Pre-Lecture Notes of MATH-6042 at CUHK: Mathematical Theory and Numerical Simulation of Homogeneous Boltzmann Equation

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Abstract

In this course, the development of the spatially homogeneous theory to the Boltzmann equation will be briefly introduced, especially for the well-posedness result of the Cauchy problem in the space of probability measure. On the other side, the numerical simulation about the homogeneous Boltzmann equation, mainly the deterministic Spectral Method will also be presented; furthermore, some corresponding stability/error analysis frameworks will be discussed in a suitable manner.

1 Personal Statement

The lecture note is based on the MATH-6042 course delivered by the author in the Term 2, 2021-2022 at CUHK. The main prerequisites are a reasonable acquaintance with functional analysis, i.e., elementary topology, Fourier transform, and so forth. Preliminary knowledge about the Boltzmann equation is literally preferred, though the brief introduction will be provided at the beginning.

Due to the current limitation of the author, most likely, there are still at places inadequacies, inconsistency of notations, inadvertently omitted references... Therefore, the lecture note will be constantly updated and frequently uploaded on the website of the author, and hopefully continue to cover up the most recent results of this topic with time evolution.

Any correction and comment will be very welcomed from the readers for further improvement of the lecture note.

2 Teaching Arrangement

So far, a rough arrangement of the 13 lectures is provided as following, where some adjustments might happen according to the actual progress:

Contents

3 From Particle System to Kinetic Equation

As widely acknowledged, the microscopic regime is modeled by the many-particle system, ranging from physics, bio-mechanics, economy, material sciences, traffic modeling to other areas. The idea simply comes from the elementary Newton's mechanics: in a system of large number of particles, the particles essentially interact with its counterparts around it.

In the macroscopic scales, where the gas and fluid are regarded as a continuum, their motion is described by the macroscopic quantities such as macroscopic mass density, bulk velocity, temperature, pressure, heat flux, and so forth. The Euler and Navior-Stokes equations, compressible or incompressible, are the most well-known governing equations proposed so far in the fluid dynamics.

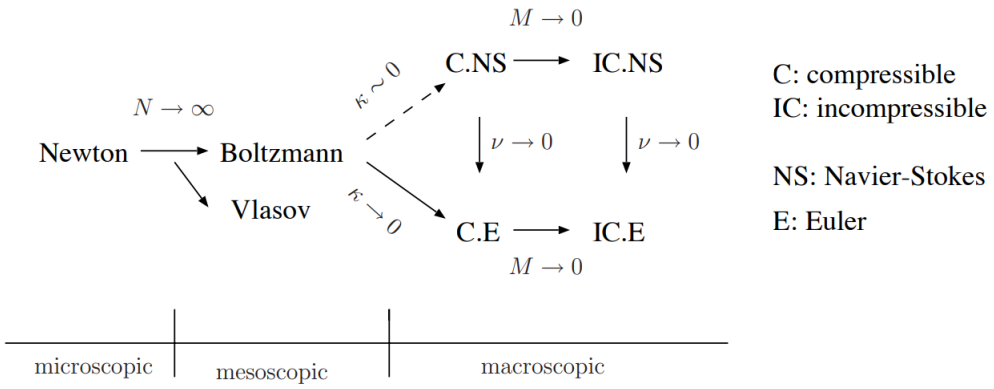

Figure 1: Multiscale Hierarchy[1]

The goal of this section is to derive the kinetic model, i.e., the Boltzmann equation, from the corresponding many-particle system. Proposed by L. Boltzmann in 1872, the Boltzmann equation is one of the fundamental and representative governing equations in kinetic theory, which describes the non-equilibrium dynamics of a gas or system comprised of a large number of particles.

3.1 Heuristic Derivation

Let the total mass be normalized to unity. Consider a binary (two-particle, say, particle 1 and particle 2) collision, with one particle having values of velocities in a range $\mathrm{d}v_1$ and another with values of velocities in a range $\mathrm{d}v_2$. In a collision, these acquire values of velocities in the ranges $\mathrm{d}v_1$ and $\mathrm{d}v_2$, respectively.

Let (v_1', v_2') be the velocities after a collision with respect to the pre-collisional velocities (v_1, v_2). By the conservation of momentum and energy:

$$v_1 + v_2 = v_1' + v_2', \quad |v_1|^2 + |v_2|^2 = |v_1'|^2 + |v_2'|^2 \tag{3.1}$$

[1]N: number of particles, κ: mean free path, μ: viscosity, M: Mach number.

one can derive that

$$v_1' = v_1 - [(v_1 - v_2)\cdot\omega]\,\omega, \quad v_2' = v_2 + [(v_1 - v_2)\cdot\omega]\,\omega, \tag{3.2}$$

where ω is the impact direction (the unit vector connecting the centers of particle 1 and particle 2). Note from Eq. (3.2) that

$$v_2' - v_1' = (v_2 - v_1) - 2\,[(v_2 - v_1)\cdot\omega]\,\omega, \tag{3.3}$$

i.e., the relative velocity undergoes a specular reflection at the impact direction.

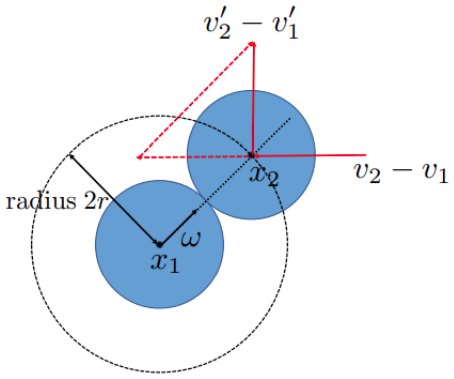

Figure 2: Velocity and impact direction during an elastic collision.

