Summer Course at PKU (July 2020)
Introduction to Kinetic Theory – Lecture Notes

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Contents

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1 Introduction

These lecture notes are a collection of materials related to various aspects of modern kinetic theory, including physical derivation, mathematical theory, and numerical methods. The main focus is on the Boltzmann-like collisional kinetic equations and their numerical approximations. To begin with, let us take a look at Figure 1 to understand the role of kinetic theory in multiscale modeling hierarchy.

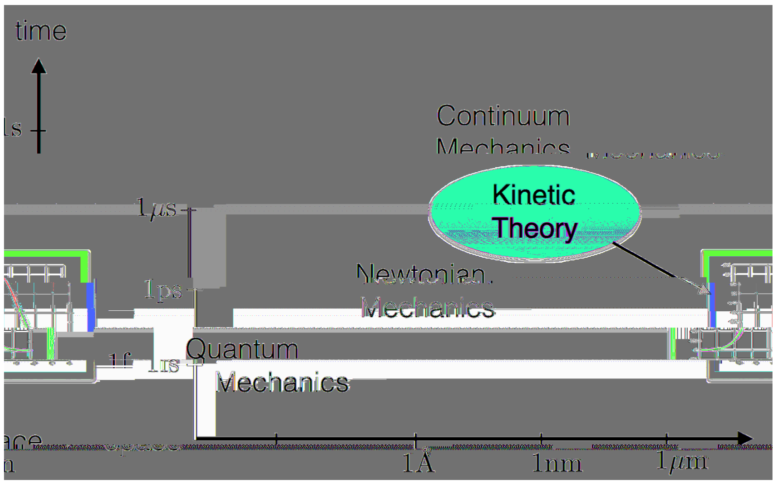

Figure 1: Role of kinetic theory in multiscale modeling hierarchy.

2 The Boltzmann equation for hard spheres

Proposed by Ludwig Boltzmann in 1872, the Boltzmann equation is one of the fundamental equations in kinetic theory. It describes the non-equilibrium dynamics of a gas or system comprised of a large number of particles. In this very first part of the course, we derive the Boltzmann equation for hard sphere molecules. For better understanding, we start with a heuristic derivation and then discuss a more formal derivation from the Liouville equation.

2.1 Heuristic derivation

This part of the presentation mainly follows [2, Chapter 1.2].

Let us start with the function $P^{(1)}(t, x_1, v_1)$, which is the one-particle *probability density function* (PDF). $P^{(1)}\, dx_1\, dv_1$ gives the probability of finding one fixed particle (say, the one labeled by 1) in an infinitesimal volume $dx_1\, dv_1$ centered at the point (x_1, v_1) of the phase space, where $x_1 \in \mathbb{R}^3$ is the position and $v_1 \in \mathbb{R}^3$ is the particle velocity.

When two particles (say, particles 1 and 2) collide, momentum and energy must be conserved (mass is always conserved). Let v_1, v_2 be the velocities before a collision and (v_1', v_2') the velocities after a collision. From

$$v_1 + v_2 = v_1' + v_2', \quad |v_1|^2 + |v_2|^2 = |v_1'|^2 + |v_2'|^2, \tag{2.1}$$

one can derive that

$$v_1' = v_1 - [(v_1 - v_2) \cdot \omega]\omega, \quad v_2' = v_2 + [(v_1 - v_2) \cdot \omega]\omega, \tag{2.2}$$

where ω is the impact direction (the unit vector connecting the centers of particles 1 and 2). Note from (2.2) that

$$v_2' - v_1' = (v_2 - v_1) - 2[(v_2 - v_1) \cdot \omega]\omega, \tag{2.3}$$

i.e., the relative velocity undergoes a specular reflection at the impact (see Figure 2).

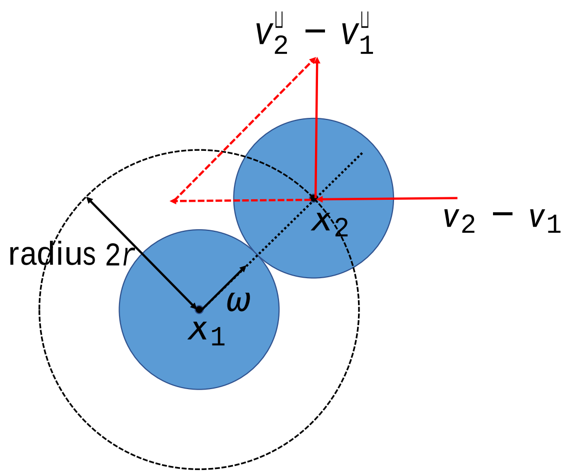

Figure 2: Illustration of particle collisions.

In the absence of collisions and external forces, $P^{(1)}$ would remain unchanged along the trajectory of particle 1. That is, $P^{(1)}$ satisfies

$$\frac{\partial P^{(1)}}{\partial t} + v_1 \cdot \nabla_{x_1} P^{(1)} = 0. \tag{2.4}$$

Now with collisions, one would expect

$$\frac{\partial P^{(1)}}{\partial t} + v_1 \cdot \nabla_{x_1} P^{(1)} = G - L, \tag{2.5}$$

where $L\, dx_1\, dv_1\, dt$ gives the probability of finding particles with position between x_1 and $x_1 + dx_1$ and velocity between v_1 and $v_1 + dv_1$ that disappear from these ranges of values because of a collision in the time interval between t and $t + \mathrm{d}t$ (L is often called the *loss* term of the collision operator), and $G\,\mathrm{d}x_1\,\mathrm{d}v_1\,\mathrm{d}t$ gives the analogous probability of finding particles entering the same range in the same time interval (G is often called the *gain* term of the collision operator). To count these probabilities, imaging particle 1 as a sphere at rest and endowed with twice the actual radius r and the other particles being the point masses with velocity $v_2 - v_1$ (see Figure 2). Fixing particle 1, there are $N - 1$ particles (assume there are a total of N particles) that will collide with it, and they are to be found in the cylinder of height $|(v_2 - v_1)\cdot\omega|\,\mathrm{d}t$ and base area $(2r)^2\,\mathrm{d}\omega$. Then

