The Kac Model Coupled to a Thermostat

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Abstract In this paper we study a model of randomly colliding particles interacting with a thermal bath. Collisions between particles are modeled via the Kac master equation while the thermostat is seen as an infinite gas at thermal equilibrium at inverse temperature β . The system admits the canonical distribution at inverse temperature β as the unique equilibrium state. We prove that any initial distribution approaches the equilibrium distribution exponentially fast both by computing the gap of the generator of the evolution, in a proper function space, as well as by proving exponential decay in relative entropy. We also show that the evolution propagates chaos and that the one particle marginal, in the large system limit, satisfies an effective Boltzmann-type equation.

Keywords Kac model · Thermostat · Approach to equilibrium · Propagation of chaos

Mathematics Subject Classifications 47A63 · 15A90

1 Introduction

The master equation approach to kinetic theory has had a revival in recent years. It was introduced by Kac [1] to model a system of N particles interacting through a Markov process. In its basic form, after waiting an exponentially distributed time, one selects randomly and

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We dedicate this article to our friend, teacher, and co-author Herbert Spohn.

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uniformly a pair of particles and lets them collide with a random scattering angle. One assumes a spatially homogeneous situation in which the state of the system is entirely specified by the velocities of the particles. The time evolution for the probability distribution of finding the system in a given state is then a *linear* master equation (albeit in very high dimensions) called the Kac master equation.

The model is based on clear probabilistic assumptions, and its simplicity allows one to focus on central issues that are very difficult to study in more fundamental models like Newtonian mechanics. Kac's main motivation was to give a rigorous derivation of the *non-linear* spatially homogeneous Boltzmann equation ([1], see also [2]). This is based on the notion of chaotic sequences (which Kac called 'sequences that have the Boltzmann property'). A derivation of the Boltzmann equation from the laws of classical mechanics is much more difficult and so far has only been achieved for situations with very few collisions [3–5].

The Kac master equation also yields some insight into the the central question of approach to equilibrium for large particle systems. Kac suggested using the gap as a measure for the rate of approach to equilibrium and he conjectured that it is bounded below by a positive constant independent of the particle number N [1]. This conjecture was first proved in [6] and shortly thereafter the gap was computed exactly [7,8].

It turns out that while the gap is a good notion for measuring the rate of approach once the system is close to equilibrium, this is not the case far away from equilibrium. The gap measures the rate at which the L^2 -norm of the deviation from equilibrium tends to zero. Since probability distributions in N variables that are close to a product have an L^2 -norm which is of the order of C^N , C > 1, one has to wait times of order N until this norm falls below a fixed number. This is clearly not physical. Furthermore, in all the exact calculations, the gap as well as the single particle marginal of the gap eigenfunction approach the corresponding quantities of the *linearized* Boltzmann equation, as $N \to \infty$.

A better notion of equilibration is in the entropic sense. It is easy to prove that the relative entropy of any state (c.f. Eq. (1.5)) is decreasing in time (note that we define entropy with opposite sign). One would expect the entropy production, i.e. the negative time derivative of the entropy, to be proportional to the entropy itself because one expects exponential decay of the entropy. The results in this direction have been disappointing. It turns out that there are states whose entropy production is inversely proportional to the particle number N. In [9] a lower bound inversely proportional to N was given while an upper bound of the same order was proven in [10]. The upper bound was achieved by estimating the entropy production of a state in which approximately half of the kinetic energy is stored in $N\delta_N$ particles and, of course, the remaining kinetic energy is stored in $N(1 - \delta_N)$ particles. It was shown in [10] that the ratio of entropy production and the entropy is bounded above by $C_{\beta}N^{-1+\beta}$ for any $\beta > 0$ provided one chooses δ_N as a suitable inverse power of N. Clearly, such a state, in which a few molecules contain half of the total kinetic energy is not observed in nature. This raises the question of how to characterize those states for which the entropy converges to zero on a reasonable time scale. Our very preliminary answer is to consider states in which an 'overwhelming' number of particles with kinetic energy per particle of the order β^{-1} are in equilibrium and only a few particles, a 'local' disturbance are out of equilibrium.

How should one describe such a state in the context of a model that is spatially homogeneous in the first place? In this paper we address this question by coupling a system of particles, 'the small system out of equilibrium' to a heat bath, 'the large system in equilibrium', i.e., we couple the Kac model to a thermostat. This idea is not new. There has been work in [11] on the (spatially inhomogeneous) Boltzmann equation coupled to a thermostat where approach to equilibrium was proved. Likewise there has been recent work in [12,13] that considered particles in an electric field interacting with external scatterers (billiard), where the thermostat is given by a deterministic friction term while the collision with the obstacles provide stochasticity.

In the present work we focus exclusively on the approach to equilibrium of a system of particles in one space dimension having unit mass interacting with a thermostat in the context of the Kac master equation. There are a number of ways to model this and the route taken here is to describe the thermostat as the interaction of particles of the Kac system with particles that are already at equilibrium, i.e., whose distribution is given by a Gaussian with inverse temperature β . Moreover we assume that the thermostat is much larger than the system so that every particle in the thermostat collides at most once with a particle in the Kac system.

Calling $f_t(\mathbf{v}), \mathbf{v} \in \mathbb{R}^N$, the probability distribution of finding the system with velocities \mathbf{v} at time t, our master equation is given by

$$\frac{\partial f}{\partial t} = -\mathscr{G}f := -\lambda N(I-Q)[f] - \mu \sum_{j=1}^{N} (I-R_j)[f].$$
(1.1)

The first term $\mathscr{G}_K := N(I - Q)$ describes the collision among the particles and has the usual Kac form

$$Q[f](\mathbf{v}) := \frac{1}{\binom{N}{2}} \sum_{i < j} \int_{0}^{2\pi} f(\mathbf{v}_{i,j}(\theta)) d\theta$$

with

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

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

while the second term $\mathscr{G}_T := \sum_{j=1}^N (I - R_j)$ describes the interaction with the thermostat where

$$R_j[f] := \int dw \int_0^{2\pi} d\theta \sqrt{\frac{\beta}{2\pi}} e^{-\frac{\beta}{2}w_j^{*2}(\theta)} f(\mathbf{v}_j(\theta, w))$$

and $\mathbf{v}_j(\theta, w) = (v_1, \dots, v_j \cos(\theta) + w \sin(\theta), \dots, v_N), w_j^*(\theta) = -v_j \sin(\theta) + w \cos(\theta).$ We use the notation

$$\int_{a}^{b} f(\theta)d\theta = \frac{1}{b-a} \int_{a}^{b} f(\theta)d\theta.$$

In contrast to Kac's original work, where the configuration space was the constant-energy sphere, here the configuration space is \mathbb{R}^N since the energy is not conserved.

As we will see, the time evolution defined by (1.1) is ergodic and has the unique equilibrium state

$$\gamma(\mathbf{v}) := \prod_j g(v_j),$$

where $g(v) = \sqrt{\frac{\beta}{2\pi}} e^{-\frac{\beta}{2}v^2}$.

As mentioned before, the approach to equilibrium can be measured in a quantitative fashion by the gap of the operator \mathcal{G} . While not self-adjoint on the space $L^2(\mathbb{R}^N, d\mathbf{v})$, a

ground state transformation can be performed that brings this operator into a self-adjoint form on the space $L^2(\mathbb{R}^N, \gamma(\mathbf{v})d\mathbf{v})$. Writing

$$f(\mathbf{v}) = \gamma(\mathbf{v})(1 + h(\mathbf{v}))$$

in Eq. (1.1) we get the new equation

$$\frac{\partial h}{\partial t} = -\mathcal{L}f := -\lambda N(I-Q)[h] - \mu \sum_{j=1}^{N} (I-T_j)[h]$$
(1.2)

where

$$T_j[h] = \int dwg(w) \oint d\theta h(\mathbf{v}_j(\theta, w)).$$

We consider h in the space $L^2(\mathbb{R}^N, \gamma(\mathbf{v})d\mathbf{v})$ with inner product $\langle h_1, h_2 \rangle := \int h_1 h_2 \gamma d\mathbf{v}$. Defining the spectral gap as

$$\Delta_N := \inf\{|\langle h, \mathscr{L}h \rangle| : ||h|| = 1, \langle h, 1 \rangle = 0\}$$

we get the following:

Proposition 1 We have

$$\Delta_N = \frac{\mu}{2}.$$

The corresponding eigenfunction is

$$h_{\Delta_N}(\mathbf{v}) := \sum_{i=1}^N \left(v_i^2 - \frac{1}{\beta} \right).$$

Thus, the spectral gap does not depend on the parameter λ of the Kac operator. To have a more precise idea of the role of λ in the equilibration process we also study the "second" spectral gap defined as

$$\Delta_N^{(2)} := \inf\{|\langle h, \mathscr{L}h\rangle| : ||h|| = 1, \langle h, 1\rangle = 0, \langle h, h_{\Delta_N}\rangle = 0\}.$$

We have the following theorem that renders the gap $\Delta_N^{(2)}$ in an explicit fashion.

