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 Introduction of Boltzmann Equation

3.1 The Spatially Homogeneous Boltzmann Equation

In the spatially homogeneous theory of the Boltzmann equation, one is interested in the solution $f(t,x,v)$ which does not depend on the x space variable. This view of point is pretty common in physics, especially when it comes to the problems focusing on the collision operator, as the collision integral operator only acts on the velocity dependence. On the other hand, the interests towards the spatially homogeneous study also arise from the numerical analysis, since almost all numerical schemes succeed from the splitting of the transport step and collision step.

In this case, the homogeneous Boltzmann equation in $\mathbb{R}^3$ reads:

$$\partial_t f(t,v) = Q(f,f)(t,v), \tag{3.1}$$

with the non-negative initial condition,

$$f(0,v) = F_0(v), \tag{3.2}$$

where the unknown $f = f(t,v)$ is regarded as the density function of a probability distribution, or more generally, a probability measure; and the initial datum F_0 is also assumed to be a non-negative probability measure on $\mathbb{R}^3$.

The right hand side of (3.1) is the so-called Boltzmann collision operator,

$$\begin{aligned} Q(f,f)(v) &= \int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B_\sigma(v-v_*,\sigma)\left[f(v')f(v'_*) - f(v)f(v_*)\right]\,\mathrm{d}\sigma\,\mathrm{d}v_* \\ &= \int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B_\omega(v-v_*,\sigma)\left[f(v')f(v'_*) - f(v)f(v_*)\right]\,\mathrm{d}\omega\,\mathrm{d}v_*, \end{aligned} \tag{3.3}$$

where (v', v'_*) and (v, v_*) represent the velocity pairs before and after a collision, which satisfy the conservation of momentum and energy:

$$v' + v'_* = v + v_*, \quad |v'|^2 + |v'_*|^2 = |v|^2 + |v_*|^2, \tag{3.4}$$

so that (v', v'_*) can be expressed in terms of (v, v_*) as

$$\begin{aligned} v' = \frac{v+v_*}{2} + \frac{|v-v_*|}{2}\sigma, \quad v'_* = \frac{v+v_*}{2} - \frac{|v-v_*|}{2}\sigma, \\ \text{or} \quad v' = v - [(v-v_*)\cdot\omega]\omega, \quad v'_* = v + [(v-v_*)\cdot\omega]\omega, \end{aligned} \tag{3.5}$$

where both of σ and ω are a vector varying over the unit sphere $\mathbb{S}^2$.

And this also easily implies the relations

$$v\cdot v_* = v'\cdot v'_*, \quad |v-v_*| = |v'-v'_*|, \quad (v-v_*)\cdot\omega = -(v'-v'_*)\cdot\omega. \tag{3.6}$$

and

$$|\langle v-v_*,\omega\rangle| = |v-v_*|\cos\alpha = |v-v_*|\cos\left(\frac{\pi-\theta}{2}\right) = |v-v_*|\sin\frac{\theta}{2}, \tag{3.7}$$

where α denotes that angle between $v-v_*$ and ω.

Next, we have a more general relation between the σ- and ω- representation in the sense that,

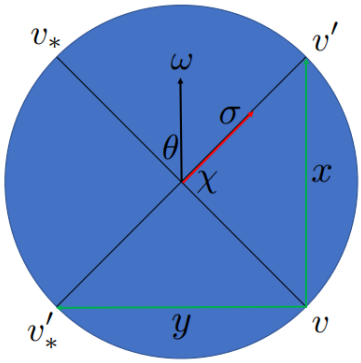

Figure 1: Velocity and unit vector during a classical elastic collision.

Lemma 3.1. *For the change of variables:*

$$\sigma = \frac{v - v_*}{|v - v_*|} - 2\left\langle \frac{v - v_*}{|v - v_*|}, \omega \right\rangle, \tag{3.8}$$

it has the Jacobian:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\omega} = 2^{d-1}\left|\left\langle \frac{v - v_*}{|v - v_*|}, \omega \right\rangle\right|^{d-2}. \tag{3.9}$$

Proof. Fix the unitary vector $\hat{q} = \frac{v-v_*}{|v-v_*|}$ and $\left\langle \frac{v-v_*}{|v-v_*|}, \omega \right\rangle = \hat{q} \cdot \omega$, then the change of variables can be regarded as a map $\sigma(\omega) : \mathbb{S}^{d-1} \longmapsto \mathbb{S}^{d-1}$ give by:

$$\sigma(\omega) = \hat{q} - 2\left(\hat{q} \cdot \omega\right)\omega. \tag{3.10}$$

Let $\mathcal{O}_{\hat{q}}$ be the orthogonal space to $\hat{q}$, α be the angle between $\hat{q}$ and ω, and θ be the angle between $\hat{q}$ and σ. In this way, one may write

$$\omega = \cos\alpha\hat{q} + \omega_o, \quad \sigma = \cos\theta\hat{q} + \sigma_o \tag{3.11}$$

where $\omega_o, \sigma_o \in \mathcal{O}_{\hat{q}}$. Using the spherical coordinates with north pole given by $\hat{q}$, the measures $\mathrm{d}\omega$ and $\mathrm{d}\sigma$ are given by

$$\mathrm{d}\omega = \sin^{d-2}\alpha \mathrm{d}\hat{\omega_o}\mathrm{d}\alpha, \quad \mathrm{d}\sigma = \sin^{d-2}\theta \mathrm{d}\hat{\sigma_o}\mathrm{d}\theta \tag{3.12}$$

where the measures $\mathrm{d}\hat{\omega_o}$ and $\mathrm{d}\hat{\sigma_o}$ are the Lebesgue measure in $\mathbb{S}^{d-2}(\hat{q})$ parameterized with the vectors ω_o, σ_o respectively. Directly from the expression of the map (by inner product $\hat{q}$ to Eq. (3.10)), we find

$$\cos\theta = \hat{q} \cdot \sigma = 1 - 2\left(\hat{q} \cdot \omega\right)^2 = 1 - 2\cos^2\alpha. \tag{3.13}$$

Then, it follows by direct differentiation that

$$-\sin\theta \mathrm{d}\theta = 4\cos\alpha\sin\alpha \mathrm{d}\alpha. \tag{3.14}$$

Now, choose a orthonormal base $\{\xi_j\}_{j=1}^{d-2}$ for $\mathcal{O}_{\hat{q}}$. Compute again using the explicit expression of the map

$$\begin{aligned}\sigma_o =& \sum_{j=1}^{d-2} (\sigma \cdot \xi_j)\, \xi_j = -2\,(\hat{q}\cdot\omega) \sum_{j=1}^{d-2} (\omega \cdot \xi_j)\, \xi_j \\ =& -2\,(\hat{q}\cdot\omega)\,\omega_o = -2\cos\alpha\omega_o.\end{aligned} \tag{3.15}$$

Thus, $\hat{\omega_o} = \hat{\sigma_o}$, and as a consequence, $\mathrm{d}\hat{\omega_o} = \mathrm{d}\hat{\sigma_o}$. Gathering these relations Eq. (3.12) and Eq. (3.14) all together, and using the basic trigomometry

$$\mathrm{d}\omega = \left(\frac{\sin\alpha}{\sin\theta}\right)^{d-3} \frac{\mathrm{d}\sigma}{4|\cos\alpha|} = \frac{\mathrm{d}\sigma}{2^{d-1}|\cos\alpha|^{d-2}}. \tag{3.16}$$

This completes the proof. □

Lemma 3.2. *Fix $\sigma \in \mathbb{S}^{d-1}$ and $q = v - v_*$, the map $u : \mathbb{R}^d \longmapsto \mathbb{R}^d$ given by*

$$u(q) = \frac{q + |q|\sigma}{2} \tag{3.17}$$

has the Jacobian:

$$\frac{\mathrm{d}u}{\mathrm{d}q} = \frac{1 + \sigma\cdot\hat{q}}{2^d}. \tag{3.18}$$

Proof. Choose an orthonormal base $\{\sigma, \xi_j\}$ with $2 \le j \le d$. Then, the coordinates of this change of variables are

$$\begin{aligned}u_1 =& u\cdot\sigma = \frac{1}{2}\,(q\cdot\sigma + |q|) = \frac{1}{2}\,(q_1 + |q|)\,, \\ u_j =& u\cdot\xi_j = \frac{1}{2}q_j, \quad j = 2, ..., d.\end{aligned} \tag{3.19}$$

Thus,

$$\frac{\partial u_1}{\partial q_1} = \frac{1}{2}\,(1 + \hat{q}\cdot\sigma)\,, \quad \frac{\partial u_j}{\partial q_l} = \frac{1}{2}\delta_{jl}, \quad j = 2, ..., d. \tag{3.20}$$

and, therefore,

$$\frac{\mathrm{d}u}{\mathrm{d}q} = \prod_{j=1}^{d} \left|\frac{\partial u_j}{\partial q_j}\right| = \frac{1 + \hat{q}\cdot\sigma}{2^d}. \tag{3.21}$$

□

3.2 The Boltzmann collision kernel.

The collision kernel B is a non-negative function that depends only on $|v - v_*|$ and cosine of the deviation angle θ, whose specific form can be determined from the intermolecular potential using classical scattering theory.

$$B(v - v_*, \sigma) = B(|v - v_*|, \cos\theta), \quad \cos\theta = \frac{\sigma\cdot(v - v_*)}{|v - v_*|}, \tag{3.22}$$

For a given impact parameter $p \geq 0$ and relative velocity $v - v_*$, let the deviation angle θ be

$$\theta(p, v - v_*) = \pi - 2p \int_{r_0}^{+\infty} \frac{\mathrm{d}r/r^2}{\sqrt{1 - \frac{p^2}{r^2} - 4\frac{U(r)}{|v-v_*|^2}}} \overset{u=p/r}{=\!=\!=} \pi - \int_0^{\frac{p}{r_0}} \frac{\mathrm{d}u}{\sqrt{1 - u^2 - \frac{4}{|v-v_*|^2} U(\frac{p}{u})}}, \tag{3.23}$$

where r_0 is the positive root of

$$1 - \frac{p^2}{r_0^2} - 4\frac{U(r)}{|v - v_*|^2} = 0, \tag{3.24}$$

then the collision kernel B is implicitly defined by

$$B(v - v_*, \sigma) = B(|v - v_*|, \cos\theta) = \underbrace{\frac{p}{\sin\theta}\frac{\mathrm{d}p}{\mathrm{d}\theta}}_{\text{scattering cross section}} |v - v_*|. \tag{3.25}$$