$$L\,\mathrm{d}x_1\,\mathrm{d}v_1\,\mathrm{d}t = (N-1)\int_{\mathbb{R}^3}\int_{S^2_-} P^{(2)}(t; x_1; v_1; x_1 + 2r\omega; v_2)|(v_2 - v_1)\cdot\omega|\,\mathrm{d}t \\ (2r)^2\,\mathrm{d}\omega\,\mathrm{d}v_2\,\mathrm{d}x_1\,\mathrm{d}v_1; \tag{2.6}$$

where $P^{(2)}$ is the two-particle PDF, and S^2_- is the hemisphere corresponding to $(v_2 - v_1)\cdot\omega < 0$. Therefore,

$$L = (N-1)(2r)^2\int_{\mathbb{R}^3}\int_{S^2_-} P^{(2)}(t; x_1; v_1; x_1 + 2r\omega; v_2)|(v_2 - v_1)\cdot\omega|\,\mathrm{d}\omega\,\mathrm{d}v_2. \tag{2.7}$$

Similarly,

$$G = (N-1)(2r)^2\int_{\mathbb{R}^3}\int_{S^2_+} P^{(2)}(t; x_1; v_1; x_1 + 2r\omega; v_2)|(v_2 - v_1)\cdot\omega|\,\mathrm{d}\omega\,\mathrm{d}v_2; \tag{2.8}$$

where S^2_+ is the hemisphere corresponding to $(v_2 - v_1)\cdot\omega > 0$.

Now we make two crucial assumptions:

> Assume $N \to \infty$, $r \to 0$, but Nr^2 is finite. This is the so-called *Boltzmann-Grad limit*.
>
> Assume $P^{(2)}(t; x_1; v_1; x_2; v_2) = P^{(1)}(t; x_1; v_1)P^{(1)}(t; x_2; v_2)$ for two particles that are about to collide. This is the *molecular chaos assumption*.

Then L becomes

$$\begin{aligned} L &= N(2r)^2\int_{\mathbb{R}^3}\int_{S^2_-} P^{(2)}(t; x_1; v_1; x_1; v_2)|(v_2 - v_1)\cdot\omega|\,\mathrm{d}\omega\,\mathrm{d}v_2 \\ &= N(2r)^2\int_{\mathbb{R}^3}\int_{S^2_-} P^{(1)}(t; x_1; v_1)P^{(1)}(t; x_1; v_2)|(v_2 - v_1)\cdot\omega|\,\mathrm{d}\omega\,\mathrm{d}v_2; \end{aligned} \tag{2.9}$$

where we used the assumption 1 in the first equality and assumption 2 in the second equality. For G, we have

$$
\begin{aligned}
G &= (N-1)(2r)^2 \int_{\mathbb{R}^3}\int_{S^2_+} P^{(2)}(t,x_1,v_1',x_1+2r\omega,v_2')|(v_2-v_1)\cdot\omega|\,\mathrm{d}\omega\,\mathrm{d}v_2 \\
&= N(2r)^2 \int_{\mathbb{R}^3}\int_{S^2_+} P^{(1)}(t,x_1,v_1')P^{(1)}(t,x_1,v_2')|(v_2-v_1)\cdot\omega|\,\mathrm{d}\omega\,\mathrm{d}v_2 \\
&= N(2r)^2 \int_{\mathbb{R}^3}\int_{S^2_-} P^{(1)}(t,x_1,v_1')P^{(1)}(t,x_1,v_2')|(v_2-v_1)\cdot\omega|\,\mathrm{d}\omega\,\mathrm{d}v_2,
\end{aligned}
\tag{2.10}
$$

where the first equality is because $P^{(2)}$ is continuous at a collision, the second equality is obtained for the same reason as above for L (since $(v_2-v_1)\cdot\omega > 0$ implies $(v_2'-v_1')\cdot\omega < 0$), and the third one is a simple change of variable $\omega \to -\omega$.

Putting together G and L, we have

$$
\begin{aligned}
\frac{\partial P^{(1)}}{\partial t}+v_1\cdot\nabla_{x_1}P^{(1)} = N(2r)^2\int_{\mathbb{R}^3}\int_{S^2_-}&|(v_2-v_1)\cdot\omega| \\
&[P^{(1)}(t,x_1,v_1')P^{(1)}(t,x_1,v_2') - P^{(1)}(t,x_1,v_1)P^{(1)}(t,x_1,v_2)]\,\mathrm{d}\omega\,\mathrm{d}v_2.
\end{aligned}
\tag{2.11}
$$

In this course we will often consider the one-particle *number distribution function* f (i.e., $f = NP^{(1)}$), then f satisfies (changing $x_1 \to x$, $v_1 \to v$, $v_2 \to v_*$, $\omega \to -\omega$)

$$
\frac{\partial f}{\partial t} + v\cdot\nabla_x f = (2r)^2\int_{\mathbb{R}^3}\int_{(v-v_*)\cdot\omega<0}|(v-v_*)\cdot\omega|[f'f_*' - ff_*]\,\mathrm{d}\omega\,\mathrm{d}v_*, \tag{2.12}
$$

where f, f_*, f', f_*' are short hand notations for $f(t,x,v)$, $f(t,x,v_*)$, $f(t,x,v')$, $f(t,x,v_*')$, and

$$
v' = v - [(v-v_*)\cdot\omega]\omega, \quad v_*' = v_* + [(v-v_*)\cdot\omega]\omega. \tag{2.13}
$$

Equation (2.12) is the Boltzmann equation for hard spheres.