Now the total number of collisions per unit time per unit volume is taken to be

$$\underbrace{\{\text{Number of particles/unit volume}\}}_{P^{(1)}(t,x_1,v)_1\,\mathrm{d}v_1} \times \underbrace{\{\text{Probabilty of them suffering a collision}\}}_{p} \tag{3.4}$$

where $P^{(1)}(t, x_1, v_1)$ is the one-particle probability density function, i.e.,

$$P^{(1)}(t, x_1, v_1) := \int_{(\mathbb{R}^3\times\mathbb{R}^3)^{N-1}} P(t, x_1, v_1, ..., x_N, v_N)\,\mathrm{d}x_2\,\mathrm{d}v_2 ...\,\mathrm{d}x_N\,\mathrm{d}v_N \tag{3.5}$$

giving the probability of finding one fixed particle (particle 1) in an infinitesimal volume $\mathrm{d}x_1\mathrm{d}v_1$ 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.

And one takes the probability p of suffering a collision proportional to

$$\underbrace{\{\text{Number of particles/unit volumn}\}}_{P^{(1)}(t,x,v_1)\,\mathrm{d}v} \times \{\mathrm{d}v_1' \times \mathrm{d}v_2'\}. \tag{3.6}$$

Thus, the

$$\frac{\text{Total number of collisions}}{(\text{Unit volume})(\text{Unit time})} = \mathcal{B}(v_1', v_2'; v_1, v_2)P^{(2)}(t, x_1, v_1, x_2, v_2)\mathrm{d}v_1\mathrm{d}v_2\mathrm{d}v_1'\mathrm{d}v_2' \tag{3.7}$$

where $\mathcal{B}(v_1', v_2'; v_1, v_2)$ is derived from the analytical mechanics by solving the collision problem assuming a given inter-molecular force. Moreover, the symmetry for $\mathcal{B}(v_1', v_2'; v_1, v_2)$ is achieved via the "Principle of detailed balancing" which asserts that

$$\mathcal{B}(v_1', v_2'; v_1, v_2) = \mathcal{B}(v_1, v_2; v_1', v_2'). \tag{3.8}$$

This is formally discussed in some physics references. Suffice it to say the following: in the equilibrium, the number of collisions $(v_1, v_2) \longmapsto (v_1', v_2')$ is equal to the number of collisions $(-v_1', -v_2') \longmapsto (-v_1, -v_2)$. This follows from the symmetry of the equations of classical mechanics under time reversal, and is adopted in non-equilibrium setting as well. Thus, under such a mapping we expect to get

$$\mathcal{B}(v_1', v_2'; v_1, v_2) = \mathcal{B}(-v_1, -v_2; -v_1', -v_2'). \tag{3.9}$$

and then the stated result.

Remark 3.1. *This symmetric property is also assumed based on the micro-reversible of collisions, which can be understood in a purely deterministic way: microscopic dynamics are time-reversible; or in a probabilistic way: the probability that velocities (v_1', v_2') are changed into (v_1, v_2) in a collision process, is the same as the probability that (v_1, v_2) are changed into (v_1', v_2')*

Intuitively speaking, the movement of particles can be divided into the following two scenario cases:

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

$$\frac{\partial P^{(1)}}{\partial t} + v_1 \cdot \nabla_{x_1} P^{(1)} = 0 \tag{3.10}$$

• With the collisions, one would expect

$$\frac{\partial P^{(1)}}{\partial t} + v_1 \cdot \nabla_{x_1} P^{(1)} = Q = \underbrace{G}_{\text{"gain"}} - \underbrace{L}_{\text{"loss"}} \tag{3.11}$$

where $L\,\mathrm{d}x_1\,\mathrm{d}v_1\,\mathrm{d}t$ denotes the probability of finding particles with position between x_1 and $x_1 + \mathrm{d}x_1$ and velocity between v_1 and $v_1 + \mathrm{d}v_1$ that disappear from these ranges of values due to a collision in the time interval between t and $t + \mathrm{d}t$.

L is often called the loss term, indicating that every such collision transfers it out of a particular range $\mathrm{d}v_1$: for binary collisions, given $\mathrm{d}v$, the total number of collisions $(v_1, v_2) \longmapsto (v_1', v_2')$ with all possible values of v_2, v_1', v_2' occurring in the volume $\mathrm{d}x_1$ during the time interval $\mathrm{d}t$ is

$$L\mathrm{d}x_1\mathrm{d}v_1\mathrm{d}t = \mathrm{d}x_1\mathrm{d}v_1\,\mathrm{d}t \int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{R}^3} \mathcal{B}(v_1', v_2'; v_1, v_2) P^{(2)}(t, x_1, v_1, x_2, v_2)\,\mathrm{d}v_1'\,\mathrm{d}v_2'\,\mathrm{d}v_2 \tag{3.12}$$

Similarly, G is often called the gain 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 $\mathrm{d}x_1\mathrm{d}v_1$ in the same

time interval $\mathrm{d}t$, or brings into the range $\mathrm{d}v_1$ molecules which originally has values outside that range: given v_1, these are collisions $(v_1', v_2') \longmapsto (v_1, v_2)$ with all possible v_2, v_1', v_2', and

$$G\mathrm{d}x_1\mathrm{d}v_1\mathrm{d}t = \mathrm{d}x_1\mathrm{d}v_1\,\mathrm{d}t \int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{R}^3} \mathcal{B}(v_1, v_2; v_1', v_2') P^{(2)}(t, x_1, v_1', x_2, v_2')\,\mathrm{d}v_1'\,\mathrm{d}v_2'\,\mathrm{d}v_2 \quad (3.13)$$

Hence, by Eq. (3.8) the collision operator Q can be written in general case:

$$Q = \int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{R}^3} \mathcal{B}(v_1, v_2; v_1', v_2') \left[P^{(2)}(t, x_1, v_1', x_2, v_2') - P^{(2)}(t, x_1, v_1, x_2, v_2)\right]\,\mathrm{d}v_1'\,\mathrm{d}v_2'\,\mathrm{d}v_2 \quad (3.14)$$

