A QUICK INTRODUCTION TO KINETIC THEORY

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Abstract. The purpose of these notes is to advertise kinetic theory to beginning graduate students with an interest in analysis and differential equations. Kinetic theory is a very active area of research in mathematics, yet there are few introductory expositions to the field. These notes provide an overview of some fundamental examples in kinetic theory, while including sufficient detail to make it apparent that the subject has real mathematical depth.

The notes explore several themes. The first chapter consists of a set of examples from statistical physics. The second chapter is an introduction to the Boltzmann equation, including its derivation from the BBGKY hierarchy. The third chapter concerns the analysis of an exactly solvable example – Smoluchowski's coagulation equation. The final chapter includes an exactly solvable particle system introduced by Kac to illustrate Zermelo's paradox.

Contents

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1. Examples of kinetic models

Kinetic theory provides an effective description of the dynamics of a large system of interacting particles. The central idea is to replace a detailed description of the dynamics in the state space by evolution equations for population densities. For instance, the dynamics of N identical particles on the line is typically given by a deterministic or stochastic rule for the evolution of states $\mathbf{x} = (x_1, \dots, x_n) \in \mathbb{R}^N$. In a kinetic model of such a system, the unknown is a number density $f(x,t)$. Here $x \in \mathbb{R}$ and $f(x,t)$ denotes the typical number of particles at time t whose positions are x. The link between the particle system and the kinetic equations are as follows. For any $-\infty < a < b < \infty$

$$\frac{1}{b-a}\int_a^b f(x,t)\,dx \approx \frac{1}{N}\sum_{i=1}^{N} \mathbf{1}_{(a,b)}(x_i(t)). \tag{1.1}$$

Given the rule for the evolution of $\mathbf{x}(t)$, our task is to rigorously derive and analyze an evolution equation for $f(x,t)$. An important aspect of the theory are the probabilistic assumptions – implicit and explicit – that allow us to replace the particle dynamics with an averaged description of population densities.

Kinetic theory has traditionally been tied to foundational questions in physics – in particular, the derivation of thermodynamics from Newton's laws. A particularly beautiful description of these ideas may be found in Kac's book [7]. However, the range of kinetic theory is much broader. Today we view it as a set of ideas that provides a consistent method of averaging over interacting particles in widely different contexts. Thus, while the examples below are mainly drawn from statistical physics, this should simply be seen as a reflection of my personal taste. New particle systems continue to arise in applications, often in unexpected ways. For instance, kinetic theory has been used to describe collective behavior in social networks [17].

1.1. The Boltzmann equation.

The subject of kinetic theory, or more broadly statistical mechanics, was founded by Boltzmann, Clausis and Maxwell in the period 1850-1875. At the time, the atomic hypothesis – the view that matter consists of atoms – was not fully accepted. Their goal was to describe the macroscopic properties of matter from an atomic hypothesis. In particular, their work provided a consistent explanation for the laws of an ideal gas –Boyle's, Charles' law, and Gay-Lussac's law – that had been established empirically in the preceding centuries. Their work also illustrated the subtle relation between irreversibility, disorder and the second law of thermodynamics. Roughly speaking, in our extremely abbreviated presentation, the empirical laws can be obtained from the equilibrium solutions of the Boltzmann equation, while irreversibility is inextricably tied to the time evolution of solutions to the Boltzmann equation. In this lecture, we introduce the

Boltzmann equation, along with a heuristic derivation. A more careful derivation is presented in Chapter 3 and the question of foundations is illustrated in Chapter 5.

Let $\mathbb{T}^d$ denote the d-dimensional torus. We consider N identical hard spheres of diameter $0 < \delta \ll 1$ in $\mathbb{T}^d$, $d \geq 2$ that interact through elastic collisions. The adjective 'hard' means that the spheres are not allowed to overlap. Thus, the centers, $\{x_i\}_{i=1}^N$ of the particles must satisfy the constraint

$$|x_i - x_j| \geq \delta, \quad 1 \leq i < j \leq N. \tag{1.2}$$

Let $\mathcal{M}_\delta^N \subset \mathbb{T}^{dN}$ denote the set of points satisfying this constraint. The state space of our system consists of vectors $(\mathbf{x}, \mathbf{v}) \in \mathcal{M}_\delta^N \times \mathbb{R}^{dN}$ describing the positions and velocities of the centers of each particle

$$\mathbf{x} = (x_1, \ldots, x_N), \quad \mathbf{v} = (v_1, \ldots, v_N). \tag{1.3}$$

The particles stream freely between collisions, that is

$$\dot{x}_i = v_i, \quad \dot{v}_i = 0, \quad i = 1, \ldots N, \tag{1.4}$$

and the velocity jumps at each collisions. The jump condition at collisions is determined as follows.

When two spheres A and B with incoming velocities v and w collide elastically, the outgoing velocities, denoted v' and w', are determined by conservation of momentum and energy:

$$v + w = v' + w', \quad |v|^2 + |w|^2 = |v'|^2 + |w'|^2. \tag{1.5}$$

The solution to these equations has an elegant expression. Let $l \in S^{d-1}$ denote the unit vector connecting the center of sphere A to B. Then (as shown in Section 2 below)

$$v' = v - ((v - w) \cdot l)\, l, \quad w' = w + ((v - w) \cdot l)\, l. \tag{1.6}$$

Let $A_l : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ denote the linear transformation $(v, w) \mapsto (v', w')$ defined by (1.6) above. The transformation A_l is reversible: that is, $A_l(v', w') = (v, w)$ and $\det(A_l) = -1$ (see Lemma 2.1 below). Further, $A_l = A_{-l}$. We will use these properties below.

Thus, when two spheres, say j and k, collide in the direction l at time t , equation (1.5) must be augmented with the jump condition

$$(v_j(t_+), v_k(t_+)) = A_l(v_j(t_-), v_k(t_-)), \quad v_i(t_+) = v_i(t_-),\ i \neq j, k. \tag{1.7}$$

It is not apparent that we have a well-defined particle system! For instance, by arranging N particles on a line in 'pathological' initial conditions, it is possible to arrange for triple collisions, as well as higher order collisions. In fact, viewed as a classical dynamical system, the analysis of the hard sphere gas is very subtle. But it is reasonable to assume that for a very dilute gas, binary collisions are dominant. This is the regime described by the Boltzmann equations. We replace a detailed description of the states $(\mathbf{x}, \mathbf{v})$ with a number density $f(x, v, t)$, $(x, v) \in \mathbb{T}^d \times \mathbb{R}^d$ in the dilute limit $N \to \infty$, $\delta \to 0$, $N\delta^{d-1} \to c > 0$. [1] In this limit, the fraction of space occupied by the particles vanishes, because this volume is proportional to $N\delta^d$. However, as we see below, the scaling $N\delta^{d-1} \to c > 0$ ensures that the frequency of collisions betweens particles remains $O(1)$.

[1]The Boltzmann equation conserves the total number of particles, and it may always be normalized to a probability density. However, we prefer the term number density to probability density since in many kinetic applications f is not a probability density.

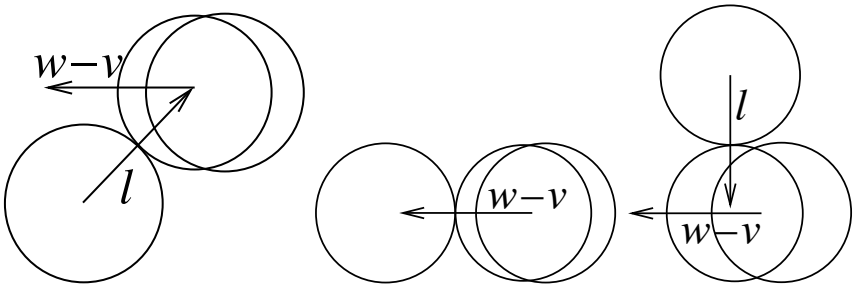


FIGURE 1. **The influence of l on the rate of collisions.** Without loss of generality, we may assume that the sphere on the right moves with the velocity difference $w-v$ and that the sphere on the left is stationary. A collision occurs in time dt if the sphere on the right intersects the collision cylinder with volume $\delta^{d-1}dl(w-v)\cdot l dt$. The factor $\delta^{d-1}dl$ is the base of the cylinder, and $(w-v)\cdot l dt$ is its length.

It is simplest to describe the Boltzmann equation under the assumption that f does not depend on x. This corresponds to the assumption that the particles are equally distributed in space. If at time t, the centers of two spheres are as shown in Figure 1, and $(v-w)\cdot l > 0$, these particles collide in the time interval $[t, t+dt]$. Let $n_A \approx Nf(v,t)$ denote the particles with velocity v and $n_B = Nf(w,t)$ denote the number of particles with velocity B. Each such collision creates $n_A n_B$ particles with velocities v' and w' in the time interval $[t, t+dt]$. Since, the collision process is reversible, analogous collisions between n'_A and n'_B particles with velocity v' and w' create $n'_A n'_B$ particles with velocity v and w. Summing over all collisions, collecting the factors of N and using the scaling $N\delta^{d-1} = 1$, we obtain the Boltzmann equation for the hard-sphere gas

$$\partial_t f(v,t) = \int_{\mathbb{R}^d}\int_{S^{d-1}} \left(f(v',t)f(w',t) - f(v,t)f(w,t)\right)\left((v-w)\cdot l\right)_+ \, dl\, dw. \tag{1.8}$$

This collision kernel admits some slightly different formulations because $A_l = A_{-l}$ and uniform measure on S^{d-1} under $l \mapsto -l$. This symmetry may be used to replace the kernel $((v-w)\cdot l)_+$ by the kernel $((w-v)\cdot l)_+$ (in each case, the integrand is non-zero only on a hemisphere). Similarly, we may replace the kernel $((v-w)\cdot l)_+$ by $|(v-w)\cdot l|$ at the cost of a factor of $1/2$:

$$\partial_t f = Q(f,f) := Q_+(f,f) - Q_-(f,f), \tag{1.9}$$

where the collision kernel Q has been split into birth and death terms, Q_+ and Q_- respectively, given by

$$Q_-(f,f)(v,t) = \frac{1}{2}\int_{\mathbb{R}^d}\int_{S^{d-1}} f(v,t)f(w,t)\,|(v-w)\cdot l|\, dl\, dw, \tag{1.10}$$

$$Q_+(f,f)(v,t) = \frac{1}{2}\int_{\mathbb{R}^d}\int_{S^{d-1}} f(v',t)f(w',t)\,|(v-w)\cdot l|\, dl\, dw, \tag{1.11}$$

where $(v',w') = A(v,w)$. In (1.10), the term $f(v,t)$ does not depend on either variable of integration w, and the term $f(w,t)$ is independent of l. However, the collision term has a symmetric appearance when it is written as above.

Finally, here is the non-homogeneous Boltzmann equation for $f(x, v, t)$. The free streaming of each equation gives rise to the transport term $v \cdot \nabla f$ and if we assume that the combined effect of streaming and collisions is additive (again, a reasonable assumption in the dilute limit), we find

$$\partial_t f + v \cdot \nabla_x f = Q(f, f), \tag{1.12}$$

with the collision kernel defined in (1.9)–(1.11). We will derive (1.12) from the BBGKY hierarchy in Chapter 3.

1.2. **Kac's caricature of the Boltzmann equation.** Much of the modern mathematical interest in the Boltzmann equations was stimulated by Mark Kac's work in the 1950s [7]. He emphasized the importance of a careful examination of the probabilistic assumptions that underly Boltzmann's theory, and introduced several simplified examples that yield interesting insights into the Boltzmann equation. One such model, is a caricature of the Boltzmann equation based on a stochastic particle system that conserves energy, but not momentum. In the previous section, we introduced the Boltzmann equation in space dimension $d \geq 2$. The restriction $d \geq 2$ is necessary, because when $d = 1$ the hard sphere gas is trivial! In one-dimensional collisions, the particles exchange velocity upon collision, and the overall effect of the collision is simply an exchange in particle labels. However, it would greatly simplify the analysis of the Boltzmann equation if we could identify a simple one-dimensional model. Kac's idea was to retain some key assumptions of the Boltzmann theory – binary collisions and an angle dependent collision kernel, and conservation of energy – in order to obtain an integral equation of Boltzmann type that could be analyzed in detail.

In order to define Kac's model, we first define a discrete Markov chain, and then an associated continuous time Markov process. The states of the model are velocity vectors $\mathbf{v} \in \mathbb{R}^N$ such that $\sum_{i=1}^N |v_i|^2 = 2EN$ for some fixed energy $E > 0$ that is independent of N. Each state $\mathbf{v}$ jumps to a new state $\mathbf{v}'$ defined as follows. A pair of indices (j, k) such that $j < k$ is chosen with equal probability from all $\binom{N}{2}$ pairs and an angle $\theta \in [0, 2\pi)$ is chosen with uniform probability. The state $\mathbf{v}'$ has coordinates

$$\begin{pmatrix} v_j' \\ v_k' \end{pmatrix} = B(\theta) \begin{pmatrix} v_j \\ v_k \end{pmatrix}, \quad B(\theta) = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}, \tag{1.13}$$

and $v_i' = v_i$ for $i \neq j, k$.

This rule for obtaining new velocities is a one-dimensional analog of the collision rule (1.6) with $\theta \in S^1$ playing the role of $l \in S^{d-1}$, and $B(\theta) : \mathbb{R}^2 \to \mathbb{R}^2$ playing the role of the linear transformation $A : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$. As in the case of elastic collisions, energy is conserved

$$|\mathbf{v}'|^2 = \sum_{i=1}^N |v_i'|^2 = \sum_{i=1}^N |v_i|^2 = |\mathbf{v}|^2 = 2EN. \tag{1.14}$$

The above procedure defines a discrete time Markov chain. Each orbit of the chain is a set of states $\mathbf{v}_0, \mathbf{v}_1, \ldots, \mathbf{v}_n, \ldots$ where $\mathbf{v}_{n+1}$ is obtained from $\mathbf{v}_n$ by the rules above. Finally, we may convert the Markov chain to a continuous time Markov process by assuming that the transition rates are a constant multiple of the transition probabilities defined above.

Kac's kinetic equation describes the $N \to \infty$ limit of this Markov process. Summing over binary collisions as in the Boltzmann equation,

$$\partial_t f = Q(f,f) = Q_+(f,f) - Q_-(f,f), \tag{1.15}$$

where the collision kernel is defined by

$$Q_+(f,f)(v,t) = \int_{\mathbb{R}} \int_0^{2\pi} f(v\cos\theta + w\sin\theta, t) f(-v\sin\theta + w\cos\theta, t)\, d\theta\, dw, \tag{1.16}$$

and

$$Q_-(f,f)(v,t) = \int_{\mathbb{R}} \int_0^{2\pi} f(v,t) f(w,t)\, d\theta\, dw. \tag{1.17}$$

1.3. **Smoluchowski's coagulation equations.** The basic kinetic description of clustering was introduced by Smoluchowski in 1917 to model the coagulations of colloids. The same kinetic description has been used to model clustering in a wide range of applications such as the formation of clouds; the formation of smoke, dust and haze; gravitational accretion; and the evolution of animal populations, such as schools of fish. Colloids are suspensions of small particles in a fluid. The particles are small enough that they are subject to Brownian motion, but sufficiently larger than the atomic scale that they admit a classical description (the typical size of a colloidal particle is between $10^{-8} - 10^{-6} m$). Smoluchowski assumed that the colloidal particles would execute Brownian motions, sticking together when they meet. He postulated a kinetic equation for the number density $f(x,t)$ of particles of mass x per unit volume. [2] Smoluchowski's coagulation equations are

$$\partial_t f = Q(f,f) = Q_+(f,f) - Q_-(f,f), \tag{1.18}$$

where the birth and death terms are of the form

$$Q_+(f,f)(x,t) = \frac{1}{2} \int_0^x f(x',t) f(x-x',t) K(x', x-x')\, dx', \tag{1.19}$$

$$Q_-(f,f)(x,t) = \int_0^x f(x,t) f(x',t) K(x,x')\, dx'. \tag{1.20}$$

All the details of the interaction of particles have been lumped into the symmetric rate kernel $K(x,y)$ which describes the rate at which a particle of size x meets a particle of size y. Each time a particle of size x collides with another particle, it becomes larger. This explains the form of the death term. Similarly, a particle of size x is created each time a particle of size x', with $0 \le x' \le x$ meets a particle of size $x - x'$. In order to avoid double-counting, it is necessary to introduce the factor of $1/2$ in the growth term.

