

MATHEMATICS OF KINETIC THEORY

Lecture Notes for AMSC 698L, Fall 2012

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Course Plan. We introduce the Boltzmann equation and other kinetic equations. From these we give formal derivations of the compressible Euler and compressible Navier-Stokes systems. These approximations can be justified using Hilbert and Chapman-Enskog expansions. We give moment-based formal derivations of the acoustic system, an incompressible Stokes system, an incompressible Navier-Stokes system, and an incompressible Euler system. We develop theories of global solutions for these systems and show that they govern different fluid dynamical limits for DiPerna-Lions solutions of the Boltzmann equation.

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I. MAXWELL-BOLTZMANN THEORY

Statistical mechanics is the study of how macroscopic phenomena arise from microscopic dynamics. It may be naturally divided into two branches — one dealing with equilibrium systems, and the other with non-equilibrium systems. Properties of systems in equilibrium are defined by averaging over suitable ensembles (micro-canonical, canonical, or grand canonical). This paradigm provides both a qualitative and quantitative understanding of such systems. For example, it illuminates the basic structure of the classical theory of thermodynamics and yields useful expressions for equations of state of real materials. On the other hand, non-equilibrium phenomena are not understood as well. A notable exception is offered by the kinetic theory of rarefied gases, the foundation of which was laid by Maxwell [8, 9] and Boltzmann [2] in the nineteenth century. In fact, their theory spurred the subsequent development of equilibrium statistical mechanics.

At the time, most scientists viewed gases as continua. In founding modern kinetic theory, Maxwell ([8] in 1860 and [9] in 1866) and Boltzmann ([2] in 1872) were testing a molecular theory of gases. They developed a recipe to construct a kinetic equation, now called the Boltzmann equation, from the Newtonian equations that govern binary collisions of molecules; they then derived the Navier-Stokes system from the kinetic equation in regimes where collisional effects are dominant. The resulting formulas for viscosity and thermal conductivity were found to be independent of density. This result surprised many at first, but it proved to be consistent with experiments carried out first by Maxwell and subsequently by others.

While this early success encouraged its proponents, kinetic theory was very controversial at the time for two main reasons. First, the notion of molecule was not generally accepted at the time. Second, neither the Navier-Stokes system nor the Boltzmann equation is reversible, while Newtonian mechanics is. It was therefore unclear how such theories of gases could arise from any microscopic dynamics governed by Newtonian mechanics. Indeed, because continua were not viewed as arising from an underlying microscopic molecular picture, the fact the Navier-Stokes system is not reversible did not pose a problem for scientists. Rather, it seemed to provide evidence against the existence of an underlying microscopic molecular picture.

Of course, the existence of atoms and molecules became generally accepted around 1906. Newtonian mechanics was superseded by quantum mechanics two decades later. However, because quantum mechanics is also reversible, kinetic theory still had to face the question of how an irreversible macroscopic dynamics can arise from a reversible microscopic dynamics. Roughly speaking, the answer has two parts. First, the underlying microscopic dynamics is chaotic (i.e. it has sensitive dependence on data). Second, the macroscopic equations are derived in limits where the number of molecules becomes infinite. Maxwell first suggested that chaos played a role in the answer while Kelvin first suggested that limits played a role. These early key insights did not make the problem much easier. A hundred years passed before Landford [6] first rigorously established the validity of the Boltzmann equation for classical hard spheres. The problem remains open in general.

While this theoretical gap remains, overwhelming experimental and computational evidence has led to a general acceptance of the validity of the Boltzmann equation, and of kinetic theory in general. During the 1900's kinetic theory was applied to many problems. These include modeling photon transport in planetary and stellar atmospheres [5, 10, 11], neutron transport in nuclear reactors and stars [3], air flow in hypersonic flight [1], carrier transport in semiconductor devices [7], and charged particle transport in plasmas.

1. RAREFIED GASES AND THE BOLTZMANN EQUATION

Roughly speaking, rarefied gases are ones for which fluid descriptions break down. However, the theory of rarefied gases did not grow out of an attempt to explain observations of these regimes. Rather, it grew out of efforts to test the theory that heat is atomic motion.