Theorem 2 $\Delta_N^{(2)}$ is given by the lower root a_2 of the quadratic equation

$$x^{2} - \left(\lambda\Lambda_{N} + \frac{13}{8}\mu\right)x + \mu\left(\lambda\Lambda_{N} + \frac{5}{8}\mu\right) - \frac{3}{8}\lambda\Lambda_{N}\mu\left(\frac{3}{N+2}\right) = 0, \quad (1.3)$$

where $\Lambda_N = \frac{1}{2} \frac{N+2}{N-1}$. The corresponding eigenfunction is an even polynomial of degree 4 in all the v_i .

As $N \to \infty$ one finds for the gap

$$\Delta_{\infty}^{(2)} = \min\left\{\frac{\lambda}{2} + \frac{5}{8}\mu, \mu\right\}.$$
(1.4)

As explained before, a deeper way of understanding the approach to equilibrium is to consider the entropy production. In the model at hand one is indeed in the lucky situation that the interaction with the thermostat yields a decay rate for the entropy, uniformly in N. The relative entropy of a state f with respect to the equilibrium state γ is defined as

$$S(f|\gamma) := \int_{\mathbb{R}^N} f(\mathbf{v}) \log \frac{f(\mathbf{v})}{\gamma(\mathbf{v})} d\mathbf{v}.$$
 (1.5)

Theorem 3 Let f_t be the solution of the master equation (1.1) with initial condition f_0 . Then

$$S(f_t|\gamma) \le e^{-\rho t} S(f_0|\gamma),$$

where

$$\rho = \frac{\mu}{2}.$$

The central concept for the derivation of the Boltzmann equation is that of a chaotic sequence. More precisely, given a distribution $f^{(N)}(\mathbf{v})$ with $\mathbf{v} \in \mathbb{R}^N$, we can define the k particle marginal as

$$f_k^{(N)}(v_1,\ldots,v_k) = \int f^{(N)}(\mathbf{v}) \prod_{i=k+1}^N dv_i.$$

Definition 4 A sequence of probability distributions $\{f^{(N)}(\mathbf{v})\}_{N=1}^{\infty}$ on \mathbb{R}^N is said to be **chaotic** if, $\forall k \ge 1$, we have

$$\lim_{N \to \infty} f_k^{(N)}(v_1, \dots, v_k) = \lim_{N \to \infty} \prod_{j=1}^k f_1^{(N)}(v_j),$$

where the above limit is taken in the weak sense.

Consider now a chaotic family of initial conditions $f^{(N)}(\mathbf{v})$ for Eq. (1.1). With a simple generalization of the proof by Kac [1] (see also [2]), we can show that the solution at time t, $f_t^{(N)}(\mathbf{v})$, is also chaotic. This property is called propagation of chaos. It follows that if we define

$$\overline{f}_t(v_1) = \lim_{N \to \infty} \int f_t^{(N)}(\mathbf{v}) \, dv_2 \cdots dv_N,$$

Equation (1.1) gives rise to the effective evolution for \overline{f}_t , that is

Theorem 5 $\overline{f}_t(v)$ is the solution of the following 'Boltzmann Equation':

$$\frac{\partial \overline{f}_t(v)}{\partial t} = 2\lambda \oint d\theta \int dw \Big[\overline{f}_t(v\cos\theta + w\sin\theta) \overline{f}_t(-v\sin\theta + w\cos\theta) - \overline{f}_t(v) \overline{f}_t(w) \Big] \\ + \mu \Big[\int dw \oint d\theta g(-v\sin\theta + w\cos\theta) \overline{f}_t(v\cos\theta + w\sin\theta) - \overline{f}_t(v) \Big]$$

with $\overline{f}_0(v)$ as initial condition.

Our proof of propogation of chaos, following the argument in [1], does not establish the validity of the above equation *uniformly* in t. One can hope to achieve this by adapting, to our model, the argument in [14], where propagation of chaos uniform in t is shown for the Kac model.

One can linearize the above Boltzmann equation about the ground state and study the operator associated with this evolution. It turns out that the Hermite polynomials diagonalize both the collision part and the thermostat, with the *n*th degree polynomial $H_n(v)$ yielding eigenvalues $2\lambda(1 - 2s_n)$ and $\mu(1 - s_n)$, respectively, where $s_n := \int_{0}^{2\pi} \cos^n \theta d\theta$. Thus, the gap is $\frac{\mu}{2}$, and the "second" gap is $\frac{\lambda}{2} + \frac{5}{8}\mu$, which correspond to the $N \to \infty$ limit of the respective gaps found at the Master equation level (Theorem 2). Incidentally, the eigenvalue μ found in the latter (see Eq. (1.4)) does not appear here since the single-particle marginal of the corresponding eigenfunction vanishes in the limit.

Remark As we will see, the proof of Theorem 3 (in particular, Proposition 15) also proves that the relative entropy associated with the Boltzmann equation decays at the same rate ρ .

It is interesting to note that if we define the total kinetic energy K(f) as

$$K(f) := \frac{1}{2} \sum_{i=1}^{N} \int_{\mathbb{R}^N} v_i^2 f(v_1, \dots, v_N) dv_1 \cdots dv_N$$

we get, using Eq. (1.1), that

$$\begin{aligned} \frac{dK}{dt} &= -\mu NK + \frac{\mu}{2} \sum_{j} \int dw d\mathbf{v} \oint d\theta \left(\sum_{k} v_{k}^{2} \right) g(w_{j}^{*}(\theta)) f(\mathbf{v}_{j}(\theta, w)) \\ &= -\mu NK + \frac{\mu}{2} \sum_{j} \left(\sum_{k \neq j} \int d\mathbf{v} v_{k}^{2} f(\mathbf{v}) \\ &+ \int dw d\mathbf{v} g(w) f(\mathbf{v}) \oint d\theta (v_{j} \cos(\theta) + w \sin(\theta))^{2} \right), \end{aligned}$$

where the Kac collision gives no contribution as it preserves the total kinetic energy. This yields

$$\frac{dK}{dt} = -\frac{\mu}{2} \left(K - \frac{N}{2\beta} \right). \tag{1.6}$$

One can interpret Eq. (1.6) as Newton's law of cooling. This law, however, is usually stated in terms of the *temperature* of the system at time *t*, i.e.,

$$\frac{1}{2}T(t) := \frac{K(t)}{N}.$$
(1.7)

It is far from clear that Eq. (1.7) can be used to define the temperature of a state far from equilibrium. To make such an identification one would have to show that the full distribution $f_t(\mathbf{v})$ is close, in a meaningful sense, to a Maxwellian with temperature T(t). In general we see no reason why this should be true. We believe, however, that in the case of an 'infinitely slow' transformation, i.e. the case where μ is very small relative to λ , the collisions provide enough 'mixing' to guide the evolution along Maxwellians.

The plan of the paper is the following. In Sect. 2.1 the gap is computed and in Sect. 2.2 the rate of decay of the relative entropy is established. In Sect. 3 we show propagation of chaos and we finish with a few remarks.

2 Approach to Equilibrium: Proof of Statements

Before proceeding with the study of the approach to equilibrium, we observe that by choosing appropriate units of energy, we can set $\beta = 1$ without loss of generality.

2.1 Approach to Equilibrium in L^2

In this section we study the lower part of the spectrum of the operator \mathscr{L} defined in Eq. (1.2) acting on the Hilbert space $\mathcal{X} = L^2(\mathbb{R}^N, \gamma(\mathbf{v})d\mathbf{v})$. To distinguish the action of the thermostat from that of the Kac collisions we define the operators

$$\mathscr{L}_T := \sum_{j=1}^N (I - T_j) \qquad \qquad \mathscr{L}_K := N(I - Q)$$

so that

$$\mathscr{L} = \mu \mathscr{L}_T + \lambda \mathscr{L}_K.$$

It is easy to see that the operator \mathscr{L} for the evolution of *h* is self-adjoint on \mathscr{X} . Moreover \mathscr{L} preserves the subspace of \mathscr{X} formed by the functions symmetric under permutation of the variables.

