varrho^{(1)} = \rho \qquad \text{and} \qquad \lim_{N\to\infty} \varrho^{(k)} = \bigotimes^k \rho \ .$$

$$\varrho^{(k)} = \mathrm{Tr}_{k+1,\dots,N}\varrho$$

Theorem (Propagation of Chaos)

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

This density matrix $\rho(t)$ satisfies a quantum version of the Kac-Boltzmann equation

Quantum Wild convolution operator

Let $(\mathcal{C}, U, \nu)$ be a collision specification, The corresponding *quantum Wild convolution* is the bilinear form sending (A, B) to $A \star B$ where

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

Theorem

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

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

Example B revisited:

In this example, let $(\mathcal{C}, U, \nu)$ be the collision specification from example B. Let $a, b \in [0,1]$ and let $w, z \in \mathbb{C}$ satisfy $|z|, |w| \leq 1$ so that with

$$\rho_1 = \begin{bmatrix} a & z \\ \overline{z} & 1-a \end{bmatrix} \qquad \text{and} \qquad \rho_2 = \begin{bmatrix} b & w \\ \overline{w} & 1-b \end{bmatrix},$$

ρ_1 and ρ_2 are two generic density matrices. Then using the basis from the second example to identify $\mathbb{C}^2 \otimes \mathbb{C}^2$ with $\mathbb{C}^4$,

$$\rho_1 \otimes \rho_2 = \begin{bmatrix} ab & zb & aw & zw \\ \overline{z}b & b(1-a) & \overline{z}w & w(1-a) \\ a\overline{w} & z\overline{w} & a(1-b) & z(1-b) \\ \overline{zw} & (1-a)\overline{w} & (1-b)\overline{z} & (1-a)(1-b) \end{bmatrix}.$$

Then

$$\mathcal{Q}(\rho_1 \otimes \rho_2) = \begin{bmatrix} ab & \frac{1}{8}zb & \frac{1}{8}aw & \frac{1}{2}zw \\ \frac{1}{8}\overline{z}b & \frac{1}{2}(a+b)-ab & 0 & \frac{1}{4}w(1-a) \\ \frac{1}{8}a\overline{w} & 0 & \frac{1}{2}(a+b)-ab & \frac{1}{4}z(1-b) \\ \frac{1}{2}\overline{zw} & \frac{1}{4}(1-a)\overline{w} & \frac{1}{4}(1-b)\overline{z} & (1-a)(1-b) \end{bmatrix}.$$

Note that Tr_2, the partial trace over the second factor, is obtained by adding up the two diagonal 2×2 blocks, and Tr_1, the partial trace over the first factor, is obtained by taking the trace in each 2×2 block. Therefore,

$$\rho_1 \star \rho_2 = \begin{bmatrix} \frac{1}{2}(a+b) & \frac{z}{8}(2-b) \\ \frac{\overline{z}}{8}(2-b) & 1-\frac{1}{2}(a+b) \end{bmatrix}.$$

In particular, taking $\rho = \rho_1$,

$$\rho \star \rho = \begin{bmatrix} a & \frac{z}{8}(2-a) \\ \frac{\bar{z}}{8}(2-a) & 1-a \end{bmatrix},$$

which is nonlinear in ρ. Note also, that in contrast with the classical case, the quantum Wild convolution is not commutative; $\rho_1 \star \rho_2 \neq \rho_2 \star \rho_1$ when $z(2-b) \neq w(2-a)$.

The Quantum Kac Boltzmann equation has a unique global solution

$$\rho(t) = e^{-2t}\rho_0 + \int_0^t e^{2(s-t)}\rho(s) \star \rho(s)\mathrm{d}s$$

The QKBE is nonlinear in general and preserves positivity and the trace

What can be done in this framework:

Steady states for the QKBE

Collision invariants

Linearized QKB equation

What should be done in this framework:

Approach to equilibrium

Compute the gap.

Study approach to equilibrium in entropy.

Dear Heinz,

All the best wishes for your further activities, mathematical and otherwise

Steady states for the QKBE

Fix an ergodic collision specification.

$$h = \sum_{e \in \mathrm{Spec}(h)} e P_e$$

Steady states are precisely the states ρ with $\rho = \rho \star \rho$

Gibbs state is a steady state

$$\rho_\beta \otimes \rho_\beta = Z_\beta^{-2} e^{-\beta H_2} \in \mathcal{A}_2$$

$$S(\rho) = -\mathrm{Tr}[\rho \log \rho]$$

Theorem (steady states)

Let h have the spectral resolution as a above, and let ρ be a density matrix such that $\rho = \rho \star \rho$ and $S(\rho) < \infty$. Then ρ has the form

$$\rho = \sum_{e \in \mathrm{Spec}(h)} \lambda_e P_e \tag{4}$$

for non-negative numbers $\{\lambda_e \ : \ e \in \mathrm{Spec}(h)\}$ such that $\sum_{e \in \mathrm{Spec}(h)} \mathrm{Tr}[P_e]\lambda_e = 1$. Moreover, if $\{e_i, e_j, e_k, e_\ell\} \subset \mathrm{Spec}(h)$ then

$$e_i + e_j = e_k + e_\ell \quad \Rightarrow \quad \log \lambda_{e_i} + \log \lambda_{e_j} = \log \lambda_{e_k} + \log \lambda_{e_\ell} \ . \tag{5}$$

Conversely, every such density matrix ρ is a steady state.