In the mid 1800's most scientists did not believe in atoms. Solids, liquids, and gases were viewed as continua rather than as being made up of atoms. Heat was viewed as another continuum called *caloric* that was attracted to matter but repelled from itself. Indeed, Fourier viewed his heat equation as describing the motion of caloric through matter. By the 1840's came the realization that heat is a form of energy, and the articulation of energy conservation laws that included heat — what subsequently became called the first law of thermodynamics. By the 1850's came several formulations of what subsequently became called the second law of thermodynamics, yet the entropy had not yet been identified as playing a central role. Atoms were almost nowhere to be seen.

Of course, there were atomic theories of heat before the 1850's. In 1738 Daniel Bernoulli used a simple one-speed atomic model to derive Boyle's law — namely, that pressure is proportional to density when the temperature is held fixed. Moreover, he showed that the constant of proportionality was proportional to the square of the speed, which he identified with temperature. This work was largely ignored. John Herrepath in 1821 and John James Waterston in 1846 advanced similar theories. Their work could not get published in the leading journals of the day. James Joule read one of Herrepath's articles and in 1848 wrote an article defending it. This influenced August Krönig to put forth a very similar theory in 1856. These later theories did not advance things much further than Bernoulli's largely forgotten early work. While these works did explain the ideal gas law, other theories did so too. They did not make any testable predictions of unknown phenomena. Moreover, the specific heats that they yielded were lower than those observed in gases. In short, there was little reason for the atomic theory of heat to be embraced.

Things began to change in the late 1850's when Rudolf Clausius became a champion of atomic theory. Clausius was a leading theorist of his day. He was inspired to begin publishing his ideas after reading Krönig's work. In 1857 Clausius explained how the rotational and vibrational degrees of freedom in molecules might account for the higher specific heats observed in gases. He was the first to realize the importance of intermolecular collisions, and in 1858 introduced the concept of *mean free path*. This work caught the attention of James Clerk Maxwell in 1859.

Maxwell understood that the mean free path was connected to diffusivity, viscosity, and thermal conductivity — all of which could be measured. In order to make this connection, in 1860 he developed a theory for the distribution of velocities of monatomic gas molecules in local equilibrium [8] — the famous Maxwellian distribution. He used this distribution to develop a theory for diffusivity, viscosity, and thermal conductivity in a gas of hard spheres. He obtained expressions for the viscosity and thermal conductivity coefficients that were independent of the density. This result was counterintuitive because it was known to be false in liquids. However, by 1866 this prediction was shown to be consistent with experiments carried out first by Maxwell and subsequently by others. The atomic view of matter had its first big success.

In 1866 Maxwell published a vast improvement on his 1860 theory [9]. His new theory is based on the first kinetic equation — what subsequently has been called the Maxwell equation of change. We will derive this equation in this chapter. Along the way we will see how Clausius's concept of the mean free path led to it and how it led to the Boltzmann equation.

1.1. Gaseous Regimes. In order to indicate how kinetic equations arise from microscopic Newtonian physics, we will examine the following idealized setting. We consider a gas of N identical molecules of mass m in a D -dimensional macroscopic domain $\Omega \subset \mathbb{R}^D$ of volume V . We will consider any $D \geq 2$. Of course, the two cases we have in mind are $D = 3$ for real gases and $D = 2$ for certain computational models.

We will assume that the molecules interact through a binary intermolecular force determined by a potential that depends only on the intermolecular distance. We will assume that this force becomes infinitely repulsive as two molecules approach each other. We will also assume that this force is characterized by a range of interaction R . Roughly speaking, two molecules will have a “significant” interaction if and only if their centers of mass pass within a distance R of each other. For example, if the molecules are hard spheres of radius R_o then $R = 2R_o$. Because there is some arbitrariness in indentifying what constitutes a “significant” interaction, for the moment we will not give a precise definition of R for a general intermolecular potential.

1.1.1. Ideal Gas Regimes. There are three natural characteristic length scales in this situation.

- First, there is the macroscopic length scale Λ_{MACRO} , which will be defined as $V^{\frac{1}{D}}$. All geometric features of the domain Ω are assumed to be characterized by this length scale.
- Second, there is the typical intermolecular spacing Λ_{MOL} , which will be on the order of $(V/N)^{\frac{1}{D}}$ when the density of molecules is fairly uniform throughout the domain Ω .
- Third, there is the characteristic range of interaction R .