To begin, we report some known or simple results on the spectra of \mathscr{L}_K and \mathscr{L}_T . We say that a function $h(\mathbf{v})$ is *radial* if it depends only on $r^2 = \sum_i v_i^2$. We call \mathscr{X}_r the subspace of \mathscr{X} of radial functions, and \mathscr{X}^{\perp} the subspace of functions orthogonal to the constant function, i.e. $\mathscr{X}^{\perp} = \{h \in \mathscr{X} \mid \langle h, 1 \rangle = 0\}$. We have

Lemma 6 •
$$\mathscr{L}_K \ge 0, \, \mathscr{L}_T \ge 0.$$

• $\mathscr{L}_K[h] = 0 \Leftrightarrow h \in \mathcal{X}_r, \, and \, \mathscr{L}_T[h] = 0 \Leftrightarrow h = constant.$

Proof All claims follow from the following observations:

$$2\langle (I-Q)h,h\rangle = \frac{1}{\binom{N}{2}} \sum_{i
$$2\langle \sum_j (I-T_j)h,h\rangle = \sum_j \left(\oint d\theta \int d\mathbf{v} dwg(w)\gamma(\mathbf{v}) |h(\mathbf{v}_j(\theta,w)) - h(\mathbf{v})|^2 \right) \ge 0,$$$$

the first of which is an identity due to Kac [1].

Notice that the Kac operator alone acting on \mathbb{R}^N has a degenerate ground state.

From the above Lemma, we see that the unique equilibrium state corresponding to Eq. (1.2) is $h(\mathbf{v}) = 1$. The following Theorem is a direct consequence of the results in [7].

Theorem 7 [7] We have that

$$\Lambda_N := \inf\{|\langle h, \mathscr{L}_K h\rangle| : ||h|| = 1, h \perp \mathcal{X}_r\} = \frac{1}{2} \frac{N+2}{N-1}$$

and the corresponding eigenfunction is $\sum_{j=1}^{N} v_j^4 - \frac{3}{N+2} \left(\sum_{j=1}^{N} v_j^2 \right)^2$.

To study the spectrum of \mathscr{L}_T we use the Hermite polynomials $H_{\alpha}(v)$ with weight g(v). More precisely, for α integer, we set

$$H_{\alpha}(v) = (-1)^{\alpha} e^{\frac{v^2}{2}} \frac{d^{\alpha}}{dv^{\alpha}} e^{-\frac{v^2}{2}}$$

so that

- 1. $H_{\alpha}(v)$ is a polynomial of degree α . Moreover $H_{\alpha}(-v) = (-1)^{\alpha} H_{\alpha}(v)$.
- 2. The coefficient of v^{α} in H_{α} is 1.
- 3. The H_{α} are orthogonal in $L^2(\mathbb{R}, gdv)$. More precisely

$$\int H_{\alpha_1}(v)g(v)H_{\alpha_2}(v)dv = \sqrt{2\pi}\alpha_1!\delta_{\alpha_1,\alpha_2}.$$

Lemma 8 $H_{\alpha}(v_j)$ form an orthogonal basis of eigenfunctions for the operator T_j and $T_j H_{\alpha} = s_{\alpha} H_{\alpha}$ with $s_{\alpha} = 0$ if α is odd while

$$s_{2\alpha} = \int_{0}^{2\pi} d\theta \cos^{2\alpha} \theta = \frac{(2\alpha)!}{2^{2\alpha} \alpha!^2}$$

Proof We drop the subscript *j* here for ease of notation. First, we observe that

$$\int T[H_{\alpha}(v)]H_{n}(v)g(v)dv = \int dwdvg(v)g(w)H_{n}(v) \oint d\theta H_{\alpha}(v\cos\theta + w\sin\theta)$$
$$= \int dwdvg(v)g(w)H_{\alpha}(v) \oint d\theta H_{n}(v\cos\theta + w\sin\theta).$$

Since $T[H_{\alpha}(v)]$ is a polynomial in v of degree α , the first line implies that $\int T[H_{\alpha}(v)]H_n(v)$ g(v)dv = 0 if $n > \alpha$. Likewise, the second line implies that $\int T[H_{\alpha}(v)]H_n(v)g(v)dv = 0$ if $\alpha > n$. Thus,

$$T[H_{\alpha}(v)] = c_{\alpha}H_{\alpha}(v).$$

By equating the coefficients of v^{α} in the above, we get that $c_{\alpha} = \int \cos^{\alpha} \theta = s_{\alpha}$.

Note that $s_{2(\alpha+1)} < s_{2\alpha}$ and $s_{2\alpha} \rightarrow 0$ as $\alpha \rightarrow \infty$. Since \mathscr{L}_T is just the direct sum of $(I - T_j)$ we get

Corollary 9 The functions

$$H_{\underline{\alpha}}(\mathbf{v}) := \prod_{i=1}^{N} H_{\alpha_i}(v_i),$$

where $\underline{\alpha} = (\alpha_1, \dots, \alpha_N)$, is an eigenfunction of \mathscr{L}_T with eigenvalue

$$\sigma_{\underline{\alpha}} := \sum_i (1 - s_{\alpha_i}).$$

The set $\{H_{\underline{\alpha}}\}_{\underline{\alpha}\geq 0}$ form an orthogonal basis of eigenfunctions for \mathscr{L}_T in \mathcal{X} . In particular $\mathscr{L}_T > 0$ on \mathcal{X}^{\perp} .

To study the spectral gap, we need to understand the action of \mathscr{L}_K on products of Hermite polynomials $H_{\underline{\alpha}}$. We first state and prove the following lemma which helps us restrict our investigation to even polynomials.

Lemma 10

Any eigenfunction of μL_T + λL_K is either even or odd in each variable v_i.
If E is an eigenvalue of μL_T + λL_K, with an eigenfunction that is odd in some v_i, we have that E ≥ 2λ + μ.

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Proof The first part can be seen by noting that the operator $\mu \mathscr{L}_T + \lambda \mathscr{L}_K$ commutes with the reflection operator $S_j[h](\mathbf{v}) := h(\ldots, -v_j, \ldots)$. For the second part, say $(\mu \mathscr{L}_T + \lambda \mathscr{L}_K)h = Eh$, with $S_1[h] = -h$. Then $T_1[h] = 0$. In addition, for any $i \neq 1$,

$$\begin{aligned} \oint d\theta h(\mathbf{v}_{i,1}(\theta)) &= \oint d\theta h(v_i \cos \theta + v_1 \sin \theta, \dots, -v_i \sin \theta + v_1 \cos \theta, \dots) \\ &= \oint d\theta h(\sqrt{v_i^2 + v_1^2} \cos (\varphi - \theta), \dots, \sqrt{v_i^2 + v_1^2} \sin (\varphi - \theta), \dots) \\ &= \oint d\theta h(\sqrt{v_i^2 + v_1^2} \cos \theta, \dots, \sqrt{v_i^2 + v_1^2} \sin \theta, \dots) \\ &= \oint d\theta h(-\sqrt{v_i^2 + v_1^2} \cos \theta, \dots, \sqrt{v_i^2 + v_1^2} \sin \theta, \dots) \quad (\text{taking } \theta \to \pi - \theta) \\ &= 0 \quad (\text{using that } S_1[h] = -h). \end{aligned}$$

Thus,

$$\lambda Nh - \lambda \frac{N}{\binom{N}{2}} \sum_{i < j, i, j \neq 1} \oint d\theta h(\mathbf{v}_{i, j}(\theta)) + N\mu h - \mu \sum_{i \neq 1} T_i[h] = Eh$$

or

$$(\lambda N + \mu N - E) \le \lambda \frac{N}{\binom{N}{2}} \binom{N-1}{2} + \mu (N-1),$$

which proves the claim.

We will thus restrict our attention to the space of functions that are even in all variables v_i and show that the eigenfunction for Δ_N and $\Delta_N^{(2)}$ lie in this space. To this end we define

$$L_{2l} = \operatorname{span}\Big\{H_{2\underline{\alpha}}\Big|\sum_{i=1}^{N} 2\alpha_i = 2l\Big\}.$$

Moreover we set

$$|\underline{\alpha}| = \sum_{i=1}^{N} \alpha_i$$

and

$$\Xi := \{ \underline{\alpha} : \sum_{i < j} \alpha_i \alpha_j \neq 0 \}$$
, that is the set of $\underline{\alpha}$ in which at least two entries are non-zero.