It is often convenient to integrate ω over the whole sphere S^2 rather than hemisphere, which yields

$$
\frac{\partial f}{\partial t} + v\cdot\nabla_x f = 2r^2\int_{\mathbb{R}^3}\int_{S^2}|(v-v_*)\cdot\omega|[f'f_*' - ff_*]\,\mathrm{d}\omega\,\mathrm{d}v_*. \tag{2.14}
$$

2.2 Formal derivation from the Liouville equation (BBGKY hierarchy)

In this section, we give a formal derivation of the Boltzmann equation starting from the Liouville equation. The rigorous derivation was an open and challenging problem for a long time. In 1973, Lanford showed that, although for a very short time, the Boltzmann equation can be derived from the mechanical systems.

This part of the presentation mainly follows [1, Chapter 3.2], where one can also find the rigorous treatise.

Consider N hard spheres of radius r. Let x_i, v_i denote the position and velocity of particle i, then the state of the system is given by

$$(x_1, v_1, \ldots, x_N, v_N) \in \Omega^N \times \mathbb{R}^{3N} = \Omega;$$

where

$$\Omega^N = \{(x_1, \ldots, x_N) \mid |x_i - x_j| > 2r, i \neq j\},$$

$$\partial\Omega = \{(x_1, v_1, \ldots, x_N, v_N) \mid |x_i - x_j| = 2r, i \neq j\},$$

since the particles cannot overlap.

Let $P^{(N)}(t, x_1, v_1, \ldots, x_N, v_N)$ be the N-particle PDF, then $P^{(N)}$ satisfies the Liouville equation

$$\frac{\partial P^{(N)}}{\partial t} + \sum_{i=1}^{N} v_i \cdot \nabla_{x_i} P^{(N)} = 0. \tag{2.15}$$

Define the s-particle PDF as

$$P^{(s)}(t, x_1, v_1, \ldots, x_s, v_s) = \int P^{(N)} \, \mathrm{d}x_{s+1} \, \mathrm{d}v_{s+1} \ldots \mathrm{d}x_N \, \mathrm{d}v_N, \tag{2.16}$$

then integrating (2.15) one obtains

$$\frac{\partial P^{(s)}}{\partial t} + I_1 + I_2 = 0, \tag{2.17}$$

with

$$\begin{aligned} I_1 &= \sum_{i=1}^{s} \int v_i \cdot \nabla_{x_i} P^{(N)} \, \mathrm{d}x_{s+1} \, \mathrm{d}v_{s+1} \ldots \mathrm{d}x_N \, \mathrm{d}v_N, \\ I_2 &= \sum_{i=s+1}^{N} \int v_i \cdot \nabla_{x_i} P^{(N)} \, \mathrm{d}x_{s+1} \, \mathrm{d}v_{s+1} \ldots \mathrm{d}x_N \, \mathrm{d}v_N. \end{aligned} \tag{2.18}$$

For I_2, applying the divergence theorem (one can refer to Figure 2 again but with (x_1, v_1) replaced by (x_i, v_i), (x_2, v_2) by (x_j, v_j), and ω by ω_{ij}), one has

$$\begin{aligned} I_2 = &\sum_{j=1}^{s} \sum_{i=s+1}^{N} (2r)^2 \int v_i \cdot \omega_{ij} P^{(N)}(t, x_1, v_1, \ldots, x_{i-1}, v_{i-1}, x_j - 2r\omega_{ij}, v_i, \ldots, x_N, v_N) \\ &\qquad \mathrm{d}\omega_{ij} \, \mathrm{d}x_{s+1} \ldots \mathrm{d}x_{i-1} \, \mathrm{d}x_{i+1} \ldots \mathrm{d}x_N \, \mathrm{d}v_{s+1} \ldots \mathrm{d}v_N \\ &+ \sum_{\substack{j=s+1, \\ j \neq i}}^{N} \sum_{i=s+1}^{N} (2r)^2 \int v_i \cdot \omega_{ij} P^{(N)}(t, x_1, v_1, \ldots, x_{i-1}, v_{i-1}, x_j - 2r\omega_{ij}, v_i, \ldots, x_N, v_N) \\ &\qquad \mathrm{d}\omega_{ij} \, \mathrm{d}x_{s+1} \ldots \mathrm{d}x_{i-1} \, \mathrm{d}x_{i+1} \ldots \mathrm{d}x_N \, \mathrm{d}v_{s+1} \ldots \mathrm{d}v_N. \end{aligned} \tag{2.19}$$

The second sum in the above equation is completely zero by the Liouville theorem (it is the integral of $\sum_{i=s+1}^{N} v_i \cdot \nabla_{x_i} P^{(N)}$ relative to the dynamics of the last $N-s$ particles). Using the symmetry of $P^{(N)}$, the first term can be further reduced to

$$
\begin{aligned}
I_2 &= (N-s)(2r)^2 \sum_{j=1}^{s} \int v_{s+1} \cdot \omega_{s+1,j} P^{(N)}(t, x_1, v_1, \dots, x_s, v_s, x_j - 2r\omega_{s+1,j}, v_{s+1}, \dots, x_N, v_N) \\
&\qquad\qquad \mathrm{d}\omega_{s+1,j}\, \mathrm{d}x_{s+2} \dots \mathrm{d}x_N\, \mathrm{d}v_{s+1} \dots \mathrm{d}v_N \\
&= (N-s)(2r)^2 \sum_{j=1}^{s} \int v_{s+1} \cdot \omega_{s+1,j} P^{(s+1)}(t, x_1, v_1, \dots, x_s, v_s, x_j - 2r\omega_{s+1,j}, v_{s+1})\, \mathrm{d}\omega_{s+1,j}\, \mathrm{d}v_{s+1}.
\end{aligned}
\tag{2.20}
$$

For I_1, it can be shown that (see below)

$$
\begin{aligned}
I_1 = \sum_{i=1}^{s} v_i \cdot \nabla_{x_i} P^{(s)} - (N-s)(2r)^2 \sum_{j=1}^{s} \int v_j \cdot \omega_{s+1,j} \\
P^{(s+1)}(t, x_1, v_1, \dots, x_s, v_s, x_j - 2r\omega_{s+1,j}, v_{s+1})\, \mathrm{d}\omega_{s+1,j}\, \mathrm{d}v_{s+1},
\end{aligned}
\tag{2.21}
$$

where the second term is due to the integration domain depends on x_i.