This theorem says in particular that if ρ is a steady state solution of the QKBE for an ergodic collision specification, then $\rho = f(h)$ for some real valued function on $\mathrm{Spec}(h)$. This may be the only restriction. Indeed if h is such that whenever $e_j + e_k = e_\ell + e_m$ then either $e_j = e_\ell$ and $e_k = e_m$ or else $e_j = e_m$ and $e_k = e_\ell$, then there is no restriction, and in this case, if $\rho = f(h)$, then $\rho \star \rho = \rho$.

On the other hand, suppose h has evenly spaced eigenvalues and there are at least three of them. To be specific, suppose that $\dim(\mathcal{H}) = n \geq 3$, and $\mathrm{Spec}(h) = \{0, 1, \dots, n-1\}$. Then for each $j = 1, \dots n-2$, $e_{j-1} + e_{j+1} = 2e_j$, and hence $\lambda_{e_j} = \sqrt{\lambda_{e_{j-1}} \lambda_{e_{j+1}}}$. This means that for some $\beta \in \mathbb{R}$, $\rho = Z_\beta^{-1} e^{-\beta h}$. (In finite dimension, negative temperatures are allowed.) In general, the more ways a given eigenvalue E of H_2 can be written as a sum of eigenvalues of h, the more constraints there are on the set of steady state solutions of the QKBE.

Steady states and collision invariants

Let h be a self adjoint operator on $\mathcal{H}$. The set $\mathfrak{S}_{\infty,h}(\mathcal{H})$ consists of those density matrices such that (4) and (5) are satisfied. The set $\mathfrak{S}_{\infty,h}(\mathcal{H})^\circ$ consist of those $\rho \in \mathfrak{S}_{\infty,h}(\mathcal{H})$ that are strictly positive. The set of *collision invariants* is the set of self adjoint operators A of the form $A = \log\rho$, $\rho \in \mathfrak{S}_{\infty,h}(\mathcal{H})^\circ$.

Theorem

Let $\rho_\infty \in \mathfrak{S}_{\infty,h}(\mathcal{H})^\circ$. Then for all $\rho \in \mathfrak{S}(\mathcal{H})$,

$$\mathrm{Tr}[\log(\rho_\infty)\rho] = \mathrm{Tr}[\log(\rho_\infty)\rho \star \rho]\ . \tag{6}$$

In particular, for every solution $\rho(t)$ of the QKBE, and every collision invariant A, $\mathrm{Tr}[A\rho(t)]$ is independent of t. Moreover, for each $\rho_\infty \in \mathfrak{S}_{\infty,h}(\mathcal{H})$ the relative entropy $D(\rho(t)\|\rho_\infty)$ is strictly monotone decreasing along any solution that is not a steady state solution.

Linearized QKBE

$$M(v) = (2\pi)^{-1/2} e^{-v^2/2}$$

$$\int \rho(v) v^2 dv = \int M(v) v^2 dv = 1 \tag{7}$$

$$\rho = M(1+f) \ , f \text{ small} \tag{8}$$

$$\int v^2 f(v) M(v) dv = 0 \ , \ S(\rho) \approx S(M) - \frac{1}{2} \int f^2 M dv$$

Thus, expect the linearized KBE to be a dissipative equation on $L^2(\mathbb{R}, M dv)$.

$$\frac{d}{dt}S(\rho + tA)\Big|_{t=0} = \mathrm{Tr}[\log(\rho)A]$$

$$[B]^{-1}A = \int_0^\infty \frac{1}{sI_{\mathcal{H}} + B} A \frac{1}{sI_{\mathcal{H}} + B} ds$$

$$[B]A = \int_0^1 B^s A B^{1-s} ds$$

$$\frac{d^2}{dt^2}S(\rho + tA)\Big|_{t=0} = \mathrm{Tr}[A[\rho]^{-1}A]$$

Bogoliubov-Kubo-Mori inner product with reference state ρ

$$\langle A, B\rangle_{BKM} = \mathrm{Tr}[A^*[\rho]^{-1}B]$$

Fix a strictly positive steady state ρ_∞ in such a way that for ρ close to ρ_∞

$$\mathrm{Tr}[\log(\widehat{\rho}_\infty)\rho] = \mathrm{Tr}[\log(\widehat{\rho}_\infty)\rho_\infty]$$

for all positive steady states $\widehat{\rho}_\infty$. This is in analogy to (7).

Define in analogy to (8)

$$A = [\rho_\infty]^{-1}(\rho - \rho_\infty)$$

Linearized QKBE

$$\frac{d}{dt}X = \mathcal{K}X$$

$$\mathcal{K}X = 2\left([\rho_\infty]^{-1}[\rho_\infty \star X + X \star \rho_\infty] - X\right)$$

$$X = [\rho_\infty]A$$

Linearized QKBE at ρ_∞

Theorem

Let $\mathcal{K}$ be the linearized Kac-Boltzmann operator at a steady state ρ_∞. Let $\langle \cdot, \cdot \rangle_{BKM}$ be the corresponding inner product on $\mathcal{B}(\mathcal{H})$. Then for all $A, B \in \mathcal{B}(\mathcal{H})$,

$$\langle B, \mathcal{K}A \rangle_{BKM} = \langle \mathcal{K}B, A \rangle_{BKM} \quad \text{and} \quad \langle A, \mathcal{K}A \rangle_{BKM} \leq 0\ . \tag{9}$$

Moreover $\langle A, \mathcal{K}A \rangle_{BKM} = 0$ if and only if A is in the linear span of the collision invariants.