Lemma 11 In each L_{2l} the eigenvalues of \mathscr{L}_T are given by $\sigma_{2\underline{\alpha}} = \sum_j (1 - s_{2\alpha_j})$, where $|\underline{\alpha}| = l$. It follows that

- The smallest eigenvalue in each L_{2l} is $1 s_{2l}$ and the corresponding eigenfunctions are precisely linear combinations of $H_{2\alpha}(\mathbf{v})$ with $\underline{\alpha} = (0, \dots, l, \dots, 0)$.
- $\min_{\underline{\alpha}\in\Xi} \sigma_{2\underline{\alpha}} = 1$. Morover, the minimum is reached when two of the α_i 's are 1 and the rest are 0.

Proof To prove the first statement, we start by observing that the function $J(x) := \int_{0}^{2\pi} \cos^{2x} \theta d\theta$ is strictly convex in x. Consider $\underline{\alpha}$ such that $|\alpha| = l$. We need to show that

$$\sum J(\alpha_i) \le J(l) + (N-1)J(0)$$

and that equality is attained if and only if $\underline{\alpha} = (0, \dots, l, \dots, 0)$. By convexity, we have that

$$J(\alpha_i) = J\left(\frac{\alpha_i}{l}l + \sum_{j \neq i} \frac{\alpha_j}{l}0\right)$$
$$\leq \frac{\alpha_i}{l}J(l) + \sum_{j \neq i} \frac{\alpha_j}{l}J(0).$$

Summing the above over *i*, we get the result.

The second claim follows from the monotonicity of the $s_{2\alpha}$ and the fact that $s_2 = \frac{1}{2}$.

Proof of Proposition 1 By Corollary 9 and Lemma 11, we have that $\mathscr{L}_T \geq 1/2$ and thus $\mathscr{L} \geq 1/2$ on \mathscr{X}^{\perp} . On the other hand, $\mathscr{L}[\sum H_2(v_i)] = \mathscr{L}_T[\sum H_2(v_i)] = \frac{\mu}{2}(\sum H_2(v_i))$ since $\sum H_2(v_i)$, being a radial function is annihilated by the Kac part. Thus, $\Delta_N = \mu/2$ and $h_{\Delta_N} = \sum_{i=1}^N H_2(v_i) \in L_2$.

To compute $\Delta_N^{(2)}$ we need to better understand the action of \mathscr{L}_K on the L_{2l} . This is done in the following Lemma, which is actually a generalization of Lemma 8.

Lemma 12 Let A be a self-adjoint operator on $L^2(\mathbb{R}^N, \gamma(\mathbf{v})d\mathbf{v})$ that preserves the space P_{2l} , of homogeneous even polynomials in v_1, \ldots, v_N of degree 2l. If

$$A(v_1^{2\alpha_1}\cdots v_N^{2\alpha_N}) = \sum_{|\underline{\beta}|=|\underline{\alpha}|} c_{\underline{\beta}} v_1^{2\beta_1}\cdots v_N^{2\beta_N},$$

we get

$$A(H_{2\alpha_1}(v_1)\cdots H_{2\alpha_N}(v_N)) = \sum_{|\underline{\beta}|=|\underline{\alpha}|} c_{\underline{\beta}} H_{2\beta_1}(v_1)\cdots H_{2\beta_N}(v_N).$$

Proof First, we observe that $A(L_{2l}) \subset L_{2l}$. Indeed, if $f \in L_{2m}$ and $g \in L_{2l}$ with m < l, we have $\langle Ag, f \rangle = \langle g, Af \rangle = 0$ because Af contains only monomials of degree at most 2m. This means that

$$A(H_{2\alpha_1}(v_1)\cdots H_{2\alpha_N}(v_N)) = \sum_{|\underline{\beta}|=|\underline{\alpha}|} k_{\underline{\beta}} H_{2\beta_1}(v_1)\cdots H_{2\beta_N}(v_N)$$

and because

$$A(v_1^{2\alpha_1}\cdots v_N^{2\alpha_N}) = \sum_{|\underline{\beta}|=|\underline{\alpha}|} c_{\underline{\beta}} v_1^{2\beta_1}\cdots v_N^{2\beta_N},$$

we get that $c_{\underline{\beta}} = k_{\underline{\beta}}$ for any $\underline{\beta}$ by equating the coefficients of the term of maximal degree $v_1^{2\beta_1} \cdots v_N^{2\beta_N}$.

Remark • Since \mathscr{L}_K preserves the spaces P_{2l} , the above Lemma applies to it. Thus, the action of \mathscr{L}_K on products of Hermite polynomials $H_{2n}(v_i)$ can be deduced from its action on products of monomials v_i^{2n} , and the latter turns out to be simpler.

• Note that L_{2l} is invariant under \mathscr{L}_K and thus is invariant under \mathscr{L} .

In preparation for the proof of Theorem 2 we note that Theorem 7 implies that

$$\langle h, \mathscr{L}_K h \rangle \geq \langle h, \Lambda_N (I - B) h \rangle$$

where B is the orthogonal projection on radial functions, that is

$$B[h](\mathbf{v}) = \int_{S^{N-1}(|\mathbf{v}|)} h(\mathbf{w}) d\sigma(\mathbf{w}).$$

where $S^{N-1}(r)$ is the sphere of radius r in \mathbb{R}^N with normalized surface measure $d\sigma(\mathbf{v})$. Setting $\mathscr{L}_R := \Lambda_N(I - B)$ we have

$$\langle h, \mathscr{L}h \rangle \ge \langle h, (\mu \mathscr{L}_T + \lambda \mathscr{L}_R)h \rangle$$

so that

$$\Delta_N^{(2)} \ge \inf\{\langle h, (\mu \mathscr{L}_T + \lambda \mathscr{L}_R)h\rangle : ||h|| = 1, h \perp L_0, L_2\},$$
(2.1)

where we have replaced the operator \mathscr{L}_K with the much simpler projection \mathscr{L}_R . Note, the same reasoning as before shows that the space L_{2l} is invariant under \mathscr{L}_R . For later use we define

$$\Gamma(\underline{\alpha}) = \int_{S^{N-1}(1)} v_1^{2\alpha_1} \cdots v_N^{2\alpha_N} d\sigma_1(\mathbf{v}).$$

Theorem 13 The smallest eigenvalue a_l of the operator

$$\mathscr{L}_S := \mu \mathscr{L}_T + \lambda \mathscr{L}_R$$

restricted to the space L_{2l} satisfies the estimates

$$a_l \geq x_l$$
,

where x_l is the smaller of the two solutions of the equation

$$x^{2} - (\lambda \Lambda_{N} + (2 - s_{2l})\mu) x + (1 - s_{2l})\mu^{2} + \lambda \Lambda_{N}\mu = \lambda \Lambda_{N}\mu s_{2l}N\Gamma(l, 0, \dots 0).$$
(2.2)

Proof The equation for the eigenvalue x of $\mu \mathscr{L}_T + \lambda \mathscr{L}_R$ gives

$$\mu \sum T_j h + \lambda \Lambda_N B h = (N\mu + \lambda \Lambda_N - x)h.$$

Observe that if $|\underline{\alpha}| = l$, $B[v_1^{2\alpha_1} \cdots v_N^{2\alpha_N}]$ is an homogeneous radial polynomial of degree 2*l* so that we have

$$B[v_1^{2\alpha_1}\cdots v_N^{2\alpha_N}](r) = \Gamma(\underline{\alpha})r^{2l} = \Gamma(\underline{\alpha})\sum_{|\underline{\beta}|=l}\frac{l!}{\beta_1!\cdots\beta_N!}v_1^{2\beta_1}\cdots v_N^{2\beta_N},$$

in particular

$$\sum_{|\underline{\alpha}|=l} \frac{l!}{\alpha_1! \cdots \alpha_N!} \Gamma(\underline{\alpha}) = 1.$$
(2.3)