Putting together I_1 and I_2, (2.17) becomes

$$
\begin{aligned}
\frac{\partial P^{(s)}}{\partial t} + \sum_{i=1}^{s} v_i \cdot \nabla_{x_i} P^{(s)} = (N-s)(2r)^2 \sum_{j=1}^{s} \int (v_j - v_{s+1}) \cdot \omega_{s+1,j} \\
P^{(s+1)}(t, x_1, v_1, \dots, x_s, v_s, x_j - 2r\omega_{s+1,j}, v_{s+1})\, \mathrm{d}\omega_{s+1,j}\, \mathrm{d}v_{s+1}.
\end{aligned}
\tag{2.22}
$$

This is the so-called *BBGKY hierarchy for hard spheres* (the equation of P^s depends on P^{s+1}), named after Bogoliubov, Born, Green, Kirkwood, and Yvon. In particular, taking $s = 1$ in (2.22) gives

$$
\begin{aligned}
&\frac{\partial P^{(1)}}{\partial t} + v_1 \cdot \nabla_{x_1} P^{(1)} = (N-1)(2r)^2 \int (v_1 - v_2) \cdot \omega_{21} P^{(2)}(t, x_1, v_1, x_1 - 2r\omega_{21}, v_2)\, \mathrm{d}\omega_{21}\, \mathrm{d}v_2 \\
&= (N-1)(2r)^2 \int (v_2 - v_1) \cdot \omega_{12} P^{(2)}(t, x_1, v_1, x_1 + 2r\omega_{12}, v_2)\, \mathrm{d}\omega_{12}\, \mathrm{d}v_2 \\
&= (N-1)(2r)^2 \int_{(v_2-v_1)\cdot\omega_{12}>0} |(v_2 - v_1) \cdot \omega_{12}| P^{(2)}(t, x_1, v_1, x_1 + 2r\omega_{12}, v_2)\, \mathrm{d}\omega_{12}\, \mathrm{d}v_2 \\
&\qquad - (N-1)(2r)^2 \int_{(v_2-v_1)\cdot\omega_{12}<0} |(v_2 - v_1) \cdot \omega_{12}| P^{(2)}(t, x_1, v_1, x_1 + 2r\omega_{12}, v_2)\, \mathrm{d}\omega_{12}\, \mathrm{d}v_2.
\end{aligned}
\tag{2.23}
$$

This is the same as equation (2.5) with (2.8) and (2.7) derived in the previous section. The rest of the derivation is the same. That is, the first BBGKY hierarchy yields the Boltzmann equation.

It remains to prove (2.21). Note that in the two-particle case,

$$\begin{aligned}
&v_1\cdot\nabla_{x_1}\int_{|x_1-x_2|>2r} P^{(2)}(t,x_1,v_1,x_2,v_2)\,\mathrm{d}x_2\,\mathrm{d}v_2\\
&=\lim_{t\to 0}\frac{1}{t}\left[\int_{|x_1+tv_1-x_2|>2r} P^{(2)}(t,x_1+tv_1,v_1,x_2,v_2)\,\mathrm{d}x_2\,\mathrm{d}v_2-\int_{|x_1-x_2|>2r} P^{(2)}(t,x_1,v_1,x_2,v_2)\,\mathrm{d}x_2\,\mathrm{d}v_2\right]\\
&=\lim_{t\to 0}\frac{1}{t}\left[\int_{|x_1-x_2|>2r} P^{(2)}(t,x_1+tv_1,v_1,x_2+tv_1,v_2)\,\mathrm{d}x_2\,\mathrm{d}v_2-\int_{|x_1-x_2|>2r} P^{(2)}(t,x_1,v_1,x_2,v_2)\,\mathrm{d}x_2\,\mathrm{d}v_2\right]\\
&=\lim_{t\to 0}\frac{1}{t}\left[\int_{|x_1-x_2|>2r} P^{(2)}(t,x_1+tv_1,v_1,x_2+tv_1,v_2)\,\mathrm{d}x_2\,\mathrm{d}v_2-\int_{|x_1-x_2|>2r} P^{(2)}(t,x_1+tv_1,v_1,x_2,v_2)\,\mathrm{d}x_2\,\mathrm{d}v_2\right]\\
&\quad+\frac{1}{t}\left[\int_{|x_1-x_2|>2r} P^{(2)}(t,x_1+tv_1,v_1,x_2,v_2)\,\mathrm{d}x_2\,\mathrm{d}v_2-\int_{|x_1-x_2|>2r} P^{(2)}(t,x_1,v_1,x_2,v_2)\,\mathrm{d}x_2\,\mathrm{d}v_2\right]\\
&=\int_{|x_1-x_2|>2r}(v_1\cdot\nabla_{x_2}+v_1\cdot\nabla_{x_1})P^{(2)}(t,x_1,v_1,x_2,v_2)\,\mathrm{d}x_2\,\mathrm{d}v_2\\
&=(2r)^2\int v_1\cdot\omega_{21}P^{(2)}(t,x_1,v_1,x_1-2r\omega_{21},v_2)\,\mathrm{d}\omega_{21}\,\mathrm{d}v_2+\int v_1\cdot\nabla_{x_1}P^{(2)}(t,x_1,v_1,x_2,v_2)\,\mathrm{d}x_2\,\mathrm{d}v_2.
\end{aligned}\tag{2.24}$$