For coagulation of colloidal particles, Smoluchowski derived the rate kernel

$$K(x,y) = \left(x^{1/3} + y^{1/3}\right)\left(x^{-1/3} + y^{-1/3}\right). \tag{1.21}$$

This kernel is certainly less intuitive than the kernel for the Boltzmann equation, but perhaps the following heuristic explanation will help. The factor of $1/3$ appears because we assume the particles are spherical with constant density – then since x is the mass, $x^{1/3}$ is the typical length scale of a particle. The factors $x^{1/3}$ and $y^{1/3}$ in the rate correspond to a greater collision cross-section for larger particles. The factors $x^{-1/3}$ and $y^{-1/3}$ arise from the Stokes-Einstein relation for the diffusion

[2] Its more suggestive to write m for mass, but these equations apply in other contexts, and since the variable x is 'standard' notion for a variable, we will use x instead.

constant of a spherical particle – large particles move slower. It is hard to analyze (1.18) with this kernel and Smoluchowski used the following dubious approximation

$$K(x,y) = \left(x^{1/3} + y^{1/3}\right)\left(x^{-1/3} + y^{-1/3}\right) \stackrel{?}{=} 2, \tag{1.22}$$

obtained by ignoring the cross-terms $x^{1/3}y^{-1/3}$ and $x^{-1/3}y^{1/3}$!

We will not view this as an approximation. Instead, we will view the kernel $K = 2$ as an example that is of interest in its own right. This is because Smoluchowski's equation (1.18) appears in a diverse range of applications and in each application kernels are derived in a similar heuristic manner. In order to establish the validity of these approximations, it is necessary to gain some insight into the behavior of solutions to (1.18). As we will see below, the kernel $K = 2$, and two other kernels, $K(x,y) = x + y$ and $K(x,y) = xy$, are exactly solvable. Further, they may be rigorously associated to particle systems that have nothing to do with the coagulation of colloids [1, 13].

1.4. **Mean curvature networks.** The main question in the theory of the Boltzmann equation and in Kac's caricature is to understand the relaxation to equilibrium. That is, we expect typical initial conditions to approach an equilibrium solution, and we would like to prove this fact. In contrast, clustering transfers mass to larger and larger scales, so the coagulation equations do not have non-trivial equilibria with finite mass [3] The growth of large domains, at the expense of smaller domains, is a central feature of the kinetics of phase transitions, where it is called *domain coarsening*. It is also common in nature – a froth of soap bubbles, or the head of a glass of beer – gradually coarsens in time as small bubbles pop.

In materials science, it has long been known that the properties of metals and alloys depend on their microstructure. A polycrystalline material consists of crystalline domains called grains that meet at grain boundaries. Within each crystalline domain, the atoms of the metal or alloy are aligned in a well-defined lattice. There is a lattice mismatch between grains at each grain boundary. This mismatch gives rise to a surface tension, and the grain boundaries move in order to decrease the surface energy, and over time the domains coarsen.

Let us now describe the simplest formulation of this problem. The natural evolution of the polycrystalline material is a gradient flow that minimizes the surface energy [4]. If we assume that the material is two-dimensional and that the surface tension is isotropic (i.e. that it does not depend upon the angle at which two grains meet), then the surface energy is simply the perimeter of the grain boundaries. The gradient descent of this energy is motion by curvature of each curve along with the *Herring boundary condition* – all grain boundaries meet at equal angles at triple junctions. This boundary condition may be understood intuitively –all junctions of higher valence are unstable, since a small perturbation can reduce the surface energy (e.g. see the picture on the right in Figure 4).

The evolution of such a grain boundary network is illustrated in Figure 3. At first glance, Figure 3 suggests that this problem is too complex to be amenable to kinetic theory. Indeed, what are the underlying populations? For the hard sphere

[3]This roughly corresponds to the economic maxim that 'the rich get richer and the poor get poorer'. In fact, the coagulation equations have been used to model the decrease in the number of financial insititutions as big banks swallow smaller banks.

[4]The precise formulation of this, and related gradient flows, may be found in an excellent set of lecture notes by Pego [16].

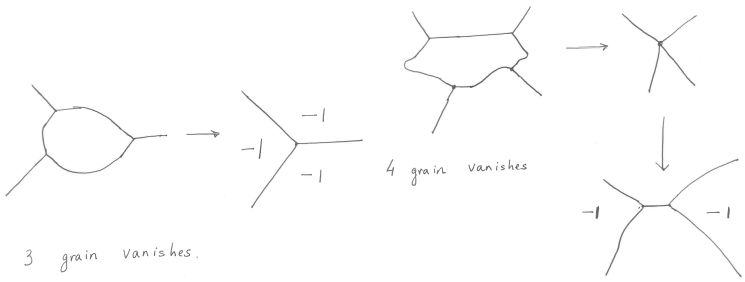


FIGURE 2. Vanishing of grains and the change in the number of sides of their neighbors. The mutation events of Figure 4 depend on the topology of the vanishing grain.

gas or spherical colloids, a kinetic description is natural – we simply count particles with a given velocity (hard spheres) or mass (colloids). But how do we account for the varying shapes of grains?

A kinetic description works in this problem because of a surprising simplification discovered by Von Neumann and Mullins. The topology of two-dimensional grains is easy to describe – each grain is an n-gon, with $n \geq 2$. The geometry varies, but is irrelevant, when one considers the evolution of area. As noted by Von Neumann (with an incorrect proof!), and proved more carefully by Mullins, if a grain boundary network evolves smoothly, the area $A(t)$ of an n-gon in the network grows linearly in time (in a suitable time scale) according to the relation [15, 18]

$$\frac{dA}{dt} = n - 6. \tag{1.23}$$

Thus, all grains with fewer than 6 sides shrink and vanish in finite time.

While surprising at first sight, the formula is easy to derive. The rate of change of area of an n-gon with bounding curves $\{\Gamma_i\}_{i=1}^n$, is obtained by integrating the change in area swept out by each bounding curve in a small interval of time. The area swept out by an arc Γ with length element ds if it moves with normal velocity v is simply

$$\frac{dA}{dt} = \int_\Gamma v\, ds \tag{1.24}$$

Now in angular coordinates $ds = \kappa^{-1} d\theta$, and for motion by curvature $v = \kappa$, thus the rate of change of area, is simply the jump in the tangent across the endpoints of the arc. By the Herring boundary condition, these jumps sum to $2\pi/3(n-6)$ for an n-gon. Rescaling time, we obtain (1.23).

The Mullins-von Neumann rule allows a natural kinetic description of the grain boundary system. We consider a set of populations, $\{f_n(x,t)\}_{n=2}^\infty$, that count the number of (topological) n-gons with area x at time t. This corresponds to extracting 'particles' from the detailed description of Figure 3 as shown in Figure 4. Our analog of collisions are 'vanishing events' when an n-gon, with $n \geq 2$ has zero area. When a grain vanishes, as shown in Figure 2, the number of sides of its neighbors can change, while the area of the neighboring grains varies smoothly. In terms of the particle system of Figure 4, this means that the particles 'mutate' from one n-gonal

species to another. The complexity of the kinetic equations lies in assigning rates to this process of mutation.

In the 1980s and 1990s several physicists and material scientists suggested kinetic equations for this model, that differ in the mutation rules [3, 4, 11]. These equations have the common form

(1.25)
$$\partial_t f_n + (n-6)\partial_x f_n = \sum_{l=2}^{5}(l-6)f_l(0_+,t)\left(\sum_{m=2}^{\infty} A_{lm}(t)f_m(x,t)\right), \quad n=2,\dots,\infty.$$

Here $x \in [0,\infty)$. There is no boundary condition on the left-moving particles ($n = 2,\dots,5$) and the right-moving particles $n \geq 6$ satisfy $f_n(0,t) = 0$. The left-hand side of equation (1.25) describes the free streaming of the area of grains given by the Mullins-von Neumann rule. It is the analog of the transport term $v \cdot \nabla f$ in the non-homogeneous Boltzmann equation (1.12). On the right hand side of (1.25), we again have a binary collision term, that accounts for the mutation between species each time a grain vanishes. It involves an interaction between the rates at which grains vanish, $(l-6)f_l(0,t)$, $l = 2,\dots,5$, and the mutations between topological 'species'. The mutation rates are given by matrix $A_{lm}(t)$ describes the rates at which species mutate into one another. In each model, it is derived from ad hoc geometric assumptions about the manner in which an l-gonal cell vanishes from the system.

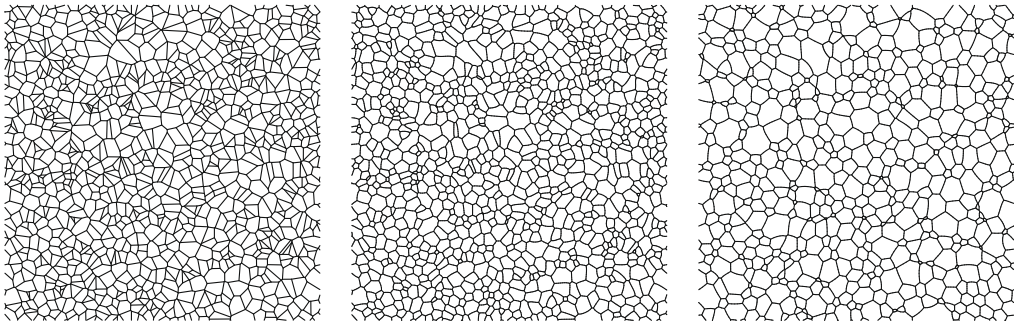
Grain boundary evolution and equation (1.25) represent an important aspect of modern kinetic theory. In many applications, the collision rules can be very subtle, and the number of particles not very large (10^6 grains in a polycrystalline network is much less than 10^{23} hard spheres in an ideal gas). There is plenty of room for mathematicians to contribute to this area, since it is necessary to clarify the validity of assumptions that underly a model. For instance, in light of extensive computations on the evolution of grain boundary networks, it is conceivable that the 'best' model could be determined by parametric estimation of computational data. Further, the analysis of the derivation of the kinetic equations, even the simplest setting, requires some care when we seek quantitative estimates for the difference between the finite N system and the kinetic equations [8].

1.5. **The impatient customer queue.** In order to get a feel for these equations, let us introduce the simplest model in its class. We consider a system of N-particles at positions $x_i \in (0,\infty)$, that moves to the left with unit velocity. When a particle hits zero, it is removed from the system, along with another particle chosen uniformly from the remaining particles. If we view the points as customers in a queue, then we see that one impatient customer leaves the queue each time the first customer reaches the top of the line. So we call this model the impatient customer queue. The kinetic equation in this case is

$$\partial_t f(x,t) - \partial_x f(x,t) = -\frac{f(0,t)}{M(t)} f(x,t), \quad 0 < x < \infty, \tag{1.26}$$

$$M(t) = \int_0^\infty f(x,t)\,dx. \tag{1.27}$$

This equation may be solved exactly. There are two effects – transport to the left at constant rate and a nonlinear decay. For simplicity, let us first ignore the



(a) t=0, 1000 grains. (b) t=0.0001, 982 grains (c) t=0.001, 571 grains

FIGURE 3. **Grain boundary networks.** The evolution of a network of smooth embedded curves in $\mathbb{R}^2$ all of which meet at equal angles in triple-junctions. Each curve evolves by motion by mean curvature. As time increases the number of domains decrease and the typical size of a domain grows. While the domains with fewer than 6 sides vanish as their area shrinks by Von Neumann's rule, new domains with fewer than 6 sides may be nucleated at times when a grain vanishes. Numerical simulations of Lazar, MacPherson, and Srolovitz [10].

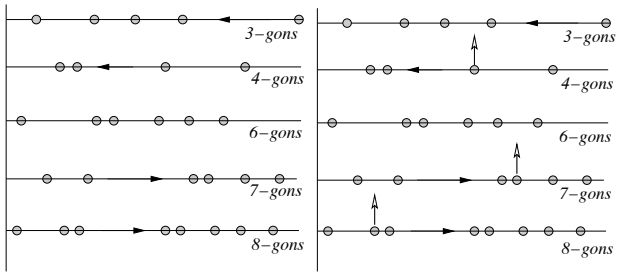


FIGURE 4. **Evolution of grain areas.** The areas of each grain may be extracted from the evolution of the network and plotted as above (not all grain populations are shown). By the Mullins-Von Neumann rule, these particles move at constant speed to the left or right depending on n. Each time a left-moving particle hits zero, there is a mutation, since this causes changes in the number of edges of neighboring grains as shown in Figure 4. For example, when a 3-grain vanishes, three neighboring grains lose a side, so the points associated to these grains jump to the tier corresponding to n-gons with one fewer side .

nonlinearity and consider the linear equation

$$\partial_f - \partial_x f = -r(t)f(x,t), \quad 0 \le x < \infty, t > 0, \tag{1.28}$$

with a prescribed rate of decay $r(t) \ge 0$. This equation may be solved by the method of characteristics. Each characteristic $x(t; x_0)$ that emerges from x_0 at

time zero, is a straight line $x(t;x_0) = x_0 - t$, provided $0 \le t < x_0$. Along this characteristic

$$\frac{df}{dt} = -r(t)f, \tag{1.29}$$

which is easily solved. Thus, the solution to (1.28) is

$$f(x,t) = e^{\int_0^t r(s)\,ds} f_0(x+t), \tag{1.30}$$

where $f_0(x)$ denotes the initial data $f(x,0)$. Now let us consider the *nonlinear* equation (1.26). Observe that it is invariant under the linear scaling $f \mapsto cf$ for any $c \in \mathbb{R}$. By rescaling the initial data, we may assume without any loss of generality that

$$\int_0^\infty f_0(x)\,dx = 1. \tag{1.31}$$

We observe that the solution to (1.26) is also a solution to the linear equation (1.28) if $r(t) = f(0,t)/M(t)$. Thus, it is reasonable to make the ansatz (1.30), and after some playing around, we find the following solution formula.

Theorem 1.1. *Assume $f_0 \in L^1_+ \cap C^1$ and $M(0) = 1$. There exists a unique solution to (1.26) with $f(x,0) = f_0(x)$. The solution is given by the formula*

$$f(x,t) = \rho(t) f_0(x+t), \quad \rho(t) = \int_t^\infty f_0(s)\,ds. \tag{1.32}$$

Proof. The solution formula is easy to check. First, assume that f_0 is smooth and strictly positive and $f(x,t)$ is given by (1.32). Then the total number of particles is

$$M(t) = \int_0^\infty f(x,t)\,dt = \rho(t) \int_0^\infty f_0(x+t)\,dx = \rho(t)^2. \tag{1.33}$$

We differentiate the expression for $f(x,t)$ in equation (1.32) to find

$$\partial_t f - \partial_x f = -f_0(t) f_0(x+t) \overset{(1.32)}{=} -\frac{f(0,t)f(x,t)}{\rho(t)^2} = -\frac{f(0,t)}{M(t)} f(x,t). \tag{1.34}$$

When f_0 has compact support, the solution formula (1.32) continues to hold for all t, and $f(x,t) \equiv 0$ when $t \ge t_*$, where $t_* = \inf\{x \,|\, \int_x^\infty f_0(r)\,dr = 0\}$. □

Observe that the solution formula continues to hold for any $f \in L^1_+$.

