Improved Approach to Equilibrium using the Kac Model

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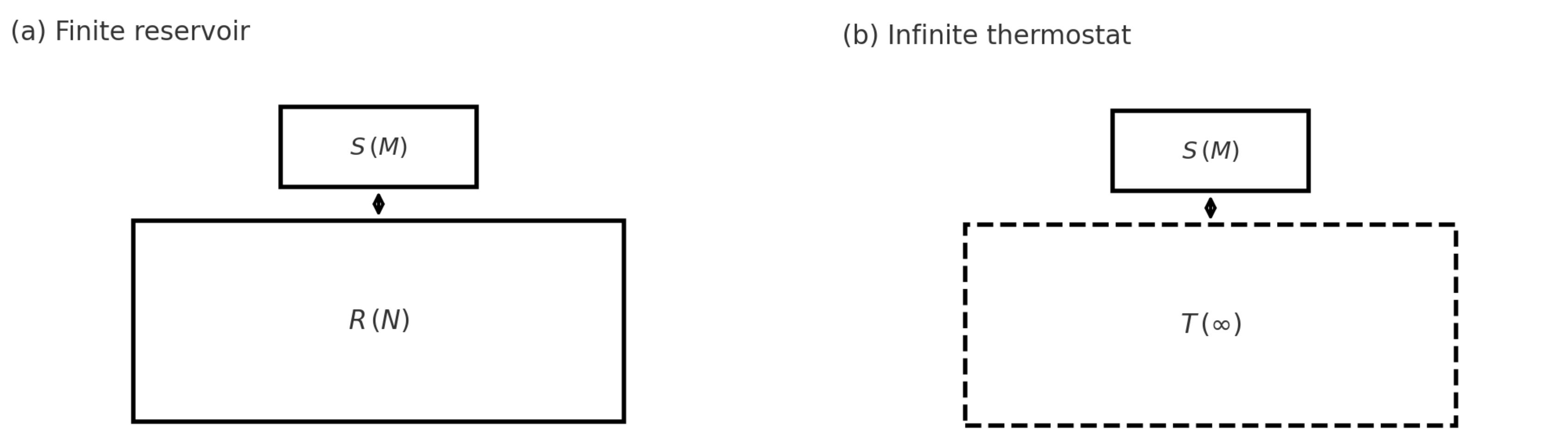
Introduction

- In 1954, Marc Kac created the Kac Model, a simplified one-dimensional model for the collisions of particles in a gas. His motivation for doing this was to rigorously show that Boltzmann's assumption of molecular chaos propagates in time; this assumption leads to a derivation of the Boltzmann Equation.
- Although the Kac Model was designed for proving propagation of chaos, we use it for a different purpose: studying approach to equilibrium for different kinds of systems. For this project, we compare two such systems.
- In the Finite Reservoir system (FR-system), a system of M particles interacts with a reservoir of N particles, with $M << N$. In the Thermostated system (T-system), a system of M particles interacts with a Maxwellian thermostat of infinite particles. Previous work has shown that the FR-system can approximate the T-system uniformly in time, and our goal was to improve the bound on this approximation.



Defining our Evolution Generators

An M-particle Kac system has the state $f(\vec{v})$, the probability density for the particles having velocities $\vec{v} = (v_1, ..., v_M)$. Particles i and j have a fixed chance to collide such that v_i and v_j become $v_i \cos\theta - v_j \sin\theta$ and $v_i \sin\theta + v_j \cos\theta$, where θ can be any angle from 0 to 2π. The generator for the Kac evolution is:

$$L_S[f] = \frac{\lambda_S}{M-1} \sum_{i<j} (R_{ij}^S[f] - f)$$

Here $R_{ij}^S[f]$ is the rotational average of f over all possible pre-collision velocities:

$$R_{ij}^S[f](\vec{v}) = \frac{1}{2\pi} \int_0^{2\pi} f(\vec{v}_{ij}(\theta))\, d\theta$$

where $\vec{v}_{ij}(\theta) = (v_1, ..., v_i \cos\theta + v_j \sin\theta, ..., -v_i \sin\theta + v_j \cos\theta, ..., v_M)$

The FR-system evolves from collisions within the system, within the reservoir, and between system and reservoir. The system evolution is generated by L_S, while the reservoir and interaction evolutions have similar generators L_R and L_I. Thus the total generator for the FR-system is $\boxed{L = L_S + L_R + L_I}$.