For example, in the case of **Inverse Power Law Potentials** $U(r) = r^{-(\ell-1)} = r^{-\frac{1}{s}}$ with $2 < \ell < \infty$ or $0 < s = \frac{1}{\ell-1} < 1$, where r is the distance between two interacting particles, B can be separated as the kinetic part and angular part:

$$B(v - v_*, \sigma) = B(|v - v_*|, \cos\theta) = b(\cos\theta)\Phi(|v - v_*|),^{1} \tag{3.26}$$

where, for $d = 3$, the kinetic part

$$\Phi(|v - v_*|) = |v - v_*|^\gamma = \begin{cases} \gamma > 0, \text{ Hard potential,} \\ \gamma = 0, \text{ Maxwellian gas,} \\ \gamma < 0, \text{ Soft potential.} \end{cases} \qquad \gamma = 1 - 4s = \frac{\ell - 5}{\ell - 1} > -3,^{2}$$

and the angular part

$$\sin^{d-2}\theta b(\cos\theta)\big|_{\theta \to 0^+} \sim K\theta^{-1-\nu}, \quad 0 < \nu = \frac{2}{\ell - 1} = 2s < 2. \tag{3.27}$$

The kernel (3.26) encompasses a wide range of potentials, among which we mention three extreme cases [8]:

(i) $\gamma = 1$ corresponds to the hard spheres, where B is only proportional to $|v - v_*|$,

$$B(|v - v_*|, \cos\theta) = K|v - v_*|, \quad K > 0; \tag{3.28}$$

(ii) $\ell = 2$, $\gamma = -3$, $\nu = 2$ corresponds to the Coulomb interaction, where B is given by the famous Rutherford formula,

$$B(|v - v_*|, \cos\theta) = \frac{1}{|v - v_*|^3 \sin^4(\theta/2)}; \tag{3.29}$$

(iii) $\ell = 5$, $\gamma = 0$, $\nu = \frac{1}{2}$ corresponds to the literally physical Maxwellian gas, where B does not depend on relative velocity $|v - v_*|$,

$$B(|v - v_*|, \cos\theta) = b\left(\frac{v - v_*}{|v - v_*|} \cdot \sigma\right) = b(\cos\theta). \tag{3.30}$$

[1] In this case, the cross section is approximate to $\sim \frac{p}{\sin\theta}\frac{\mathrm{d}p}{\mathrm{d}\theta}|v - v_*| \sim \left(\sin\frac{\theta}{2}\right)^{-2-2s} |v - v_*|^{1-4s}$.

[2] This is why we usually assume $\gamma + 2s > -1$, since $\gamma + 4s = 1$ and $0 < s < 1$.

However, instead of this very special case above, we are interested in the more general case $B = b(\cos\theta)$, not depending on $|v - v_*|$ that,

$$\gamma = 0, \quad 0 < \nu < 2, \tag{3.31}$$

which is called Maxwellian molecules type.

The range of deviation angle θ, namely the angle between pre- and post-collisional velocities, is a full interval $[0, \pi]$, but it is customary to restrict it to $[0, \pi/2]$ mathematically, replacing $b(\cos\theta)$ by its "symmetrized" version [21]:

$$[b(\cos\theta) + b(\cos(\pi - \theta))]\, \mathbf{1}_{0 \le \theta \le \frac{\pi}{2}}, \tag{3.32}$$

which amounts more or less to forbidding the exchange of particles.

Another physically interesting example that is not explicit at all has been called **Debye-Yukawa Potential** $U(r) = \mathrm{e}^{-r}/r$, also asymptotically behaving as $\theta \to 0$:

$$\sin^{d-2}\theta B(|v - v_*|, \cos\theta)\Big|_{\theta \to 0^+} \sim K|v - v_*|\theta^{-1}|\log\theta^{-1}|. \tag{3.33}$$

3.3 Cutoff VS Non-cutoff

As it has been long known, the main difficulty in establishing the well-posedness result for Boltzmann equation is that the singularity of the collision kernel b is not locally integrable in $\sigma \in \mathbb{S}^2$. To avoid this, H. Grad gave the integrable assumption on the collision kernel b_c by a "**Cutoff** " near singularity:

$$\int_{\mathbb{S}^2} b_c\left(\frac{v - v_*}{|v - v_*|} \cdot \sigma\right) \mathrm{d}\sigma = 2\pi \int_0^{\frac{\pi}{2}} b_c(\cos\theta)\sin\theta\, \mathrm{d}\theta < \infty. \tag{3.34}$$

However, the full singularity condition for the collision kernel with **Non-cutoff Assumption** is implicitly defined for the angular collision part $b(\cos\theta)$, which asymptotically behaves as $\theta \to 0^+$,

$$\sin\theta b(\cos\theta)\big|_{\theta \to 0^+} \sim K\theta^{-1-\nu}, \quad 0 < \nu = \frac{2}{\ell - 1} = 2s < 2 \quad \text{and} \quad K > 0, \tag{3.35}$$

or in "symmetrized" manner,

$$\exists \alpha_0 \in (0, 2], \quad \text{such that} \quad \int_0^{\frac{\pi}{2}} \sin^{\alpha_0}\left(\frac{\theta}{2}\right) b(\cos\theta)\sin\theta \mathrm{d}\theta < \infty, \tag{3.36}$$

which can handle the strongly singular kernel b in Eq. (3.35) with some $0 < \nu < 2$ and $\alpha_0 \in (\nu, 2]$. Besides, we further illustrate that the non-cutoff assumption Eq. (3.36) can be rewritten as

$$(1 - \tau)^{\frac{\alpha_0}{2}} b(\tau) \in L^1[0, 1), \quad \text{for } \alpha_0 \in (0, 2], \tag{3.37}$$

by means of the transformation of variable $s = \cos\theta$ in the symmetric version of b. As mentioned in [15, Remark 1], the full non-cutoff assumption Eq. (3.36), or equivalently Eq. (3.37), is the extension of the mild non-cutoff assumption of the collision kernel b used in [14], namely,

$$(1 - \tau)^{\frac{\alpha_0}{4}} (1 + \tau)^{\frac{\alpha_0}{4}} b(\tau) \in L^1(-1, 1), \quad \text{for } \alpha_0 \in (0, 2]. \tag{3.38}$$

3.4 The Weak Formulation and Conservation Law

To derive the weak formulation, a universal tool (so-called *Pre-postcollisional change of variables*) is frequently used, which is an involutive change of variables with unit Jacobian,

$$(v, v_*, \sigma) \to (v', v'_*, \hat{q}), \tag{3.39}$$

where $\hat{q}$ is the unit vector along the relative velocity $q := v - v_*$,

$$\hat{q} = \frac{v - v_*}{|v - v_*|}. \tag{3.40}$$

Lemma 3.3. *For a fixed ω, the Jacabian matrix induced from $(v, v_*) \to (v', v'_*)$ satisfies*

$$\left| \frac{\partial(v', v'_*)}{\partial(v, v_*)} \right| = -1 \tag{3.41}$$

Proof. Considering the relation between the pre-and post-collision velocities:

$$v' = v - a\omega, \quad v'_* = v + a\omega \tag{3.42}$$

where

$$a = [(v - v_*) \cdot \omega] = \sum_{i=1}^{3} (v_i - v_{*i})\omega_i \text{ with } a_{v_j} = \frac{\partial a}{\partial v_j} = \omega_j, \quad a_{v_{*j}} = \frac{\partial a}{\partial v_{*j}} = -\omega_j \tag{3.43}$$

then we can rewrite the Jacobian $\left| \frac{\partial(v', v'_*)}{\partial(v, v_*)} \right|$ in 3×3 blocks:

$$\left| \frac{\partial(v', v'_*)}{\partial(v, v_*)} \right| = \begin{pmatrix} \frac{\partial v'_i}{\partial v_j} & \frac{\partial v'_{*i}}{\partial v_j} \\ \frac{\partial v'_i}{\partial v_{*j}} & \frac{\partial v'_{*i}}{\partial v_{*j}} \end{pmatrix} = \begin{pmatrix} \delta_{ij} - \omega_i a_{v_j} & \omega_i a_{v_j} \\ -\omega_i a_{v_{*j}} & \delta_{ij} + \omega_i a_{v_{*j}} \end{pmatrix} \tag{3.44}$$

Now add the fourth column to the first column, add the fifth column to the second column, and add the sixth column to the third column. Then, we have

$$\left| \frac{\partial(v', v'_*)}{\partial(v, v_*)} \right| = \begin{pmatrix} I & \omega_i a_{v_j} \\ I & \delta_{ij} + \omega_i a_{v_{*j}} \end{pmatrix} \tag{3.45}$$

Next subtract the first row from the fourth row, subtract the second row from the fifth row, and subtract the third row from the sixth row. This leads to

$$\left| \frac{\partial(v', v'_*)}{\partial(v, v_*)} \right| = \begin{pmatrix} I & \omega_i a_{v_j} \\ 0 & \delta_{ij} + \omega_i b_j \end{pmatrix} \tag{3.46}$$

where $b_j = a_{v_{*j}} - a_{v_j}$. Thus, $\left| \frac{\partial(v', v'_*)}{\partial(v, v_*)} \right| = \det(\delta_{ij} + \omega_i b_j)$ which is now a 3×3 matrix computation.

Since $b_j = a_{v_{*j}} - a_{v_j} = -2\omega_j$,

$$\begin{aligned}\left|\frac{\partial(v', v_*')}{\partial(v, v_*)}\right| &= \det(\delta_{ij} + \omega_i b_j) \\ &= \begin{vmatrix} 1-2\omega_1^2 & -2\omega_1\omega_2 & -2\omega_1\omega_3 \\ -2\omega_2\omega_1 & 1-2\omega_2^2 & -2\omega_2\omega_3 \\ -2\omega_3\omega_1 & -2\omega_2\omega_3 & 1-2\omega_3^2 \end{vmatrix} \\ &= \left(1-2\omega_1^2\right)\left[(1-2\omega_2^2)(1-2\omega_3^2) - 4\omega_2^2\omega_3^2\right] \\ &\quad + 2\omega_1\omega_2\left[-2\omega_1\omega_2(1-2\omega_3^2) - 4\omega_2^2\omega_3^2\right] \\ &\quad - 2\omega_1\omega_3\left[4\omega_1\omega_2^2\omega_3 + 2\omega_1\omega_3(1-2\omega_2^2)\right] \\ &= -1\end{aligned} \tag{3.47}$$

which implies the absolute value of the Jacobian $\left|\frac{\partial(v', v_*')}{\partial(v, v_*)}\right|$ is unity. □

Remark 3.4. *For the inelastic collision, where the restitution coefficient e is chosen as a suitable function of the impact velocity, i.e., $e = e(|[(v - v_*) \cdot \omega]|)$ as well as the following assumptions:*

- *The mapping $r \in \mathbb{R}_+ \longmapsto e(r) \in (0, 1]$ is absolutely continuous.*
- *The mapping $r \in \mathbb{R}_+ \longmapsto \vartheta(r) := re(r)$ is strictly increasing.*

Then, the Jacobian of the following transformation

$$v' = v - \frac{1+e}{2}([(v - v_*) \cdot \omega])\omega, \quad v_*' = v_* + \frac{1+e}{2}([(v - v_*) \cdot \omega])\omega \tag{3.48}$$

can be computed as, since $[(v - v_*) \cdot \omega] = q \cdot \omega$

$$\left|\frac{\partial(v', v_*')}{\partial(v, v_*)}\right| = e(|q \cdot \omega|) + |q \cdot \omega|\frac{\mathrm{d}e(|q \cdot \omega)|}{\mathrm{d}r} = \frac{\mathrm{d}\vartheta(|q \cdot \omega|)}{\mathrm{d}r} > 0. \tag{3.49}$$