Analogously,

$$\begin{aligned}
&\sum_{i=1}^{s} v_i\cdot\nabla_{x_i}\int P^{(N)}\,\mathrm{d}x_{s+1}\,\mathrm{d}v_{s+1}\dots\mathrm{d}x_N\,\mathrm{d}v_N\\
&=\sum_{i=1}^{s}\int\left(\sum_{k=s+1}^{N} v_i\cdot\nabla_{x_k}+v_i\cdot\nabla_{x_i}\right)P^{(N)}\,\mathrm{d}x_{s+1}\,\mathrm{d}v_{s+1}\dots\mathrm{d}x_N\,\mathrm{d}v_N\\
&=\sum_{i=1}^{s}\Bigg[(N-s)(2r)^2\int v_i\cdot\omega_{s+1,i}P^{(N)}(t,x_1,v_1,\dots,x_s,v_s,x_i-2r\omega_{s+1,i},v_{s+1},\dots,x_N,v_N)\\
&\qquad\mathrm{d}\omega_{s+1,i}\,\mathrm{d}v_{s+1}\,\mathrm{d}x_{s+2}\dots\mathrm{d}x_N\,\mathrm{d}v_N+\int v_i\cdot\nabla_{x_i}P^{(N)}\,\mathrm{d}x_{s+1}\,\mathrm{d}v_{s+1}\dots\mathrm{d}x_N\,\mathrm{d}v_N\Bigg].
\end{aligned}\tag{2.25}$$

This implies

$$\begin{aligned}
&\sum_{i=1}^{s} v_i\cdot\nabla_{x_i}P^{(s)}-\sum_{i=1}^{s}(N-s)(2r)^2\int v_i\cdot\omega_{s+1,i}P^{(s+1)}(t,x_1,v_1,\dots,x_s,v_s,x_i-2r\omega_{s+1,i},v_{s+1})\,\mathrm{d}\omega_{s+1,i}\,\mathrm{d}v_{s+1}\\
&=\sum_{i=1}^{s}\int v_i\cdot\nabla_{x_i}P^{(N)}\,\mathrm{d}x_{s+1}\,\mathrm{d}v_{s+1}\dots\mathrm{d}x_N\,\mathrm{d}v_N,
\end{aligned}\tag{2.26}$$

which is (2.21).

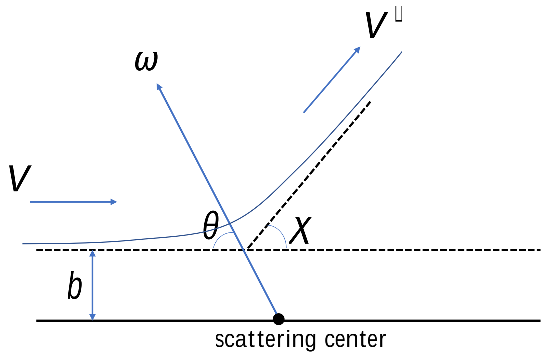

Figure 4: Illustration of particle scattering in a repulsive potential field (notation consistent with Figure 3). b is the impact parameter, χ is the scattering angle, $V = v - v_*$ and $V' = v' - v'_*$.

where

$$B_\omega(|V|, |\cos\theta|) = \frac{1}{2}|V|\frac{b}{\sin\theta}\left|\frac{\mathrm{d}b}{\mathrm{d}\theta}\right|, \tag{3.6}$$

and

$$v' = v - [(v - v_*)\cdot\omega]\omega, \quad v'_* = v_* + [(v - v_*)\cdot\omega]\omega. \tag{3.7}$$

This is what we are going to refer to as the ω-representation.

Another parametrization of the Boltzmann equation that uses the unit vector σ along V' reads

$$\frac{\partial f}{\partial t} + v\cdot\nabla_x f = \int_{\mathbb{R}^3}\int_{S^2} B_\sigma(|V|, \cos\chi)[f'f'_* - ff_*]\,\mathrm{d}\sigma\,\mathrm{d}v_*, \tag{3.8}$$

where

$$B_\sigma(|V|, \cos\chi) = |V|\Sigma(|V|, \chi), \qquad \Sigma(|V|, \chi) = \frac{b}{\sin\chi}\left|\frac{\mathrm{d}b}{\mathrm{d}\chi}\right|, \tag{3.9}$$

$\Sigma(|V|, \cos\chi)$ is the *differential cross section* with $0 < \chi < \pi$, and

$$v' = \frac{v + v_*}{2} + \frac{|v - v_*|}{2}\sigma, \quad v'_* = \frac{v + v_*}{2} - \frac{|v - v_*|}{2}\sigma. \tag{3.10}$$

This is what we are going to refer to as the σ-representation. In particular, the hard sphere collision kernel under this representation reads $B_\sigma(|V|, \cos\chi) = r^2|V|$.

Now for a general (repulsive) intermolecular potential $\phi(r)$ (r is the distance between two particles), b is related to χ implicitly as follows

$$\chi = \pi - 2\int_0^{r_0}\frac{\mathrm{d}r}{\left[1 - r^2 - \frac{4\phi(br^{-1})}{m|V|^2}\right]^{1/2}}, \tag{3.11}$$

where m is the single particle mass, and r_0 is the positive root to the equation

$$1 - r^2 - \frac{4\phi(br^{-1})}{m|V|^2} = 0. \tag{3.12}$$

Let's take a close look of the inverse power law potential

$$(r) = \frac{K}{r^{s-1}}; \quad 2 < s \quad 1; \quad K \text{ is some positive constant}. \tag{3.13}$$

Then (3.11) becomes

$$= \quad 2\int_0^{r_0} \frac{\mathrm{d}r}{\left[1 \quad r^2 \quad \frac{4Kr^{s-1}}{m|V|^2 b^{s-1}}\right]^{1/2}} = \quad 2\int_0^{r_0} \frac{\mathrm{d}r}{\left[1 \quad r^2 \quad \left(\frac{r}{\beta}\right)^{s-1}\right]^{1/2}}; \tag{3.14}$$

with $:= \left(\frac{m|V|^2}{4K}\right)^{\frac{1}{s-1}} b$. Thus the collision kernel B_σ is

$$B_\sigma = jVj\frac{b}{\sin}\left|\frac{\mathrm{d}b}{\mathrm{d}}\right| = jVj\left(\frac{4K}{mjVj^2}\right)^{\frac{2}{s-1}}\frac{}{\sin}\left|\frac{\mathrm{d}}{\mathrm{d}}\right| = \left(\frac{4K}{m}\right)^{\frac{2}{s-1}} jVj^{\frac{s-5}{s-1}}\frac{}{\sin}\left|\frac{\mathrm{d}}{\mathrm{d}}\right|. \tag{3.15}$$