Ideal or *perfect gas* regimes are ones in which these length scales are ordered as

$$(1.1) \quad R \ll \Lambda_{MOL} \ll \Lambda_{MACRO} .$$

In other words, ideal gas regimes are ones in which

$$(1.2) \quad NR^D \ll V, \quad \text{and} \quad 1 \ll N .$$

With each molecule we associate a *sphere of interaction* that has radius R and is centered at its center of mass. Because the volume of each sphere of interaction is $|\mathbb{S}^{D-1}|R^D$, the first condition in (1.2) states that the volume occupied by the union of these N spheres is a small fraction of the entire volume V of Ω .

A molecule is said to be moving *freely* if it lies outside all the spheres of interaction of the other molecules. If we assume that the centers of mass are located randomly in Ω then it is clear that in ideal gas regimes most molecules will not be interacting, but rather will be traveling freely between collisions. The volume $V_{\text{ex}} = |\mathbb{S}^{D-1}|NR^D$ is called the *excluded volume* because it is the volume of the fraction of Ω that is not available for free molecular motion. The ratio V_{ex}/V is called the *excluded volume fraction*.

Two molecules will be interacting directly if their centers of mass lie within each other’s sphere of interaction. If neither of the two molecules is interacting with any other molecule then the interaction is said to be *binary*. If we again assume that the centers of mass are located randomly in Ω then it can be shown that in ideal gas regimes most interactions will be binary. Our analysis will therefore neglect the effects of interactions involving more than two molecules.

We will see that in ideal gas regimes the pressure p and temperatue T of a gass are related by the ideal gas law:

$$pV = k_B NT ,$$

where k_B is the Boltzmann constant. Corrections to this law, such as that given by the Van der Waals equation of state, explicitly involve the notion of excluded volume fraction.

Remark. Ideal gas regimes are common. For example, a monatomic gas at room temperature and atmospheric pressure has about 10^{19} molecules per cubic centimeter, while the range of intermolecular forces is on the order of 10^{-8} centimeters. We then find that

$$\Lambda_{MOL} \approx (1/10^{19})^{\frac{1}{3}} = 10^{-\frac{19}{3}} \text{ centimeters,}$$

while $R = 10^{-8}$ centimeters, whereby $R/\Lambda_{MOL} \approx 10^{-\frac{5}{3}}$ and the excluded volume fraction is about $4 \cdot 10^{-5}$.

1.1.2. *Mean Free Path.* In 1858 Clausius introduced a fourth important length scale that can be derived from N , V and R . The *mean free path* is a length typical of the distance a molecule travels freely between collisions. He obtained a rough estimate of this distance as follows. As a molecule travels a distance λ , its sphere of interaction sweeps out a cylinder of radius R with a hemispherical “caps” on each end. If we assume that $R \ll \lambda$ then we can neglect the contribution of the caps and approximate the volume of the cylinder by $|\mathbb{S}^{D-2}|R^{D-1}\lambda$. The molecule will interact with another molecule if and only if that other molecule enters this cylinder. This event becomes likely when the volume of the cylinder becomes equal to the volume in which one typically expects to find a molecule, which is V/N . In other words, an interaction becomes likely when λ satisfies

$$|\mathbb{S}^{D-2}|R^{D-1}\lambda = \frac{V}{N} = \Lambda_{MOL}^D.$$

We define this value of λ to be the mean free path Λ_{MFP} , which is therefore given by

$$(1.3) \quad \Lambda_{MFP} = \frac{V}{|\mathbb{S}^{D-2}|NR^{D-1}}.$$

With this definition our assumption that $R \ll \Lambda_{MFP}$ in the above argument is equivalent to assuming we are in an ideal gas regime. Indeed, one sees from definition (1.3) that

$$\frac{R}{\Lambda_{MFP}} = \frac{|\mathbb{S}^{D-2}|NR^D}{V} = |\mathbb{S}^{D-2}| \left(\frac{R}{\Lambda_{MOL}} \right)^D.$$

It then immediately follows that

$$\frac{\Lambda_{MOL}}{\Lambda_{MFP}} = \frac{R}{\Lambda_{MFP}} \frac{\Lambda_{MOL}}{R} = |\mathbb{S}^{D-2}| \left(\frac{R}{\Lambda_{MOL}} \right)^{D-1}.$$

Hence, in ideal gas regimes one has the ordering of length scales

$$(1.4) \quad R \ll \Lambda_{MOL} \ll \Lambda_{MFP}$$

Notice that these three length scales become comparable as one leaves the ideal gas regimes. In fact, a more careful analysis would have shown that Λ_{MFP} vanishes as R and Λ_{MOL} become comparable. However, because we are restrict our considerations to ideal gas regimes, the above analysis suffices.