Writing a generic function f in L_{2l} as

$$f = \sum_{|\underline{\alpha}|=l} c_{\underline{\alpha}} H_{2\underline{\alpha}}$$

the eigenvalue equation becomes:

$$\mu \sum_{|\underline{\alpha}|=l} \sum_{j} s_{2\alpha_{j}} c_{\underline{\alpha}} H_{2\underline{\alpha}} + \lambda \Lambda_{N} \left[\sum_{|\underline{\alpha}|=l} c_{\underline{\alpha}} \Gamma(\underline{\alpha}) \right] \sum_{|\underline{\alpha}|=l} \frac{l!}{\alpha_{1}! \cdots \alpha_{N}!} H_{2\underline{\alpha}}$$
$$= (N\mu + \lambda \Lambda_{N} - x) \sum_{|\underline{\alpha}|=l} c_{\underline{\alpha}} H_{2\underline{\alpha}}, \qquad (2.4)$$

where we have used that the projection *B* satisfies the hypothesis of Lemma 12. Thus for every $\underline{\alpha}$

$$\left(\mu\sigma_{2\underline{\alpha}} + \lambda\Lambda_N - x\right)c_{\underline{\alpha}} = K\lambda\Lambda_N \frac{l!}{\alpha_1!\cdots\alpha_N!},\tag{2.5}$$

where we set $\sum_{|\underline{\alpha}|=l} c_{\underline{\alpha}} \Gamma(\underline{\alpha}) = K$. Consider first the case $K \neq 0$, that is $(x - \lambda \Lambda_N - \mu \sigma_{2\underline{\alpha}}) \neq 0$ for every $\underline{\alpha}$. Rearranging, multiplying both sides by $\Gamma(\underline{\alpha})$, and adding we get

$$\frac{1}{\lambda\Lambda_N} = \sum_{|\underline{\alpha}|=l} \frac{1}{\lambda\Lambda_N + \mu\sigma_{2\underline{\alpha}} - x} \Gamma(\underline{\alpha}) \frac{l!}{\alpha_1! \cdots \alpha_N!}.$$
(2.6)

With x moving in from $-\infty$, the first singularity of the right side of Eq. (2.6) occurs when

$$x = \min_{|\underline{\alpha}|=l} \left(\lambda \Lambda_N + \mu \sigma_{2\underline{\alpha}} \right) = \lambda \Lambda_N + \mu (1 - s_{2l}),$$

where the last equality follows from Lemma 11. The right side of Eq. (2.6) is a positive increasing function of x until the first singularity. Thus, the smallest eigenvalue is less than $\lambda \Lambda_N + \mu (1 - s_{2l})$. For $0 < x < \lambda \Lambda_N + \mu (1 - s_{2l})$ we get

$$\frac{1}{\lambda\Lambda_N} = \frac{1}{\lambda\Lambda_N + (1 - s_{2l})\mu - x} N\Gamma(l, 0, \dots 0) + \sum_{\substack{|\underline{\alpha}| = l \\ \underline{\alpha} \in \Xi}} \frac{1}{(\lambda\Lambda_N + \mu\sigma_{2\underline{\alpha}} - x)} \Gamma(\underline{\alpha}) \frac{l!}{\alpha_1! \cdots \alpha_N!}$$

$$\leq \frac{1}{\lambda\Lambda_N + (1 - s_{2l})\mu - x} N\Gamma(l, 0, \dots 0) + \frac{1}{\lambda\Lambda_N + \mu - x} \sum_{\substack{|\underline{\alpha}| = l \\ \underline{\alpha} \in \Xi}} \Gamma(\underline{\alpha}) \frac{l!}{\alpha_1! \cdots \alpha_N!}$$

$$\leq \frac{1}{\lambda\Lambda_N + (1 - s_{2l})\mu - x} N\Gamma(l, 0, \dots 0) + \frac{1}{\lambda\Lambda_N + \mu - x} [1 - N\Gamma(l, 0, \dots 0)].$$
(using eq. (2.3))

It is easily seen that the equation

$$\frac{1}{\lambda\Lambda_N} = \frac{1}{\lambda\Lambda_N + (1 - s_{2l})\mu - x} N\Gamma(l, 0, \dots 0) + \frac{1}{\lambda\Lambda_N + \mu - x} [1 - N\Gamma(l, 0, \dots 0)]$$
(2.7)

and (2.2) are equivalent and hence the smallest eigenvalue $a_l \ge x_l$.

Note that necessarily $x_l < \lambda \Lambda_N + \mu(1 - s_{2l})$. Thus, if K = 0, $a_l = \lambda \Lambda_N + \mu \sigma_{2\underline{\alpha}}$ for some $\underline{\alpha}$ and hence $a_l \ge \lambda \Lambda_N + \mu(1 - s_{2l}) > x_l$ which proves the theorem.

Proof of Theorem 2 Since symmetric functions are preserved under \mathscr{L} , the space of symmetric Hermite polynomials in L_4 with orthonormal basis $\left\{\sqrt{\frac{2}{N(N-1)}}\sum_{i\neq j}H_2(v_i)H_2(v_j),\right\}$

 $\sqrt{\frac{2}{3N}} \sum H_4(v_i)$ gives rise to two eigenfunctions. The action of $\mu \mathscr{L}_T + \lambda \mathscr{L}_K$ on this space is represented by the following matrix

$$\begin{pmatrix} \mu + \frac{3\lambda}{2(N-1)} & \frac{-\sqrt{3}\lambda}{2\sqrt{N-1}} \\ \frac{-\sqrt{3}\lambda}{2\sqrt{N-1}} & \frac{5\mu}{8} + \frac{\lambda}{2} \end{pmatrix}$$
(2.8)

whose characteristic Eq. is (1.3) and smallest eigenvalue is thus a_2 . Hence, we immediately have $\Delta_N^{(2)} \leq a_2$.

To see the opposite inequality recall that x_l is the smaller of the two solutions of the Eq. (2.7) Since for $l \ge 2$, $s_{2l} \le s_4 = \frac{3}{8}$ and $\Gamma(l, 0, ..., 0) \le \Gamma(2, 0, ..., 0) = \frac{3}{N(N+2)}$ we get from (2.7)

$$\Delta_N^{(2)} \ge a_2.$$

The eigenfunction corresponding to the "second" gap $\Delta_N^{(2)}$ is given by $\sum_{|\underline{\alpha}|=2} c_{\underline{\alpha}} H_{2\underline{\alpha}} \in L_4$, where $c_{\underline{\alpha}}$ are symmetric under exchange of indices (see Eq. (2.5)). In fact, Eq. (2.5) characterizes the symmetric eigenfunctions of $\mu \mathscr{L}_T + \lambda \mathscr{L}_R$ when $K \neq 0$ and the non-symmetric eigenfunctions when K = 0. This means that solutions x of Eq. (2.6) correspond to symmetric eigenfunctions alone. Hence, the unique eigenfunction (by extension, also that of $\mu \mathscr{L}_T + \lambda \mathscr{L}_K$) corresponding to a_2 is symmetric, which is the physically interesting case.

We eventually do get the optimal bound a_2 due to the following reason: The space of symmetric functions in L_4 is spanned by the set $\{\sum_{i \neq j} H_2(v_i)H_2(v_j), \sum H_4(v_i)\}$, which can also be spanned by two functions, one of which is radial (of degree 4) and the other perpendicular to the radial one. The latter gives the gap Λ_N for \mathscr{L}_K . Hence, the action of \mathscr{L}_K and \mathscr{L}_R on the space of symmetric functions in L_4 is precisely the same.

In the limit $N \to \infty$, the off-diagonal elements of the matrix (2.8) vanish. Therefore, in this limit, the eigenvalues x_2^{\pm} tend to $\frac{\lambda}{2} + \frac{5}{8}\mu$ and μ , which corresponds to the simultaneous diagonalization of operators \mathscr{L}_T and \mathscr{L}_K .

2.2 Approach to Equilibrium in Entropy

It is well known that

$$S(f|\gamma) = 0 \Leftrightarrow f = \gamma,$$

where $S(f|\gamma)$ is defined as in Eq. (1.5). In this section we will prove that $S(f_t|\gamma)$ decays to 0 exponentially as $t \to \infty$, if f_t is the solution of the Master equation (1.1). Indeed Theorem 3 immediately follows from the following proposition.