2. Basic properties of the Boltzmann equation

In this chapter we explore the properties of the Boltzmann equation for the hard sphere gas more carefully. The Boltzmann equation describes the evolution of a distribution of velocities through collisions. The central question in the theory of the Boltzmann equation is to understand the decay to equilibrium caused by the 'mixing properties' of collisions.

2.1. **The geometry of elastic collisions.** Let us first explain how conservation of momentum and energy (equation (1.5)) is sufficient to determine the post-collision velocities v' and w'. Given $l \in S^{d-1}$, let P_l and $P_{l^\perp}$ denote the orthogonal projections onto the span of l and its orthogonal complement respectively. That is, $P_l u = (u \cdot l)l$ and $P_{l^\perp} u = u - (u \cdot l)l$ for each $u \in \mathbb{R}^d$. The main insight is that in an elastic collision between two hard spheres, we must have

$$P_l(v' - w') = -P_l(v - w), \quad P_{l^\perp}(v' - w') = P_{l^\perp}(v - w). \tag{2.1}$$

Therefore, we find that the first post-collision velocity is

$$\begin{aligned} v' &= \frac{1}{2}(v' + w') + \frac{1}{2}(v' - w') = \frac{1}{2}(v + w) + \frac{1}{2}(P_l + P_{l^\perp})(v' - w') \\ &= \frac{1}{2}(P_l + P_{l^\perp})(v + w) + \frac{1}{2}(-P_l + P_{l^\perp})(v - w) = P_{l^\perp} v + P_l w. \end{aligned} \tag{2.2}$$

In a similar manner, we see that

$$w' = P_l v + P_{l^\perp} w. \tag{2.3}$$

Equations (2.1) and (2.2) are clearly equivalent to equation (1.5). This transformation may be represented geometrically by the *collision sphere* shown in Figure 5(a). Observe, however, that $A_l = A_{-l}$ since $P_l = P_{-l}$, a fact that is not obvious from the construction in Figure 5.s

The linear transformation $A_l : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$, $(v, w) \mapsto (v', w')$ may be represented by the matrix

$$A_l = \begin{pmatrix} P_{l^\perp} & P_l \\ P_l & P_{l^\perp} \end{pmatrix}, \tag{2.4}$$

where $P_l = ll^T$, $P_{l^\perp} = I_d - P_l$, and I_d denotes the $d \times d$ identity matrix.

Lemma 2.1. *For each $l \in S^{d-1}$, $\det(A_l) = -1$ and $A_l^{-1} = A_l$.*

Proof. The projections P_l and $P_{l^\perp}$ satisfy the relations

$$P_l^2 = P_l, \quad P_{l^\perp}^2 = P_{l^\perp}, \quad \text{and} \quad P_l P_{l^\perp} = P_{l^\perp} P_l = 0. \tag{2.5}$$

It immediately follows that $A_l^{-1} = A_l$. Further,

$$A_l = I_{2d} - uu^T, \quad u = \begin{pmatrix} l \\ -l \end{pmatrix}, \tag{2.6}$$

and by the Sherman-Morrison formula for determinants of rank-one updates

$$\det(A_l) = 1 - u^T u = 1 - 2l^T l = -1. \tag{2.7}$$

□

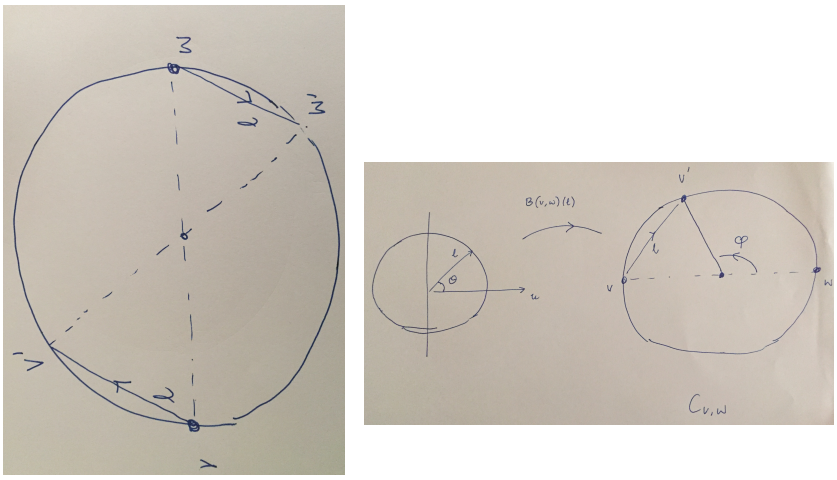


FIGURE 5. (a) The collision sphere $C_{v,w}$ is the sphere in R^d with center $(v+w)/2$ and diameter $|v-w|$. For each $l \in S^{d-1}$, the outgoing velocities v' and w' are represented by the points shown on $C_{v,w}$. Clearly, $C_{v,w} = C_{v',w'}$. (b) Given v and w, the set of possible $v'(l)$ is parametrized by $l \in H_+$. The pushforward of uniform measure on the hemisphere under the map $l \mapsto B_{v,w}(l)$ is uniform measure on $C_{v,w}$.

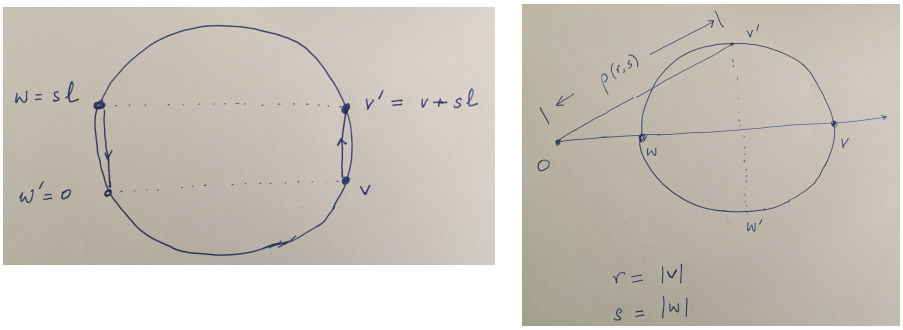


FIGURE 6. The collision spheres $C_{v,w}$ used in the proof of Theorem 2.4 (a) A normalized C^2 collision invariant is radial. (b) A normalized radial C^2 collision invariant vanishes.

In the above calculation, we assumed that $l \in S^{d-1}$ was fixed in order to obtain a linear transformation A_l. We now fix v and w and consider the effect of varying l. In order to simplify the calculation, let $u \in S^{d-1}$ be the unit vector $u = (v-w)/|v-w|$. Let H_+ denote the hemisphere $\{l \in S^{d-1} \,|\, l \cdot u \geq 0\}$ and define the map

$$B_{v,w} : H_+ \to C_{v,w}, \quad l \mapsto v' = v + P_l(w-v). \tag{2.8}$$

Lemma 2.2. *If l is distributed uniformly on H_+, then $B_{v,w}(l)$ is uniformly distributed on $C_{v,w}$.*

Proof. Let θ and φ be the angular coordinates shown in Figure 5(b). We claim that $\varphi = 2\theta$.

This is seen as follows. We separate l into its components parallel and perpendicular to u, writing $l = P_u l + P_{u^\perp} l$, where $P_u l = (u \cdot l)u = \cos\theta\, u$. It then follows from the definition of $v' = B_{v,w}(l)$ that

$$B_{v,w}(l) - \frac{1}{2}(v+w) = \rho\left(\left(\cos^2\theta - \frac{1}{2}\right)u + \cos\theta P_{u^\perp} l\right). \tag{2.9}$$

Finally, the trigonometric identity $2\cos^2\theta - 1 = \cos 2\theta$, and the definition of φ, imply that $\cos\varphi = \cos 2\theta$. Therefore, $\varphi = 2\theta$ on the domain $\theta \in [0, \pi/2]$.

Equation (2.9) also shows that the map from H_+ to $C_{v,w}$ is symmetric in the azimuthal direction. More precisely, if l is uniformly distributed on H_+, then $P_{u^\perp} l$ is uniformly distributed on the $d-2$ dimensional sphere with radius $\sin\theta$, and $B_{v,w}(l)$ is uniformly distributed on the $d-2$ dimensional sphere with radius $(\rho/2)\sin\varphi$. Thus, we may average over the azimuthal direction.

The volume of an infinitesimal shell in H_+ is $\omega_{d-2}(\sin\theta)^{d-2}\, d\theta$ where ω_k denotes the k-dimensional volume of the unit sphere S^k (thus, $\omega_0 = 2$, $\omega_1 = 2\pi$, etc.). Since $\varphi = 2\theta$ and $B_{v,w}(l)$ lies on a sphere with radius $\rho/2$, the volume of its image is $\omega_{d-2}(\rho/2)^{d-1}(\sin\varphi)^{d-2}\, d\varphi/2$. Aside from a normalizing factor, this is again the pushforward of uniform measure on S^{d-1}. □

2.2. **Collision invariants.** Let us first state a useful moment identity for the Boltzmann equation. For suitable test functions φ, let

$$\langle f, \varphi\rangle(t) := \int_{\mathbb{R}^d} f(v,t)\varphi(v)\, dv. \tag{2.10}$$

Lemma 2.3. *Assume $f(v,t)$ is a classical solution to the homogeneous solution Boltzmann equation (1.9). Then*

$$\begin{aligned}&\frac{d}{dt}\langle f, \varphi\rangle \\ &= \frac{1}{8}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{S^{d-1}} \mathcal{L}\varphi(v,w)\left(f(v')f(w') - f(v)f(w)\right)|(v-w)\cdot l|\, dv\, dw,\end{aligned} \tag{2.11}$$

where $\mathcal{L}$ denotes the linear operator

$$\mathcal{L}\varphi(v,w) = \varphi(v) + \varphi(w) - \varphi(v') - \varphi(w'). \tag{2.12}$$

Proof. Since φ is independent of time,

$$\frac{d}{dt}\langle f, \varphi\rangle = \int_{\mathbb{R}^d} \varphi(v)\partial_t f(v,t)\, dv = \int_{\mathbb{R}^d} \varphi(v) Q(f,f)(v,t)\, dv.$$

In all the calculations that follow, we suppress the dependence on t for brevity. [5] We substitute for the collision $Q(f,f)$ to find that

$$\begin{aligned}
&\int_{\mathbb{R}^d} \varphi(v) Q(f,f)(v)\, dv \\
&= \frac{1}{2}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{S^{d-1}} \varphi(v)\left(f(v')f(w') - f(v)f(w)\right)|(v-w)\cdot l|\; dl\, dw\, dv \\
&= \frac{1}{4}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{S^{d-1}} \left(\varphi(v)+\varphi(w)\right)\left(f(v')f(w') - f(v)f(w)\right)|(v-w)\cdot l|\; dl\, dw\, dv \\
&= -\frac{1}{4}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{S^{d-1}} \left(\varphi(v')+\varphi(w')\right)\left(f(v')f(w') - f(v)f(w)\right)|(v-w)\cdot l|\; dl\, dw\, dv.
\end{aligned}$$

The second equality follows from the symmetry of the integrand. The last equality follows from Lemma 2.1. □

The advantage of this formulation is that it makes the fundamental conservation laws of the Boltzmann equation apparent. We choose $\varphi(v) = 1$, v_i, $1 \le i \le d$, and $|v|^2$ to see that the Boltzmann equation conserves the total number, total momentum and total energy

$$\int_{\mathbb{R}^d} f(v,t)\, dv, \quad \int_{\mathbb{R}^d} v f(v,t)\, dv, \qquad \frac{1}{2}\int_{\mathbb{R}^d} |v|^2 f(v,t)\, dv. \tag{2.13}$$

These collision invariants are to be expected and serve as a useful consistency check of the model. Indeed, the number, momentum and energy are conserved at every binary collision between hard spheres. Equation (2.13) reflects this property of the hard sphere system, much as mass conservation was built into (4.2).

More generally, we say that φ defines a *collision invariant* if it satisfies the functional equation

$$\mathcal{L}\varphi(v,w) = 0, \quad v, w \in \mathbb{R}^d, l \in S^{d-1}. \tag{2.14}$$

A remarkable feature of the Boltzmann equation is that the *only* collision invariants are linear combinations of the ones in equation (2.13).

Theorem 2.4. *Assume $\varphi \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$ is a collision invariant. Then there exist constants $(a,b,c) \in \mathbb{R}\times\mathbb{R}^d\times\mathbb{R}$ such that*

$$\varphi(v) = a + b\cdot v + c|v|^2, \quad v \in \mathbb{R}^d. \tag{2.15}$$

Proof. 1. We first prove the theorem under the assumption that φ is a C^2 function. The general case when φ is only L^1_{loc}, may be reduced to the case of C^2 collision invariants by mollification. This step is outlined at the end.
2. Normalization. Assume that $\varphi \in C^2$ is a collision invariant. Without loss of generality, we may assume that

$$\varphi(0) = 0, \quad \nabla\varphi(0) = 0, \quad \triangle\varphi(0) = 0. \tag{2.16}$$

Indeed, if φ is a collision invariant that does not satisfy (2.16), we replace it by

$$\varphi - \varphi(0) - \nabla\varphi(0)\cdot v - \frac{1}{2}\triangle\varphi(0)|v|^2.$$

[5] That is, we have written $f(v)$ for $f(v,t)$. Time only appears as a parameter in the collision operator, and it is convenient to suppress the t dependence in order to understand the properties of the collision operator.

3. A normalized C^2 collision invariant is radial. We fix $v \in \mathbb{R}^d$ and choose $l \in S^{d-1}$ such that $v \cdot l = 0$. Let $w = sl$ for $s \in \mathbb{R}$. This gives a collision sphere $C_{v,w}$ as shown in Figure 6(a) with $v' = v + ls$ and $w' = 0$. Since φ is a collision invariant, we find that

$$\varphi(v + ls) - \varphi(v) = \varphi(ls) - \varphi(0).$$

Dividing by s and letting $s \to 0$, we obtain the identity

$$\nabla\varphi(v) \cdot l = \nabla\varphi(0) \cdot l = 0.$$

Since this holds for each $l \in S^{d-1}$ that is orthogonal to v, it follows that $\nabla\varphi(v)$ is parallel to v for each $v \in \mathbb{R}^d$.

4. A radial C^2 collision invariant is constant. We now write $\varphi(v) = \psi(r)$ where $r = |v|$. We fix $0 < s < r$ and consider the collision sphere $C_{v,w}$ with $|w| = s$ as shown in Figure 6(b). We then find that

$$|v'|^2 = |w'|^2 = \frac{1}{4}(r+s)^2 + \frac{1}{4}(r-s)^2 = \frac{1}{2}(s^2 + r^2) := \rho^2(r,s). \tag{2.17}$$

Since ψ is a collision invariant

$$\psi(s) + \psi(r) = 2\psi(\rho(r,s)).$$

We differentiate this expression with respect to s, and use (2.17) to obtain the identity

$$\frac{\psi'(s)}{s} = \frac{\psi'(\rho)}{\rho}. \tag{2.18}$$

Letting $s \to 0$, we find the identity

$$\frac{\psi'(\rho)}{\rho} = \psi''(0) = 0, \quad \rho = \frac{r}{\sqrt{2}}.$$

Thus, $\psi(r) = \psi(0) = 0$.