The Knudsen number Kn is defined to be the ratio of the mean free path over the characteristic macroscopic length scale:

$$(1.5) \quad \text{Kn} = \frac{\Lambda_{MFP}}{\Lambda_{MACRO}}.$$

Upon comparing (1.1) with (1.4), we see that the Knudsen number is the key dimensionless parameter for characterizing different regimes of an ideal gas.

Definition 1.1. *An ideal gas is said to be in a fluid regime when $\text{Kn} \ll 1$, and in a kinetic or rarefied regime otherwise. An ideal gas is said to be in a collisionless regime when $\text{Kn} \gg 1$, and in a collisional regime otherwise.*

We therefore have identified three regimes to consider:

$$(1.6) \quad \begin{aligned} \text{Kn} \ll 1 &\quad \implies \quad (\text{collisional}) \text{ fluid regime,} \\ \text{Kn} \sim 1 &\quad \implies \quad \text{collisional kinetic regime,} \\ \text{Kn} \gg 1 &\quad \implies \quad \text{collisionless (kinetic) regime.} \end{aligned}$$

Because all fluid regimes are collisional, and all collisionless regimes are kinetic, the words in parentheses are usually dropped.

Remark. Fluid regimes are common in our every day experience. For the example of air at room temperature and atmospheric pressure one finds that

$$\Lambda_{MFP} \approx V/(NR^{D-1}) \approx 1/(10^{20}10^{-16}) = 10^{-4} \text{ centimeters.}$$

While this is much larger than either Λ_{MOL} ($= 10^{-\frac{20}{3}}$) or R ($= 10^{-8}$), for most situations we encounter, it is far smaller than a macroscopic length scale. However, at altitudes where there are 10^{16} molecules per cubic centimeter one finds that $\Lambda_{MFP} \approx 1$ centimeter, which is certainly macroscopic.

1.2. Ideal Gas Limits. Equations governing ideal gas regimes arise formally in limits where

$$(1.7) \quad \begin{aligned} N &\rightarrow \infty, \\ m &\rightarrow 0, \quad \text{such that } Nm \rightarrow \text{finite}, \\ R &\rightarrow 0, \quad \text{such that } NR^D \rightarrow 0. \end{aligned}$$

You should understand that Ω is being held fixed when taking this limit, whereby V is also fixed. The first constraint above states that the total mass Nm in the system remains finite. The second constraint above states that the excluded volume fraction, $|\mathbb{S}^{D-1}|NR^D/V$, vanishes, which is consistent with the characterization of ideal gas regimes given in (1.1). We will call any limit satisfying (1.7) an *ideal gas limit*.

One obtains the equations that govern fluid, collisional kinetic, and collisionless regimes respectively if in addition to satisfying (1.7) the limit also satisfies

$$(1.8) \quad NR^{D-1} \rightarrow \begin{cases} 0, & \text{for the collisionless regime,} \\ \text{finite,} & \text{for the collisional kinetic regime,} \\ \infty, & \text{for the fluid regime.} \end{cases}$$

This is consistent with the characterization of these regimes given in (1.6). In particular, limits for collisional kinetic regimes are characterized by a Knudsen number $\text{Kn} \in (0, \infty)$ such that

$$\frac{\Lambda_{MFP}}{\Lambda_{MACRO}} = \frac{V^{1-\frac{1}{D}}}{|\mathbb{S}^{D-2}|NR^{D-1}} \rightarrow \text{Kn}.$$

The Knudsen number Kn provides a measure of how close a collisional kinetic regime is to a fluid regime.