Proposition 14 Let f_0 be a probability density on \mathbb{R}^N with finite relative entropy and f_t the solution of the Master equation (1.1) with initial condition f_0 . We have

$$\frac{dS(f_t|\gamma)}{dt} \le -\rho S(f_t|\gamma),\tag{2.9}$$

where

$$\rho = \frac{\mu}{2}.$$

The left-hand side of the inequality (2.9) is the entropy production and can be computed as

$$\frac{dS(f_t|\gamma)}{dt} = \int \frac{\partial f_t}{\partial t} \log \frac{f_t}{\gamma} + \int \frac{\partial f_t}{\partial t} = -\int (\lambda \mathscr{G}_K + \mu \mathscr{G}_T)[f_t] \log \frac{f_t}{\gamma}$$

because $\int f_t = 1$. Thus, Proposition 14 will follow if we prove that for any density f with finite relative entropy, we have

$$-\int (\lambda \mathscr{G}_K + \mu \mathscr{G}_T)[f] \log \frac{f}{\gamma} \le -\rho \int f \log \frac{f}{\gamma}$$

Since the relative entropy decreases along the Kac flow, i.e. $\int \mathscr{G}_K[f] \log \frac{f}{\gamma} \ge 0$ (see [1]), it is enough to show that

$$-\int \mu \mathscr{G}_{T}[f] \log \frac{f}{\gamma} \le -\rho \int f \log \frac{f}{\gamma}.$$
(2.10)

We first prove the above for the case N = 1. In this case, $\mathscr{G}_T = (I - R)$.

Proposition 15 Let f be a probability density on \mathbb{R} . Then

$$\int R[f](v)\log\frac{f(v)}{g(v)}dv = \int dvdw \oint d\theta f(v^*)g(w^*)\log\frac{f(v)}{g(v)} \le \frac{1}{2}\int dvf(v)\log\frac{f(v)}{g(v)},$$

where $v^* = v \cos \theta + w \sin \theta$, $w^* = -v \sin \theta + w \cos \theta$ and g(v) is the Gaussian $\frac{1}{\sqrt{2\pi}} e^{-\frac{v^2}{2}}$.

Calling f(v) = g(v)G(v), we need to prove that

$$\int dv \, g(v) T[G](v) \log G(v) \le \frac{1}{2} \int dv \, g(v) G(v) \log G(v), \tag{2.11}$$

where

$$T[G](v) := \int dwg(w) \int_{0}^{2\pi} d\theta G(v\cos\theta + w\sin\theta).$$

The idea will be to show the above inequality by proving that

$$\int dv \, g(v) T[G](v) \log T[G](v) \le \frac{1}{2} \int dv \, g(v) G(v) \log G(v).$$
(2.12)

We will be invoking the following well-known property of the Ornstein–Uhlenbeck process, see [15–19].

Theorem 16 Let P_s be the semigroup generated by the 1-dimensional Ornstein–Uhlenbeck process, that is, $U_s = P_s[U_0]$ is the solution of the Fokker–Planck equation

$$\frac{\partial U_s(v)}{\partial s} = U_s''(v) - vU_s'(v)$$

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with initial condition U_0 . For every density G we have

$$\int g(v)dv P_s[G](v) \log(P_s[G](v)) \le e^{-2s} \int g(v)dv G(v) \log G(v).$$

Remark The semigroup, which can be represented explicitly as

$$P_{s}[G](v) = \int dwg(w)G(e^{-s}v + \sqrt{1 - e^{-2s}}w), \qquad (2.13)$$

is self-adjoint in $L^2(\mathbb{R}, g(v)dv)$.

r

We are now ready to prove Proposition 15.

Proof of Proposition 15 To connect the Ornstein–Uhlenbeck process P_s with the operator T we set

$$\overline{T}[G](v) := \int dwg(w) \oint_{0}^{\pi/2} d\theta G(v\cos\theta + w\sin\theta) = \frac{2}{\pi} \int_{0}^{\infty} ds \frac{\mathrm{e}^{-s}}{\sqrt{1 - \mathrm{e}^{-2s}}} P_{s}[G](v),$$

where we use Eq. (2.13) and the change of variables $cos(\theta) = e^{-s}$. It follows that

$$\int dv g(v)\overline{T}[G]\log\overline{T}[G]$$

$$= \int dv g(v) \left(\frac{2}{\pi} \int_{0}^{\infty} ds \frac{e^{-s}}{\sqrt{1 - e^{-2s}}} P_{s}[G]\right) \log \left(\frac{2}{\pi} \int_{0}^{\infty} ds' \frac{e^{-s'}}{\sqrt{1 - e^{-2s'}}} P_{s'}[G]\right)$$

$$\leq \int dv g(v) \left(\frac{2}{\pi} \int_{0}^{\infty} ds \frac{e^{-s}}{\sqrt{1 - e^{-2s}}} P_{s}[G]\log P_{s}[G]\right) \quad \text{(using convexity of x log x)}$$

$$\leq \frac{2}{\pi} \int_{0}^{\infty} ds \frac{e^{-s}}{\sqrt{1 - e^{-2s}}} e^{-2s} \int dv g(v) G \log G \quad \text{(using Theorem 16)}$$

$$= \frac{1}{2} \int dv g(v) G \log G.$$

The next step is to prove the corresponding result for the operator T. Let $G = G_e + G_o$ where G_e is even, i.e. $G_e(v) = G_e(-v)$, and G_o is odd, i.e. $G_o(-v) = -G_o(v)$. Observe that T[G] is even, $T[G_o] = 0$ and $\overline{T}[G_e] = T[G_e]$. While the first two identities follow directly from the definitions, the last one also uses the fact that $\int dwg(w) \int_{\frac{\pi}{2}}^{\frac{\pi}{2}} d\theta G_e(v \cos \theta + w \sin \theta) = \int dwg(w) \int_{0}^{\frac{\pi}{2}} d\theta G_e(-v \cos \theta - w \sin \theta)$ under the change of variables $\theta \to \pi - \theta$ and $w \to -w$. Thus,

$$\int dv g(v)T[G](v) \log T[G](v) = \int dv g(v)T[G_e](v) \log T[G_e](v)$$
$$= \int dv g(v)\overline{T}[G_e](v) \log \overline{T}[G_e](v)$$
$$\leq \frac{1}{2} \int dv g(v)G_e(v) \log G_e(v)$$
$$\leq \frac{1}{2} \int dv g(v)G(v) \log G(v),$$

where, in the last inequality, we have used that $G_e(v) = (G(v) + G(-v))/2$ and Jensen's inequality. Now that we have established (2.12), we proceed to derive (2.11) from it as follows:

$$\int dv g(v) e^{(T-I)t} G \log(e^{(T-I)t} G)$$

$$\leq e^{-t} \sum_{k=0}^{\infty} \frac{t^k}{k!} \int dv g(v) T^k[G](v) \log T^k[G](v) \quad \text{(by convexity)}$$

$$\leq e^{-t} \sum_{k=0}^{\infty} \left(\frac{t}{2}\right)^k \frac{1}{k!} \int dv g(v) G(v) \log G(v) \quad \text{(by the previous computation)}$$

$$= e^{-\frac{t}{2}} \int dv g(v) G(v) \log G(v).$$

From the first order terms in the Taylor expansion about t = 0, we get (2.11).

The following lemma will help extend the result to N > 1.

Lemma 17 Let $f(\mathbf{v})$ be a probability density on \mathbb{R}^N and let its marginal over the *j*th variable be denoted by $f_j(\hat{\mathbf{v}}_j) = \int f(\mathbf{v}) dv_j$, where $\hat{\mathbf{v}}_j = (v_1, \dots, v_{j-1}, v_{j+1}, \dots, v_N)$. Then we have

$$\sum_{j=1}^{N} \int f_j \log f_j d\hat{\mathbf{v}}_j \le (N-1) \int f \log f d\mathbf{v}.$$

Proof We first observe that from the Loomis–Whitney inequality [20], that is $\int_{\mathbb{R}^N} F_1(\hat{\mathbf{v}}_1) \cdots F_N(\hat{\mathbf{v}}_N) \leq ||F_1||_{L^{N-1}} \cdots ||F_N||_{L^{N-1}}$ for $F_j \in L^{N-1}(\mathbb{R}^{N-1})$, it follows that

$$Z := \int \prod_{j=1}^{N} f_j^{\frac{1}{N-1}} d\mathbf{v} \le 1.$$
 (2.14)

Thus we have

$$\int f \log\left[\frac{f}{\prod f_j^{\frac{1}{N-1}}}\right] d\mathbf{v} = Z \int \frac{f}{\prod f_j^{\frac{1}{N-1}}} \log\left[\frac{f}{\prod f_j^{\frac{1}{N-1}}}\right] \frac{\prod f_j^{\frac{1}{N-1}}}{Z} d\mathbf{v}$$
$$\geq Z \left[\int \frac{f}{Z} d\mathbf{v}\right] \log\left[\int \frac{f}{Z} d\mathbf{v}\right] = -\log Z,$$

where we have used Jensen's inequality and the convexity of $x \log(x)$. The Lemma follows easily from the above inequality and (2.14).