On the other hand, since $\sigma = (v' - v_*')/|v' - v_*'|$, the change of variables (3.39) formally amounts to the change of (v, v_*) and (v', v_*'). Hence, under suitable integrability conditions on the measurable function F,

$$\begin{aligned}&\int_{\mathbb{S}^2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} B(|v - v_*|, \hat{q} \cdot \sigma)F(v, v_*, v', v_*')\,\mathrm{d}v\,\mathrm{d}v_*\,\mathrm{d}\sigma \\ =&\int_{\mathbb{S}^2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} B(|v - v_*|, \hat{q} \cdot \sigma)F(v, v_*, v', v_*')\,\mathrm{d}v'\,\mathrm{d}v_*'\,\mathrm{d}\sigma \\ =&\int_{\mathbb{S}^2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} B(|v - v_*|, \hat{q} \cdot \sigma)F(v', v_*', v, v_*)\,\mathrm{d}v\,\mathrm{d}v_*\,\mathrm{d}\sigma,\end{aligned} \tag{3.50}$$

where the fact $|v' - v_*'| = |v - v_*|, \sigma \cdot \hat{q} = \hat{q} \cdot \sigma$ is used to keep the arguments of collision kernel $B(v - v_*, \sigma) = B(|v - v_*|, \hat{q} \cdot \sigma)$ unchanged. Note that the change of variables $(v, v_*) \to (v', v_*')$ *works for a fixed ω but is illegal for any given σ.*

With the help of this micro-reversiblity of velocity from (v, v) to (v', v_*'), which leaves the collision kernel B invariant, we can obtain the following weak form for the Boltzmann collision operator.

Proposition 3.5. *For any test function ϕ that is an arbitrarily continuous function of the velocity v,*

$$\begin{aligned}\int_{\mathbb{R}^3} Q(f,f)\phi \,\mathrm{d}v &= \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(v-v_*,\omega)(f'f'_* - ff_*)\phi \,\mathrm{d}\omega \,\mathrm{d}v_* \,\mathrm{d}v \\ &= \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(v-v_*,\omega)ff_*(\phi' - \phi) \,\mathrm{d}\omega \,\mathrm{d}v_* \,\mathrm{d}v \\ &= \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(v-v_*,\omega)ff_*(\phi' + \phi'_* - \phi - \phi_*) \,\mathrm{d}\omega \,\mathrm{d}v_* \,\mathrm{d}v \\ &= \frac{1}{4}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(v-v_*,\omega)(f'f'_* - ff_*)(\phi + \phi_* - \phi' - \phi'_*) \,\mathrm{d}\omega \,\mathrm{d}v_* \,\mathrm{d}v.\end{aligned} \tag{3.51}$$

Proof. **Step 1:** Swap v and v^*, as $B(v-v_*,\omega) = B(|v-v_*|,\omega)$ is invariant, and notice that

$$\begin{aligned}v' =& v - [\omega\cdot(v-v_*)]\omega \to v_* - [\omega\cdot(v_*-v)]\omega = v'_* \\ v'_* =& v + [\omega\cdot(v-v_*)]\omega \to v + [\omega\cdot(v_*-v)]\omega = v'\end{aligned} \tag{3.52}$$

we have

$$\begin{aligned}\int_{\mathbb{R}^3} Q(f,f)\phi \,\mathrm{d}v &= \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(v-v_*,\omega)(f'f'_* - ff_*)\phi \,\mathrm{d}\omega \,\mathrm{d}v_* \,\mathrm{d}v \\ &\xLeftrightarrow{v\leftrightarrow v_*} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(v-v_*,\omega)(f'f'_* - ff_*)\phi_* \,\mathrm{d}\omega \,\mathrm{d}v_* \,\mathrm{d}v \\ &\xLeftrightarrow{\text{add and divided}} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(|v-v_*|,\omega)(f'f'_* - ff_*)\frac{\phi+\phi_*}{2} \,\mathrm{d}\omega \,\mathrm{d}v_* \,\mathrm{d}v\end{aligned} \tag{3.53}$$

Step 2: Apply the pre-post velocity transformation $(v,v_*) \longmapsto (v',v'_*)$ for a fixed ω with the unit Jacobian $\mathrm{d}v\mathrm{d}v_* = \mathrm{d}v'\mathrm{d}v'_*$, and $B(|v-v_*|,\omega)$ is still invariant, since by the conservation of momentum and energy as in Eq. (3.4)

$$|v-v_*|^2 = 2|v|^2 + 2|v_*|^2 - |v+v_*|^2 = |v'-v'_*|^2. \tag{3.54}$$

we continue with Eq. (3.53) above that

$$\begin{aligned}&\xLeftrightarrow{(v,v_*)\longmapsto(v',v'_*)} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(|v-v_*|,\omega)\left|\frac{\partial(v,v_*)}{\partial(v',v'_*)}\right| \\ &\qquad \left[f'f'_* - f\big(v(v',v'_*)\big)f\big(v_*(v',v'_*)\big)\right]\frac{\phi\big(v(v',v'_*)\big) + \phi\big(v_*(v',v'_*)\big)}{2} \,\mathrm{d}\omega \,\mathrm{d}v'_* \,\mathrm{d}v'\end{aligned} \tag{3.55}$$

where, by the definition Eq. (3.5)

$$\begin{aligned}&v' - v'_* = v - v_* - 2[(v-v_*)\cdot\omega]\omega \\ \Longrightarrow\ &(v'-v'_*)\cdot\omega = (v-v_*)\cdot\omega - 2[(v-v_*)\cdot\omega] = -(v-v_*)\cdot\omega\end{aligned} \tag{3.56}$$

we can invert these to find $v(v',v'_*)$ and $v_*(v',v'_*)$:

$$\begin{aligned}v = v' + [(v-v_*)\cdot\omega]\omega \Leftrightarrow v' - [(v'-v'_*)\cdot\omega]\omega \equiv v(v',v'_*) \\ v_* = v' - [(v-v_*)\cdot\omega]\omega \Leftrightarrow v'_* + [(v'-v'_*)\cdot\omega]\omega \equiv v_*(v',v'_*)\end{aligned} \tag{3.57}$$

Then, rename (v', v'_*) by (v, v_*),

$$\begin{aligned}
&\Longleftrightarrow \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(|v'-v'_*|,\omega)\Big(ff_* - f\big(\underbrace{v-[(v-v_*)\cdot\omega]\omega}_{:=v'}\big)f\big(\underbrace{v_*+[(v-v_*)\cdot\omega]\omega}_{:=v'_*}\big)\Big)\\
&\qquad\qquad \frac{\phi\big(v-[(v-v_*)\cdot\omega]\omega\big)+\phi\big(v_*+[(v-v_*)\cdot\omega]\omega\big)}{2}\,\mathrm{d}\omega\,\mathrm{d}v_*\,\mathrm{d}v\\
&\Longleftrightarrow \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(|v-v_*|,\omega)(ff_*-f'f'_*)\frac{\phi'+\phi'_*}{2}\,\mathrm{d}\omega\,\mathrm{d}v_*\,\mathrm{d}v
\end{aligned} \tag{3.58}$$

Step 3: By adding the last equality in Eq. (3.53) and that in Eq. (3.58), and divided to obtain

$$\xLeftrightarrow{\text{add and divided}} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(v-v_*,\omega)(f'f'_*-ff_*)\frac{\phi+\phi_*-\phi'-\phi'_*}{4}\,\mathrm{d}\omega\,\mathrm{d}v_*\,\mathrm{d}v \tag{3.59}$$

Step 4: The second equality in Eq. (3.51) is obtained by changing $(v, v_*) \longmapsto (v', v'_*)$ only to the gain term. □

Remark 3.6. *There is another proof based on the bilinear form of the collision operator $Q^*(f,g)$ as following:*

$$Q^*(g,f) = \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(v-v_*,\omega)(g'f'_*+f'g'_*-gf_*-fg_*)\,\mathrm{d}\omega\,\mathrm{d}v_*\,\mathrm{d}v \tag{3.60}$$

Then Q^* is symmetric and $Q^*(f,f) = Q(f,f)$.

Similarly, for suitable test function ϕ,

$$\begin{aligned}
&\int_{\mathbb{R}^3} Q^*(g,f)\phi\,\mathrm{d}v\\
\xLeftrightarrow{Def}\ &\frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(|v-v_*|,\omega)(g'f'_*+f'g'_*-gf_*-fg_*)\phi\,\mathrm{d}\omega\,\mathrm{d}v_*\,\mathrm{d}v\\
\xLeftrightarrow{Step1: v\leftrightarrow v_*}\ &\frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(|v-v_*|,\omega)(g'f'_*+f'g'_*-gf_*-fg_*)\phi_*\,\mathrm{d}\omega\,\mathrm{d}v_*\,\mathrm{d}v\\
\xLeftrightarrow{Step2: (v,v_*)\longmapsto(v',v'_*)}\ &\frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(|v'-v'_*|,\omega)(gf_*+fg_*-g'f'_*-f'g'_*)\phi'\,\mathrm{d}\omega\,\mathrm{d}v'_*\,\mathrm{d}v'\\
\xLeftrightarrow{Step1: v\leftrightarrow v_*}\ &\frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(|v-v_*|,\omega)(gf_*+fg_*-g'f'_*-f'g'_*)\phi'_*\,\mathrm{d}\omega\,\mathrm{d}v'_*\,\mathrm{d}v'
\end{aligned} \tag{3.61}$$

By taking $g = f$, adding the four choices and divided, we finally get the same quadratic form:

$$\int_{\mathbb{R}^3} Q(f,f)\phi\,\mathrm{d}v = \frac{1}{4}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(v-v_*,\omega)(f'f'_*-ff_*)(\phi+\phi_*-\phi'-\phi'_*)\,\mathrm{d}\omega\,\mathrm{d}v_*\,\mathrm{d}v. \tag{3.62}$$

3.5 Boltzmann's H–Theorem and Equilibrium State

Recall the weak formulation (3.51) of the Boltzmann equation as in (3.5), there is an immediate consequence for a solution f to the Boltzmann equation that, whenever ϕ

satisfies the functional equation,

$$\forall (v, v_*, \sigma) \in \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2, \qquad \phi(v') + \phi(v'_*) = \phi(v) + \phi(v_*), \tag{3.63}$$

then, we at least formally have,

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathbb{R}^3} f(t,v)\phi(v)\,\mathrm{d}v = \int_{\mathbb{R}^3} Q(f,f)\phi\,\mathrm{d}v = 0, \tag{3.64}$$

and this kind of ϕ is usually called the *collision invariant*.