1.2.1. *Kinetic Density.* It is reasonable to expect that in such limits the molecules will fill out the continuum Ω . Indeed, with sufficient additional technical assumptions one can prove that the state of the gas is described by a mass density F over the single-molecule phase space $\mathbb{R}^D \times \Omega$. A point (v, x) in $\mathbb{R}^D \times \Omega$ designates a possible velocity v and position x for a single fluid molecule. At any instant of time t , one understands $F(v, x, t) dv dx$ to give the mass of molecules that occupy the infinitesimal volume $dv dx$ about the point (v, x) . More precisely, if A is any measurable subset of $\mathbb{R}^D \times \Omega$ then the definite integral of F over A , denoted

$$\iint_A F(v, x, t) dv dx,$$

gives the mass of fluid molecules with states in A at time t . Similarly, the momentum and kinetic energy of fluid molecules with states in A at time t are respectively given by

$$\iint_A v F(v, x, t) dv dx, \quad \iint_A \frac{1}{2}|v|^2 F(v, x, t) dv dx.$$

Because F is a mass density, it is nonnegative. At this point our discussion is formal, so we will forgo mathematical details like stating explicitly that the function F and set A are measurable with respect to $dv dx$.

One can construct various spatial densities from the phase-space density F . For example, the mass, momentum, and energy densities of the gas over Ω are respectively given by

$$(1.9) \quad \rho = \int_{\mathbb{R}^D} F dv, \quad \rho u = \int_{\mathbb{R}^D} v F dv, \quad \frac{1}{2}\rho|u|^2 + \rho\varepsilon = \int_{\mathbb{R}^D} \frac{1}{2}|v|^2 F dv.$$

Here $\rho(x, t)$ is the mass density, $u(x, t)$ is the bulk velocity, and $\varepsilon(x, t)$ is the specific internal energy. There is no contribution from the intermolecular potential to the energy density because the interaction range R vanishes faster than the intermolecular spacing Λ_{MOL} in an ideal gas limit, whereby fraction of molecules interacting vanishes in the limit.

1.2.2. *Collisionless Limit.* When a gas is so dilute that molecular collisions can be neglected, its dynamics is governed by the collisionless limit. When no forces of any kind act on the molecules, each molecule will move with a constant velocity until it hits the boundary of Ω . Therefore, within the interior of Ω we expect that the kinetic density F will satisfy

$$(1.10) \quad \partial_t F + v \cdot \nabla_x F = 0.$$

When Ω has no boundaries (like, for example, \mathbb{R}^D or \mathbb{T}^D), then the solution of this equation with initial data F^{in} is simply given by $F(v, x, t) = F^{in}(v, x - vt)$.

1.2.3. *Fluid Limit.* In fluid regimes we expect the gas to be described by the fluid variables, $\rho(x, t)$, $u(x, t)$, and $\varepsilon(x, t)$, governed by a gas dynamics system (say Euler or Navier-Stokes) with the pressure given by an ideal gas equation of state.

Maxwell argued [8] that in fluid regimes F would have the form

$$(1.11) \quad F(v, x, t) = \frac{\rho(x, t)}{(2\pi\theta)^{\frac{D}{2}}} \exp\left(-\frac{|v - u(x, t)|^2}{2\theta(x, t)}\right),$$

where $\rho(x, t) \in \mathbb{R}_+$, $u(x, t) \in \mathbb{R}^D$, and $\theta(x, t) \in \mathbb{R}_+$. In words, the velocity distribution at (x, t) is given by an isotropic Gaussian density with weight $\rho(x, t)$, mean $u(x, t)$, and variance $\theta(x, t)$, which is related to the temperature by $\theta = k_B T/m$. The specific energy ε and the pressure p are given by $\varepsilon = \frac{D}{2}\theta$ and $p = \rho\theta$. The last relation is a restatement of the ideal gas law.

Maxwell's argument that $F(v, x, t)$ is given by (1.7) was based only on notions of symmetry and randomness. It goes as follows. Fix (x, t) . Suppose we are in the Galilean frame in which $u(x, t) = 0$. In this frame the action of the (many) collisions will make the distribution isotropic. The density F must therefore have the form $F(v) = \Phi(|v|^2)$ for some function Φ . He then argues that the distributions of the velocity in orthogonal directions should be independent. This means that if $v = (v_1, v_2, \dots, v_D)$ then F must have the form $F(v) = \Psi(v_1^2)\Psi(v_2^2)\dots\Psi(v_D^2)$ for some function Ψ . If we combine these assertions, we see that the functions Φ and Ψ must satisfy the functional relation

$$\Phi(|v|^2) = \Psi(v_1^2) \Psi(v_2^2) \dots \Psi(v_D^2).$$

If one assumes that Φ and Ψ are smooth, it is easy to argue that they must be exponentials. The form (1.11) then follows from the normalization (1.9).