5. Mollification for $\varphi \in L^1_{\mathrm{loc}}$. We first observe that each translation of a collision sphere is a collision sphere. Thus, if φ is a collision invariant, and

$$\varphi(v) + \varphi(w) = \varphi(v') + \varphi(w'), \quad v, w \in \mathbb{R}^d, l \in S^{d-1},$$

then for each $u \in \mathbb{R}^d$ we also have

$$\varphi(v-u) + \varphi(w-u) = \varphi(v'-u) + \varphi(w'-u), \quad v, w \in \mathbb{R}^d, l \in S^{d-1}. \tag{2.19}$$

Let k be a C^∞ mollification kernel (that is, $k \geq 0$ and $\int_{\mathbb{R}^d} k(v)\,dv = 1$) and for each $\varepsilon > 0$ set $k_\varepsilon(v) = \varepsilon^{-d}k(v/\varepsilon)$. Consider the functions $\varphi_\varepsilon = \varphi * k_\varepsilon$. It follows from (2.19) that φ_ε is a C^∞ collision invariant for each $\varepsilon > 0$. It follows from steps 2–4 that $\varphi_\varepsilon = a_\varepsilon + b_\varepsilon \cdot v + c_\varepsilon|v|^2$ for some constants $a_\varepsilon \in \mathbb{R}$, $b_\varepsilon \in \mathbb{R}^d$ and $c_\varepsilon \in \mathbb{R}$.

The span of the functions $\{1, v, |v|^2\}$, denoted $\mathcal{V}$, is a closed, finite-dimensional subspace of L^1_{loc}. Since $\varphi_\varepsilon \in \mathcal{V}$ for all $\varepsilon > 0$, and $\varphi_\varepsilon \to \varphi$ in L^1_{loc} as $\varepsilon \to 0$, it follows that $\varphi \in \mathcal{V}$. □

Remark 2.5. The fact that collision invariants are so 'rigid' is closely tied to the properties of the Cauchy-Hamel functional equation

$$\varphi(x) + \varphi(y) = \varphi(x+y), \quad x, y \in \mathbb{R}, \varphi : \mathbb{R} \to \mathbb{R}. \tag{2.20}$$

Every linear function $\varphi(x) = ax$, with $a = \varphi(1)$, is a solution to (2.15). Further, if $\varphi(x)$ is known to be continuous, then since (2.20) implies $\varphi(p/q) = p/q\varphi(1)$ for every rational number $p/q \in \mathbb{Q}$, we may use the continuity of φ to see that

$\varphi(x) = \varphi(1)x$ for every $x \in \mathbb{R}$. It is a deeper fact that (2.15) admits only linear solutions, even if φ is assumed only to be measurable. [6]

2.3. **Maxwellian distributions.** Boltzmann and Maxwell made the profound discovery that the only equilibrium solutions to the Boltzmann equation, i.e. solutions such that $\partial_t f = Q(f, f) = 0$ are constant multiples of the Maxwellian (or Gaussian) distributions

$$f_\sigma(v) = \exp\left(-\frac{|v|^2}{2\sigma}\right). \tag{2.21}$$

In order to see that $Q(f_\sigma, f_\sigma) \equiv 0$, we observe that

$$f_\sigma(v')f_\sigma(w') = \exp\left(-\frac{|v'|^2 + |w'|^2}{2\sigma}\right) = \exp\left(-\frac{|v|^2 + |w|^2}{2\sigma}\right) = f_\sigma(v)f_\sigma(w),$$

by conservation of energy in each collision. Similarly, the only equilibrium solution to Kac's model is of the form (2.21).

How could one possibly guess that these are equilibrium solutions? The answer is that these distributions are the $N \to \infty$ limit of the natural equilibrium measures for the hard sphere gas and Kac's model. Both the hard sphere gas and Kac's model have no 'preferred directions', and it is intuitively reasonable that the uniform measure on the sphere is invariant. That is, imagine that the initial velocity vector $\mathbf{v}_0$ for Kac's model is chosen uniformly on $\sqrt{N}S^{N-1}$. Then at time t, the (random) velocity vector $\mathbf{v}(t)$ has the same law as $\mathbf{v}_0$. For the hard sphere gas, this is a consequence of Liouville's theorem for Hamiltonian systems. A Hamiltonian system on $\mathbb{R}^{2m}$ with Hamiltonian $H(x, y)$ takes the form

$$\dot{x} = \nabla_y H(x, y), \quad \dot{y} = -\nabla_x H(x, y).$$

Its flow map Φ_t has the property that $\det(D\Phi_t) = 1$ for all t. Thus, the flow preserves Lebesgue measure. Given a compact energy surface, $H(x, y) = c$, it follows that the restriction of Lebesgue measure to this energy surface is invariant under Φ_t. The hard sphere gas is *not* described by a smooth Hamiltonian system like the one above, since the velocity jumps at collisions. Nevertheless, the energy surface $|\mathbf{v}|^2 = C$ is invariant under the flow and the restriction of Lebesgue measure to this sphere is the uniform measure. Further, the fact that the Jacobian of the transformation $(v, w) \to A(v, w)$ is 1 means that this measure is invariant under collisions too.

Now it is a beautiful fact that the uniform measure on the sphere $\sqrt{n}S^{n-1}$ as $n \to \infty$ converges to the standard Gaussian measure on $\mathbb{R}^{\mathbb{N}}$. We formalize this idea by considering the convergence of marginal distributions. Let normalized uniform measure on the sphere $\sqrt{n}S^{n-1}$ be denoted by $\mathbb{P}_n$. Then a simple geometric argument shows that for any $a \in [\sqrt{n}, \sqrt{n}]$,

$$\mathbb{P}_n\left(a \le x_1\right) = \frac{\int_a^{\sqrt{n}} (n - x^2)^{(n-3)/2}\, dx}{\int_{-\sqrt{n}}^{\sqrt{n}} (n - s^2)^{(n-3)/2}\, ds} = \frac{\int_a^{\infty} (1 - \frac{x^2}{n})_+^{(n-3)/2}\, dx}{\int_{-\infty}^{\infty} (1 - \frac{s^2}{n})_+^{(n-3)/2}\, ds}. \tag{2.22}$$

The pointwise limit of the integrand is easily computed:

$$\lim_{n\to\infty} \left(1 - \frac{x^2}{n}\right)_+^{(n-3)/2} = e^{-x^2/2}, \quad x \in (-\infty, \infty). \tag{2.23}$$

[6] There are pathological non-measurable solutions to this equation.

Further, we may write

$$\left(1-\frac{x^2}{n}\right)_+^{n/2} = \exp\left(\frac{n}{2}\log\left(1-\frac{x^2}{n}\right)\right)\mathbf{1}_{|x|\leq\sqrt{n}}, \tag{2.24}$$

and use the expansion $\log(1-z) = -(z+z^2/2+\ldots)$ to see that $(1-\frac{x^2}{n})_+^{n/2} \leq e^{-x^2/2}$ for $x \in \mathbb{R}$. Therefore, by the dominated convergence theorem,

$$\lim_{n\to\infty} \mathbb{P}_n\left(a \leq x_1\right) = \frac{1}{\sqrt{2\pi}}\int_a^\infty e^{-x^2/2}\,dx, \quad a \in (-\infty,\infty). \tag{2.25}$$

Similarly, for each integer k, if we consider the first k-components $(x_1,\ldots,x_k)$ of $(x_1,\ldots,x_n)$, we find that

(2.26)

$$\lim_{n\to\infty} \mathbb{P}_n\left(a_1 \leq x_1, a_2 \leq x_2, \ldots, a_k \leq x_k\right) = \frac{1}{(2\pi)^{k/2}}\prod_{j=1}^k \int_{a_j}^\infty e^{-x_j^2/2}\,dx_j \quad a_j \in (-\infty,\infty).$$

2.4. **The H-theorem.** Boltzmann observed the following astonishing property of his equation. Given a density $f : \mathbb{R}^3 \to \mathbb{R}_+$, let us define the Boltzmann entropy

$$H[f] = \int_{\mathbb{R}^d} f(v)\log f(v)\,dv. \tag{2.27}$$

Theorem 2.6 (The H-theorem)**.** *Assume $f(v,t)$ is a classical solution to the homogeneous Boltzmann equation (1.9). Then for all t in the interval of existence*

$$\frac{dH[f(\cdot,t)]}{dt} \leq 0, \tag{2.28}$$

with equality only if f is a Maxwellian.

Proof. We find that

$$\begin{aligned}
\frac{dH[f]}{dt} &= \int_{\mathbb{R}^d}\left(1+\log f(v)\right)Q(f,f)(v)\,dv = \int_{\mathbb{R}^d}\log f(v) Q(f,f)(v)\,dv,\\
&= \frac{1}{8}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{S^{d-1}} \mathcal{L}(\log f)\left(f(v')f(w') - f(v)f(w)\right)|(w-v)\cdot l|\;dl\,dv\,dw\\
&= \frac{1}{8}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{S^{d-1}} \log\frac{f(v)f(w)}{f(v')f(w')}\left(f(v')f(w') - f(v)f(w)\right)|(w-v)\cdot l|\;dl\,dv\,dw \leq 0,
\end{aligned}$$

by the elementary inequality

$$(a-b)\log\frac{b}{a} \leq 0, \quad a,b>0. \tag{2.29}$$

Equality holds only if $a=b$ in (2.29). But this means that $\log f(v,t)$ is a collision invariant. Since all collision invariants are of the form (2.15), equality holds in (2.28) if and only if

$$f(v,t) = f(v) = C\exp\left(a+b\cdot v + c|v|^2\right), \quad a\in\mathbb{R}, b\in\mathbb{R}^3, c<0, C>0. \tag{2.30}$$

□

Here is why this theorem is astonishing. For any finite N, the dynamics of the hard-sphere gas is reversible in time. However, in the limit $N\to\infty$, the effective dynamics modeled by the Boltzmann equation is irreversible. Clearly, there is something subtle going on. In order to understand this question better, we now

turn to the derivation of the Boltzmann equation from the hard-sphere gas via the BBGKY hierarchy.

3. The BBGKY hierarchy for the hard sphere gas

3.1. **The Liouville equation.** The first step in the derivation of the Boltzmann equation is to introduce the Liouville equation. While the ordinary differential equations (1.4) with the jump condition (1.7) describes the evolution of one initial configuration, the Liouville equation describes the evolution of a probability density $f_N(\mathbf{x}, \mathbf{v}, t)$ on the phase space $\mathcal{M}_\delta^N \times \mathbb{R}^{dN}$. Collisions correspond to boundary conditions for f_N on the boundary $\partial\mathcal{M}_\delta^N \times \mathbb{R}^{dN}$. In order to state these boundary conditions, we must first examine the boundary $\partial\mathcal{M}_\delta^N$ more carefully.

Let $\partial^*\mathcal{M}_\delta^N$ denote the set of points $\mathbf{x} \in \mathbb{T}^{dN}$ such that $|x_j - x_k| = \delta$ for exactly one pair of indices $1 \leq j < k \leq N$, and $|x_m - x_n| > \delta$ for all other indices $1 \leq m < n \leq N$. The set $\partial^*\mathcal{M}_\delta^N$ consists of the boundary points that correspond to binary collisions between one pair of spheres. The set $\partial\mathcal{M}_\delta^N \backslash \partial^*\mathcal{M}_\delta^N$ has zero $dN-1$ dimensional measure. We do not prove this fact, but it should be intuitive. The boundary $\partial\mathcal{M}_\delta^N$ is an algebraic variety described by equalities of the form $|x_j - x_k| = \delta$ for pairs of indices j and k. Each equality $|x_j - x_k| = \delta$ describes a variety of codimension 1, or dimension $dN-1$. Points in the set $\partial\mathcal{M}_\delta^N \backslash \partial^*\mathcal{M}_\delta^N$, are degenerate in the sense that for such point p equalities hold, with $p > 1$. Thus, $\partial\mathcal{M}_\delta^N \backslash \partial^*\mathcal{M}_\delta^N$ is a finite union of varieties of codimension p, with $p > 1$, and thus has $dN-1$ dimensional measure zero.

We will assume that f_N has a density so that the boundary condition needs to be stated only on $\partial^*\mathcal{M}_\delta^N$. Then the Liouville equation for the hard sphere gas is the partial differential equation

$$\partial_t f_N + \sum_{i=1}^{N} v_i \cdot \nabla_{x_i} f_N = 0, \quad \mathbf{x} \in \mathcal{M}_\delta^N, \mathbf{v} \in \mathbb{R}^{dN}, t > 0. \tag{3.1}$$

At each boundary point $\mathbf{x} \in \partial^*\mathcal{M}_\delta^N$ where (j,k) is the unique pair of indices with $j < k$ such that $|x_j - x_k| = \delta$, we augment (3.1) with the boundary condition

$$f_N(\mathbf{x}, \mathbf{v}', t) = f_N(\mathbf{x}, \mathbf{v}, t), \quad \mathbf{x} \in \partial^*\mathcal{M}_\delta^N, \tag{3.2}$$

where the velocity vector $\mathbf{v}'$ is defined by

$$\mathbf{v}' = (v_1, \ldots, v_j', \ldots, v_k', \ldots, v_N), \quad (v_j', v_k') = A_{l_{jk}}(v_j, v_k), \quad l_{jk} = \frac{x_k - x_j}{|x_k - x_j|}. \tag{3.3}$$

3.2. **Marginal densities.** The probability density $f_N(\mathbf{x}, \mathbf{v}, t)$ provides a far more detailed description than we need. We're typically interested only in observables that depend only on low-dimensional marginal densities of f_N. In order to define the marginals, we first introduce a fundamental symmetry assumption.

Let S_k denote the permutation group of order k. Given $\pi \in S_N$, we set

$$\pi(\mathbf{x}) = (x_{\pi_1}, \ldots, x_{\pi_N}), \pi(\mathbf{v}) = (v_{\pi_1}, \ldots, v_{\pi_N}). \tag{3.4}$$

We say that f_N is *exchangeable* if

$$f_N(\pi(\mathbf{x}), \pi(\mathbf{v})) = f_N(\mathbf{x}, \mathbf{v}), \quad \pi \in S_N, (\mathbf{x}, \mathbf{v}) \in \mathcal{M}_\delta^N \times \mathbb{R}^{dN}. \tag{3.5}$$

In all that follows, we assume that (3.5) holds.

For each integer $k \leq N$ let us denote

$$\mathbf{x}_k = (x_1, \ldots, x_k), \quad \mathbf{v}_k = (v_1, \ldots, v_k). \tag{3.6}$$

We then define the k-point marginal density of f_N by

$$f_{k,N}(\mathbf{x}_k, \mathbf{v}_k, t) = \int_{\mathbb{T}^{d(N-k)}} \int_{\mathbb{R}^{d(N-k)}} \mathbf{1}_{\mathcal{M}_\delta^N}(\mathbf{x}) f_N(\mathbf{x}, \mathbf{v}, t) \prod_{j=k+1}^{N} dx_j\, dv_j. \tag{3.7}$$

For $k \geq 2$, the domain of $f_{k,N}$ is the set of $(x_1, \ldots, x_k)$ such that $|x_l - x_m| > \delta$, $1 \leq l < m \leq k$. The symmetry of f_N under S_N extends to $f_{k,N}$: for each permutation $\pi \in S_k$, we have

$$f_{k,N}(\pi_k(\mathbf{x}_k), \pi_k(\mathbf{v}_k)) = f_{k,N}(\mathbf{x}_k, \mathbf{v}_k), \quad \pi_k(\mathbf{x}_k) = (x_{\pi_1}, \ldots, x_{\pi_k}).$$

The BBGKY hierarchy is a linear system of evolution equations for $\{f_{k,N}\}_{k=1}^N$ listed in equations (3.25) and (3.26) below. In order to explain the derivation of these equations from the Liouville equation, we first begin with a special case that contains some of the key steps of the general calculation.