For a monatomic gas, we write

$$\frac{\mathcal{B}(v_1, v_2; v_1', v_2')\,\mathrm{d}v_1'\,\mathrm{d}v_2'}{|v_1 - v_2|} = B(|v_1 - v_2|, \omega)\mathrm{d}\omega \quad (3.15)$$

which is called the differential collision cross section, containing the δ-functions

$$\delta\left(v_1' + v_2' - v_1 - v_2\right) \cdot \delta\left(\frac{|v_1'|^2 + |v_2'|^2 - |v_1|^2 - |v_2|^2}{2}\right) \quad (3.16)$$

that expresses the conservation of momentum and energy. Assume these have been removed, then the $B(|v_1 - v_2|, \omega)\mathrm{d}\omega$ becomes scattering cross section, such that

$$Q = \int_{\mathbb{R}^3} B(|v_1 - v_2|, \omega) \left[P^{(2)}(t, x_1, v_1', x_2, v_2') - P^{(2)}(t, x_1, v_1, x_2, v_2)\right]\,\mathrm{d}\omega\,\mathrm{d}v_2. \quad (3.17)$$

3.2 Formal Derivation of Hard-Sphere Model

Usually, the cross section $B(|v_1 - v_2|, \omega)$ cannot be explicitly calculated, except for some special cases, now we are about to take the hard-sphere model as an example to derive the more usual form of the Boltzmann equation.

For the hard-sphere model, to count these probability of "gain" and "loss" effects, we imagine particle 1 as a sphere at rest and endowed with twice the actual radius r and other particles being the point masses with velocity $v_2 - v_1$. Fixing the particle 1, it will be to found in the cylinder of height $|(v_2 - v_1)\cdot\omega|\mathrm{d}t$ and base area $\mathrm{d}S = (2r)^2\mathrm{d}\omega$ (where $\mathrm{d}\omega$ is the area of the surface element of the unit sphere of ω). Then,

$$\begin{aligned} l\mathrm{d}x_1\,\mathrm{d}v_1\mathrm{d}t = \mathrm{d}x_1\mathrm{d}v_1 \int_{\mathbb{R}^3}\int_{\mathbb{S}^2_-} & P^{(2)}(t, x_1, v_1, x_1 + 2r\omega, v_2) \\ & \times \underbrace{|(v_2 - v_1)\cdot\omega|\mathrm{d}t}_{\text{Cylinder of height}}\,\underbrace{(2r)^2\,\mathrm{d}\omega}_{\text{Base area}}\,\mathrm{d}v_2 \end{aligned} \quad (3.18)$$

where l indicates the contribution of another fixed particle, say particle 2, and $P^{(2)}$ is the two-particle probability density function of particle 1 and 2, and $\mathbb{S}^2_-$ is the hemi-sphere corresponding to $(v_2 - v_1)\cdot\omega < 0$.

Since there are another $N - 1$ identical particles, if assuming that there are in total of N particles and multiple collisions are disregarded, that will collide with particle 1.

Therefore,

$$L = (N-1)(2r)^2 \int_{\mathbb{R}^3} \int_{\mathbb{S}^2_-} P^{(2)}(t, x_1, v_1, x_1 + 2r\omega, v_2)|(v_2 - v_1) \cdot \omega| \, \mathrm{d}\omega \, \mathrm{d}v_2 \tag{3.19}$$

similarly, for G, what we are look for particles that have velocities (v_1, v_2) after collision, and hence we have to integrate over the hemi-sphere $\mathbb{S}^2_+$ corresponding to $(v_2 - v_1) \cdot \omega > 0$ (the particles are moving away one from the other after the collision) to obtain:

$$G = (N-1)(2r)^2 \int_{\mathbb{R}^3} \int_{\mathbb{S}^2_+} P^{(2)}(t, x_1, v_1, x_1 + 2r\omega, v_2)|(v_2 - v_1) \cdot \omega| \, \mathrm{d}\omega \, \mathrm{d}v_2. \tag{3.20}$$

We could thus write the right-hand side of Eq. (3.11) as a single expression:

$$G - L = (N-1)(2r)^2 \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} P^{(2)}(t, x_1, v_1, x_1 + 2r\omega, v_2)|(v_2 - v_1) \cdot \omega| \, \mathrm{d}\omega \, \mathrm{d}v_2. \tag{3.21}$$

where $\mathbb{S}^2$ is the entire unit sphere.

So far, the derivation of Eq. (3.21) has been formal and can be justified with full rigor. Although, Eq. (3.21) is correct, it turns out more convenient to keep the gain and loss terms separated and make further simplification. To achieve this, we need the following to crucial assumptions:

- (i) *Boltzmann-Grad Limit*: Assume Nr^2 is finite, as $N \to \infty, r \to 0$.
- (ii) *Molecular Chaos*: 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.

Remark 3.2. *(i) The Boltzmann-Grad Limit Assumption actually implies that the gases are sufficiently dilute, but not too much, so that only binary interactions play a significant role, and a typical particle collides about once in a unit time.*

To understand the idea, let us say that we have a box whose volume is $L^3 = 1m^3$ at room temperature and atmospheric pressure. Then $N \approx 10^{20}$ and $2r \approx 10^{-8}cm$. Then $(N-1)(2r)^2 \approx N(2r)^2 = 10^4 cm^2 = 1m^2 = L^2$ is a sizable quantity, while we can neglect the difference between x_1 and $x_1 + 2r\omega$. This means that the Eq. (3.21) to be written can be rigorously valid only in the so-called Boltzmann-Grad Limit, with Nr^2 is finite, as $N \to \infty, r \to 0$, i.e.,

$$N(2r)^3 << L^3, \quad N(2r)^2 = O(L^2) \tag{3.22}$$

where r can be regarded as the typical range of microscopic interaction, and L is the typical macroscopic length scale.