Since the mass, momentum and energy are conserved during the classical elastic collisions, it is natural to find that the functions $1, v_j, 1 \le j \le 3$, and $|v|^2$ and any linear combination of them are the collision invariants, which can be actually shown as the only collision invariants. Together with the weak form, this leads to the formal conservation law of the Boltzmann equation,

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathbb{R}^3} f(t,v) \begin{pmatrix} 1 \\ v_j \\ |v|^2 \end{pmatrix} \mathrm{d}v = \int_{\mathbb{R}^3} Q(f,f)(t,v) \begin{pmatrix} 1 \\ v_j \\ |v|^2 \end{pmatrix} \mathrm{d}v = 0, \qquad 1 \le j \le 3. \tag{3.65}$$

In particular, at a given time t, one can define the local density ρ, the local macroscopic velocity u, and the local temperature T, by

$$\rho = \int_{\mathbb{R}^3} f(t,v)\,\mathrm{d}v, \quad \rho u = \int_{\mathbb{R}^3} f(t,v) v\,\mathrm{d}v, \quad \rho|u|^2 + d\rho T = \int_{\mathbb{R}^3} f(t,v)|v|^2\,\mathrm{d}v, \tag{3.66}$$

then the equilibrium is the **Maxwellian Equilibrium Distribution**,

$$\mathcal{M}(v) = \mathcal{M}^f(v) = \frac{1}{(2\pi T)^{d/2}}\,\mathrm{e}^{-\frac{|v-u|^2}{2T}}. \tag{3.67}$$

If not caring about the integrability issues, we select the test function $\phi = \log f$ into the weak form (3.51), and consider the properties of the logarithm function, to find that

$$\begin{aligned} -\int_{\mathbb{R}^3} Q(f,f)\ln f\,\mathrm{d}v =& D(f) \\ =& \frac{1}{4}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(v-v_*,\sigma)(f'f'_* - ff_*)\ln\frac{f'f'_*}{ff_*} \ge 0 \end{aligned} \tag{3.68}$$

due to the fact that the function $(X,Y) \longmapsto (X-Y)(\ln X - \ln Y)$ is always non-negative. Thus, if we introduce Boltzmann's H–functional,

$$H(f) = \int_{\mathbb{R}^3} f\ln f\,\mathrm{d}v, \tag{3.69}$$

then the $H(f)$ will evolve in time because of the collisional effect that

$$\frac{\mathrm{d}}{\mathrm{d}t} H(f(t,\cdot)) = -D(f(t,\cdot)) \le 0, \tag{3.70}$$

which is the well-known Boltzmann's H–Theorem: the H–functional, or entropy, is non-increasing with time evolution.

And the equality holds if and only if $\ln f$ is a collision invariant, i.e., $f = \exp(a + b\cdot v + c|v|^2)$ with a, b, c being all constants. In the following Lemma, we will show that the collision invariant satisfying (3.63) must be of form given as $\ln f = a + b\cdot v + c|v|^2$ if ϕ is assumed to be continuous.

Lemma 3.7. *Let ϕ be continuous and satisfy*

$$\phi(v') + \phi(v'_*) = \phi(v) + \phi(v_*), \quad \forall (v, v_*, \sigma) \in \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2. \tag{3.71}$$

Then there exists constants $a, c \in \mathbb{R}$ and a constant vector $b \in \mathbb{R}^3$ such that

$$\phi(v) = a + b \cdot v + c|v|^2. \tag{3.72}$$

Proof. By hypothesis,

$$\phi(v) + \phi(v_*) = F(|v|^2 + |v_*|^2, v + v_*) \tag{3.73}$$

for some function F. Define

$$\begin{aligned} \phi_\pm(v) =& \phi(v) \pm \phi(-v); \\ F_\pm(|v|^2 + |v_*|^2, v + v_*) =& F(|v|^2 + |v_*|^2, v + v_*) \pm F(|v|^2 + |v_*|^2, -v - v_*). \end{aligned} \tag{3.74}$$

From above, $\phi(-v) + \phi(-v_*) = F(|v|^2 + |v_*|^2, -v - v_*)$. Hence,

$$\phi_\pm(v) + \phi_\pm(v_*) = F_\pm(|v|^2 + |v_*|^2, v + v_*). \tag{3.75}$$

Clearly, we have $\phi_\pm(-v) = \pm\phi_\pm(v)$ and so forth.

Put $v_* = -v$ in (3.75):

$$\pm\, \phi_\pm(v) + \phi_\pm(v) = F_\pm(2|v|^2, 0). \tag{3.76}$$

Thus,

$$2\phi_+(v) = F_+(2|v|^2, 0) \tag{3.77}$$

so $g_+(v)$ depends only on $|v|^2$. Write $\phi_+(v) = \zeta(|v|^2)$. From the equation (3.75), then F_+ depends only on $|v|^2 + |v_*|^2$ (see the observation below), and hence,

$$\zeta(|v|^2) + \zeta(|v_*|^2) = F_+(|v|^2 + |v_*|^2). \tag{3.78}$$

Set $v_* = 0$, we have $\zeta(|v|^2) + \zeta(0) = F_+(|v|^2)$. Hence,

$$\zeta(|v|^2 + |v_*|^2) + \zeta(0) = F_+(|v|^2 + |v_*|^2) = \zeta(|v|^2) + \zeta(|v_*|^2). \tag{3.79}$$

Set $g(|v|^2) = \zeta(|v|^2) - \zeta(0)$. By the following Lemma 3.8, $g(|v|^2) = c|v|^2$ for some constant c. Thus,

$$\phi_+(v) = \zeta(|v|^2) = g(|v|^2) + \zeta(0) = c|v|^2 + \zeta(0). \tag{3.80}$$

as desired.

For the function ϕ_-, we have,

$$\phi_-(v) + \phi_+(v_*) = F_-(|v|^2 + |v_*|^2, v + v_*). \tag{3.81}$$

First we take v_* perpendicular v; then $|v + v_*|^2 = |v|^2 + |v_*|^2$ so F_- depends on the second argument only. We can write

$$\phi_-(v) + \phi_-(v_*) = h(v + v_*). \tag{3.82}$$

Set $v_* = 0$:

$$\phi_-(v) + \phi_-(0) = h(v), \tag{3.83}$$

or

$$g_-(v) = h(v) \tag{3.84}$$

so that

$$\phi_-(v) + \phi_-(v_*) = h(v + v_*) = \phi_-(v + v_*). \tag{3.85}$$

Therefore, we are done if v_* is perpendicular to v.

To avoid this extra hypothesis: let v, v_* be arbitrary, choose a vector z such that

$$z \cdot v = z \cdot v_* = 0, \quad |z|^2 = |v \cdot v_*| \quad (e.g.,\ z = \pm cv \times v_*) \tag{3.86}$$

By the above considerations,

$$\begin{aligned} \phi_-(v + z) =& \phi_-(v) + \phi_-(z) \\ \phi_-(v \mp z) =& \phi_-(v) \mp \phi_-(z) \end{aligned} \tag{3.87}$$

The sign in the second expression is chosen as follows: we take the minus sign if $v \cdot v_* > 0$, the plus sign if $v_* \cdot v < 0$.

Now

$$\begin{aligned} (v + z) \cdot (v_* \mp z) =& v \cdot v_* \mp v \cdot z + z \cdot v_* \mp |z|^2 \\ =& v \cdot v_* \mp |z|^2 = 0 \end{aligned} \tag{3.88}$$

by this choice if sign. Therefore,

$$\phi_-(v + z) + \phi_-(v_* \mp z) = \phi_-(v + v_* + z \mp z) = \phi_-(v + z) + \phi_-(z \mp z) \tag{3.89}$$

due to the fact that $(v + v_*) \perp (z \mp z)$.

By using the relationship (3.87) on the left hand side, we get,

$$\phi_-(v) + \phi_-(z) + \phi_-(v_*) \mp \phi_-(z) = \phi_-(v + v_*) + \phi_-(z \mp z). \tag{3.90}$$

If $v \cdot v_* > 0$, we take the minus sign: $\phi_-(v) + \phi_-(v_*) = \phi_-(v + v_*)$. Put $v_* = v$, we obtain $2\phi_-(v) = \phi_-(2v)$. Hence,

$$2\phi_-(z) = \phi_-(2z). \tag{3.91}$$

Put this in (3.90), using the bottom sign:

$$\phi_-(v) + 2\phi_-(z) + \phi_-(v_*) = \phi_-(v + v_*) + \phi_-(2z). \tag{3.92}$$

Therefore,

$$\phi_-(v) + \phi_-(v_*) = \phi_-(v + v_*) \tag{3.93}$$

so that

$$\phi_- = b \cdot v \quad \text{for some constant vector} b. \tag{3.94}$$

Above we used the following observation: in order to deduce (3.78) from (3.75), we show that no non-constant function of $v + v_*$ can be constructed from the arguments $|v|^2$ and $|v_*|^2$. For, suppose that

$$g(v + v_*) = \phi(|v|^2, |v_*|^2). \tag{3.95}$$

Put $v_* = 0$:

$$g(v) = \phi(|v|^2, 0) = h(|v|^2) \tag{3.96}$$

hence,

$$h(|v + v_*|^2) = h(|v|^2 + |v_*|^2 + 2v \cdot v_*). \tag{3.97}$$

Thus, $g(v + v_*) = h(|v + v_*|^2)$ implies that

$$h(|v|^2 + |v_*|^2 + 2v \cdot v_*) = \phi(|v|^2, |v_*|^2). \tag{3.98}$$

When $v \cdot v_* = 0$ and $|v_*|^2 = t|v|^2$, we have,

$$\begin{aligned} \text{Left-hand side} =& h(|v|^2 + |v_*|^2 + 2v \cdot v_*) = h((1 + t)|v|^2); \\ \text{Right-hand side} =& \phi(|v|^2, |v_*|^2) = \phi(|v|^2, t|v|^2) \end{aligned} \tag{3.99}$$

However, when $v_* = t^{\frac{1}{2}} v$,

$$\begin{aligned} \text{Left-hand side} =& h(|v|^2 + |v_*|^2 + 2v \cdot v_*) = h((t^{\frac{1}{2}} + 1)^2|v|^2); \\ \text{Right-hand side} =& \phi(|v|^2, |v_*|^2) = \phi(|v|^2, t|v|^2) \end{aligned} \tag{3.100}$$

So for these two different choices of arguments, the right hand sides are equal. But the left hand sides are not. Hence, h must be constant.

□

To complete the proof above, we have to show the following Lemma 3.8 used in the proof above:

Lemma 3.8. *Let $x \in \mathbb{R}^d$. Let f be continuous at one point x_0 and satisfy*

$$g(x) + g(y) = g(x + y), \quad \forall x, y \in \mathbb{R}^d. \tag{3.101}$$

Then $g(x) = b \cdot x$ for some constants $b \in \mathbb{R}^d$.

Proof. We claim that g is homogeneous of degree one:

$$g(\alpha x) = \alpha g(x), \quad \forall x \in \mathbb{R}^d, \ \alpha \in \mathbb{R}. \tag{3.102}$$

Indeed, assume this temporarily and consider any orthogonal basis $\{e_k\}_{k=1}^n$ for all $\mathbb{R}^d$. Let $x \in \mathbb{R}^d$. Then,

$$\begin{aligned} g(x) =& g\left(\sum_{k=1}^d (x \cdot e_k)e_k\right) = \sum_{k=1}^d g((x \cdot e_k)e_k) \\ =& \sum_{k=1}^d (x \cdot e_k)g(e_k) = x \cdot \sum_{k=1}^d g(e_k)e_k = x \cdot b \end{aligned} \tag{3.103}$$

as desired.