Since can be solved implicitly from (3.14) to yield $= \ (\ )$, (3.15) implies that

$$B_\sigma = b_s(\cos \ )jVj^{\frac{s-5}{s-1}}; \quad b_s(\cos \ ) = \left(\frac{4K}{m}\right)^{\frac{2}{s-1}}\frac{}{\sin}\left|\frac{\mathrm{d}}{\mathrm{d}}\right|. \tag{3.16}$$

When $s = 5$, B_σ is a function of only which will lead to many simpli cations (usually referred to as Maxwell molecules). The hard sphere kernel can be considered as a special case of (3.16) when $s = 1$. Furthermore, (3.16) shows that the velocity dependence in the collision kernel behaves like $jVj^{\frac{s-5}{s-1}+2}$. When jVj is small, this is integrable if $\frac{s-5}{s-1} + 2 > 1$, i.e. $s > 2$. Note that $s = 2$ corresponds to the Coulomb potential. Therefore, the Boltzmann equation should not be used to describe the Coulomb interaction[1].

Based on (3.16), it is common in the kinetic literature to distinguish the kernel by its velocity dependence:

$$B_\sigma = b_\lambda(\cos \ )jVj^\lambda; \quad 3 < \quad 1; \tag{3.17}$$

where > 0 is called the *hard potential*, < 0 is the *soft potential*, and $= 0$ is the *Maxwell kernel*.

Let's analyze a bit the asymptotic behavior of w.r.t. . When 1, (3.14) can be approximated as

$$2\int_0^{\beta} \frac{\mathrm{d}r}{\left[1 \quad \left(\frac{r}{\beta}\right)^{s-1}\right]^{1/2}} = \quad 2 \quad \int_0^1 \frac{\mathrm{d}u}{(1 \quad u^{s-1})^{1/2}} = \quad 2 \ A(s); \tag{3.18}$$

[1] In this limit, one should consider the so-called Landau operator which is a diffusive type operator. We will come back to this later in the course.

so when $\; ! \; 0$, $\; ! \;$, and $\left|\frac{d\beta}{d\chi}\right|$ is well behaved. When $\;\; 1$, (3.14) can be approximated as

$$2\int_0^1 \frac{1 + \frac{1}{2}(1 \quad r^2)^{-1}\left(\frac{r}{\beta}\right)^{s-1}}{(1 \quad r^2)^{1/2}}\, dr = \frac{A(s)}{\;\; s-1};\tag{3.19}$$

so when $\; ! \; 1$, $\; ! \; 0$, and

$$\left|\frac{d}{d}\right| \qquad {}^{-\frac{2}{s-1}-1};\tag{3.20}$$

i.e., the collision kernel contains a nonintegrable singularity at $\; = 0$ for all $s > 2$ (except $s = 1$). This can be avoided either by cutting o , so that the potential is zero for large , or by the less physical, but mathematically more tractable, method of directly cutting o near 0, that is, eliminating grazing collisions from the collision term. This is the so-called *Grad's angular cut-off* assumption.

4 Basic properties of the Boltzmann equation

In this section, we derive some basic properties of the Boltzmann equation, which we rewrite here for clarity[2]

$$\frac{@f}{@t} + v \quad r_x f = Q(f; f); \quad x\ 2 \qquad \mathbb{R}^d; \quad v\ 2\ \mathbb{R}^d; \quad d \quad 2:\tag{4.1}$$

$Q(f; f)$ is the so-called *collision operator*, which is a quadratic integral operator acting only in the velocity space. In fact, it is convenient to introduce a bilinear form of Q as (in both - and $!$- representations):

$$\begin{aligned} Q(g; f)(v) &= \int_{\mathbb{R}^d}\int_{S^{d-1}} B_\sigma(jv \quad v_*j; \cos \quad)[g'_* f' \quad g_* f]\, d \quad dv_* \\ &= \int_{\mathbb{R}^d}\int_{S^{d-1}} B_\omega(jv \quad v_*j; j\cos \quad j)[g'_* f' \quad g_* f]\, d!\, dv_*; \end{aligned}\tag{4.2}$$

where

$$v' = \frac{v + v_*}{2} + \frac{jv \quad v_*j}{2} \quad ; \quad v'_* = \frac{v + v_*}{2} \quad \frac{jv \quad v_*j}{2} \quad ; \quad \cos \quad = \quad (\widehat{v \quad v_*});\tag{4.3}$$

$$v' = v \quad [(v \quad v_*) \quad !]!; \quad v'_* = v_* + [(v \quad v_*) \quad !]!; \quad j\cos \quad j = j! \quad (\widehat{v \quad v_*})j:\tag{4.4}$$

Note that the physically relevant case is the dimension $d = 3$ as we considered in previous sections. Here we assume $d \quad 2$ for mathematical generality.

We rst derive a very important formula of the collision operator using the $!$-representation.

[2]We have deliberately ignored the forcing term like $F(x) \cdot \nabla_v f$ in the discussion so far. With this term, the equation is the so-called Vlasov equation. We will come back to this later in the course.