3.3. **The evolution equation when $N = 2$ and $k = 1$.** In this case, the set $\mathcal{M}_\delta^N = \{(x_1, x_2) \in \mathbb{T}^{2d} || x_1 - x_2| > \delta\}$, so that

$$f_{1,N}(x_1, v_1, t) = \int_{|x_2 - x_1| > \delta} \int_{\mathbb{R}^d} f_{2,N}(x_1, x_2, v_1, v_2, t)\, dv_2\, dx_2. \tag{3.8}$$

(In fact, here $f_{1,N} = f_{1,2}$ and $f_{2,N} = f_2$, since $N = 2$ but we keep the notation above for comparison with the case when N is large). Therefore, using the Liouville equation (3.1) we have

$$\begin{aligned}
\partial_t f_{1,N}(x_1, v_1, t) &= \int_{|x_2 - x_1| > \delta} \int_{\mathbb{R}^d} \partial_t f_{2,N}(x_1, x_2, v_1, v_2, t)\, dv_2\, dx_2 \\
&= -\int_{|x_2 - x_1| > \delta} \int_{\mathbb{R}^d} (v_1 \cdot \nabla_{x_1} f_{2,N} + v_2 \cdot \nabla_{x_2} f_{2,N})\, dv_2\, dx_2 \\
&= -v_1 \cdot \int_{|x_2 - x_1| > \delta} \int_{\mathbb{R}^d} \nabla_{x_1} f_{2,N} dx_2 dv_2 - \int_{|x_2 - x_1| > \delta} \int_{\mathbb{R}^d} \nabla_{x_2} \cdot (f_{2,N} v_2) dv_2\, dx_2 \\
&:= (a) + (b).
\end{aligned}$$

Let's first consider the term (b). Since the boundary of the domain $\{x_2 \in \mathbb{R}^d : |x_1 - x_2| > \delta\}$ is the sphere of diameter δ centered at x_1, we apply the Gauss-Green theorem to obtain

$$(b) = \delta^{d-1} \int_{\mathbb{R}^d} \int_{S^{d-1}} (v_2 \cdot l)\, f_{2,N}(x_1, x_1 + \delta l, v_1, v_2)\, dl dv_2, \tag{3.9}$$

where l is the outward unit normal to the sphere S^{d-1}. The sign change above is due to the fact that $-l$ is the outward normal to the domain $\{|x_2 - x_1| > \delta\}$. In a similar manner, we may pull the derivative ∇_{x_1} out of the integral in (a) at the price of introducing a boundary integral. That is,

$$\begin{aligned}
(a) = -v_1 \cdot \nabla_{x_1} &\int_{|x_1 - x_2| > \delta} \int_{\mathbb{R}^d} f_{2,N}(x_1, x_2, v_1, v_2)\, dx_2\, dv_2 \\
&-\delta^{d-1} \int_{\mathbb{R}^d} \int_{S^{d-1}} (v_1 \cdot l)\, f_{2,N}(x_1, x_1 + \delta l, v_1, v_2)\, dl dv_2.
\end{aligned} \tag{3.10}$$

By the definition (3.8), the first term on the right hand side is simply $-v_1 \cdot \nabla_{x_1} f_{1,N}$. Thus, combining (3.9) and (3.10) we see that $f_{1,N}$ satisfies the equation

$$\begin{aligned} \partial_t f_{1,N} + v_1 \cdot \nabla_{x_1} f_{1,N} \\ = \delta^{d-1} \int_{\mathbb{R}^d} \int_{S^{d-1}} ((v_2 - v_1) \cdot l)\, f_{2,N}(x_1, x_1 + \delta l, v_1, v_2)\, dl dv_2. \end{aligned} \tag{3.11}$$

In order to organize the boundary integrals that arise when we extend this calculation to N hard spheres, it is helpful to observe that for sufficiently smooth f_N equation (3.11) may also be obtained in the following way. Let $\chi_\delta : [0, \infty) \to \{0, 1\}$ denote the step function $\chi_\delta(s) = \mathbf{1}_{s>\delta}$. Then

$$\partial_t f_{1,N} = -\int_{\mathbb{T}^d} \int_{\mathbb{R}^d} \chi_\delta(|x_1 - x_2|)\, (v_1 \cdot \nabla_{x_1} f_{2,N} + v_2 \cdot \nabla_{x_2} f_{2,N})\, dv_2\, dx_2, \tag{3.12}$$

and we may rewrite the integrand as

$$\begin{aligned} \chi_\delta(|x_1 - x_2|)\, (v_1 \cdot \nabla_{x_1} f_{2,N} + v_2 \cdot \nabla_{x_2} f_{2,N}) = v_1 \cdot \nabla_{x_1} (\chi_\delta(|x_1 - x_2|) f_{2,N}) \\ + \nabla_{x_2} \cdot (v_2 \chi_\delta(|x_1 - x_2|) f_{2,N}) + f_{2,N}(v_1 - v_2) \cdot \nabla_{x_2} \chi_\delta(|x_1 - x_2|), \end{aligned} \tag{3.13}$$

where $\nabla_{x_1} \chi_\delta(|x_1 - x_2|) = -\nabla_{x_2} \chi_\delta(|x_1 - x_2|)$ is interpreted as a vector valued measure concentrated on the sphere $|x_1 - x_2| = \delta$. When integrated over $\mathbb{T}^d \times \mathbb{R}^d$, the first term on the right hand side yields the transport term $-v_1 \cdot \nabla_{x_1} f_{1,N}$, the second term vanishes, and the third yields the boundary integral on the right hand side of (3.11).

3.4. **The evolution equation for $f_{1,N}$.** Let us now proceed to the calculation with N hard spheres. We use the Liouville equation to obtain

$$\begin{aligned} \partial_t f_{1,N}(x_1, v_1, t) &= \int_{\mathbb{T}^{d(N-1)}} \int_{\mathbb{R}^{d(N-1)}} \mathbf{1}_{\mathcal{M}_\delta^N}(\mathbf{x}) \partial_t f_N \prod_{k=2}^N dv_k\, dx_k \\ &= -\int_{\mathbb{T}^{d(N-1)}} \int_{\mathbb{R}^{d(N-1)}} \mathbf{1}_{\mathcal{M}_\delta^N}(\mathbf{x}) \sum_{j=1}^N v_j \cdot \nabla_{x_j} f_N \prod_{k=2}^N dv_k\, dx_k. \end{aligned} \tag{3.14}$$

As in equation (3.13), we rewrite each term in the integrand in (3.14) as the difference

$$\mathbf{1}_{\mathcal{M}_\delta^N}(\mathbf{x}) v_j \cdot \nabla_{x_j} f_N = \nabla_{x_j} \cdot \left(v_j \mathbf{1}_{\mathcal{M}_\delta^N}(\mathbf{x}) f_N \right) - f_N v_j \cdot \nabla_{x_j} \mathbf{1}_{\mathcal{M}_\delta^N}(\mathbf{x}). \tag{3.15}$$

When (3.15) is substituted in (3.14) the first term on the right hand side gives the transport term $-v_1 \cdot \nabla_{x_1} f_{1,N}$ when $j = 1$ and vanishes when $j \neq 1$. Thus,

$$\begin{aligned} \partial_t f_{1,N} + v_1 \cdot \nabla_{x_1} f_{1,N} \\ = \sum_{j=1}^N \int_{\mathbb{T}^{d(N-1)}} \int_{\mathbb{R}^{d(N-1)}} f_N \left(v_j \cdot \nabla_{x_j} \mathbf{1}_{\mathcal{M}_\delta^N}(\mathbf{x}) \right) \prod_{k=2}^N dv_k\, dx_k. \end{aligned} \tag{3.16}$$

Each term on the right hand side gives a boundary integral that we compute as follows. The characteristic function $\mathbf{1}_{\mathcal{M}_\delta^N}(\mathbf{x})$ may be expressed as the product

$$\mathbf{1}_{\mathcal{M}_\delta^N}(\mathbf{x}) = \prod_{1 \le l < m \le N} \chi_\delta(|x_l - x_m|). \tag{3.17}$$

Thus, for each index j, the gradient $\nabla_{x_j} \mathbf{1}_{\mathcal{M}_\delta^N}(\mathbf{x})$ is a sum

$$\nabla_{x_j} \mathbf{1}_{\mathcal{M}_\delta^N}(\mathbf{x}) = \left(\sum_{l \neq j} \frac{\nabla_{x_j} \chi_\delta(|x_l - x_j|)}{\chi_\delta(|x_l - x_j|)} \right) \mathbf{1}_{\mathcal{M}_\delta^N}(\mathbf{x}). \tag{3.18}$$

When substituted in equation (3.14), each term above gives an integral

$$\int_{\mathbb{T}^{d(N-1)}} \int_{\mathbb{R}^{d(N-1)}} f_N \mathbf{1}_{\mathcal{M}_\delta^N}(\mathbf{x}) \frac{v_j \cdot \nabla_{x_j} \chi_\delta(|x_l - x_j|)}{\chi_\delta(|x_l - x_j|)} \prod_{k=2}^{N} dv_k \, dx_k. \tag{3.19}$$

There are three cases to consider: (i) $j = 1$, $l \neq 1$ (ii) $l = 1$, $j \neq 1$ and (iii) $j \neq 1$, $l \neq 1$. In case (i), we may integrate over all $N - 2$ indices k that are not equal to l to obtain that the integral in (3.19) is

$$\int_{\mathbb{T}^d} \int_{\mathbb{R}^d} v_1 \cdot \nabla_{x_1} \chi_\delta(|x_1 - x_l|) f_{2,N}(x_1, x_l, v_1, v_l) \, dv_l dx_l. \tag{3.20}$$

Similarly, in case (ii) we integrate over all $N - 2$ indices not equal to j to obtain the integral

$$\int_{\mathbb{T}^d} \int_{\mathbb{R}^d} v_j \cdot \nabla_{x_j} \chi_\delta(|x_1 - x_j|) f_{2,N}(x_1, x_j, v_1, v_j) \, dv_j dx_j. \tag{3.21}$$

In case (iii), we integrate over $N - 3$ indices k not equal to j or l to obtain

$$\int_{\mathbb{T}^{2d}} \int_{\mathbb{R}^{2d}} v_j \cdot \nabla_{x_j} \chi_\delta(|x_1 - x_j|) f_{3,N}(x_1, x_j, x_l, v_1, v_j, v_l) \, dv_j dv_l \, dx_j dx_l. \tag{3.22}$$

Finally, we sum over j and l and substitute in (3.16). Each integral of the form (3.22) has an equal and opposite term that it cancels with, and it is only the terms of the type (3.20) and (3.21) that contribute. For each index $j \neq 1$, the integral (3.21) is identical to (3.9). Similarly, the integrand (3.20) is identical to the second integral in (3.10). Since there are $N - 1$ such terms, we obtain

$$\begin{aligned} &\partial_t f_{1,N} + v_1 \cdot \nabla_{x_1} f_{1,N} \\ &= (N-1)\delta^{d-1} \int_{\mathbb{R}^d} \int_{S^{d-1}} ((w - v) \cdot l) \, f_{2,N}(x_1, x_1 + \delta l, v_1, w) \, dl dw. \end{aligned} \tag{3.23}$$

This is the first equation in the BBGKY hierarchy for a system of N hard spheres. The main point is that we do not have a closed equation for $f_{1,N}$, since the right hand side depends on $f_{2,N}$. Thus, in order to solve for $f_{1,N}$, we need an equation for $f_{2,N}$. The reader is invited to check that the equation for $f_{2,N}$ is of a similar form: a linear transport term on the left hand side, with a source term that depends linearly on $f_{3,N}$:

$$\begin{aligned} &\partial_t f_{2,N} + v_1 \cdot \nabla_{x_1} f_{2,N} + v_1 \cdot \nabla_{x_2} f_{2,N} \\ &= (N-2)\delta^{d-1} \int_{\mathbb{R}^d} \int_{S^{d-1}} ((w - v_1) \cdot l) \, f_{3,N}(x_1, x_2, x_1 + \delta l, v_1, v_2, w) \, dl dw \\ &+ (N-2)\delta^{d-1} \int_{\mathbb{R}^d} \int_{S^{d-1}} ((w - v_2) \cdot l) \, f_{3,N}(x_1, x_2, x_2 + \delta l, v_1, v_2, w) \, dl dw. \end{aligned} \tag{3.24}$$

Proceeding in this manner, we obtain a *hierarchy* of *linear* equations for $f_{k,N}$, $1 \leq k < N$,

$$\partial_t f_{k,N} + \sum_{j=1}^{k} v_j \cdot \nabla_{x_j} f_{k,N} \\ = (N-k)\delta^{d-1} \sum_{j=1}^{k} \int_{\mathbb{R}^d} \int_{S^{d-1}} ((w - v_j) \cdot l)\, f_{k+1,N}(x_1, \ldots, x_k, x_j + \delta l, v_1, \ldots, v_k, w)\, dl dw. \tag{3.25}$$

For $k \geq 2$, $f_{k,N}$ also satisfies a boundary condition that is analogous to (3.2). At each boundary point where $|x_m - x_n| = \delta$ for exactly one pair of indices $1 \leq m < n \leq k$, we have (ignoring the x and t dependence)

$$f_{k,N}(v_1, \ldots, v_m, \ldots, v_n, \ldots, v_k) = f_{k,N}(v_1, \ldots, v'_m, \ldots, v'_n, \ldots, v_k), \\ (v'_m, v'_n) = A_{l_{mn}}(v_m, v_n)), \quad l_{mn} = \frac{x_n - x_m}{|x_n - x_m|}. \tag{3.26}$$

This is the BBGKY hierarchy for the hard sphere system. [7]

This hierarchy simplifies in the Boltzmann-Grad scaling limit $N \to \infty$ and $\delta \to 0$ with $N\delta^{d-1} \to 1$. Writing f_k for the $N \to \infty$ limit of $f_{k,N}$, we see that the limit of the BBGKY hierarchy (3.25)–(3.26) is the hierarchy

$$\partial_t f_k + \sum_{j=1}^{k} v_j \cdot \nabla_{x_j} f_k \\ = \sum_{j=1}^{k} \int_{\mathbb{R}^d} \int_{S^{d-1}} ((w - v_j) \cdot l)\, f_{k+1}(x_1, \ldots, x_k, x_j, v_1, \ldots, v_k, w)\, dl dw, \tag{3.27}$$

along with the boundary condition

$$f_k(v_1, \ldots, v_m, \ldots, v_n, \ldots, v_k) = f_k(v_1, \ldots, v'_m, \ldots, v'_n, \ldots, v_k), \\ (v'_m, v'_n) = A_l(v_m, v_n)), \quad l \in S^{d-1}, \tag{3.28}$$

for each pair $m < n$ where $x_m = x_n$. (In order to see that (3.28) is the limit of (3.26), hold $l = l_{mn}$ fixed in (3.25) and take $\delta \to 0$.) Equations (3.27)–(3.28) are called the Boltzmann hierarchy.