It remains to establish (3.102). g is actually everywhere continuous by

$$g(0) = 0,\ g(x+h) - g(x) = g(h) = g(x_0+h) - g(x_0). \tag{3.104}$$

Next, for $n \in \mathbb{N}$,

$$g\left(\sum_{i=1}^{n} x_i\right) = \sum_{i=1}^{n} g(x_i). \tag{3.105}$$

We take $x_i = x$ for all i to obtain $g(nx) = ng(x)$. Now, we put $n \to m \in \mathbb{N}$ and $x \to \frac{1}{m}x$, and then obtain $g(x) = mg\left(\frac{x}{m}\right)$, i.e.,

$$g\left(\frac{x}{m}\right) = \frac{1}{m}g(x) \tag{3.106}$$

and hence,

$$g\left(\frac{n}{m}x\right) = ng\left(\frac{x}{m}\right) = \frac{n}{m}g(x) \tag{3.107}$$

i.e.,

$$g(\alpha x) = \alpha g(x), \quad \forall x \in \mathbb{R}^d,\ 0 < \alpha \in \mathbb{Q}. \tag{3.108}$$

and thus, for all $x \in \mathbb{R}^d, 0 < \alpha \in \mathbb{R}$. By hypothesis, $g(0) = 0$ and $g(-x) = -f(x)$. Hence,

$$g(x) + g(y) = g(x+y), \quad \forall x, y \in \mathbb{R}^d. \tag{3.109}$$

□

Remark 3.9. *Note that, on the one hand, if we restrict $\phi \in C^2$, there is a relatively easier proof for the Lemma 3.7 above; on the other hand, the Lemma 3.7 holds, even if the function ϕ is only assumed to be measurable rather than continuous: however, when passing from continuous to (possibly) discontinuous functions, one should insist on the fact that the equation* (3.63) *is satisfied almost everywhere and not everywhere in $\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2$.*

3.6 Boundary Conditions

When the Boltzmann equation is posed over a spatial domain with a boundary, it must be supplemented with boundary conditions, and the boundary effect can dominate the solution when mean-free-paths are comparable to length scales in the spatial domain.

There are many kinds of boundaries:

- Physical boundaries: Wall of a container, Piston that confines gas...
- Open boundaries: Mouth of a valve, Nozzle though which gas is either injected into or expelled from the domain...
- Moving boundaries: Move in a prescribed way independent of the gas, or in a unprescribed way that is influenced by the gas, e.g., a piston can have a prescribed position as a function of time, or it can exert a prescribed containing force on the gas and move accordingly...

- Free boundaries: Being free to take on a wide variety of shapes in response to the gas, e.g., a confining membrane or liquid surface...
- Artificial boundaries: Make a problem computationally manageable, e.g., computing the aerodynamics of a reentering spacecraft...

However, introducing the appropriate boundary conditions is a nontrivial task. Beyond complicating the well-posedness problem, the most mathematically natural boundary conditions are not necessarily the best suited to describing physical scenarios. Mathematically, boundary conditions such as **Specular-reflection** (particles bounce off the walls at an angle equal to the pre-collision angle) and **Bounce-back** (particles bounce off the walls with reversed momenta) are convenient, but they are not always good physical models. A good boundary condition takes into account the fine details of the gas-surface interaction. A commonly studied example of such a boundary condition is **Maxwellian diffusion**, in which particles are absorbed and re-emitted by the boundary according to a probability distribution which maintains thermodynamic equilibrium between the particles and the boundary...

We will first present the basic set-up of the most physical boundaries – (Perfectly) Reflecting Boundaries, at which every molecule striking it is reflected back in some altered state. Molecules are neither created nor destroyed at such a boundary. Each molecule that strikes such a boundary will certainly have its momentum changed, and possibly its energy too. The walls of a container that physically confine a gas are often modeled as (Perfectly) Reflecting Boundaries.

Let $\partial\Omega|_R$ denote the part of $\partial\Omega$ which is a (Perfectly) Reflecting Boundaries. We will begin with considering the case where $\partial\Omega|_R$ is stationary, and at each point $x \in \partial\Omega|_R$, there is a unique tangent plane with outward unit normal $n(x) \in \mathbb{S}^{d-1}$.

Molecules with velocities v such that

$$\begin{cases} n(x) \cdot v > 0 : \text{moving towards the boundary} \\ n(x) \cdot v < 0 : \text{moving away from the boundary into the domain} \end{cases} \tag{3.110}$$

For every $t > 0$, we must specify boundary values for $F(t, x, v)$ on the set of incoming velocities along $\partial\Omega|_R$ denoted by

$$\Gamma_R^- := \left\{(x, v) \in \partial\Omega|_R \times \mathbb{R}^d : n(x) \cdot v < 0\right\} \tag{3.111}$$

in terms of the boundary values for for $F(t, x, v)$ on the set of outgoing velocities along $\partial\Omega|_R$ denoted by

$$\Gamma_R^+ := \left\{(x, v) \in \partial\Omega|_R \times \mathbb{R}^d : n(x) \cdot v > 0\right\} \tag{3.112}$$

Remark 3.10. *In the ideal gas regimes, most of the gas molecules that intersect with the reflecting boundary will not be influenced by other gas molecules. The relationship giving $f(t, x, v)$ on Γ_R^- in terms of $f(t', x', v')$ on $[0, t] \times \Gamma_R^+$ will therefore be taken to be linear.*

We will also assume that the spatial and temporal scales over which most molecules interact with the boundary are comparable with the spatial and temporal scales of an intermolecular interaction, which are neglected in our kinetic model. The linear relationship

giving giving $f(t,x,v)$ on Γ_R^- in terms of $f(t',x',v')$ on $[0,t]\times\Gamma_R^+$ will therefore be taken to be local in space and time.

In other words, $f(t,x,v)$ on Γ_R^- will be related linearly to $f(t,x,v')$ on Γ_R^+.

Finally, we will assume e the boundary material is in local thermal equilibrium characterized by a so-called wall temperature $T_W := T_W(t,x)$. This temperature can either be prescribed or be influenced by the gas. The assumption that a boundary is in local thermal equilibrium is usually good because the molecules of the boundary material are usually far denser than those of the gas.

Indeed, the molecules of a solid boundary material are in constant contact and behave collectively. Therefore they typically interact with each other many times between their interactions with gas molecules. Plus, the molecules of the boundary material also generally are heavier than those of the gas. Therefore their momentum and energy are changed less by interactions with gas molecules than by interactions with each other.

- The rate at which molecules of mass m with velocity v' **strike** a differential area $\mathrm{d}A(x)$ of the boundary surface with outward normal unit vector $n(x)$ is given by:
$$\frac{1}{m}\left[n(x)\cdot v'\right] f(t,x,v')\,\mathrm{d}v'\,\mathrm{d}A(x) \tag{3.113}$$
- The rate at which molecules of mass m with velocity v **moving away from** the differential area $\mathrm{d}A(x)$ of the boundary surface with outward normal unit vector $n(x)$ is given by:
$$\frac{1}{m}|n(x)\cdot v| f(t,x,v)\,\mathrm{d}v\,\mathrm{d}A(x) \tag{3.114}$$

If we let $R(v,v')$ be the probability density that a molecule which strikes the boundary surface with velocity v' will move away from it with velocity v, then we can express the general reflection boundary condition as

$$|n(x)\cdot v| f(t,x,v) = \int_{n(x)\cdot v'>0} \left[n(x)\cdot v'\right] R(v,v') f(t,x,v')\,\mathrm{d}v', \quad \text{for every } (x,v)\in\Gamma_R^-, \tag{3.115}$$

where the so-called re-distribution kernel $R(v,v')$ satisfies

- Con. (1): $R(v,v')\geq 0$ for every $n(x)\cdot v<0$ and $n(x)\cdot v'>0$;
- Con. (2): $\int_{n(x)\cdot v<0} R(v,v')\,\mathrm{d}v = 1$ for every $n(x)\cdot v'>0$;
- Con. (3): $|n(x)\cdot v| M(v;T_W) = \int_{n(x)\cdot v'>0}\left[n(x)\cdot v'\right] R(v,v') M(v';T_W)\,\mathrm{d}v'$ for every $n(x)\cdot v'<0$.

where $T_W(t,x)$ is the wall temperature and the so-called wall Maxwellian distribution $M(v;T_W)$ is given by
$$M(v;T_W) = \mathcal{M}(v;1,0,T_W). \tag{3.116}$$
Note that, here we have suppressed the fact that $R(v,v')$ can depend on (t,x), typically through the normal $n(x)$ and/or the wall temperature $T_W(t,x)$.

Remark 3.11. *(i) Con. (1) and Con. (2) state that, for each v', the kernel $R(v, v')$ is a probability density in v over $n(x) \cdot v < 0$, which is another way of saying the boundary is perfectly reflecting.*

(ii) Con. (3) states that the boundary condition (3.115) *is satisfied when f is a local Maxwellian in the form that $f(t, x, v) = \rho(t, x)M(v; T_W(t, x))$ for some mass density ρ.*

(iii) Con. (3) is sometimes replaced by the so-called detail-balance condition: for every $n(x) \cdot v < 0$ and $n(x) \cdot v' > 0$,

$$[n(x) \cdot v']\, R(v, v')M(v'; T_W) = R(v', v)\, |n(x) \cdot v|\, M(v; T_W). \tag{3.117}$$

This statement of symmetry holds for many re-distribution kernel models, which is also easily checked that this condition plus Con. (2) implies Con. (3).

3.6.1 Specular Reflection Model R_S

If the boundary is modeled as a smooth hard surface, then a molecule striking it with velocity v' will be elastically reflected with a velocity v given by

$$v = v' - 2\,[n(x) \cdot v']\, n(x) = \big(I - 2n(x)n^T(x)\big)\, v'. \tag{3.118}$$

This is called specular reflection. Each such reflection conserves the energy of molecule $|v|^2 = |v'|^2$, and also conserves the tangential momentum of molecule, as $v - v'$ is always in the normal direction.

Now consider $f(t, x, v)$ at a point $(x, v) \in \Gamma_R^-$. By the Eq. (3.118), a molecule with reflected velocity v can only have been produced by striking the surface with velocity v' given by

$$v' = v - 2\,[n(x) \cdot v']\, n(x) = \big(I - 2n(x)n^T(x)\big)\, v, \quad \text{for every } (x, v) \in \Gamma_R^-. \tag{3.119}$$

The so-called **specular reflection boundary condition** therefore reads:

$$f(t, x, v) = f(t, x, v - 2\,[n(x) \cdot v']\, n(x)) \quad \text{for every } (x, v) \in \Gamma_R^-. \tag{3.120}$$

In this case, the corresponding re-distribution kernel R_S is given by

$$R_S(v, v') = \delta(v' - v + 2\,[n(x) \cdot v]\, n(x)). \tag{3.121}$$

This kernel satisfies the Con. (1)-(3) and the detailed-balance symmetry (3.117). Of course, on molecular length scales, no surface is smooth. Consequently, few reflections will be truly specular. Therefore, this boundary condition represents an ideal scenario.