Proposition 4.1. *(Boltzmann's lemma) For any functions $\varphi(v)$, $f(v)$ such that the integrals make sense, one has*

$$
\begin{aligned}
\int_{\mathbb{R}^d} Q(f,f)\,\varphi\,\mathrm{d}v &= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{S^{d-1}} B_\omega(|v-v_*|,|\cos\theta|)[f'f'_* - f f_*]\frac{\varphi+\varphi_*-\varphi'-\varphi'_*}{4}\,\mathrm{d}\omega\,\mathrm{d}v\,\mathrm{d}v_* \\
&= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{S^{d-1}} B_\omega(|v-v_*|,|\cos\theta|) f f_*[\varphi'-\varphi]\,\mathrm{d}\omega\,\mathrm{d}v\,\mathrm{d}v_*.
\end{aligned}
\tag{4.5}
$$

Proof.

$$
\begin{aligned}
\int_{\mathbb{R}^d} Q(f,f)\,\varphi\,\mathrm{d}v &= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{S^{d-1}} B_\omega(|v-v_*|,|\cos\theta|)[f'f'_* - f f_*]\,\varphi\,\mathrm{d}\omega\,\mathrm{d}v\,\mathrm{d}v_* \\
&= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{S^{d-1}} B_\omega(|v-v_*|,|\cos\theta|)[f'f'_* - f f_*]\,\varphi_*\,\mathrm{d}\omega\,\mathrm{d}v\,\mathrm{d}v_* \\
&= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{S^{d-1}} B_\omega(|v-v_*|,|\cos\theta|)[f'f'_* - f f_*]\frac{\varphi+\varphi_*}{2}\,\mathrm{d}\omega\,\mathrm{d}v\,\mathrm{d}v_* \\
&= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{S^{d-1}} B_\omega(|v-v_*|,|\cos\theta|)[f f_* - f'f'_*]\frac{\varphi'+\varphi'_*}{2}\,\mathrm{d}\omega\,\mathrm{d}v\,\mathrm{d}v_* \\
&= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{S^{d-1}} B_\omega(|v-v_*|,|\cos\theta|)[f'f'_* - f f_*]\frac{\varphi+\varphi_*-\varphi'-\varphi'_*}{4}\,\mathrm{d}\omega\,\mathrm{d}v\,\mathrm{d}v_*,
\end{aligned}
\tag{4.6}
$$

where in the second line we swapped v and v_* (hence v' and v'_*); in the fourth line we changed (v,v_*) to (v',v'_*) (hence (v',v'_*) becomes (v,v_*)) for a fixed ω and used the fact that $\mathrm{d}v\,\mathrm{d}v_* = \mathrm{d}v'\,\mathrm{d}v'_*$ (the transform has the unit Jacobian).

The second equality in (4.5) is obtained by changing (v,v_*) to (v',v'_*) only to the gain term. □

4.1 Collision invariants and local conservation laws

Definition 4.2. *A collision invariant is a continuous function $\varphi = \varphi(v)$ such that for each $v,v_* \in \mathbb{R}^d$ and $\omega \in S^{d-1}$, one has*

$$
\varphi + \varphi_* = \varphi' + \varphi'_*. \tag{4.7}
$$

Since during collisions, mass, momentum and energy are conserved, it is obvious that functions 1, v, and $|v|^2$, and any linear combination of them are the collision invariants. In fact, it can be shown that these are the *only* collision invariants (this is a non-trivial result, for proof one may refer to [3, p. 36-42]).

Using the Boltzmann's lemma, it is clear that

Corollary 4.3.

$$
\int_{\mathbb{R}^d} Q(f,f)\,\mathrm{d}v = \int_{\mathbb{R}^d} Q(f,f)\,v\,\mathrm{d}v = \int_{\mathbb{R}^d} Q(f,f)|v|^2\,\mathrm{d}v = 0. \tag{4.8}
$$

Using the Corollary 4.3, if we multiply the Boltzmann equation (4.1) by m, mv, $m|v|^2/2$, and integrate w.r.t. v, we obtain

$$\begin{cases} \partial_t \displaystyle\int_{\mathbb{R}^d} mf \,\mathrm{d}v + \nabla_x \cdot \int_{\mathbb{R}^d} mvf \,\mathrm{d}v = 0; \\ \partial_t \displaystyle\int_{\mathbb{R}^d} mvf \,\mathrm{d}v + \nabla_x \cdot \int_{\mathbb{R}^d} mv \otimes vf \,\mathrm{d}v = 0; \\ \partial_t \displaystyle\int_{\mathbb{R}^d} \frac{1}{2} m|v|^2 f \,\mathrm{d}v + \nabla_x \cdot \int_{\mathbb{R}^d} \frac{1}{2} mv|v|^2 f \,\mathrm{d}v = 0. \end{cases} \tag{4.9}$$

These are the local *conservation laws* (conservation of mass, momentum, and energy).

To better view the connection of f (number distribution function) and macroscopic quantities such as density, temperature, etc., let us define

$$n = \int_{\mathbb{R}^d} f \,\mathrm{d}v; \qquad \rho = mn; \quad u = \frac{1}{n}\int_{\mathbb{R}^d} vf \,\mathrm{d}v; \tag{4.10}$$

where n is the *number density*, ρ is the *mass density*, and u is the *bulk velocity*. Further, with the *peculiar velocity*

$$c = v - u; \tag{4.11}$$

we define

$$T = \frac{1}{dRn}\int_{\mathbb{R}^d} |c|^2 f \,\mathrm{d}v; \quad \mathbb{P} = \int_{\mathbb{R}^d} mc \otimes cf \,\mathrm{d}v; \quad q = \int_{\mathbb{R}^d} \frac{1}{2} mc|c|^2 f \,\mathrm{d}v; \tag{4.12}$$

where T is the *temperature*, $\mathbb{P}$ is the *stress tensor*, and q is the *heat flux vector*. $R = k_B/m$ is the gas constant (k_B is the Boltzmann's constant).