For the T-system, the system-thermostat interaction has the generator:

$$L_T[f] = \mu \sum_i (T_i[f] - f)$$

where

$$T_i[f] = \int e^{-\pi x^2} \frac{1}{2\pi} \int_0^{2\pi} f(\vec{v}_i(x,\theta))\, dx$$

and $\vec{v}_i(x,\theta) = (v_1, ..., v_i \cos\theta + x \sin\theta, ..., v_M)$. Thus the total generator for the T-system is $\boxed{\bar{L} = L_S + L_T}$.

Distance Between States

We call the initial state of the system h_0. Using our generators, we can write our evolution equations: $h_t = e^{Lt} h_0$ for the FR-system and $\bar{h}_t = e^{\bar{L}t} h_0$ for the T-system. In order to compare h_t and $\bar{h}_t$, we define an L_2 space with inner product given by:

$$(f,g) = \int f(\vec{v},\vec{w})\, g(\vec{v},\vec{w})\, \Gamma(\vec{v},\vec{w})\, d\vec{v}\, d\vec{w}$$

where $\Gamma(\vec{v},\vec{w}) = e^{-\pi(|\vec{v}|^2 + |\vec{w}|^2)}$. Defining the L_2 norm as $||f||_2 = \sqrt{(f,f)}$, our task is to put a uniform bound on $||(e^{Lt} - e^{\bar{L}t})h_0||_2$.

Previous Results vs. Our Result

In Bonetto *et al.* (2017) it was proved that:

$$||(e^{Lt} - e^{\bar{L}t})h_0||_2 \le \frac{M}{\sqrt{N}}(1 - e^{-\frac{\mu}{2}t})||h_0 - 1||_2$$

On the other hand, Bonetto *et al.* (2017) also includes a proof that as $t \to \infty$, the difference between states obeys:

$$||h_\infty - 1||_2 \le \sqrt{\frac{M}{N-2}}||h_0 - 1||_2$$

Thus, the uniform bound over all time is clearly very inefficient, since it only bounds the final steady state difference by a factor of $M/\sqrt{N}$, which is much larger than for the true steady states; see the figure below for a rough visualization of this problem.

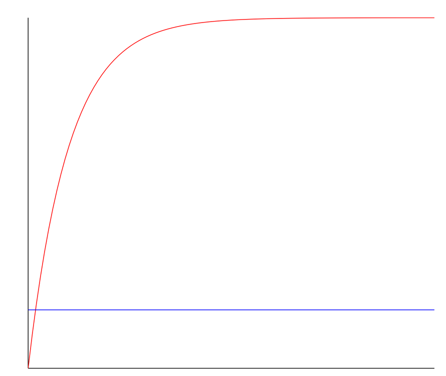


Figure 1. Rough visualization of old bounds; red is the uniform bound and blue is the asymptote for final state.

Our work rectifies this problem: we proved the following bound, which is uniform in time and has the desired behavior as $t \to \infty$:

$$\boxed{||(e^{Lt} - e^{\bar{L}t})h_0||_2 \le [\sqrt{\frac{M}{N-2}}(1 - e^{-cMt}) + \frac{M}{\sqrt{N}}\frac{\mu/2}{\kappa - \mu/2}(e^{-\frac{\mu}{2}t} - e^{-\kappa t})]\; ||h_0 - 1||_2}$$

where $-\kappa$ is the largest negative eigenvalue of L and $-cM$ is the smallest eigenvalue of $\bar{L}$.