3.6.2 Isotropic Reflection Model (Bounce-back) R_I

If the boundary is modeled as a rough hard surface, then a molecule striking it with velocity v' will be elastically reflected to have velocity $v = |v'|o$, where o is an arbitrary unit vector such that $n(x) \cdot o < 0$. Each such reflection conserves the energy of the molecule $|v|^2 = |v'|^2$.

The vector o should be drawn from a probability distribution that depends on $n(x)$ and the direction $o' = v'/|v'|$. When the microscopic dynamic is rotationally invariant, the underlying probability density will be a function of the cosines, namely $o \cdot o', o \cdot n(x)$ and $o' \cdot n(x)$. Rather than deriving such probability density from a model for the molecule structure of the surface, we will simply draw o from the uniform distribution. This is called isotropic reflection.

Now consider $f(t, x, v)$ at a point $(x, v) \in \Gamma_R^-$. A molecule reflected with velocity v can only have been produced by striking the surface with velocity $v' = |v|o'$, where o' is a unit vector such that $n(x) \cdot o' > 0$. By (3.113), molecules strike the surface at a rate proportional to $n(x) \cdot o'$.

Therefore, the so-called **isotropic reflection boundary condition** reads:

$$f(t, x, v) = \frac{1}{c} \int_{n(x)\cdot o'>0} [n(x) \cdot o']\, f(t, x, |v|o')\, \mathrm{d}o' \tag{3.122}$$

for every $(x, v) \in \Gamma_R^-$, where the constant c is given by

$$c = \int_{n(x)\cdot o'>0} n(x) \cdot o'\, \mathrm{d}o'. \tag{3.123}$$

The corresponding re-distribution kernel R_I is given by

$$R_I(v, v') = \frac{|n(x) \cdot v|}{c|v|^d} \delta(|v'| - |v|). \tag{3.124}$$

This kernel satisfies the Con. (1)-(3) and the detailed-balance symmetry (3.117).

Remark 3.12. *(i) The microscopic roughness being modeled here is not in contradiction with our assumption that $\partial\Omega$ varies on the scales of a mean-free-path or longer.*

(ii) In particular, if coincidentally $o = -n(x)$ and $o' = v'/|v'| = n(x)$, the isotropic reflection actually becomes the bounce-back scenario that

$$f(t, x, -v) = f(t, x, v) \tag{3.125}$$

for every $(x, v) \in \Gamma_R^-$. This condition simply means that particles arriving with a certain velocity on the wall will bounce back with an opposite velocity, which sometimes could lead to more relevant conclusions than specular reflection, because ot allows for some transfer of tangential momentum during collisions.

3.6.3 Diffuse (Thermal) Reflection Model R_D

If the boundary is modeled as a rough surface at a co-called wall temperature $T_W = T_W(t, x)$ such that a molecule striking it with velocity v' will be thermalized and re-emitted with a velocity v drawn from the Maxwellian distribution $M(v; T_W)$.

The so-called **diffuse (thermal) reflection boundary condition** therefore reads:

$$f(t, x, v) = M(v; T_W) \int_{n(x)\cdot v'>0} [n \cdot v'] f(t, x, v')\, \mathrm{d}v' \tag{3.126}$$

for every $(x, v) \in \Gamma_R^-$. The corresponding re-distribution kernel R_D is given by

$$R_D(v, v') = |n(x) \cdot v| M(v; T_W) \tag{3.127}$$

This kernel satisfies the Con. (1)-(3) and the detailed-balance symmetry (3.117).

3.6.4 Simple Mixed Model

We can build more realistic models of perfectly reflecting boundaries by simply taking convex combinations of the idealized kernels given above:

$$R(v, v') = \alpha_S R_S(v, v') + \alpha_I R_I(v, v') + \alpha_D R_D(v, v'), \tag{3.128}$$

where the so-called accommodation coefficients $\alpha_S, \alpha_I, \alpha_D \geq 0$ with $\alpha_S + \alpha_I + \alpha_D = 1$. They are the probabilities that a molecule striking the surface will undergo specular, isotropic, or diffuse reflection. This kernel satisfies the Con. (1)-(3) and the detailed-balance symmetry (3.117).

Remark 3.13. *(i) In 1879, Maxwell proposed such a model with $\aleph_I = 0$, in which case α_D is the so-called the Maxwell accommodation coefficient. This Maxwell model was the only one used to model reflecting boundaries until the late 1960s. Its major shortcoming is that it has only the one free parameter α_D, which is not enough to capture all important boundary phenomena.*

(ii) Better models of reflecting boundaries were developed so that simulations could better match experimental observations. The Cercignani-Lampis model is among the best examples of such developments. It has two free parameters, which is the number needed to capture most important boundary phenomena.

3.6.5 Non-Reflection Boundary Condition (Stationary, Absorbing-Emitting Boundary Condition)

Perfectly emitting-absorbing boundaries are ones at which every molecule striking it is absorbed, while molecules are emitted from it in a prescribed way that only depends on properties like the velocity, orientation, and temperature of the boundary.

Let $\partial\Omega|_A$ denote that the part of $\partial\Omega$ which is a perfectly absorbing-emitting boundary. We will start with considering the case where $\partial\Omega|_A$ is stationary, and assume that at each point $x \in \partial\Omega|_A$ there is a unique tangent plane with outward unit normal $n(x) \in \mathbb{S}^{d-1}$. For every $t > 0$, we must specify boundary value of $f(t, x, v)$ on the set

$$\Gamma_A^- = \left\{(x, v) \in \partial\Omega|_A \times \mathbb{R}^d : n(x) \cdot v < 0\right\}. \tag{3.129}$$

The boundary condition will have the form

$$f(t, x, v) = g^{\text{boundary}}(t, x, v), \quad \text{for every } (x, v) \in \Gamma_A^-, \tag{3.130}$$

where $g^{\text{boundary}}(t, x, v)$ is a specified density of emitted molecules. For example:

- At a perfectly absorbing boundary, we set

$$g^{\text{boundary}}(t,x,v) = 0, \tag{3.131}$$

for every $(v,x) \in \Gamma_A^-$.

- At the boundary of a reservoir of gas molecules in the local thermal equilibrium characterized by a mass density $\rho^{\text{boundary}}(t,x)$ and a temperature $T^{\text{boundary}}(t,x)$, we set

$$g^{\text{boundary}}(t,x,v) = \mathcal{M}(v;\rho^{\text{boundary}}(t,x),0,T^{\text{boundary}}(t,x)), \tag{3.132}$$

for every $(v,x) \in \Gamma_A^-$.

3.6.6 Non-Reflection Boundary Condition (Moving Boundary Condition)

There are two kinds of moving boundaries:

- (i) Ones whose **motion is prescribed**: An example of a prescribed moving boundary is a piston with a predetermined position in a cylinder or the surface of an airfoil being controlled by a pilot.
- (ii) Ones whose motion depends on the state of the gas – so called **free boundaries**: An example of a free boundary is a piston applying a position-dependent force in a cylinder or a liquid-gas interface. A moving piston often is modeled as a rigid body; an airfoil often is modeled as flexible structure; while a liquid-gas interface typically is deformable.

We will consider the Boltzmann equation over a prescribed spatial domain $\Omega(t)$. Let $\partial\Omega|_R(t)$ denote that part of $\partial\Omega(t)$ which is a perfectly reflecting boundary. We will assume that at each point $x \in \partial\Omega|_R(t)$, there is a unique tangent plane with outward unit vector $n(t,x)$ and a velocity $u_W(t,x)$ at which the boundary is moving.

Molecules with velocities v such that $n(t,x)\cdot(v-u_W(t,x)) > 0$ are moving towards the boundary into domain. For every $t > 0$, we must specify boundary values for $f(t,x,v)$ on the set of incoming velocities along $\partial\Omega|_R(t)$ in term in terms of the boundary values for $f(t,x,v)$ on the set of outgoing velocities along $\partial\Omega|_R(t)$, in other words, for each $t > 0$, we must specify $f(t,x,v)$ on the set

$$\Gamma_R^-(t) := \left\{(x,v) \in \partial\Omega|_R(t) \times \mathbb{R}^d : n(t,x)\cdot(v-u_W(t,x)) < 0\right\}, \tag{3.133}$$

in terms of $f(t',x',v')$ for $t' \in [0,t]$ on the set

$$\Gamma_R^-(t) := \left\{(x,v) \in \partial\Omega|_R(t) \times \mathbb{R}^d : n(t,x)\cdot(v-u_W(t,x)) > 0\right\}. \tag{3.134}$$

The rate at which molecules of mass m with velocity v' are impinging a differential area $\mathrm{d}A(x)$ with outward normal $n(t,x)$ moving with velocity $u_W(t,x)$ is given by

$$\frac{1}{m} n(t,x)\cdot(v'-u_W(t,x)) f(t',x',v')\,\mathrm{d}v'\,\mathrm{d}A(x). \tag{3.135}$$

The rate at which molecules of mass m with velocity v' are moving away a differential area $\mathrm{d}A(x)$ with outward normal $n(t,x)$ moving with velocity $u_W(t,x)$ is given by

$$\frac{1}{m}|n(t,x)\cdot(v-u_W(t,x))|f(t,x,v)\,\mathrm{d}v\,\mathrm{d}A(x). \tag{3.136}$$

Now we assume that the motion of the boundary is sufficiently slow that its motion can be considered uniform during on a time scale over which most molecules interact with the it. We can then model: for every $(x,v)\in\Gamma_R^-(t)$,

$$\begin{aligned}&|n(t,x)\cdot(v-u_W(t,x))|f(t,x,v)\\ &=\int_{n(t,x)\cdot(v-u_W(t,x))>0} R(v-u_W(t,x),v'-u_W(t,x))\,[n(t,x)\cdot(v-u_W(t,x))]\,f(t,x,v')\,\mathrm{d}v'\end{aligned} \tag{3.137}$$

where the re-distribution kernel R is as before.

3.7 Formal Derivation of Macroscopic Equation (Hydrodynamic Limit)

Following the Boltzmann weak formulation and the invariant property of the collision operator, in this subsection, we attempt to derive the macroscopic description supplied by continuum gas dynamics from the mesoscopic description supplied by the kinetic theory.