(ii) The Molecular Chaos Assumption actually implies that the velocities of two particles which are about to collide are uncorrelated. Since the volume occupied by the particles is about $N(2r)^3 \approx 10^{-4}cm^3$, the collisions between two pre-selected particles is a rather rare event. Or, roughly speaking, this means that if we randomly pick up two particles at position x, which have not collided yet, then the joint distribution of their velocities will be given by a tensor product (in velocity space) of f with itself.

Note that this assumption also implies an asymmetry between past and future: indeed, in general if the pre-collisional velocities are uncorrelated, then post-collisional velocities have to be correlated.

Then, L becomes

$$\begin{aligned} L =& N(2r)^2 \int_{\mathbb{R}^3} \int_{\mathbb{S}^2_-} P^{(2)}(t, x_1, v_1, x_1, v_2) |(v_2 - v_1) \cdot \omega| \, \mathrm{d}\omega \, \mathrm{d}v_2 \\ =& N(2r)^2 \int_{\mathbb{R}^3} \int_{\mathbb{S}^2_-} P^{(1)}(t, x_1, v_1) P^{(1)}(t, x_1, v_2) |(v_2 - v_1) \cdot \omega| \, \mathrm{d}\omega \, \mathrm{d}v_2, \end{aligned} \tag{3.23}$$

where we used the Assumption (i) in the first equality and Assumption (ii) in the second equality.

Then, we insert the G the information that the $P^{(2)}$ is continuous at a collision, i.e., for $i = 1, j = 2$, we integrate with respect to the positions and velocities of the remaining $N - 2$ particles,

$$P^{(2)}(t, x_1, v_1, x_2, v_2) = P^{(2)}(t, x_1, \underbrace{v_1 - [(v_1 - v_2) \cdot \omega] \, \omega}_{v_1'}, x_2, \underbrace{v_2 + [(v_1 - v_2) \cdot \omega] \, \omega)}_{v_2'} \tag{3.24}$$

because the transformation v_1', v_2' maps the hemi-sphere $\mathbb{S}^2_+$ onto $\mathbb{S}^2_-$; if $|x_1 - x_2| = 2r$ where we write $q_{1,2} = v_1 - v_2$ and $\omega = -\omega_{1,2}$.

Only in this way, for G, we have,

$$\begin{aligned} G =& (N-1)(2r)^2 \int_{\mathbb{R}^3} \int_{\mathbb{S}^2_+} P^{(2)}(t, x_1, v_1, x_1 + 2r\omega, v_2) |(v_2 - v_1) \cdot \omega| \, \mathrm{d}\omega \, \mathrm{d}v_2 \\ =& N(2r)^2 \int_{\mathbb{R}^3} \int_{\mathbb{S}^2_+} P^{(1)}(t, x_1, v_1') P^{(1)}(t, x_1, v_2') |(v_2 - v_1) \cdot \omega| \, \mathrm{d}\omega \, \mathrm{d}v_2 \\ =& N(2r)^2 \int_{\mathbb{R}^3} \int_{\mathbb{S}^2_-} P^{(1)}(t, x_1, v_1') P^{(1)}(t, x_1, v_2') |(v_2 - v_1) \cdot \omega| \, \mathrm{d}\omega \, \mathrm{d}v_2, \end{aligned} \tag{3.25}$$

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 simple change of variable $\omega \longmapsto -\omega$.

Putting together G and L, we have,

$$\begin{aligned} \frac{\partial P^{(1)}}{\partial t} + v_1 \cdot \nabla_{x_1} P^{(1)} = N(2r^2) \int_{\mathbb{R}^3} \int_{\mathbb{S}^2_-} & |(v_2 - v_1) \cdot \omega| \\ & \times \left[P^{(1)}(t, x_1, v_1') P^{(1)}(t, x_1, v_2') - P^{(1)}(t, x_1, v_1) P^{(1)}(t, x_1, v_2) \right] \mathrm{d}\omega \, \mathrm{d}v_2. \end{aligned} \tag{3.26}$$

In the following note, we will mainly consider the one-particle number probability distribution function f, i.e., $f(t, x, v) = NP^{(1)}(t, x_1, v_1)$, by changing $x_1 \longmapsto x, v_1 \longmapsto v, v_2 \longmapsto v_*, \omega \longmapsto -\omega$, then the Boltzmann equation for hard-sphere model reads:

$$\partial_t f + v \cdot \nabla_x f = (2r)^2 \int_{\mathbb{R}^3} \int_{\mathbb{S}^2_-} |(v - v_*) \cdot \omega| \, [f' f_*' - f f_*] \, \mathrm{d}\omega \, \mathrm{d}v_*, \tag{3.27}$$

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

It is often convenient to integrate ω over the whole unit sphere rather than hemi-sphere by inserting a $1/2$ factor, which yields,

$$\partial_t f + v \cdot \nabla_x f = 2r^2 \int_{\mathbb{R}^3} \int_{\mathbb{S}^2_-} |(v - v_*) \cdot \omega| \left[f' f'_* - f f_* \right] \mathrm{d}\omega \, \mathrm{d}v_*. \tag{3.28}$$

3.3 Formal Derivation of Liouville Equation (BBGKY Hierarchy)

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

3.3.1 Liouville Equation

Under the dynamics: we denote the $\mathbf{x}_i$ by x_i, $\mathbf{v}_i$ by v_i, and $\mathbf{F}_i$ by F_i for convenience,

$$\begin{cases} m\dot{v}_i(t) = F_i \\ \dot{x}_i(t) = v_i \end{cases} \tag{3.29}$$

with the initial date given.