For future reference, let us also record separately the first equation in the hierarchy, which is the limit of (3.23):

$$\partial_t f_1 + v_1 \cdot \nabla_{x_1} f_1 = \int_{\mathbb{R}^d} \int_{S^{d-1}} ((w - v) \cdot l)\, f_2(x_1, x_1, v_1, w)\, dl dw, \tag{3.29}$$

with the boundary condition

$$f_2(x_1, x_1, v, w) = f_2(x_1, x_1, v', w'), \quad (v', w') = A_l(v, w), \quad l \in S^{d-1}. \tag{3.30}$$

[7] For Bogoliubov, Born, Green, Kirkwood and Yvon.

3.5. **Propagation of chaos.** The Boltzmann equation is a single *nonlinear* equation for the density $f(x,v,t)$. The Boltzmann hierarchy, however, is an infinite system of *linear* equations for the k-point densities $f_k(\mathbf{x}_k,\mathbf{v}_k,t)$. The two models are related by a factorization property we saw in Section 2.3: As $n\to\infty$, uniform measure on $\sqrt{n}S^{n-1}$ converges to Gaussian measure on the product space $\mathbb{R}^{\mathbb{N}}$. This is an example of an asymptotic factorization of an exchangeable density. It is somewhat simpler to convey the essence of this situation in probabilistic language.

A finite sequence of random variables $X_1,\dots,X_k$ is exchangeable if the joint law of $(X_1,\dots,X_k)$ is the same as that of $(X_{\pi_1},\dots,X_{\pi_k})$ for each $\pi\in S_k$. An infinite sequence $X_1,X_2,\dots$, is exchangeable if for each k and each $\pi\in S_k$ the joint law of $(X_1,\dots,X_k)$ is the same as that of $(X_{\pi_1},\dots,X_{\pi_k})$. Clearly, if the sequence is iid, it is exchangeable. A fundamental theorem of De Finetti provides a converse – the law of an infinite sequence of exchangeable random variables is a convex combination of iid laws. De Finetti's theorem is an example of a Choquet theorem expressing each point in a convex set as a linear combination of extreme points in the set. In our context, laws of exchangeable infinite sequences form a convex set, and the laws of iid sequences form the extreme points in this set.

This abstract structure underlies the reduction of the hard sphere gas to the Boltzmann equation. In the Boltzmann-Grad limit, the Boltzmann hierarchy describes the marginals of an exchangeable distribution on $\mathbb{T}^{d\mathbb{N}}\times\mathbb{R}^{d\mathbb{N}}$. By De Finetti's theorem, the extreme points of this set of distributions are given by iid laws. The Boltzmann equation describes the evolution of iid laws under the assumption that the initial data is a law of this type. That is, if we assume that at time $t=0$, $f_k(\cdot,\cdot,0)$ is an iid product measure for each k, then for all t in the interval of existence, $f_k(\cdot,\cdot,t)$ remains an iid product measure, and the evolution of the 1-point marginal is described by the Boltzmann equation.

In order to see this connection between the Boltzmann hierarchy and the Boltzmann equation, let us denote the first marginal by $f(x,v,t)$ and make the ansatz

$$f_k(\mathbf{x}_k,\mathbf{v}_k,t)=\prod_{j=1}^{k} f(x_j,v_j,t),\quad k\in\mathbb{N}. \tag{3.31}$$

Let us write x and v instead of x_1 and v_1 in (3.29), and substitute $f_2(x,x,v,w,t)=f(x,v,t)f(x,w,t)$ into the right hand side. Further, we split the integral according to whether $(w-v)\cdot l>0$ or $(w-v)\cdot l<0$. On the set where $(w-v)\cdot l>0$, we use the boundary condition (3.30), to write

$$f_2(x,x,v,w,t)=f_2(x,x,v',w',t)=f(x,v',t)f(x,w',t). \tag{3.32}$$

On the set where $(w-v)\cdot l<0$, we set $(w-v)\cdot l=-\left((w-v)\cdot(-l)\right)_+$, and use

$$f_2(x,x,v,w,t)=f(x,v,t)f(x,w,t), \tag{3.33}$$

instead of (3.32). Finally, we use the symmetry of S^{d-1} under the map $l\to -l$ to write the right hand side of (3.29) as

$$\begin{aligned}
&\int_{\mathbb{R}^d}\int_{S^{d-1}}\left((w-v)\cdot l\right) f_2(x,x,v,w)\,dl\,dw\\
&=\int_{\mathbb{R}^d}\int_{S^{d-1}}\left((w-v)\cdot l\right)_+ f(x,v',t)f(x,w',t)\,dl\,dw\\
&-\int_{\mathbb{R}^d}\int_{S^{d-1}}\left((w-v)\cdot l\right)+-f(x,v,t)f(x,w,t)\,dl\,dw.
\end{aligned}$$

Thus, (3.29) has reduced to the Boltzmann equation (1.8). Observe that the 'arrow of time' has been introduced by our decision to introduce the boundary conditions as above, thus distinguishing between pre- and post-collision states.

Finaly, we also have to check that substituting the ansatz (3.31) into the k-the equation in the Boltzmann hierarchy does not cause any inconsistency. That is, for each k, not just $k = 1$, we must obtain the Boltzmann equation. This is an interesting calculation that is left to the reader.

A rigorous proof of the persistence of the factorization property (termed *propagation of chaos* by Kac) goes as follows. First, one establishes local well-posedness for the Boltzmann hierarchy for a class of initial data including factorized initial data. Second, one establishes local well-posedness for the Boltzmann equation. Since product laws of the form (3.31) solve the Boltzmann hierarchy (3.27)–(3.28) when f solves the Boltzmann equation (1.8), and the solution to the hierarchy is unique, it follows that the factorization property persists in time. A complete account of this approach may be found in [5, Ch.5].

4. An introduction to coagulation

4.1. **Moment identity for the coagulation equations and gelation.** We now turn to Smoluchowski's coagulation equations. In the scientific literature on coagulation, it is traditional to treat separately the cases when the mass distribution is continuous and discrete. While we have presented equations (1.18)–(1.20) under the assumption that $f(x,t)$ is a density, it is just as natural to assume that the mass distribution is discrete. Indeed, if we begin with all particles of size 1, then the solution must always consists of particles of integer size. From the mathematical standpoint, it is efficient to treat both cases together using some simple measure theory.

Let μ_t denote the measure with density $f(x,t)$ (if it has a density) and for a suitable test function φ, let

$$\langle \mu_t, \varphi \rangle = \int_0^\infty \varphi(x) \mu_t(dx). \tag{4.1}$$

We may integrate by parts to obtain the identity

$$\frac{d}{dt}\langle \mu_t, \varphi \rangle = \frac{1}{2} \int_0^\infty \int_0^\infty (\varphi(x+y) - \varphi(x) - \varphi(y))\, K(x,y)\, \mu_t(dx)\, \mu_t(dy). \tag{4.2}$$

Equation (4.2) allows us to treat discrete and continuous coagulation in a unified way and is the basis for a rigorous well-posedness theorem.

But before stating a rigorous result, let us first get a feel for the coagulation equations. Intuitively, coagulation is a process that transfers mass from small scales to large scales. In order to see the mass transport, it is helpful to consider the evolution of moments of μ_t. For each $p \geq 0$, let

$$m_p(t) = \langle \mu_t, x^p \rangle. \tag{4.3}$$

We call $m_0(t)$ the *total number* and $m_1(t)$ the *total mass*. Plugging $\varphi(x) = x^p$ with $p = 0$ and 1 into (4.2) we find immediately that

$$\dot{m_0} < 0, \quad \dot{m_1} = 0. \tag{4.4}$$

Thus, the total number decreases in time, while the mass stays constant. Of course, both of these must be true, since they are 'built into' the model. More generally, we see that

$$\dot{m_p} < 0, \quad p < 1, \qquad \dot{m_p} > 0, \quad p > 1. \tag{4.5}$$

Most kernels in applications are homogeneous with degree γ. That is,

$$K(\alpha x, \alpha y) = \alpha^\gamma K(x,y), \quad \alpha, x, y > 0. \tag{4.6}$$

For example, Smoluchowski's kernel (1.21) is homogeneous with degree 0. The solvable kernels $K(x,y) = 2$, $x+y$, and xy have degree $\gamma = 0$,1 and 2 respectively. When a kernel has $\gamma > 0$, (4.6) says that the clustering of large particles happens at a faster rate than smaller particles. This has an unexpected consequence: if γ is too large, we may have runaway growth and (1.18)–(1.20) may not be globally well-posed. Let us illustrate this point with an example.

Let $\delta_1(dx)$ denote the Dirac mass with a unit atom at $x = 1$. Consider the solution μ_t to (1.18)–(1.20) when $K = xy$ and $\mu_0(dx) = \delta_1(dx)$. When we substitute

$\varphi(x) = 1$ and x^2 in (4.2) we find that the integral factors into two parts, and we obtain the identities

$$\dot{m}_0 = -\frac{1}{2}m_1^2, \quad \dot{m}_2 = m_2^2. \tag{4.7}$$

Since $m_2(0) = 1$ we find that

$$m_2(t) = \frac{1}{1-t}. \tag{4.8}$$

Thus, if there is a solution to Smoluchowski's equation with $K = xy$ on the interval $[0, 1]$ then its second moment blows-up at time 1. At first sight, this seems like a problem that one may fix, since the mass $m_1(t)$ may remain finite, even when $m_2(t)$ diverges. But if the mass is conserved (as it should be, according to (4.4)) we would find that

$$m_0(t) = 1 - \frac{t}{2}, \quad \text{so that} \quad m_0(2) = 0. \tag{4.9}$$

But then $\mu_2 = 0$ contradicting $m_1 = 1$. In summary, there is no global mass-conserving solution to Smoluchowski's coagulation equations when $K(x, y) = xy$. The reader is invited to check what goes wrong with (4.4) when $m_2 = \infty$.

This phenomenon – blow-up of higher moments and absence of global solutions – is known as *gelation*. This term originates in polymer chemistry, where gelation corresponds to the growth of a giant chain molecule from individual units (monomers). There are general results in the literature regarding well-posedness of (1.18)–(1.20). Roughly, gelation occurs for a large class of homogeneous kernels if and only if $\gamma > 1$.

4.2. **Bernstein transforms and solution formulas.** Despite the fact that Smoluchowski's equation is nonlinear, when $K = 2$, $x + y$ or xy, it may be solved using the Laplace transform. In fact, we will use a modified Laplace transform, that we term the Bernstein transform, defined by

$$\varphi(q, t) = \int_0^\infty \left(1 - e^{-qx}\right) \mu_t(dx), \quad q \in \mathbb{C}_+. \tag{4.10}$$

The reason for this choice is explained below.

Assume $K = 2$. We substitute $\varphi(x) = 1 - e^{-qx}$ in (4.2), and use the factorization

$$(1 - e^{-q(x+y)}) - (1 - e^{-qx}) - (1 - e^{-qy}) = -\left(1 - e^{-qx}\right)\left(1 - e^{-qy}\right), \tag{4.11}$$

to obtain the simple ordinary differential equation

$$\partial_t \varphi(q, t) = -\varphi^2(q, t), \quad q \in \mathbb{C}_+, \tag{4.12}$$

with solution

$$\varphi(q, t) = \frac{\varphi_0(q)}{1 + t\varphi_0(q)}, \quad q \in \mathbb{C}_+, t > 0. \tag{4.13}$$

Here φ_0 denotes the Bernstein transform of the initial data μ_0.

What has happened, of course, is that the factorization (4.11) and the fact that $K = 2$ allows us to separate the double integral in (4.2) into two independent

factors. A similar calculation applies to the kernels $K = x + y$ and $K = xy$. When $K = x + y$ we find that the integrals factor again, and we have

$$\partial_t \varphi(q,t) = -\left(\int_0^\infty (1-e^{-qx}) x \mu_t(dx)\right)\left(\int_0^\infty (1-e^{-qy})\mu_t(dy)\right) = -\varphi(q,t)\left(\int_0^\infty (1-e^{-qx}) x\mu_t(dx)\right). \tag{4.14}$$

Since $xe^{-qx} = \partial_q(1-e^{-qx})$, the integral on the right hand side may be written as a q-derivative. Let us also assume that the initial data has been normalized so that

$$\int_0^\infty x\mu_0(dx) = 1. \tag{4.15}$$

Then by conservation of mass (strictly speaking, this must be established, but let's assume it first and derive the equation for $\varphi(q,t)$), we find that

$$\partial_q \varphi(0,t) = \int_0^\infty x\mu_t(dx) = 1. \tag{4.16}$$

We then find that the Bernstein transform satisfies

$$\partial_t \varphi - \varphi \partial_q \varphi = -\varphi, \quad q \in \mathbb{C}_+, t > 0. \tag{4.17}$$

Aside from the decay term on the right hand side, we see that this is the inviscid Burgers equation in the right-half plane. It may be (formally) solved by the method of characteristics. Let $q(t;q_0)$ denote the characteristic that starts at q_0 at time 0. Along characteristics we find the ordinary differential equations

$$\frac{d\varphi}{dt} = -\varphi, \quad \frac{dq}{dt} = -\varphi. \tag{4.18}$$

Thus, the forward map $q \mapsto q(t;q_0)$ is given by

$$q(t;q_0) = q_0 - (1-e^{-t})\varphi_0(q_0). \tag{4.19}$$

Assume for a moment that this map has a unique inverse (i.e. characteristics do not intersect), denoted by $q_0(q,t)$. We then find the implicit solution formula

$$\varphi(q,t) = e^{-t}\varphi_0(q_0(q,t)), \quad q \in \mathbb{C}_+. \tag{4.20}$$

We invite the reader to compute a similar solution formula for the case $K = xy$ (the answer may be found in [12]).

These solution formulas are appealing, but there is still work to be done. In order that the Bernstein functions define a solution to Smoluchowski's equation, we must show that the Bernstein transforms given by (4.13) and (4.20) have a unique inverse that is a positive measure μ_t with $m_1(t) = m_1(0)$. This involves an interesting detour into classical analysis.

4.3. **Completely monotone functions and Bernstein functions.** Let us now approach the problem with greater rigor. Assume μ is a finite measure on $[0,\infty)$, and observe that its Laplace transform

$$\eta(q) = \int_0^\infty e^{-qx}\mu(dx), \quad q \in \mathbb{C}_+, \tag{4.21}$$

satisfies the following inequalities:

$$(-1)^k \partial_q^k \eta(q) \geq 0, \quad q \in (0,\infty), \quad k \in \mathbb{N}. \tag{4.22}$$

These inequalities are strict unless μ has an atom at zero. We will show that the class of positive functions that satifies these inequalities is very rigid. In fact, we won't even assume that η is C^∞, by working instead with finite-differences from the right. For any measurable function $g : (0,\infty) \to \mathbb{R}$ we define the difference operators

$$D_h g(q) = \frac{1}{h}\left(g(q+h) - g(q)\right). \tag{4.23}$$

Definition 4.1. A measurable function $\eta : (0,\infty) \to (0,\infty)$ is *completely monotone* if the following inequalities hold:

$$(-1)^k D_h^k(q) \geq 0, \quad q, h \in (0,\infty), \quad k \in \mathbb{N}. \tag{4.24}$$

Here is one version of a celebrated theorem of Bernstein.