Finally, the *pressure* p is defined as

$$p = \frac{1}{d}\mathrm{tr}(\mathbb{P}) = \rho RT. \tag{4.13}$$

With the above definitions, we can recast the local conservation laws (4.9) using macroscopic quantities:

$$\begin{cases} \partial_t \rho + \nabla_x \cdot (\rho u) = 0; \\ \partial_t(\rho u) + \nabla_x \cdot (\rho u \otimes u + \mathbb{P}) = 0; \\ \partial_t E + \nabla_x \cdot (Eu + \mathbb{P}u + q) = 0; \end{cases} \tag{4.14}$$

where $E = \frac{d}{2}\rho RT + \frac{1}{2}\rho u^2$ is the total energy. The system (4.14) is completely equivalent to (4.9), hence to the Boltzmann equation. Note that this system is not closed because $\mathbb{P}$ and q, generally speaking, cannot be represented in terms of ρ, u, and T.

4.2 Boltzmann's H-theorem and Maxwellian

Proposition 4.4. *(Boltzmann's H-theorem)*

$$\int_{\mathbb{R}^d} Q(f,f)\ln f\,\mathrm{d}v \le 0, \tag{4.15}$$

and the equality holds if and only if $f = \exp(a + b\cdot v + c|v|^2)$.

Proof. Taking $\varphi = \ln f$ in the Boltzmann's lemma yields

$$\int_{\mathbb{R}^d} Q(f,f)\ln f\,\mathrm{d}v = -\frac{1}{4}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{S^{d-1}} B_\omega[f'f'_* - ff_*][\ln(f'f'_*) - \ln(ff_*)]\,\mathrm{d}\omega\,\mathrm{d}v\,\mathrm{d}v_* \le 0, \tag{4.16}$$

where the inequality is due to $\ln x$ is a monotonically increasing function, so $(x-y)(\ln x - \ln y) \ge 0$ for any $x, y > 0$. The equality holds iff $\ln f$ is a collision invariant, i.e., $f = \exp(a + b\cdot v + c|v|^2)$, with a, b, c being some constants. □

If a function f is of the form $\exp(a + b\cdot v + c|v|^2)$, it can be rewritten as

$$f = \exp\left(c\left|v + \frac{b}{2c}\right|^2 - \frac{|b|^2}{4c} + a\right). \tag{4.17}$$

For f to be integrable, c must be negative. Choosing $c' = -c$, $b' = -\frac{b}{2c}$, $a' = \exp(-\frac{|b|^2}{4c} + a)$ gives

$$f = a'\exp(-c'|v - b'|^2). \tag{4.18}$$

Using the definition of n, u and T given in the previous section, we can see that[3]

$$f = \frac{n}{(2\pi RT)^{d/2}}\exp\left(-\frac{|v-u|^2}{2RT}\right) := M. \tag{4.19}$$

(4.19) is called the *Maxwellian*.

Corollary 4.5. *The following statements are equivalent.*

$$\int_{\mathbb{R}^d} Q(f,f)\ln f\,\mathrm{d}v = 0 \iff f = M \iff Q(f,f) = 0. \tag{4.20}$$

Corollary 4.6.

$$\partial_t\int_{\mathbb{R}^d} f\ln f\,\mathrm{d}v + \nabla_x\cdot\int_{\mathbb{R}^d} vf\ln f\,\mathrm{d}v = -D(f) \le 0, \tag{4.21}$$

where

$$D(f) = \frac{1}{4}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{S^{d-1}} B_\omega[f'f'_* - ff_*][\ln(f'f'_*) - \ln(ff_*)]\,\mathrm{d}\omega\,\mathrm{d}v\,\mathrm{d}v_*. \tag{4.22}$$

[3]Note the Gaussian integrals $\int_{-\infty}^{\infty} e^{-\alpha v^2}\,\mathrm{d}v = \left(\frac{\pi}{\alpha}\right)^{\frac{1}{2}}$, $\int_{-\infty}^{\infty} v^2 e^{-\alpha v^2}\,\mathrm{d}v = \frac{1}{2\alpha}\left(\frac{\pi}{\alpha}\right)^{\frac{1}{2}}$.

If we assume f decays fast enough as $x \to \infty$, or is periodic in x, then (4.21) upon further integration in x yields

$$\frac{\mathrm{d}}{\mathrm{d}t} H(t) \leq 0, \tag{4.23}$$

where $H(t) := \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} f \ln f \,\mathrm{d}v\,\mathrm{d}x$ is the *H function*. (4.23) shows that H is always non-increasing and reaches its minimum value iff f reaches the Maxwellian (local equilibrium). This is consistent to the second law of thermodynamics.

4.3 Boundary condition

The commonly used boundary condition for the Boltzmann equation consists of the following: for a boundary point $x \in \partial\Omega$ and outward pointing normal $n(x)$,

- Inflow boundary:

$$f(t,x,v) = \frac{n_0}{(2\pi RT_0)^{d/2}} \exp\left(-\frac{|v-u_0|^2}{2RT_0}\right), \quad v\cdot n < 0, \tag{4.24}$$

  where $n_0(t,x)$, $u_0(t,x)$, and $T_0(t,x)$ are the prescribed density, velocity and temperature.

- Maxwell diffusive boundary:

$$f(t,x,v) = \rho_w(t,x) f_w(t,x,v), \quad (v-u_w)\cdot n < 0, \tag{4.25}$$

  with

$$f_w(t,x,v) = \exp\left(-\frac{|v-u_w|^2}{2RT_w}\right), \tag{4.26}$$

  where $u_w(t,x)$ and $T_w(t,x)$ are the wall velocity and temperature. $\rho_w(t,x)$ is determined by

$$\rho_w(t,x) = -\frac{\int_{(v-u_w)\cdot n\geq 0}(v-u_w)\cdot n f\,\mathrm{d}v}{\int_{(v-u_w)\cdot n<0}(v-u_w)\cdot n f_w\,\mathrm{d}v}. \tag{4.27}$$

- Reflective boundary:

$$f(t,x,v) = f(t,x,v-2[(v-u_w)\cdot n]n), \quad (v-u_w)\cdot n < 0. \tag{4.28}$$

References

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[3] C. Cercignani, R. Illner, and M. Pulvirenti. *The Mathematical Theory of Dilute Gases*. Springer-Verlag, 1994.