Here "the point at x_i with velocity v_i" means "the point between x_i and $x_i + \mathrm{d}x_i$ with velocity between v_i and $v_i + \mathrm{d}v_i$". And the trajectory is

$$\begin{cases} x_i = x_i(t) \\ v_i = \dot{x}_i(t) \end{cases} \tag{3.30}$$

Let $P^{(N)}(t, x_1, v_1, ..., x_N, v_N)$ be the N-particle (empirical) probability density function,

$$\begin{aligned} P^{(N)}(t, x_1, v_1, ..., x_N, v_N) =& \delta(x_1 - x_1(t))\delta(x_2 - x_2(t))...\delta(x_N - x_N(t)) \\ & \cdot \delta(v_1 - \dot{x}_1(t))\delta(v_2 - \dot{x}_2(t))...\delta(v_N - \dot{x}_N(t)). \end{aligned} \tag{3.31}$$

Derive the Liouville equation from the following calculation:

$$\begin{aligned} \frac{\partial P^{(N)}}{\partial t} =& -\sum_{j=1}^{N} \prod_{k=1, k\neq j}^{N} \delta(x_k - x_k(t))\delta(v_k - \dot{x}_k(t)) \cdot \frac{\partial}{\partial x_j} \delta(x_j - x_j(t))\delta(v_j - \dot{x}_j(t)) \cdot \dot{x}_j \\ & -\sum_{j=1}^{N} \prod_{k=1, k\neq j}^{N} \delta(x_k - x_k(t))\delta(v_k - \dot{x}_k(t)) \cdot \delta(x_j - x_j(t)) \frac{\partial}{\partial v_j} \delta(v_j - \dot{x}_j(t)) \cdot \ddot{x}_j \end{aligned} \tag{3.32}$$

Note that

$$\dot{x}_j(t)\delta(v_j - \dot{x}_j(t)) = v_j \delta(v_j - \dot{x}_j(t)) \tag{3.33}$$

and

$$\begin{cases} \ddot{x}_j = \dfrac{F_j}{m} = f_j \\ \dot{x}_j = v_j(t) \end{cases} \tag{3.34}$$

where f_j is the force per unit mass over the j-th particle. Therefore,

$$\begin{aligned}\frac{\partial P^{(N)}}{\partial t} =& -\sum_{j=1}^{N} v_j \frac{\partial}{\partial x_j}\delta(x_j - x_j(t))\delta(v_j - \dot{x}_j(t)) \prod_{k=1,k\neq j}^{N} \delta(x_k - x_k(t))\delta(v_k - \dot{x}_k(t)) \\ & -\sum_{j=1}^{N} \frac{F_j}{m}\frac{\partial}{\partial v_j}\delta(v_j - \dot{x}_j(t))\delta(x_k - x_k(t)) \prod_{k=1,k\neq j}^{N} \delta(x_k - x_k(t))\delta(v_k - \dot{x}_k(t)) \\ =& -\sum_{j=1}^{N} v_j \frac{\partial P^{(N)}}{\partial x_j} - \sum_{j=1}^{N} \frac{F_j}{m}\frac{\partial P^{(N)}}{\partial v_j}\end{aligned} \tag{3.35}$$

that is to say,

$$\frac{\partial P^{(N)}}{\partial t} + \sum_{j=1}^{N} v_j \frac{\partial P^{(N)}}{\partial x_j} + \sum_{j=1}^{N} \frac{F_j}{m}\frac{\partial P^{(N)}}{\partial v_j} = 0 \tag{3.36}$$

which is the Liouville equation, a linear, homogeneous, first-order partial differential equation.

3.3.2 BBGKY Hierarchy

Consider N hard sphere 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

$$(x_1, v_1, ..., x_N, v_N) \in \Omega^N \times \mathbb{R}^{3N} = \Lambda_{1,...,N} \tag{3.37}$$

where

$$\Omega^N = \left\{(x_1, ..., x_N) \;\middle|\; |x_i - x_j| > 2r, \quad i \neq j\right\} \tag{3.38}$$

and

$$\Omega_c^N = \left\{(x_1, ..., x_N) \;\middle|\; |x_i - x_j| < 2r, \quad i \neq j\right\} \tag{3.39}$$

in fact, if a point $(x_1, ..., x_N)$ lies in the set Ω_c^N, the i-th and j-th molecule would overlap, which is impossible since they are assumed to be hard spheres.
On the other hand, we have to introduce the boundaries, with the regions where the spheres would but not yet overlap, in order to define $\Lambda_{1,...,N}$:

$$\partial\Lambda_{1,...,N} = \left\{(x_1, v_1, ..., x_N, v_N) \;\middle|\; |x_i - x_j| = 2r, \quad i \neq j\right\}, \tag{3.40}$$

since $P^{(N)}$ is always constant along the trajectory Eq. (3.30) in $\Lambda_{1,...,N}$ (boundaries included), but the velocities $(v_1, ..., v_N)$ should undergo a discontinuous transformation there, we must impose that $P^{(N)}$ is the same at $(..., x_i, v_i, x_j, v_j...)$ and $(..., x_i, v_i', x_j, v_j'...)$, indicating points of the boundary of $\Lambda_{1,...,N}$ that are transformed one into the other by the transformation associated with an impact factor or direction (continuous at a collision):

$$P^{(N)}(..., x_i, v_i, x_j, v_j...) = P^{(N)}(..., x_i, v_i', x_j, v_j'...) \tag{3.41}$$

or more specifically, such as elastic binary collision:

$$P^{(N)}(..., x_i, v_i, x_j, v_j...) = P^{(N)}(..., x_i, v_i - (q_{i,j}\cdot\omega_{i,j})\omega_{i,j}, x_j, v_i + (q_{i,j}\cdot\omega_{i,j})\omega_{i,j}...) \tag{3.42}$$

where $q_{i,j} = v_i - v_j$ and $\omega_{i,j}$ is the unit vector directed as $x_i - x_j$.