Theorem 4.2 (Bernstein)**.** *A completely monotone function η with $\eta(0) = 1$ is the Laplace transform of a probability measure on $(0,\infty)$. In particular, it has an analytic extension to the right half plane $\mathbb{C}_+$.*

We will not prove this theorem (for proofs, see [2]). It may be seen as an instance of Choquet's theorem in functional analysis [9]. Choquet's theorem allows us to express each point in the interior of a compact convex set as a linear combination of its extreme points. In this case, the set of completely monotone functions with $\eta(0) = 1$ is a compact, convex set, whose extreme points are the exponentials e^{-ax}, $a \in [0,\infty)$. The main difficulty in the proof is to characterize the extreme points. Bernstein's theorem then follows from Choquet's theorem. Observe the surprising fact that a measurable that satisfies infinitely many inequalities is smooth, in fact analytic!

This theorem reveals that the use of the solution formulas (4.13) and (4.20) to solve Smoluchowski's equation could be delicate, since we have to establish the validity of infinitely many inequalities. Fortunately, there are simpler criterion that may be used to establish complete monotonicity, or the following closely related notion.

Definition 4.3. A function $\varphi : \mathbb{C}_+ \to \mathbb{C}$ is a Bernstein function of the first kind if it is of the form

$$\varphi(q) = aq + \int_0^\infty \left(1 - e^{-qx}\right) \mu(dx) \tag{4.25}$$

where $a \geq 0$ is a real number and μ is a positive measure on $[0,\infty)$ that satisfies the integrability condition

$$\int_0^\infty \min(1,x)\, \mu(dx) < \infty. \tag{4.26}$$

Definition 4.4. A function $\Psi : \mathbb{C}_+ \to \mathbb{C}$ is a Bernstein function of the second kind if it is of the form

$$\Psi(q) = \sigma^2 q^2 + cq + \int_0^\infty \left(e^{-qx} - 1 + qx\right) \Lambda(dx), \tag{4.27}$$

where σ and c are real numbers and Λ is a positive measure that satisfies the integrability condition

$$\int_0^\infty \min\left(x, x^2\right) \Lambda(dx) < \infty. \tag{4.28}$$

Clearly, the derivative of a Bernstein function of the first kind is completely monotone, and the derivative of a Bernstein function of the second kind is a Bernstein function of the first kind. However, note that condition (4.26) is weaker than that required to define the Laplace transform of μ, since we allow measures such that $\int_0^x \mu(ds)$ is divergent for every $x > 0$. Such generality is necessary, since it turns out that the self-similar solutions for the kernel $K = x + y$ and $K = xy$ have such a divergence. The linear term aq may be viewed as the limit of the right hand side when we consider a sequence of measures $\mu^{(n)}$ such that the measures $x^{-1}\mu^{(n)}$ converge weakly to the Dirac mass $a\delta_0$ as $n \to \infty$. In what follows, we will mainly work with Bernstein functions of the first kind.

Theorem 4.5 (Subordination)**.** *Assume φ and ψ are Bernstein functions of the first kind. Then the composition $\varphi \circ \psi$ is also a Bernstein function of the first kind.*

A variant of this theorem was first established by Bochner in the 1950s. However, the probabilistic import of the theorem was not clear at the time, and the initial analyses were quite cumbersome. The key to the theorem lies in the probabilistic interpretation of formula (4.25). For simplicity, assume first that μ is a finite measure. Let $\lambda = \int_0^\infty \mu(dx)$ and let N be a Poisson-λ random variable. That is, $\mathbb{P}(N = n) = e^{-\lambda}\lambda^n/n!$ for each integer $n \geq 0$. Let $\{X_j\}_{j=0}^\infty$ be iid random variables with distribution $\lambda^{-1}\mu$ and consider the random sum $Y = \sum_{j=1}^N X_j$ where N is independent of $\{X_j\}_{j=0}^\infty$. Then we claim that

$$e^{-\varphi(q)} = \mathbb{E}\left(e^{-qY}\right). \tag{4.29}$$

Indeed, conditioning on N we find

$$\mathbb{E}\left(e^{-qY}\right) = \sum_{n=0}^\infty \mathbb{E}\left(e^{-q\sum_{j=0}^n X_j} \,|N = n\right) \mathbb{P}\left(N = n\right) = e^{-\lambda} \sum_{n=0}^\infty \left(\mathbb{E}(e^{-qX_1}\right)^n \frac{\lambda^n}{n!}. \tag{4.30}$$

Now since X_1 has law $\lambda^{-1}\mu$, we find that

$$\left(\mathbb{E}(e^{-qX_1}\right) = \frac{1}{\lambda}\int_0^\infty e^{-qx}\mu(dx). \tag{4.31}$$

Therefore,

$$\mathbb{E}\left(e^{-qY}\right) = e^{-\lambda}e^{\int_0^\infty e^{-qx}\mu(dx)} = e^{\int_0^\infty (1-e^{-qx})\mu(dx)} = e^{-\varphi(q)}. \tag{4.32}$$

This establishes (4.29) when μ is a finite measure. The general case is obtained by approximation.

In fact, formula (4.29) underlies an important discovery in probability theory. Rather than work with a Poisson random variable, it is more natural to work with a compound Poisson process, defined as follows. Let the increasing sequence $\{T_j\}_{j=1}^\infty$ define a Poisson process with rate λ in $(0, \infty)$ and let $N_t = \sum_{j=1}^\infty \mathbf{1}_{T_j \leq t}$ denote the counting function. [8] Now define the compound Poisson process $Y_t = \sum_{j=0}^{N_t} X_j$. It consists of two parts: (i) a clock defined by N_t; (ii) independent jumps of size X_j at each jump time. A minor variation on the argument above yields the fundamental formula

$$\mathbb{E}\left(e^{-qY_t}\right) = e^{-t\varphi(q)}, \quad q \in \mathbb{C}_+, t \geq 0. \tag{4.33}$$

[8] If you've never seen a Poisson process before, its a random 'clock' whose increments $T_{j+1} - T_j$ are independent exponential random variables with rate λ.

Continuous time processes with independent increments constitute an important example of stochastic processes called Lévy processes. An increasing Lévy process is called a subordinator. Given φ, the process Y_t defined as above is a subordinator by construction. In fact, a central result in the theory of Lévy processes is that all subordinators are of this form. To summarize, a function φ is a Bernstein function of the first kind if and only if it is associated to a subordinator as above. The probabilistic import of Theorem 4.5 is that subordinators allow us to 'time-change' a Lévy process while staying within the class of Lévy processes. In the particular case, when both processes are subordinators, we obtain Theorem 4.5.

Proof of Theorem 4.5. Let Y_t and Z_t denote independent subordinators defined by the Bernstein function φ and ψ respectively, and consider the time-changed process $R_t = Z_{Y_t}$. We claim that

$$\mathbb{E}\left(e^{-qR_t}\right) = e^{-t\varphi(\psi(q))}, \quad q \in \mathbb{C}_+, t \geq 0. \tag{4.34}$$

In order to see why this formula is true, let's first rewrite equation(4.33) in the following manner

$$e^{-t\varphi(q)} = \mathbb{E}\left(e^{-qZ_t}\right) = \int_0^\infty e^{-qs}\mathbb{P}\left(Z_t \in (s, s+ds)\right). \tag{4.35}$$

Therefore, conditioning on the value of Z_t we find

$$\begin{aligned}\mathbb{E}\left(e^{-qR_t}\right) = \mathbb{E}\left(e^{-qZ_{Y_t}}\right) &= \int_0^\infty \mathbb{E}\left(e^{-qZ_s}\,|Y_t = s\right)\mathbb{P}\left(Y_t \in (s, s+ds)\right) \\ &= \int_0^\infty e^{-s\psi(q)}\mathbb{P}\left(Y_t \in (s, s+ds)\right) = e^{-t\varphi(\psi(q))}.\end{aligned} \tag{4.36}$$

□

4.4. **Well-posedness of Smoluchowski's equation.** We now have the tools necessary to show that the solution formulas define solutions to Smoluchowski's equation. We first define the appropriate notion of measure-valued solution, and then use the solution formulas (4.13) and (4.20) in combination with the results of the previous section.

We index the three solvable kernels $K = 2$, $x + y$ and xy by their degree of homogeneity $\gamma = 0$, 1 and 2 respectively. Let $\mathcal{M}_\gamma$ denote the space of measures on $(0, \infty)$ such that for each $\mu \in \mathcal{M}_\gamma$

$$m_\gamma = \int_0^\infty x^\gamma \mu(dx) < \infty. \tag{4.37}$$

Without loss of generality, we may rescale the initial data so that

$$m_\gamma(0) = \int_0^\infty x^\gamma \mu_0(dx) = 1. \tag{4.38}$$

We equip $\mathcal{M}_\gamma$ with the weak topology. [9] For each kernel, given initial data $\mu_0 \in \mathcal{M}_\gamma$, we will say that a continuous function $\mu : [0, T] \to \mathcal{M}_\gamma$, $t \mapsto \mu_t$ solves

[9]Recall that a sequence of finite measures $\mu^{(n)} \in \mathcal{M}_0$ converges weakly to μ if

$$\lim_{n\to\infty} \langle \mu^{(n)}, \varphi\rangle = \langle \mu, \varphi\rangle, \tag{4.39}$$

for every $h \in C_0((0, \infty))$. This is really weak-$*$ convergence. However, it appears so often in probability, that it is called the weak topology by probabilists, and we use their terminology. When we consider $\mathcal{M}_\gamma$, the space of test functions is modified by multiplying it by $x^{-\gamma}$.

Smoluchowski's equation with initial data μ_0 if the moment identity obtained after integrating (4.2) in time,

$$\langle \mu_t, \varphi \rangle - \langle \mu_0, \varphi \rangle = \frac{1}{2} \int_0^t \int_0^\infty \int_0^\infty (\varphi(x+y) - \varphi(x) - \varphi(y)) \, K(x,y) \, \mu_t(dx) \, \mu_t(dy), \quad t \in [0,T], \tag{4.40}$$

holds for a sufficiently rich class of test functions, denoted S_γ. The precise class required must satisfy certain smoothness assumptions, and the interested reader is referred to [12]. In the theorem below, we use the terminology $T_\gamma = +\infty$, $\gamma = 0{,}1$ and $T_\gamma = 1$, $\gamma = 2$.

Theorem 4.6. *Assume μ_0 satisfies (4.38). There exists a unique function $\mu \in C([0,T_\gamma), \mathcal{M}_\gamma)$ such that (4.40) holds for all $\varphi \in S_\gamma$.*

Proof. While we haven't precisely defined S_γ, the main point is that the functions $1 - e^{-qx}$, $q > 0$ are dense in S_γ. Thus, if the solution formulas (4.13) and (4.20) hold for $q > 0$ and $t > 0$ and these solution formulas define positive measures, we will have well-posedness. That is, the essential difficulty is to show positivity, and we will focus on it. The reader interested in the other details (showing that $\mu \in C([0,T_\gamma), \mathcal{M}_\gamma)$, uniqueness, etc.) is referred to [12].

Positivity is easiest to see for the constant kernel. Observe that

$$\frac{q}{1+q} = \int_0^\infty \left(1 - e^{-qx}\right) e^{-x} \, dx \tag{4.41}$$

is a Bernstein function. We apply Theorem 4.5 to see that $\varphi(q,t)$ is a Bernstein function.

Next consider the additive kernel. Recall that we have assumed that $\int_0^\infty s\mu_0(ds) = 1$. Thus, for $q_0 > 0$ we have the uniform estimate

$$\frac{\varphi_0(q_0)}{q_0} = \int_0^\infty \frac{1 - e^{-q_0 x}}{q_0 x} x \mu_0(dx) < 1. \tag{4.42}$$

Hence, for $0 < t < \infty$, the forward map defined by (4.19) is strictly increasing and maps $[0,\infty)$ in a one-to-one manner onto itself. Therefore, the inverse mapping $q_0(q,t)$ is well-defined. If we can show that $q_0(q,t)$ is a Bernstein function of q, we are done, since (4.20) and Theorem 4.5 combine to show that $\varphi(q,t)$ is a Bernstein function of q.

In order to show that q_0 is a Bernstein function of the first kind, we write it as the fixed point of a sequence of iterates

$$q_0^{(n)}(q,t) = q + (1 - e^{-t})\varphi_0\left(q_0^{(n-1)}(q,t)\right), \quad n \geq 0, q_0^{(0)}(q,t) = q. \tag{4.43}$$

The zeroth iterate, $q_0^{(0)}(q,t)$, is trivially Bernstein. By Theorem 4.5, the first iterate, $q_0^{(1)}$ is then the sum of two Bernstein functions, so it is a Bernstein function. Proceeding inductively, each iterate $q_0^{(n)}(q,t)$ is a Bernstein function. The limit of a sequence of Bernstein function is a Bernstein function (this may be seen by using (4.1) and (4.2), for example). Thus $q_0(q,t)$ is a Bernstein function. □

A second (slick) proof of the fact that q_0 is a Bernstein function function goes as follows. While we have only used Bernstein functions of the first kind so far, there is a striking relation between Bernstein functions of the first and second kind that plays a crucial role here: Assume Ψ is a Bernstein function of the second kind

such that $\Psi(0) = 0$ and $\Psi(\infty) = \infty$. Then the inverse function Ψ^{-1} is a Bernstein function of the first kind!

This result applies here as follows. Integrating along characteristics we see that

$$q - \varphi(q,t) = q_0 - \varphi_0(q) = \int_0^\infty \left(e^{-q_0 x} - 1 + q_0 x\right) := \Psi_0(q). \tag{4.44}$$

Thus, we may rewrite (4.19) in the form

$$q = (1 - e^{-t})\Psi_0(q_0) + e^{-t} q_0. \tag{4.45}$$

This shows that $q_0 \mapsto q(t; q_0)$ is a Bernstein function of the second kind of q_0. Thus, the inverse function $q \mapsto q_0$ is a Bernstein function of the first kind.

Why would somebody think up this proof? The answer lies in a suprising connection between Smoluchowski's equation and the study of shock clustering in Burgers equation with random initial data [13].

4.5. **Self-similar solutions for the constant kernel.** Unlike the Boltzmann equation, Smoluchowski's coagulation equations (1.18)–(1.20) have no non-singular equilibrium solutions. [10] For both the constant and additive kernels there is a global solution in time, and the natural question to ask is the following: what are the long-time asymptotics? There can be no non-trivial asymptotics unless we rescale the mass distribution. Indeed, as time increases the mass is transported to larger and larger scales, and without rescaling all we get is a giant cluster.