In order to obtain the **density**, $\rho=\rho(t,x)$, in ordinary space, we have to integrate $f(t,x,v)$ with respect to v:

$$\rho(t,x):=\int_{\mathbb{R}^3} f(t,x,v)\,\mathrm{d}v \tag{3.138}$$

The **bulk (macroscopic, mass) velocity** $u=u(t,x)$ of the gas is the average of the molecule velocities v at a certain point x and time instant t; since $f(t,x,v)$ is proportional to the probability for a molecule to have a given velocity, u is given by

$$u(t,x):=\frac{\int_{\mathbb{R}^3} f(t,x,v)v\,\mathrm{d}v}{\int_{\mathbb{R}^3} f(t,x,v)\,\mathrm{d}v}=\frac{\int_{\mathbb{R}^3} f(t,x,v)v\,\mathrm{d}v}{\rho(t,x)} \tag{3.139}$$

that is to say, the **momentum density** reads:

$$\rho(t,x)u(t,x):=\int_{\mathbb{R}^3} f(t,x,v)v\,\mathrm{d}v \tag{3.140}$$

or, for each component:

$$\rho(t,x)u_i(t,x):=\int_{\mathbb{R}^3} f(t,x,v)v_i\,\mathrm{d}v,\quad 1\le i\le 3 \tag{3.141}$$

The bulk velocity u is what we can directly perceive of the molecular motion by means of macroscopic observations; it is zero for gases in equilibrium in a box at rest. Each molecule has its own velocity v, which can be decomposed into the sum of v and another velocity

$$c(t,x,v):=v-u(t,x) \tag{3.142}$$

called the **random, peculiar, or internal velocity**; c is clearly due to the deviations of v from u, and even if a given infinitesimal region $\mathrm{d}x$ of the gas is at rest ($u = 0$), the c is not zero, which coincides with the molecules velocity v in this case. And it is clear that the average of c is zero, i.e,

$$\int_{\mathbb{R}^3} c(t,x,v) f(t,x,v)\,\mathrm{d}v = 0 \tag{3.143}$$

The quantity ρu_i that appears in Eq. (3.141) is the **i-th component of the mass flow** or of the **momentum density of the gas**. Other quantities of similar nature include:

Remark 3.14. *In the following (i)-(iii) calculation, considering Eq.* (3.143)*, note that c, c_i depend on v, whereas u, u_i, u_{ij} are independent of v.*

(i) The **momentum flow** $u_{ij}(t,x)$: for $i,j = 1,2,3$,

$$\begin{aligned} u_{ij}(t,x) :=& \int_{\mathbb{R}^3} f(t,x,v) v_i v_j \,\mathrm{d}v \\ &\iff \int_{\mathbb{R}^3} f(c_i + u_i)(c_j + u_j)\,\mathrm{d}v \\ &= \int_{\mathbb{R}^3} f c_i c_j \,\mathrm{d}v + u_i \int_{\mathbb{R}^3} f v_j \,\mathrm{d}v + u_j \int_{\mathbb{R}^3} f v_i \,\mathrm{d}v - u_i u_j \int_{\mathbb{R}^3} f \,\mathrm{d}v \\ &= p_{ij} + u_i(\rho u_j) + u_j(\rho u_i) - u_i u_j \rho \\ &= p_{ij} + \rho u_i u_j \end{aligned} \tag{3.144}$$

where

$$p_{ij} := p_{ij}(t,x) = \int_{\mathbb{R}^3} f(t,x,v) c_i c_j \,\mathrm{d}v, \quad \text{for } i,j = 1,2,3 \tag{3.145}$$

plays the role of **stress tensor** (because the microscopic momentum flow associated with it is equivalent to forces distributed on the boundary of any region of gas, according to the macroscopic description).

(ii) The **energy density per unit volume** $w(t,x)$:

$$\begin{aligned} w(t,x) :=& \frac{1}{2} \int_{\mathbb{R}^3} f(t,x,v) |v|^2 \,\mathrm{d}v \\ &\iff \frac{1}{2} \int_{\mathbb{R}^3} f \left(|u|^2 + 2c \cdot u + |c|^2 \right) \mathrm{d}v \\ &= \frac{1}{2} \int_{\mathbb{R}^3} f |u|^2 \,\mathrm{d}v + \frac{1}{2} \int_{\mathbb{R}^3} f |c|^2 \,\mathrm{d}v + u \cdot \underbrace{\int_{\mathbb{R}^3} f c \,\mathrm{d}v}_{:=0} \\ &= \frac{1}{2} \rho |u|^2 + \rho e \end{aligned} \tag{3.146}$$

where e is **internal energy per unit mass** (associated with random motions) defined by:

$$\rho e := \frac{1}{2} \int_{\mathbb{R}^3} |c|^2 f \,\mathrm{d}v \tag{3.147}$$

in addition, the **isotropic pressure** p corresponds to $\frac{1}{3}\sum_{i=1}^{3} p_{ii}$, so

$$\begin{aligned} \frac{1}{2}\sum_{i=1}^{3} p_{ii} = \rho e \quad \text{and} \quad p = \frac{1}{3}\sum_{i=1}^{3} p_{ii} \\ \Longrightarrow p = \frac{2}{3}\rho e \end{aligned} \tag{3.148}$$

the Eq. (3.148) above is the **equation of state**. For a monatomic perfect gas, $e = e(T)$ with T denoting temperature, then p/ρ is constant at constant temperature, i.e., the internal energy of gas only depends on its temperature. A perfect gas is given by

$$p = \rho R T \tag{3.149}$$

where R is gas constant (the Boltzmann constant k_B times the Avogadro number of gas particles, i.e., $k_B = R/N_A$); if further compareing the Eq. (3.146) with the Eq. (3.66), we observe that

$$p = \rho R T = \frac{2}{3}\rho e \xrightarrow{R=1} T = \frac{2}{3}e \tag{3.150}$$

with a normalized $R = 1$; or, that is to say, if we particularly select $R = \frac{2}{3}$, we can re-write

$$p = \rho R T = \frac{2}{3}\rho e \xrightarrow{R=\frac{2}{3}} T = e, \tag{3.151}$$

which means that we are able to replace the internal energy $e(t,x)$ by the temperature $T(t,x)$ in those macroscopic equations.

(iii) The **energy flow** $r_i(t,x)$: for $i = 1,2,3$,

$$\begin{aligned} r_i :=& \frac{1}{2}\int_{\mathbb{R}^3} v_i |v|^2 f(t,x,v)\,\mathrm{d}v \\ \Longleftrightarrow& \frac{1}{2}\int_{\mathbb{R}^3} (c_i + u_i)(|u|^2 + 2c\cdot u + |c|^2) f\,\mathrm{d}v \\ =& u_i \underbrace{\frac{1}{2}\int_{\mathbb{R}^3} (|u|^2 + |c|^2) f\,\mathrm{d}v}_{\frac{1}{2}\rho|u|^2 + \rho e} + \frac{1}{2}\sum_{j=1}^{3} 2u_j \underbrace{\int_{\mathbb{R}^3} c_i c_j f\,\mathrm{d}v}_{p_{ij}} + \underbrace{\frac{1}{2}\int_{\mathbb{R}^3} c_i |c|^2 f\,\mathrm{d}v}_{q_i} \\ =& u_i\left(\frac{1}{2}\rho|u|^2 + \rho e\right) + \sum_{j=1}^{3} u_j p_{ij} + q_i \end{aligned} \tag{3.152}$$

where q_i are the components of the so-called heat-flow vector:

$$q_i = \frac{1}{2}\int_{\mathbb{R}^3} c_i |c|^2 f\,\mathrm{d}v \tag{3.153}$$

The decomposition in Eq. (3.152) shows that

$$\begin{aligned} &\textbf{Microscopic energy flow} \\ =&\textbf{Macroscopic flow of energy (both kinetic and internal)} \\ &+ \textbf{Work done by stresses (per unit area and unit time)} \\ &+ \textbf{Heat flow} \end{aligned} \tag{3.154}$$

Eq. (3.152) shows that the momentum flow is described by the components of a symmetric tensor of second order, because we need to describe the flow in the i-th direction of the momentum in the j-th direction. It is to be expected that in a macroscopic description only a part of this tensor will be identified as a bulk momentum flow, because in general, $u_{i,j}$ will be different from zero even in the absence of a macroscopic motion ($u = 0$).

Remark 3.15. *As the identities derived above apply to the solution of Boltzmann equation, in particular, the Maxwellian Equilibrium Distribution necessarily holds: for the simplest global Maxwellian distribution (independent of t and x) with the collision invariant $\phi = a + b \cdot v + c|v|^2$,*

$$M^f = A\,\mathrm{e}^{a+b\cdot v+c|v|^2} = A\,\mathrm{e}^{a+2\beta u\cdot v-\beta|v|^2} = A\,\mathrm{e}^{-\beta(|v|^2-2v\cdot u-\frac{a}{\beta})} = A\,\mathrm{e}^{-\beta|v-u|^2} \tag{3.155}$$

where $c = -\beta, b = 2\beta u, a = -\beta|u|^2$ and A is a positive constant $a, c, |b|^2$ (A, β, u constitute a new set of constants).

By computing the macroscopic quantities as above for a generic (not necessarily global) Maxwellian, we find that

$$\begin{aligned}
\beta(t,x) =& \frac{3}{4e(t,x)} \overset{(3.150)}{=\!=\!=} \frac{1}{2T(t,x)} \\
A(t,x) =& \left(\frac{3}{4\pi e(t,x)}\right)^{\frac{3}{2}} \overset{(3.150)}{=\!=\!=} \frac{1}{[2T(t,x)]^{\frac{3}{2}}} \\
p_{ij} =& \frac{2}{3}\rho(t,x)e(t,x)\delta_{ij}, \quad \textit{for } i,j = 1,2,3 \\
q_i =& 0, \quad \textit{for } i = 1,2,3.
\end{aligned} \tag{3.156}$$

which is actually the Maxwellian Equilibrium Distribution defined as in Eq. (3.67).

To obtain the differential relations satisfied by the macroscopic quantities introduced above, which describes the balance of mass, momentum, and energy and have the same form as in continuum mechanics, we consider the spatially-inhomogeneous Boltzmann equation:

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = Q(f,f) \tag{3.157}$$

multiplying both sides of the Eq. (3.157) above by the collision invariants $\phi_k, k = 0,1,2,3,4$ and integrate with respect to v, we have

$$\int_{\mathbb{R}^3} \phi_k Q(f,f)\,\mathrm{d}v = 0 \tag{3.158}$$

and hence, if it is permitted to change the order by which we differentiate with respect to t integrate with respect to v:

$$\frac{\partial}{\partial t}\int_{\mathbb{R}^3} \phi_k f\,\mathrm{d}v = \sum_{i=1}^{3} \frac{\partial}{\partial x_i}\int_{\mathbb{R}^3} v_i\phi_k f\,\mathrm{d}v = 0, \quad k = 0,1,2,3,4 \tag{3.159}$$

If we take successively $k = 0, 1, 2, 3, 4$ and use the definitions introduced above, we obtain

$$\begin{cases} \dfrac{\partial}{\partial t}\rho + \displaystyle\sum_{i=1}^{3} \frac{\partial}{\partial x_i}(\rho u_i) = 0, \\ \dfrac{\partial}{\partial t}(\rho u_j) + \displaystyle\sum_{i=1}^{3} \frac{\partial}{\partial x_i}\left(\rho u_i u_j + p_{ij}\right) = 0, \quad j = 1, 2, 3 \\ \dfrac{\partial}{\partial t}\left(\dfrac{1}{2}\rho|u|^2 + \rho e\right) + \displaystyle\sum_{i=1}^{3} \frac{\partial}{\partial x_i}\left[u_i\left(\dfrac{1}{2}\rho|u|^2 + \rho e\right) + \sum_{j=1}^{3} u_j p_{ij} + q_i\right] = 0. \end{cases} \tag{3.160}$$

These equations have the so-called **conservation form**, expressing the circumstance that a certain quantity (whose density appears differentiated with respect to time) is created or destroyed in a certain region Ω because something is flowing through the boundary $\partial\Omega$.