Remark 3.3. *(i) If Ω^N does not coincide with $\mathbb{R}^{3N}$, then there are additional boundary points that at least one x_i is on $\partial\Lambda_{1,\dots,N}$. A suitable boundary condition must be assigned at these points as well, e.g., the specular reflection:*

$$v_i' = v_i - (v_i \cdot \omega_i)\omega_i \tag{3.43}$$

where ω_i is unit normal vector at x_i.

(ii) If Ω is a box, periodicity conditions are very popular, in that case one can avoid mentioning the boundaries and talk about a flat torus (after identification of opposite faces).

(iii) Another point to be mentioned is that we shall allow the symmetric initial condition $P_0^{(N)}$ upon interchange of any two particles (since the particles are identical):

$$P^{(N)}(t=0,...,x_i,v_i,x_j,v_j...) = P^{(N)}(t=0,...,x_j,v_j,x_i,v_i...) \tag{3.44}$$

the same symmetry of which is preserved for $t > 0$, as the time evolution is consistent with the symmetric property.

In this case, $P^{(N)}$ satisfies the Liouville equation without other outer force,

$$\frac{\partial P^{(N)}}{\partial t} + \sum_{i=1}^{N} v_i \frac{\partial P^{(N)}}{\partial x_i} = 0. \tag{3.45}$$

Define the s-particle probability density function as

$$P^{(s)}(t,x_1,v_1,...,x_s,v_s) = \int_{\Lambda_{s+1,\dots,N}} P^{(N)}(t,x_1,v_1,...,x_N,v_N)\,\mathrm{d}x_{s+1}\,\mathrm{d}v_{s+1}...\,\mathrm{d}x_N\,\mathrm{d}v_N, \tag{3.46}$$

then integrating Eq. (3.45) with respect to the variables $x_j, v_j (s+1 \le j \le N)$ over $\Lambda_{1,\dots,N}$, and it is convenient to keep the terms in the sum appearing in Eq. (3.45) with $i \le s$ from those with $i > s$, we can obtain that

$$\frac{\partial P^{(s)}}{\partial t} + I_1 + I_2 = 0, \tag{3.47}$$

with

$$I_1 = \sum_{i=1}^{s} \int_{\Lambda_{s+1,\dots,N}} v_i \frac{\partial P^{(N)}}{\partial x_i}\,\mathrm{d}x_{s+1}\,\mathrm{d}v_{s+1}...\,\mathrm{d}x_N\,\mathrm{d}v_N, \tag{3.48}$$

and

$$I_2 = \sum_{i=s+1}^{N} \int_{\Lambda_{s+1,\dots,N}} v_i \frac{\partial P^{(N)}}{\partial x_i}\,\mathrm{d}x_{s+1}\,\mathrm{d}v_{s+1}...\,\mathrm{d}x_N\,\mathrm{d}v_N, \tag{3.49}$$

For I_1, though it contains the integral of derivative with respect to $x_i, 1 \le i \le s$, over which one does not integrate; it is not possible, however, to simply change the order of integration and differentiation to obtain a derivative of $P^{(s)}$, because the domain has boundaries $|x_i - x_j| = 2r$ depending on x_i. Consequently, recalling Leibniz's Rule

$$\frac{\mathrm{d}}{\mathrm{d}x}\int_{b(x)}^{a(x)} u(x,y)\,\mathrm{d}y = u(x,b(x))b'(x) - u(x,a(x))a'(x) + \int_{b(x)}^{a(x)} \frac{\partial u(x,y)}{\partial x}\,\mathrm{d}y \tag{3.50}$$

and considering the boundary term for each x_i:

$$\begin{aligned}
&\int_{\Lambda_{s+1,\dots,N}} v_i \frac{\partial P^{(N)}}{\partial x_i}\,\mathrm{d}x_{s+1}\,\mathrm{d}v_{s+1}...\,\mathrm{d}x_N\,\mathrm{d}v_N \\
=&v_i\frac{\partial P^{(s)}}{\partial x_i} - \sum_{j=s+1}^{N}\int_{\partial\Lambda_{s+1,\dots,N}} v_i\omega_{i,j}P^{(s+1)}\,\mathrm{d}\mathbf{r_{i,j}}\,\mathrm{d}v_j \\
=&v_i\frac{\partial P^{(s)}}{\partial x_i} - (N-s)(2r)^2\int_{\partial\Lambda_{s+1}} v_i\omega_{i,s+1}P^{(s+1)}\,\mathrm{d}\omega_{i,s+1}\,\mathrm{d}v_{s+1}
\end{aligned} \tag{3.51}$$

where $\omega_{i,j}$ is the outer normal vector to the sphere $|x_i - x_j| = 2r$ (with center at x_j); $\mathrm{d}\mathbf{r_{i,j}} = (2r)^2\mathrm{d}\omega_{i,j}$ is the surface element on the same particle sphere; $P^{(s+1)}$ is the $(s+1)$-particle distribution function with arguments $(x_1, v_1, ..., x_s, v_s, x_j, v_j),\ s+1 \le j \le N$.