Proof of Proposition 14 We first observe that

$$\begin{split} &-\int \mathscr{G}_{T}[f] \log \frac{f}{\gamma} \\ &= \sum_{j} \int d\mathbf{v} \int dw \oint d\theta f(\mathbf{v}_{j}(\theta, w)) g(w_{j}^{*}(\theta)) \log \frac{f(\mathbf{v})}{\gamma(\mathbf{v})} - NS(f|\gamma) \\ &= \sum_{j} \int d\hat{\mathbf{v}}_{j} f_{j}(\hat{\mathbf{v}}_{j}) \int dv_{j} dw \oint d\theta \frac{f(\mathbf{v}_{j}(\theta, w))}{f_{j}(\hat{\mathbf{v}}_{j})} g(w_{j}^{*}(\theta)) \log \left(\frac{f(\mathbf{v})}{f_{j}(\hat{\mathbf{v}}_{j})g(v_{j})}\right) \\ &+ \sum_{j} \int d\mathbf{v} dw \oint d\theta f(\mathbf{v}_{j}(\theta, w)) g(w_{j}^{*}(\theta)) \log \frac{f_{j}(\hat{\mathbf{v}}_{j})}{\gamma_{j}(\hat{\mathbf{v}}_{j})} - NS(f|\gamma), \end{split}$$

where $f_j(\hat{\mathbf{v}}_j) := \int dv_j f(\mathbf{v})$ and $\gamma_j(\hat{\mathbf{v}}_j) := \int dv_j \gamma(\mathbf{v})$, as in Lemma 17. In the first term of the last line, we can undo the rotation by θ by noting that f_j and γ_j are independent of v_j . Applying Proposition 15 to $\frac{f(\mathbf{v})}{f_j(\hat{\mathbf{v}}_j)}$ (in the second line above) as a function of v_j alone we get:

$$\begin{split} -\int \mathscr{G}_{T}[f] \log \frac{f}{\gamma} &\leq \frac{1}{2} \sum_{j} \int d\mathbf{v} f(\mathbf{v}) \log \left(\frac{f(\mathbf{v})}{f_{j}(\hat{\mathbf{v}}_{j})g(v_{j})} \right) \\ &+ \sum_{j} \int d\mathbf{v} f(\mathbf{v}) \log \frac{f_{j}(\hat{\mathbf{v}}_{j})}{\gamma_{j}(\hat{\mathbf{v}}_{j})} - NS(f|\gamma) \\ &= \frac{1}{2} \sum_{j} \int d\mathbf{v} f(\mathbf{v}) \log \left(\frac{f(\mathbf{v})}{f_{j}(\hat{\mathbf{v}}_{j})g(v_{j})} \right) + \frac{1}{2} \sum_{j} \int d\mathbf{v} f(\mathbf{v}) \log \frac{f_{j}(\hat{\mathbf{v}}_{j})}{\gamma_{j}(\hat{\mathbf{v}}_{j})} \\ &+ \frac{1}{2} \sum_{j} \int d\mathbf{v} f(\mathbf{v}) \log \frac{f_{j}(\hat{\mathbf{v}}_{j})}{\gamma_{j}(\hat{\mathbf{v}}_{j})} - NS(f|\gamma) \\ &= -\frac{1}{2} NS(f|\gamma) + \frac{1}{2} \sum_{j} \int d\mathbf{v} f(\mathbf{v}) \log f_{j}(\hat{\mathbf{v}}_{j}) \\ &- \frac{1}{2} \sum_{j} \int d\mathbf{v} f(\mathbf{v}) \log \gamma_{j}(\hat{\mathbf{v}}_{j}). \end{split}$$

Using Lemma 17 for the second term, and that $\gamma_j(\hat{\mathbf{v}}_j) = \prod_{i \neq j} g(v_i)$ so that $\sum_j \int d\mathbf{v} f(\mathbf{v}) \log \gamma_j(\hat{\mathbf{v}}_j) = (N-1) \int f \log \gamma$ we get:

$$-\int \mathscr{G}_{T}[f]\log\frac{f}{\gamma} \leq -\frac{1}{2}S(f|\gamma)$$

and this proves (2.10).

Remark

• Proposition 14 yields a lower bound on the spectral gap Δ_N as follows: given a function *f* of the form

$$f = \gamma (1 + \varepsilon h)$$

with $\int h\gamma = 0$ and ϵ small, one can write

$$\varepsilon \int \gamma \frac{\partial h}{\partial t} \left(\varepsilon h - \frac{\varepsilon^2 h^2}{2} \cdots \right) \leq -\rho \int \gamma (1 + \varepsilon h) \left(\varepsilon h - \frac{\varepsilon^2 h^2}{2} \cdots \right),$$

where $\rho = \mu/2$. That is,

$$\int \gamma h \frac{\partial h}{\partial t} \leq -\rho \int \frac{\gamma h^2}{2}.$$

Thus in $L^2(\mathbb{R}^N, \gamma(\mathbf{v})d\mathbf{v})$ we get

$$\frac{d}{dt}\|h\| \le -\frac{\rho}{2}\|h\|.$$

Observe that this is very similar to the result one get from Proposition 1 but $\rho < \mu$. One may wonder whether ρ is the optimal estimate for the decay rate of the relative entropy.

• In contrast to the Kac model, the presence of the thermostat guarantees that the rate of convergence is strictly positive uniformly in *N*. It is fundamental in the above analysis that the thermostat acts on all particles. The presence of the Kac part gives no contribution to the above estimate of the exponential decay rate.

3 Propagation of Chaos

We finally turn our attention to the effective Boltzmann equation that emerges in the limit for $N \to \infty$. The fundamental step to this end is to show that the dynamics defined by Eq. (1.1) propagates chaos, which is done in this section.

Theorem 18 Let $f^{(N)}(\mathbf{v}, 0)$ be a chaotic sequence of initial densities. Then its evolution under the master equation (1.1), $f^{(N)}(\mathbf{v}, t)$, is a chaotic sequence for any fixed t. That is, if

$$\lim_{N \to \infty} \int_{\mathbb{R}^N} \varphi_1(v_1) \cdots \varphi_k(v_k) f^{(N)}(\mathbf{v}, 0) = \prod_{j=1}^k \lim_{N \to \infty} \int_{\mathbb{R}} \varphi_j(v_j) f^{(N)}(\mathbf{v}, 0)$$

for any $k \in \mathbb{N}$ and any $\phi_1(v_1), \dots, \phi_k(v_k)$ bounded and continuous, then for any t:

$$\lim_{N \to \infty} \int_{\mathbb{R}^N} \varphi_1(v_1) \cdots \varphi_k(v_k) f^{(N)}(\mathbf{v}, t) = \prod_{j=1}^k \lim_{N \to \infty} \int_{\mathbb{R}} \varphi_j(v_j) f^{(N)}(\mathbf{v}, t)$$

for any $k \in \mathbb{N}$ and any $\varphi_1(v_1), \ldots, \varphi_k(v_k)$ bounded and continuous.

The proof follows closely the McKean [2] algebraic version of Kac [1], for the Kac operator. The idea is to write $f(\mathbf{v}, t) = e^{-(\lambda \mathscr{G}_K + \mu \mathscr{G}_T)t} f(\mathbf{v}, 0)$, expand the exponential in series of *t*, and use the chaotic property of the initial sequence. The key observation is that \mathscr{G}_T is a derivation already for finite *N* (in the sense of Lemma 20). Two main ingredients are needed:

Lemma 19 The series $\sum_{l=0}^{\infty} \frac{t^l}{l!} \int \varphi_1(v_1) \cdots \varphi_k(v_k) (\lambda \mathscr{G}_K + \mu \mathscr{G}_T)^l f(\mathbf{v}, 0)$ converges absolutely if $t < \frac{1}{4\lambda + \mu}$.