The total number $m_0(t) = \varphi(\infty, t)$ and the solution formula (4.13) shows that

$$m_0(t) = \frac{m_0(0)}{1 + t m_0(0)} \sim \frac{1}{t}, \quad t \to \infty. \tag{4.46}$$

For this reason, we make the scaling ansatz

$$\varphi(q,t) = \frac{1}{t}\psi(\xi), \quad \xi = q\lambda(t), \tag{4.47}$$

where the scaling function ψ and the time scale $\lambda(t)$ are to be determined. We substitute (4.47) in (4.12) and find after a simple calculation that

$$\frac{\dot\lambda}{\lambda}\xi\psi' = \psi\left(1 - \psi\right). \tag{4.48}$$

We now separate variables to find

$$\xi\psi' = \rho\psi\left(1 - \psi\right), \quad \frac{\dot\lambda}{\rho\lambda} = 1, \tag{4.49}$$

where $\rho \in \mathbb{R}$ is a constant. Since $\psi' > 0$ we must have $\rho > 0$. We integrate (4.49), and obtain the ρ-dependent solution

$$\psi_\rho = \frac{\xi^\rho}{1 + \xi^\rho}, \quad \lambda(t) = t^{1/\rho}. \tag{4.50}$$

The function $q^{\rho-1}$ cannot be completely monotone if $\rho >$, since its first derivative would be increasing if $\rho > 1$. Thus, q^ρ could possibly be a Bernstein function only

[10] Formally, they do admit equilibria that are pure power laws, however the interpretation of these solutions requires care.

in the range $0 < \rho \leq 1$. In fact, in this range, it *is* a Bernstein function as follows from the elementary observation that for $0 < \rho < 1$

$$\int_0^\infty \frac{1 - e^{-qx}}{x^{1+\rho}}\, dx = C_\rho q^\rho, \tag{4.51}$$

where C_ρ is a ρ-dependent constant. Thus, combining (4.41) and Theorem 4.5, we see that there is a one-parameter family of self-similar solutions to (1.18)–(1.20) of the form

$$\varphi(q,t) = \frac{q^\rho}{1 + tq^\rho}, \quad 0 < \rho \leq 1. \tag{4.52}$$

At the end-point $\rho = 1$, we may invert the Bernstein transform explicitly to find that

$$\mu_t(dx) = \frac{1}{t^2} e^{-x/t}, \quad x, t > 0. \tag{4.53}$$

The density $f_1(x) = e^{-x}$ has a finite limit as $x \to 0$ and (obviously) exponential decay as $x \to \infty$. For $0 < \rho < 1$, the Bernstein transform ψ_ρ cannot be inverted in closed form. However, the density $f_\rho(x)$ can be expressed as an infinite series and we find that it has the following asymptotic properties

$$f_\rho(x) \sim \frac{1}{\Gamma(\rho) x^{1-\rho}}, \quad x \to 0, \qquad f_\rho(x) \sim \frac{1}{|\Gamma(-\rho)| x^{1+\rho}}, \quad x \to \infty. \tag{4.54}$$

In particular, *all* self-similar solutions for $\rho \neq 1$ have fat tails, in the sense that their mass is infinite. This is the first sign of rather delicate long-time asymptotics. The tails of the initial data that determine the domains of attraction of these self-similar solutions. Roughly, the solution μ_t with an initial data μ_0 can be rescaled so that the rescaled number distribution function approaches the profile f_ρ if and only if

$$\int_0^x x \mu_0(dx) \sim C x^{1-\rho}, \quad x \to \infty. \tag{4.55}$$

For precise statements, see [12].

5. Foundations

We now return to the hard sphere gas. The Boltzmann equation describes the evolution of a distribution of velocities through collisions. The central question in the theory of the Boltzmann equation is to understand the decay to equilibrium caused by the 'mixing properties' of collisions.

5.1. **Kac's example.** Boltzmann's approach to kinetic theory caused a crisis in physics. While Boltzmann's goal was to derive the laws of thermodynamics from Newtonian mechanics, the $N \to \infty$ limit had properties that violated fundamental properties of Newton's laws. For instance, the H-theorem shows that the behavior of the Boltzmann equation is irreversible, whereas Newton's laws are reversible in time (Loschmidt's paradox). From Boltzmann's standpoint, this was a desirable feature of the theory – he wanted all initial velocity distributions to approach the Maxwellians. The underlying idea is that collisions between spheres serve to rapidly mix the velocity statistics, so that the Maxwellian distribution is inevitable. Zermelo was sharply critical of this hypothesis for the following reason. An essential consequence of Liouville's theorem for Hamiltonian systems is Poincaré's recurrence theorem: every initial condition on a compact energy surface returns infinitely often to an arbitrarily small neighborhood of itself. Thus, microscopic mixing – the essential hypothesis of Boltzmann's theory – cannot be true![11]

The resolution of Zermelo's paradox lies in a careful analysis of the timescale of recurrence. We will illustrate these ideas in a simple model introduced by Kac. We consider a set B of n equally spaced points on S^1. Let a subset A consisting of m of these points be chosen uniformly. We assume that $0 < m/n < 1/2$. Each site of B is occupied by a single ball that may be either white or black. The system evolves in discrete time steps as follows. At each time step, all the balls are moved one site counterclockwise. Further, all the balls that originate in A switch color under this move, while the other balls do not change color. How do we describe the number of black and white balls at time t as $n \to \infty$, $m \to \infty$, $m/n \to \mu \in (0, 1/2)$?

To simplify matters further, let us assume that all the balls are initially white. Let $N_w(t)$ and $N_b(t)$ denote the number of white and black balls respectively at time $t \in \mathbb{N}$. Let $N_w(A, t)$ and $N_b(A, t)$ denote the number of white and black balls in A. Since each white ball in A at time t becomes a black ball at time $t + 1$, and each black ball becomes a white ball, we have the conservation laws

$$\begin{aligned} N_w(t+1) &= N_w(t) + N_b(A,t) - N_w(A,t), \\ N_b(t+1) &= N_b(t) + N_w(A,t) - N_b(A,t). \end{aligned} \tag{5.1}$$

Clearly, the total number of balls is conserved

$$N_w(t+1) + N_b(t+1) = N_w(t) + N_b(t) = n, \tag{5.2}$$

while the rescaled excess mass,

$$\rho_n(t) := \frac{1}{n}\left(N_w(t) - N_b(t)\right), \tag{5.3}$$

fluctuates according to

$$\rho(t+1) = \rho(t) + 2\frac{1}{n}\left(N_b(A,t) - N_w(A,t)\right). \tag{5.4}$$

[11] Boltzmann called this hypothesis the 'Stosszahlansatz' – the assumption of 'molecular chaos'.

The reader is encouraged to play around with this simple system by hand or on a computer. The randomness in this problem is an example of 'frozen disorder' – that is, the set A is chosen initially at random and the dynamics of the system is deterministic once A has been chosen. Nevertheless, one sees that for a typical choice of A, the configuration of white and black balls soon gets rather mixed up. The analog of Boltzmann's molecular chaos assumption in this problem is the following simple 'closure' assumption:

$$N_b(A,t) \stackrel{?}{=} \mu N_b(t), \quad N_w(A,t) \stackrel{?}{=} \mu N_w(t). \tag{5.5}$$

We call this a closure assumption because we it allows us to obtain a closed kinetic equation for $\rho(t)$ from the exact n-particle description (5.4). As in all of kinetic theory, we have collapsed a detailed description of the state of the system (here the entire configuration) to the description of a population (here the excess mass).

With assumption (5.5) we find that

$$\rho(t+1) = (1-2\mu)\rho(t), \rho(t) = (1-2\mu)^t, \quad t \in \mathbb{N}, \tag{5.6}$$

which is easily solved along with the initial condition $\rho(0) = 1$ to yield

$$\rho(t+1) = (1-2\mu)^t, \quad t \in \mathbb{N}. \tag{5.7}$$

Since we have assumed that $0 < \mu < 1/2$, we see that the excess mass decays exponentially fast. But as we explain below, the dynamics of the system is periodic with periodic $2n$, so such irreversibility is impossible! This is the analog of Zermelo's paradox in this model.

5.2. **Reversibility and irreversibility.** Here is a more precise description of the configurations and evolution. Let us index the sites by $p \in \{1, \dots, n\}$. Let $\eta \in \{-1,1\}^n$ denote each configuration, with $\eta_p = 1$ if there is a white ball at site p and $\eta_p = -1$ if the ball at site p is black. We describe the frozen disorder by the fixed vector $a \in \{-1,1\}^n$ with

$$a_p = -1, \quad p \in A, \quad a_p = 1, \quad p \in A^c. \tag{5.8}$$

Both a and η are cyclic vectors: that is $a_k := a_p$ when $k \equiv p(\mod n)$ and $1 \le p \le n$. The evolution of the system is given by

$$\eta_{p+1}(t+1) = a_p \eta_p(t), \quad 1 \le p \le n. \tag{5.9}$$

Equation (5.9) may be solved exactly to yield

$$\eta_p(t) = a_{p-1} a_{p-2} \dots a_{p-t} \eta_{p-t}(0) \tag{5.10}$$

This system is clearly periodic: since $\prod_{j=1}^n a_{p-j} = (-1)^m$ for every p, when $t = 2n$

$$\eta_p(t) = \left(\prod_{j=1}^{2n} a_{p-j} \right) \eta_p(0) = (-1)^2 \eta_p(0) = \eta_p(0). \tag{5.11}$$

When the initial condition $\eta_p(0) = 1$, $1 \le p \le n$, the state at time t is

$$\eta_p(t) = a_{p-1} a_{p-2} \dots a_{p-t}, \tag{5.12}$$

and the excess mass is given by

$$\rho_n(t) = \frac{1}{n} \sum_{p=1}^n \eta_p(t) = \frac{1}{n} \sum_{p=1}^n \prod_{j=1}^t a_{p-j}. \tag{5.13}$$

We thus see that the state of the system is a function of the disorder alone. The kinetic description and the closure approximation apply in the limit when $n \to \infty$. In this limit, we expect $\rho_n(t)$ to be close to its average,

$$\mathbb{E}\left(\rho_n(t)\right) = \frac{1}{n}\mathbb{E}\left(\sum_{p=1}^{n}\prod_{j=1}^{t} a_{p-j}\right) = \mathbb{E}\left(\prod_{j=1}^{t} a_j\right). \tag{5.14}$$

Here the expectation is over the initial disorder, that is, the choice of a subset of size m from a set of n sites. The symmetry of this law allows us to obtain the second equality above.

The closure assumption (5.5) is motivated by the following naive calculation: if the a_i had been iid random variables with expected value $\mu(-1)+(1-\mu)(1) = 1-2\mu$, then by independence

$$\mathbb{E}\left(\prod_{j=1}^{t} a_j\right) = (1-2\mu)^t,$$

establishing (5.6). This calculation is suggestive, but not quite right. The expectation actually takes the form

$$\mathbb{E}\left(\prod_{j=1}^{t} a_j\right) = \frac{1}{\binom{n}{m}}\sum_{A}\prod_{j=1}^{t} a_j \tag{5.15}$$

where $\sum_A$ denotes the fact that we sum over all subsets A of size m. In particular, the a_j are related by the constraint

$$\sum_{p=1}^{n} a_p = n - 2m. \tag{5.16}$$

Kac uses the following elegant contour integral representation to deal with this constraint. Let Γ denote the unit circle $\{|z| = 1\} \subset \mathbb{C}$. Since

$$\frac{1}{2\pi i}\oint_\Gamma \frac{1}{z^s}\, dz = \delta_{s,-1}, \quad s \in \mathbb{Z}, \tag{5.17}$$

we may set $s = 2m - n + 1 - \sum_{p=1}^{n} a_p$ to obtain the identity

$$\begin{aligned}\sum_{A}\prod_{j=1}^{t} a_{1-j} &= \sum_{a\in\{-1,1\}^n} \frac{1}{2\pi i}\oint_\Gamma \frac{a_1 a_2 \dots a_m}{z^s}\, dz \qquad (5.18)\\ &= \frac{1}{2\pi i}\oint_\Gamma \frac{dz}{z^{2m-n+1}} \sum_{a\in\{-1,1\}^n} \frac{a_1 a_2 \dots a_t}{z^{a_1+a_2+\dots+a_n}},\\ &= \frac{1}{2\pi i}\oint_\Gamma \frac{dz}{z^{2m-n+1}}\left(z+\frac{1}{z}\right)^{n-t}\left(\frac{1}{z}-z\right)^{t}. \qquad (5.19)\end{aligned}$$

One may now use the method of steepest descent to analyze $\mathbb{E}(\rho_n(t))$ in the limit $n \to \infty$ for fixed t. A similar calculation applies to the variance of $\rho_n(t)$.

A more modern approach to this problem is based on the idea of concentration inequalities [12] . Let S_n denote the symmetric group. The symmetric group is a

[12] I don't expect beginning graduate students to know these inequalities. However, since the idea of concentration of measure and the geometry of Banach spaces was extensively developed in

metric space when it is equipped with the normalized Hamming distance

$$d_H(\pi,\tau) = \frac{1}{n}\sum_{i=1}^{n} \mathbf{1}_{\{\pi_i \neq \tau_i\}}, \quad \pi,\tau \in S_n. \tag{5.20}$$

Finally, S_n carries a natural probability measure: the uniform measure assigns each permutation $\pi \in S_n$ the weight $1/n!$. We say that a function $f : (S_n, d_H) \to \mathbb{R}$ is M-Lipschitz if $|f(\pi) - f(\tau)| \leq M d_H(\pi,\tau)$ for $\pi,\tau \in S_n$. Lipschitz functions on (S_n, d_H) are 'almost constant' in the following sense.

Theorem 5.1. ***Maurey's inequality*** [14, §6.5] *Let f be an M-Lipschitz function on (S_n, d_H), and $\mathbb{Q}_n$ be the uniform measure on S_n. Then for any $\varepsilon \geq 0$*

$$\mathbb{Q}_n(\pi : |f(\pi) - \mathbb{E}_{\mathbb{Q}_n}(f)| > \varepsilon) \leq 2\exp\left(\frac{-n\varepsilon^2}{16M^2}\right). \tag{5.21}$$

Kac's estimates on the mean and variance of $\rho_n(t)$ require some careful asymptotics. In contrast, the following theorem – which is stronger than Kac's – is an almost trivial consequence of Maurey's inequality.

Let $\mathbb{P}$ denote the law of the uniformly chosen subset A of size m.

Theorem 5.2. *Assume $t \in \mathbb{N}$ and fix $\varepsilon > 0$. Then*

$$\mathbb{P}(|\rho_n(t) - \mathbb{E}(\rho_n(t))| > \varepsilon) \leq 2\exp\left(\frac{-n\varepsilon^2}{64t^2}\right). \tag{5.22}$$

In order to establish this theorem, we first observe that the set of possible subsets A of size m may be identified with $S_n/(S_m \times S_{n-m})$. More precisely, we associate to each subset A the equivalence class $[\pi] \in S_n/(S_m \times S_{n-m})$, and the assignment $a([\pi])$ as in (5.8). We lift a into S_n by defining the function $\tilde{a} : S_n \to \{-1,1\}^n$ by setting $\tilde{a}(\tau) = a([\pi])$ for each $\tau \in [\pi]$. Finally, consider the function

$$f(\tau) = \frac{1}{n}\sum_{p=1}^{m}\prod_{j=1}^{t}\tilde{a}_{p-j}(\tau) = \frac{1}{n}\sum_{p=1}^{m}\prod_{j=1}^{t} a_{p-j}([\pi]), \quad \tau \in [\pi]. \tag{5.23}$$

By construction, this function is constant on each equivalence class. It is also a Lipschitz function with Lipschitz constant $2t$. This is easiest to check for two permutations τ and $\tilde{\tau}$ that differ by a swap. In this case, $d_H(\pi,\tau) = 2/n$, and

$$|f(\tau) - f(\tilde{\tau})| \leq \frac{4t}{n},$$

since the products $\prod_{j=1}^{t}\tilde{a}_{p-j}(\tau)$ and $\prod_{j=1}^{t}\tilde{a}_{p-j}(\tilde{\tau})$ differ by 2 in at most two intervals of p each of length t. Iterating this argument, we see that f is a Lipschitz function with Lipschitz constant $2t$. Theorem 5.1 then follows by an application of Maurey's inequality.

In conclusion, the resolution of Zermelo's paradox in this simplified problem is as follows. For each choice of disorder, A, the solution $\eta(t)$ is periodic, however the length of the period is $O(n)$. There are $\binom{n}{m}$ solution curves $\rho_n(t)$ corresponding to the possible choices of disorder A. When t is held fixed, these solution curves concentrate around the deterministic decay $(1-2\mu)^t$ as $n \to \infty$ with high probability.

Israel, I found it attractive to present this application of Maurey's inequality in these lectures. I wish I understood the mysterious section $3\frac{1}{2}$ of Gromov's green book [6] better.

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