Then, after summing up from $i = 1$ to s, the I_1 can be shown that

$$\begin{aligned}
I_1 = \sum_{i=1}^{s} v_i\frac{\partial P^{(s)}}{\partial x_i} - &(N-s)(2r)^2\sum_{i=1}^{s}\int_{\partial\Lambda_{s+1}} v_i\cdot\omega_{i,s+1} \\
&\times P^{(s+1)}(t, x_1, v_1, ..., x_s, v_s, x_i + 2r\omega_{i,s+1}, v_{s+1})\,\mathrm{d}\omega_{i,s+1}\,\mathrm{d}v_{s+1},
\end{aligned} \tag{3.52}$$

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

For I_2, applying the Divergence Theorem via replacing (x_1, v_1) by (x_i, v_i), (x_2, v_2) by (x_j, v_j), and ω by $\omega_{i,j}$, one has,

$$\begin{aligned}
I_2 = &\sum_{i=s+1}^{N}\sum_{j=1}^{s}(2r)^2\int_{\Lambda_{s+1,\dots,N}} v_i\cdot\omega_{i,j}P^{(N)}(t, x_1, v_1, ..., x_{i-1}, v_{i-1}, x_j + 2r\omega_{j,i}, v_i, ..., x_N, v_N) \\
&\times\ \mathrm{d}\omega_{i,j}\,\mathrm{d}x_{s+1}...\,\mathrm{d}x_{i-1}\,\mathrm{d}x_{i+1}...\,\mathrm{d}x_N\,\mathrm{d}v_{s+1}...\,\mathrm{d}v_N \\
+\sum_{i=s+1}^{N}\sum_{j=s+1,j\neq i}^{N}&(2r)^2\int_{\Lambda_{s+1,\dots,N}} v_i\cdot\omega_{i,j}P^{(N)}(t, x_1, v_1, ..., x_{i-1}, v_{i-1}, x_j + 2r\omega_{j,i}, v_i, ..., x_N, v_N) \\
&\times\ \mathrm{d}\omega_{i,j}\,\mathrm{d}x_{s+1}...\,\mathrm{d}x_{i-1}\,\mathrm{d}x_{i+1}...\,\mathrm{d}x_N\,\mathrm{d}v_{s+1}...\,\mathrm{d}v_N,
\end{aligned} \tag{3.53}$$

where the second sum in the above equation is completely zero by the Liouville Theorem (it is actually the integral of $\sum_{i=s+1}^{N} v_i\frac{\partial P^{(N)}}{\partial x_i}$ with respect to the dynamics of the last $N-s$ particles).
Furthermore, by using the symmetry of $P^{(N)}$, the first term can be reduced to

$$\begin{aligned}
I_2 = &(N-s)(2r)^2\sum_{j=1}^{s}\int_{\partial\Lambda_{s+1}\times\Lambda_{s+2,\dots,N}} v_{s+1}\cdot\omega_{s+1,j} \\
&\times P^{(N)}(t, x_1, v_1, ..., x_{i-1}, v_{i-1}, x_j + 2r\omega_{j,i}, v_i, ..., x_N, v_N)\,\mathrm{d}\omega_{s+1,j}\,\mathrm{d}x_{s+2}...\,\mathrm{d}x_N\,\mathrm{d}v_{s+1}...\,\mathrm{d}v_N \\
= &(N-s)(2r)^2\sum_{j=1}^{s}\int_{\partial\Lambda_{s+1}} v_{s+1}\cdot\omega_{s+1,j} \\
&\times P^{(s+1)}(t, x_1, v_1, ..., x_s, v_s, x_j + 2r\omega_{j,s+1}, v_{s+1})\,\mathrm{d}\omega_{s+1,j}\,\mathrm{d}x_{s+1}.
\end{aligned} \tag{3.54}$$

Combining the I_1 and I_2 together, the Eq. (3.47) becomes,

$$\begin{aligned}\frac{\partial P^{(s)}}{\partial t}+\sum_{i=1}^{s} v_i\frac{\partial P^{(s)}}{\partial x_i} =&(N-s)(2r)^2\sum_{j=1}^{s}\int_{\partial\Lambda_{s+1}}(v_j-v_{s+1})\cdot\omega_{s+1,j}\\ &\times P^{(s+1)}(t,x_1,v_1,...,x_s,v_s,x_j-2r\omega_{s+1,j},v_{s+1})\,\mathrm{d}\omega_{s+1,j}\,\mathrm{d}v_{s+1}\end{aligned} \tag{3.55}$$

This is the so-called BBGKY hierarchy for hard-sphere model (the equation of $P^{(s)}$ depends on the $P^{(s+1)}$), named after *Bogoliubov, Born, Green, Kirkwood, and Yvon.*

The physical meaning of Eq. (3.55) is obvious: the left-hand side is a operator, generating the free motion of s particle, hence, the s-particle distribution function evolves in time according to the s-particle dynamics, corrected by the effect of the interaction with the remaining $(N-s)$ particles. The effect of this interaction is described by the right-hand side of Eq. (3.55).

In particular, taking $s=1$ in Eq. (3.55), we obtain,

$$\begin{aligned}&\frac{\partial P^{(1)}}{\partial t}+v_1\frac{\partial P^{(1)}}{\partial x_1}\\ =&(N-1)(2r)^2\int_{\partial\Lambda_2}(v_1-v_2)\cdot\omega_{2,1}P^{(2)}(t,x_1,v_1,x_1-2r\omega_{2,1},v_2)\,\mathrm{d}\omega_{2,1}\,\mathrm{d}v_2\\ =&(N-1)(2r)^2\int_{\partial\Lambda_2}(v_2-v_1)\cdot\omega_{1,2}P^{(2)}(t,x_1,v_1,x_1+2r\omega_{1,2},v_2)\,\mathrm{d}\omega_{1,2}\,\mathrm{d}v_2\\ =&(N-1)(2r)^2\int_{(v_2-v_1)\cdot\omega_{1,2}>0}|(v_2-v_1)\cdot\omega_{1,2}|P^{(2)}(t,x_1,v_1,x_1+2r\omega_{1,2},v_2)\,\mathrm{d}\omega_{1,2}\,\mathrm{d}v_2\\ &-(N-1)(2r)^2\int_{(v_2-v_1)\cdot\omega_{1,2}<0}|(v_2-v_1)\cdot\omega_{1,2}|P^{(2)}(t,x_1,v_1,x_1+2r\omega_{1,2},v_2)\,\mathrm{d}\omega_{1,2}\,\mathrm{d}v_2.\end{aligned} \tag{3.56}$$

This is the same as the Eq. (3.11) with Eq. (5.32) and Eq. (3.20) derived in the previous subsection, and the rest derivation is the same. That is, the original BBGKY hierarchy yields the Boltzmann equation.