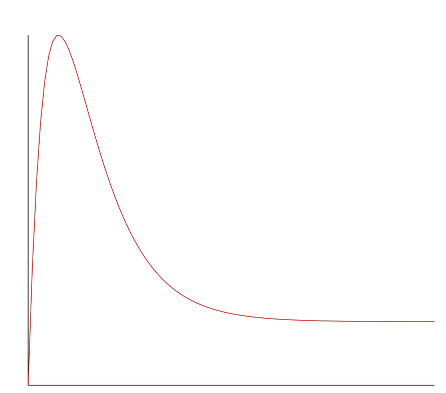


Figure 2. Rough visualization of new uniform bound.

Proof

The key ingredient in our proof is the concept of rotational invariance. We define the operator R to average f over all possible rotations of the system and reservoir velocity vectors:

$$R[f](\vec{v},\vec{w}) = \int_{S^{M+N-1}(r)} f(\vec{v'},\vec{w'})\, d\sigma_r(\vec{v'},\vec{w'})$$

where $\vec{v}$ are the system velocities, $\vec{w}$ are the reservoir velocities, and $r = \sqrt{|\vec{v}|^2 + |\vec{w}|^2}$. Importantly, by the argument in Bonetto *et al.* (2017), $||R[f]||_2 \le \sqrt{\frac{M}{N-2}}||f||_2$ for any function $f(\vec{v})$ with $(f,1) = 0$.

To start, we write

$$(e^{Lt} - e^{\bar{L}t})h_0 = (e^{Lt} - e^{\bar{L}t})u_0 = \int_0^t e^{L(t-s)}(L - \bar{L})e^{\bar{L}s}u_0\, ds$$

where $u_0 = h_0 - 1$. We then split this integral into two parts: $\{1\} = \int_0^t e^{L(t-s)}(1-R)(L-\bar{L})e^{\bar{L}s}u_0\, ds$ and $\{2\} = \int_0^t e^{L(t-s)}R(L-\bar{L})e^{\bar{L}s}u_0\, ds$. For the first integral, we take the norm:

$$||\{1\}||_2 \le \int_0^t ||e^{L(t-s)}(1-R)(L-\bar{L})e^{\bar{L}s}u_0||_2\, ds \le \int_0^t e^{-\kappa(t-s)}||(1-R)(L-\bar{L})e^{\bar{L}s}u_0||_2\, ds$$

where in the last inequality we invoke the spectral gap of L, proven in Carlen *et al.* (2003), and the fact that R is an orthogonal projector. From here, we can use the results from Bonetto *et al.* (2017) to get

$$\{1\} \le \frac{M}{\sqrt{N}}\frac{\mu/2}{\kappa - \mu/2}(e^{-\frac{\mu}{2}t} - e^{-\kappa t})||h_0 - 1||_2$$

For $\{2\}$, we take advantage of the fact that $L(R[f]) = R(L[f]) = 0$ for any function f to write

$$\{2\} = \int_0^t R(L-\bar{L})e^{\bar{L}s}u_0\, ds = \int_0^t -R\bar{L}e^{\bar{L}s}u_0\, ds = \left[-Re^{\bar{L}s}u_0\right]_0^t = R[(1 - e^{\bar{L}t})u_0]$$

By the effect of R mentioned above, we write

$$||\{2\}||_2 = ||R[(1 - e^{\bar{L}t})u_0]||_2 \le \sqrt{\frac{M}{N-2}}||(1 - e^{\bar{L}t})u_0||_2 \le \sqrt{\frac{M}{N-2}}(1 - e^{-cMt})||u_0||_2$$

Combining the inequalities for $||\{1\}||_2$ and $||\{2\}||_2$ completes the proof.□

Future Work

Some work which may be pursued further would be the extension of this result to the 3-D Kac Model, and possibly introducing the complication of a shear, so that the system may start out with an overall velocity relative to the reservoir or thermostat.

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