Proof To prove the lemma, it is enough to show that:

$$||(\lambda \mathscr{G}_{K} + \mu \mathscr{G}_{T}^{*})^{l} \phi||_{\infty} \le (4\lambda + 2\mu)^{l} m(m+1) \cdots (m+l-1) ||\phi||_{\infty}$$
(3.1)

and then follow the proof in [2]. The above statement follows from a simple induction starting from

 $|(\lambda \mathscr{G}_K + \mu \mathscr{G}_T^*)\phi(v_1, \ldots, v_m)| \le |\lambda \mathscr{G}_K \phi| + |\mu \mathscr{G}_T^* \phi| \le (4\lambda + 2\mu)m||\phi||_{\infty}.$

Calling

$$\Gamma_K \phi := 2 \sum_{i \le m} \oint d\theta (\phi(\dots, v_i \cos \theta + v_{m+1} \sin \theta, \dots) - \phi),$$

one can prove, as in [2], that if $\varphi_1(v_1), \ldots, \varphi_k(v_k)$ are bounded and continuous then:

$$\lim_{N\to\infty}\int (\lambda \mathscr{G}_K + \mu \mathscr{G}_T^*)^l [\varphi_1 \cdots \varphi_k] f^{(N)}(\mathbf{v}, 0) = \lim_{N\to\infty}\int (\lambda \Gamma_K + \mu \mathscr{G}_T^*)^l [\varphi_1 \cdots \varphi_k] f^{(N)}(\mathbf{v}, 0).$$

The main ingredient to re-sum the power series expansion and obtain the Boltzmann equation is the following "algebraic" Lemma.

Lemma 20 If
$$(\phi \otimes \psi)(v_1, \dots, v_{m+k}) := \phi(v_1, \dots, v_m)\psi(v_{m+1}, \dots, v_{m+k})$$
, then
 $(\Gamma_K + \mathscr{G}_T^*)[\phi \otimes \psi] = (\Gamma_K + \mathscr{G}_T^*)[\phi] \otimes \psi + \phi \otimes (\Gamma_K + \mathscr{G}_T^*)[\psi].$

It is now possible to prove Theorem 5 by following the proof in [2] step-by-step.

4 Conclusion and Future Work

We hope to have convinced the reader that master equations of Kac type are reasonable models for large particle systems interacting with thermal reservoirs. The main advantage is that physically relevant quantities such the first and second gap can be computed quite easily and the entropic convergence to equilibrium can be established in a quantitative fashion as well. Moreover, since propagation of chaos holds, contact is made with a Boltzmann type equation in one dimension.

There are a number of directions for future research. The generalization to threedimensional momentum-conserving collisions [21], while more complicated, should not pose any new real difficulties. There are other, more severe, assumptions made in our model that one ought to address.

For example, it is the very nature of a reservoir that it is not influenced by the interaction with the other N particles. A more realistic situation would be to consider the reservoir as finite but large. More precisely, consider an initial state of the form γF where γ is a Gaussian in M variables with inverse temperature β and F a function of N variables with kinetic energy eN. Thus, M particles are in thermal equilibrium and N particles are not in equilibrium but with finite energy per particle. Now we let this state evolve under the Kac evolution. Clearly, this state will evolve to a radial function in N + M variables as $t \to \infty$. One would expect that this function is close to a Gaussian with a temperature $(\frac{M}{\beta} + 2eN)/(M + N)$. Assuming that M >> N, is it true that the entropy has a rate of decay that is uniform in N? Note that the problem is not to get an estimate on the entropy production of the initial state. The infinitesimal time evolution is precisely the weak thermostat treated in our paper. The real issue is to quantify the entropy production at later times for which the state is no longer of this simple form.

Another important issue is how to understand non-equilibrium steady states in a wider sense. We believe that the Kac approach to kinetic theory could shed some light on this very difficult problem. The fact that the particles interact with a single heat reservoir leads to a non-self-adjoint operator that can be brought into a self-adjoint form using a ground state

transformation. It is easy to write down the master equation for a system of particles that interact with, say, two reservoirs at different temperatures. However, the generator cannot be brought into a self-adjoint form anymore and the equilibrium cannot be found though an optimization procedure, or at least not an obvious one. In particular the equilibrium is not a simple function. How, then, can one measure the approach to steady-state for such systems? Note that the steady-state is, from the point of physics, not an equilibrium state, since it mediates an energy transport from a reservoir of higher temperature to one of lower temperature. The solution of this problem would be a small step towards understanding non-equilibrium steady states.

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References

- Kac, M.: Foundations of kinetic theory. In: Proceedings of the Third Berkeley Symposium on Mathematical Statistics and Probability. 1954–1955, vol. III, pp. 171–197. University of California Press, Berkeley and Los Angeles (1956)
- McKean Jr, H.P.: Speed of approach to equilibrium for kac's caricature of a maxwellian gas. Arch. Ration. Mech. Anal. 21, 343–367 (1966)
- Lanford III, O.E.: Time evolution of large classical systems. In: Dynamical Systems, Theory and Applications (Recontres, Battelle Res. Inst., Seattle, Wash., 1974), pp. 1–111. Lecture Notes in Physics, vol. 38. Springer, Berlin (1975)
- 4. Lanford III, O.E.: On a derivation of the Boltzmann equation. In: International Conference on Dynamical Systems in Mathematical Physics (Rennes, 1975), pp. 117–137. Astérisque, No. 40. Societe Mathematique De France, Paris (1976).
- Illner, R., Pulvirenti, M.: Global validity of the Boltzmann equation for two- and three-dimensional rare gas in vacuum. Erratum and improved result: "Global validity of the Boltzmann equation for a two-dimensional rare gas in vacuum" [Comm. Math. Phys. 105(2), 1986, pp. 189–203; MR0849204 (88d:82061)] and "Global validity of the Boltzmann equation for a three-dimensional rare gas in vacuum" [ibid. 113 (1987), no. 1, 79–85; MR0918406 (89b:82052)] by Pulvirenti. Comm. Math. Phys. 121(1), 143–146 (1989). http://projecteuclid.org/getRecord?id=euclid.cmp/1104178007. Accessed 08 May 2014
- Janvresse, E.: Spectral gap for Kac's model of Boltzmann equation. Ann. Probab. 29(1), 288–304 (2001). doi:10.1214/aop/1008956330
- Carlen, E., Carvalho, M.C., Loss, M.: Many-body aspects of approach to equilibrium. In: Journées "Équations aux Dérivées Partielles" (La Chapelle sur Erdre, 2000), pp. Exp. No. XI, 12. University of Nantes, Nantes (2000)
- Maslen, D.K.: The eigenvalues of Kac's master equation. Math. Z. 243(2), 291–331 (2003). doi:10.1007/ s00209-002-0466-y
- Villani, C.: Cercignani's conjecture is sometimes true and always almost true. Commun. Math. Phys. 234(3), 455–490 (2003). doi:10.1007/s00220-002-0777-1
- Einav, A.: On Villani's conjecture concerning entropy production for the Kac master equation. Kinet. Relat. Models 4(2), 479–497 (2011). doi:10.3934/krm.2011.4.479
- Fröhlich, J., Gang, Z.: Exponential convergence to the Maxwell distribution for some class of Boltzmann equations. Commun. Math. Phys. 314(2), 525–554 (2012). doi:10.1007/s00220-012-1499-7
- Bonetto, F., Chernov, N., Korepanov, A., Lebowitz, J.L.: Nonequilibrium stationary state of a currentcarrying thermostated system. EPL 102, 15001 (2013)
- Bonetto, F., Carlen, E., Esposito, R., Lebowitz, J., Marra, R.: Propagation of chaos for a thermostated kinetic model. http://arxiv.org/abs/1305.7282
- Mischler, S., Mouhot, C.: Kac's program in kinetic theory. Invent. Math. 193(1), 1–147 (2013). doi:10. 1007/s00222-012-0422-3
- Stam, A.J.: Some inequalities satisfied by the quantities of information of fisher and shannon. Inf. Control 2, 101–112 (1959)

- 16. Gross, L.: Logarithmic sobolev inequalities. Am. J. Math. 97(4), 1061–1083 (1975)
- Bakry, D., Émery, M.: Diffusions hypercontractives. In: Séminaire de Probabilités, XIX, 1983/84. Lecture Notes in Mathematics, vol. 1123, pp. 177–206. Springer, Berlin (1985). doi:10.1007/BFb0075847
- Gross, L.: Logarithmic Sobolev inequalities and contractivity properties of semigroups. In: Dirichlet Forms (Varenna, 1992). Lecture Notes in Mathematics, vol. 1563, pp. 54–88. Springer, Berlin (1993). doi:10.1007/BFb0074091
- Toscani, G.: Entropy production and the rate of convergence to equilibrium for the Fokker–Planck equation. Quart. Appl. Math. 57(3), 521–541 (1999)
- Loomis, L.H., Whitney, H.: An inequality related to the isoperimetric inequality. Bull. Am. Math. Soc 55, 961–962 (1949)
- Carlen, E.A., Geronimo, J.S., Loss, M.: Determination of the spectral gap in the Kac model for physical momentum and energy-conserving collisions. SIAM J. Math. Anal. 40(1), 327–364 (2008). doi:10.1137/ 070695423