4 Corresponding and Relevant Materials

The following materials are, in chronological order, referred to the development of the study about the solution to spatially homogeneous Boltzmann equation as a probability measure, where the Fourier Transformation plays a critical role.

KQ: This list is not intended to be completely covered in the mini-course, which is definitely impossible, but to partly reflect the history and hopefully present a big picture about how the research of the homogeneous Boltzmann equation in probability measure sense developed: from cutoff to non-cutoff, from the Maxwellian molecule to hard/soft potential, from higher-order moments requirement to lower-order... The selection is biased in favor of personal taste.

[1] A. V. Bobylev. A class of invariant solutions of the Boltzmann equation. *Dokl. Akad. Nauk SSSR*, 231(3):571–574, 1976.

[2] A. V. Bobylev. The theory of the nonlinear spatially uniform Boltzmann equation for Maxwell molecules. *Soviet Sci. Rev. Sect. C: Math. Phys. Rev., 7*, 111–233, 1988.

[3] G. Gabetta, G. Toscani, and B. Wennberg. Metrics for probability distributions and the trend to equilibrium for solutions of the Boltzmann equation. *J. Stat. Phys.*, 81(5-6):901–934, 1995.

[4] A. Pulvirenti and G. Toscani. The theory of the nonlinear Boltzmann equation for Maxwell molecules in Fourier representation. *Ann. Mat. Pura Appl. (4)*, 171:181-204, 1996.

[5] E. A. Carlen, E. Gabetta, and G. Toscani. Propagation of smoothness and the rate of exponential convergence to equilibrium for a spatially homogeneous Maxwellian gas. *Comm. Math. Phys.*, 199(3):521–546, 1999.

[6] G. Toscani and C. Villani. Probability metrics and uniqueness of the solution to the Boltzmann equation for a Maxwell gas. *J. Stat. Phys.*, 94(3-4):619–637, 1999.

[7] A. V. Bobylev and C. Cercignani. Self-similar solutions of the Boltzmann equation and their applications. *J. Stat. Phys.*, 106(5-6):1039–1071, 2002.

[8] C. Villani. A review of mathematical topics in collisional kinetic theory. In S. Friedlander and D. Serre, editors, *Handbook of Mathematical Fluid Mechanics*, volume I, pages 71–305. North-Holland, 2002.

[9] L. Desvillettes. About the use of the Fourier transform for the Boltzmann equation. volume 2*, pages 1–99. 2003. Summer School on "Methods and Models of Kinetic Theory" (M&MKT 2002).

[10] C. Villani. Mathematics of granular materials. *J. Stat. Phys.*, 124(2-4):781–822, 2006.

[11] J. A. Carrillo, G. Toscani Contractive probability metrics and asymptotic behavior of dissipative kinetic equations. *Riv. Mat. Univ. Parma*, 7(6):75–198, 2007.

[12] A. V. Bobylev, C. Cercignani, and I. M. Gamba. On the self-similar asymptotics for generalized nonlinear kinetic Maxwell models. *Comm. Math. Phys.*, 291(3):599–644, 2009.

[13] N. Fournier and C. Mouhot. On the well-posedness of the spatially homogeneous Boltzmann equation with a moderate angular singularity. *Comm. Math. Phys.*, 289(3):803–824, 2009.

[14] M. Cannone and G. Karch. Infinite energy solutions to the homogeneous Boltzmann equation. *Comm. Pure Appl. Math.*, 63(6):747–778, 2010.

[15] Y. Morimoto. A remark on Cannone-Karch solutions to the homogeneous Boltzmann equation for Maxwellian molecules. *Kinet. Relat. Models*, 5(3):551–561, 2012.

[16] X. Lu and C. Mouhot. On measure solutions of the Boltzmann equation, part I: moment production and stability estimates. *J. Differential Equations*, 252(4):3305–3363, 2012.

[17] M. Cannone and G. Karch. On self-similar solutions to the homogeneous Boltzmann equation. *Kinet. Relat. Models*, 6(4):801–808, 2013.

[18] X. Lu and C. Mouhot. On measure solutions of the Boltzmann equation, Part II: Rate of convergence to equilibrium. *J. Differential Equations*, 258(11):3742–3810, 2015.

[19] N. Fournier. Finiteness of entropy for the homogeneous Boltzmann equation with measure initial condition. *Ann. Appl. Probab.*, 25(2):860–897, 2015.

[20] Y. Morimoto, S. Wang, and T. Yang. A new characterization and global regularity of infinite energy solutions to the homogeneous Boltzmann equation. *J. Math. Pures Appl. (9)*, 103(3):809–829, 2015.

[21] Y. Morimoto, S. Wang, and T. Yang. Measure valued solutions to the spatially homogeneous Boltzmann equation without angular cutoff. *J. Stat. Phys.*, 165(5):866–906, 2016.

[22] Y. Morimoto, T. Yang, and H. Zhao. Convergence to self-similar solutions for the homogeneous Boltzmann equation. *J. Eur. Math. Soc.*, 19(8):2241–2267, 2017.

[23] K. Qi. Measure Valued Solution to the Spatially Homogeneous Boltzmann Equation with Inelastic Long-Range Interactions. *Preprint*, 2020.

[24] A. V. Bobylev, A. Nota, J. J. L. Velázquez. Self-similar asymptotics for a modified Maxwell-Boltzmann equation in systems subject to deformations. *Comm. Math. Phys.*, 380(1):409–448, 2020.

[25] K. Qi. On the measure valued solution to the inelastic Boltzmann equation with soft potentials. *J. Stat. Phys.*, 183(27), 2021.