Remark. This argument did not convince everyone. Indeed, it did not even convince Maxwell because he published an alternative argument six years later [9]. However, he was ready to test the conclusions drawn from it against laboratory experiments.

1.2.4. *Boltzmann-Grad Limit.* The limit leading to collisional kinetic regimes in (1.8) was dubbed the Boltzmann-Grad limit by Lanford, who established it for hard spheres in 1974 [6]. More specifically, he showed that in this limit the kinetic density $F(v, x, t)$ is governed by the Boltzmann equation, which has the form

$$(1.12) \quad \partial_t F + v \cdot \nabla_x F = \frac{1}{\text{Kn}} \mathcal{B}(F, F), \quad F(v, x, 0) = F^{in}(v, x),$$

where \mathcal{B} is the so-called Boltzmann collision operator, which we give below. When Ω has boundaries, boundary conditions must be specified. While the subject of boundary conditions is critical to most applications of kinetic theory, they will be ignored here so that we can get directly to other critical topics.

Remark. Additional, more technical, requirements on the limit are needed to ensure, for example, that the total energy in the system remains finite. These will not be presented here, but can be found in [4]. We remark however that in order for NR^{D-1} to remain finite while both $N \rightarrow \infty$ and $R \rightarrow 0$, one must require that $D \geq 2$. We henceforth restrict ourselves to that case.

The collision operator \mathcal{B} in (1.12) models the rate of change of F due to the binary collisions of molecules. It has features that are not common in either the physical or mathematical literature, and so requires some explanation. We will present it formally first, postponing the explanations and interpretations until later.

The collision operator \mathcal{B} in (1.12) acts only on the v dependence of F . This means collisions are local and instantaneous, which reflects the fact that the range of interaction R vanishes in the Boltzmann-Grad limit (1.8). It formally acts on any ‘‘sufficiently nice’’ function f of v according to the formula

$$(1.13) \quad \mathcal{B}(f, f)(v) = \iint (f(v'_*)f(v') - f(v_*)f(v)) b(\omega, v_* - v) d\omega dv_*.$$

It is quadratic in F , which reflects the fact that it models only binary collisions. The contributions from collisions that are other than binary vanish in the Boltzmann-Grad limit, and so are neglected. The collision kernel $b(\omega, v_* - v)$ is an almost everywhere positive, locally integrable

function. Its precise form depends on details of the microscopic physics in a way that will be described in more detail below. The variable ω lies on the unit sphere

$$\mathbb{S}^{D-1} = \{\omega \in \mathbb{R}^D : |\omega| = 1\},$$

which is endowed with its rotationally invariant measure $d\omega$. The domain of integration in (1.13) is understood to be $\mathbb{S}^{D-1} \times \mathbb{R}^D$. This is a particular instance of the convention that every definite integral with an unspecified domain of integration is understood to be evaluated over the whole domain associated with its measure. Finally, the velocities v'_* and v' are defined for every $(\omega, v_*, v) \in \mathbb{S}^{D-1} \times \mathbb{R}^D \times \mathbb{R}^D$ by

$$(1.14) \quad v'_* = v_* - \omega \omega \cdot (v_* - v), \quad v' = v + \omega \omega \cdot (v_* - v).$$

Notice that when $D = 1$ these reduce to $v'_* = v$ and $v' = v_*$, whereby $\mathcal{B}(f, f)$ would vanish identically. This degeneration reflects the need for the restriction to $D \geq 2$.

The unprimed and primed velocities need a bit more explanation. They denote possible velocities for a pair of molecules either before and after, or after and before the molecules interact through an elastic binary collision. Elastic collisions are ones that conserve both momentum and energy. The conservation of momentum and energy for molecule pairs during such collisions is expressed as

$$(1.15) \quad \begin{aligned} v + v_* &= v' + v'_*, \\ |v|^2 + |v_*|^2 &= |v'|^2 + |v'_*|^2. \end{aligned}$$

It is clear that these equations have the trivial solution $v'_* = v_*$ and $v' = v$, which corresponds to there being no collision. Equation (1.14) represents the general nontrivial solution of the $D + 1$ equations (1.15).

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