They are also the five basic equations of continuum mechanics, however, consisting of more than five unknowns:

- ρ, e are **two** unknown scalars.
- $u = (u_1, u_2, u_3)$ and $q = (q_1, q_2, q_3)$ are vectors, including **six** unknowns components.
- $p \in M^{3\times 3}$ is symmetric matrix, including **six** unknowns components.

for a total of 14; and the known relation $\frac{1}{3}\sum_{i=1}^{3} p_{ii} = \frac{2}{3}\rho e$ leaves us with 13 unknowns.

> "*The entire purpose of kinetic theory is to relate the* 13*-scalar fields...to various circumstances of the kinetic gas.*"

To make these quantities consistent, we need to impose "constitutive equations" to link p_{ij}, q_i with ρ, u_i, e; as particular famous examples, we present:

- **The Euler Equation (ideal fluids)**
  Take $p(t, x)$ to be a scalar-valued function, and

$$p_{ij} = p(t, x)\delta_{ij}, \quad q_i = 0 \tag{3.161}$$

  Then the classical Euler equation result.

- **The Navier-Stokes Equation (viscous fluids)**
  Let $p(t, x)$ be as above and denote by ν, μ certain viscosity coefficients. One takes

$$p_{ij} = p(t, x)\delta_{ij} - \nu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \mu\sum_{k=1}^{3}\frac{\partial u_k}{\partial x_k}\delta_{ij} \tag{3.162}$$

$$q_i = -\kappa\frac{\partial T}{\partial x_i} \tag{3.163}$$

In fact, when integrating both sides of the equations with respect to x over Ω, the term differentiated with respect to x can be replaced by surface integrals over $\partial\Omega$, thanks to the Divergence Theorem. If these surface integrals turn out to be zero, then we obtain that the **total mass**:

$$M(t) = \int_\Omega \rho(t,x)\,\mathrm{d}x \tag{3.164}$$

the **total momentum**:

$$U(t) = \int_\Omega \rho(t,x)u(t,x)\,\mathrm{d}x \tag{3.165}$$

and the **total energy**:

$$E(t) = \int_\Omega \left(\frac{1}{2}\rho(t,x)|u(t,x)|^2 + \rho(t,x)e(t,x)\right)\,\mathrm{d}x \tag{3.166}$$

are conserved in Ω, the typical cases of which include:

- Ω is $\mathbb{R}^3$ and suitable conditions at infinity ensure that the fluxes of the mass, momentum, and energy flow vectors though a large sphere vanish when the radius of the sphere tends to infinity.
- Ω is a box with periodicity conditions, e.g., flat torus $\mathbb{T}^3$, because essentially there are no boundaries.
- Ω is a compact domain with the condition of (Perfectly) Reflecting Boundaries, e.g., specular reflection, then the boundary term on $\partial\Omega$ disappear in the mass and energy equation but not in the momentum equation; thus only M and E are conserved.

Remark 3.16. *For the spatially-homogeneous case, where the various quantities do not depend on x, all the spatial derivatives then disappear from Eqs.* (3.160) *and the densities $\rho, \rho v$ and $\frac{1}{2}\rho|v|^2 + \rho e$ are conserved, i.e., do not change with time.*

Now, let's formally derive the global conservation law in the case of (Perfectly) Reflecting Boundaries: for every collision invariant $\phi = \phi(v)$, we first have the local conservation law

$$\partial_t \langle f, \phi\rangle + \nabla_x \cdot \langle vf, \phi\rangle = 0 \tag{3.167}$$

Upon integrating this over Ω and applying the Divergence Theorem, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \langle f, \phi\rangle\,\mathrm{d}x = -\int_{\partial\Omega|_A} n(x)\cdot\langle vf,\phi\rangle\,\mathrm{d}A(x). \tag{3.168}$$

This will yield a global conservation law whenever the above integrals make sense and the right-hand side vanishes.

If $\partial\Omega|_R$ is perfectly reflecting and $f(t,x,v)$ satisfies a boundary condition of the general reflection form (3.115), then the normal component of the flux on the right-hand side of (3.168) becomes

$$\begin{aligned} n(x)\cdot\langle vf,\phi\rangle &= \int_{n(x)\cdot v'>0} \phi(v')[n(x)\cdot v']\,\mathrm{d}v' - \int_{n(x)\cdot v<0}\phi(v)|n(x)\cdot v|f(t,x,v)\,\mathrm{d}v \\ &= \int_{n(x)\cdot v'>0}\left[\phi(v') - \int_{n(x)\cdot v<0}\phi(v)R(v,v')\,\mathrm{d}v\right][n(x)\cdot v']f(t,x,v')\,\mathrm{d}v' \end{aligned} \tag{3.169}$$

which then implies that, by considering Con. (2),

$$n(x) \cdot \langle vf, \phi \rangle = 0, \quad \text{for every } x \in \partial\Omega|_R \tag{3.170}$$

if we set $\phi = 1$. Therefore, *the **mass** is globally conserved for every kind of reflecting boundary condition* in the form of (3.115).

However, the *same statement cannot be said for **momentum** and **energy***. In what follows, we shall show that some models of reflecting boundaries can have additional conservation laws that are consistent with the geometry of Ω:

- *Specular Reflection Model.* For the specular reflection kernel (3.121), we have

$$\phi(v') - \int_{n(x)\cdot v<0} \phi(v) R_S(v, v')\, \mathrm{d}v = \phi(v') - \phi(v' - 2[n(x)\cdot v']n(x)). \tag{3.171}$$

  Upon setting $\phi(v) = v$ and $\phi(v) = \frac{1}{2}|v|^2$, we obtain

$$\begin{aligned} v' - \int_{n(x)\cdot v<0} v R_S(v, v')\, \mathrm{d}v =& 2[n(x)\cdot v']n(x), \\ |v'|^2 - \int_{n(x)\cdot v<0} |v|^2 R_S(v, v')\, \mathrm{d}v =& 0 \end{aligned} \tag{3.172}$$

  By (3.169), we find that, for every $x \in \partial\Omega|_R$,

$$\begin{aligned} n(x)\cdot\langle v \otimes vf\rangle =& 2n(x) \int_{n(x)\cdot v'>0} [n(x)\cdot v'] f(t, x, v')\, \mathrm{d}v' \\ n(x)\cdot\left\langle vf, \frac{1}{2}|v|^2 \right\rangle =& 0. \end{aligned} \tag{3.173}$$

  which then implies that the specular reflection boundary condition (3.120) thereby only globally conserves mass and energy. Moreover, it globally conserves momentum in every direction $n_\perp(x) \in \mathbb{S}^{d-1}$ such that $n_\perp(x)\cdot n(x) = 0$ at every $x \in \partial\Omega|_R$. Such $n_\perp(x)$ will exits only for those domains Ω with a translational symmetry.

- *Isotropic Reflection Model.* For the isotropic reflection kernel (3.124), we have

$$\phi(v') - \int_{n(x)\cdot v<0} \phi(v) R_I(v, v')\, \mathrm{d}v = \phi(v') - \frac{1}{c}\int_{n(x)\cdot o>0} |n(x)\cdot o|\phi(|v'|o)\, \mathrm{d}o \tag{3.174}$$

  where c is given by (3.123). Uppon letting $\phi = v$ and $\phi = \frac{1}{2}|v|^2$, we obtain

$$\begin{aligned} v' - \int_{n(x)\cdot v<0} v R_I(v, v')\, \mathrm{d}v =& v' - \frac{1}{c}\int_{n(x)\cdot o>0} |n(x)\cdot o||v'|o\, \mathrm{d}o = v' + \frac{C}{c}|v'|n(x), \\ |v'|^2 - \int_{n(x)\cdot v<0} |v|^2 R_I(v, v')\, \mathrm{d}v =& |v'|^2 - \frac{1}{c}\int_{n(x)\cdot o>0} |n(x)\cdot o||v'|^2\, \mathrm{d}o, \end{aligned} \tag{3.175}$$

  where the constant C is given by

$$C = \int_{n(x)\cdot o'>0} |n(x)\cdot o'|\, \mathrm{d}o'. \tag{3.176}$$

By (3.169), we find that, for every $x \in \partial\Omega|_I$,

$$\begin{aligned} n(x)\cdot\langle v\otimes vf\rangle =& \int_{n(x)\cdot v'>0}\left(v'+\frac{C}{c}|v'|^2 n(x)\right)[n(x)\cdot v']f(t,x,v')\,\mathrm{d}v' \\ n(x)\cdot\left\langle vf,\frac{1}{2}|v|^2\right\rangle =& 0. \end{aligned} \tag{3.177}$$

which then implies that the isotropic reflection boundary condition (3.122) thereby only globally conserves mass and energy.

- *Diffusive (Thermal) Reflection Model.* For the diffusive (thermal) reflection kernel (3.127), we have

$$\phi(v')-\int_{n(x)\cdot v<0}\phi(v)R_D(v,v')\,\mathrm{d}v = \phi(v')-\left(\frac{2\pi}{T_W}\right)^{\frac{1}{2}}\int_{n(x)\cdot v<0}\phi(v)|n(x)\cdot v|M(v;T_W)\,\mathrm{d}v. \tag{3.178}$$

Uppon letting $\phi = v$ and $\phi = \frac{1}{2}|v|^2$, we obtain,

$$\begin{aligned} & v'-\int_{n(x)\cdot v<0} vR_D(v,v')\,\mathrm{d}v \\ =& v'-\left(\frac{2\pi}{T_W}\right)^{\frac{1}{2}}\int_{n(x)\cdot v<0} v|n(x)\cdot v|M(v;T_W)\,\mathrm{d}v \\ =& v'+\left(\frac{2\pi}{T_W}\right)^{\frac{1}{2}} n(x)\int_{n(x)\cdot v<0}|n(x)\cdot v|^2 M(v;T_W)\,\mathrm{d}v \\ =& v'+\left(\frac{\pi T_W}{2}\right)^{\frac{1}{2}} n(x), \end{aligned} \tag{3.179}$$

and

$$\begin{aligned} & |v'|^2-\int_{n(x)\cdot v<0}|v|^2 R_D(v,v')\,\mathrm{d}v \\ =& |v'|^2-\left(\frac{2\pi}{T_W}\right)^{\frac{1}{2}}\int_{n(x)\cdot v<0}|v|^2|n(x)\cdot v|M(v;T_W)\,\mathrm{d}v \\ =& |v'|^2-\left(\frac{2\pi}{T_W}\right)^{\frac{1}{2}}\int_{n(x)\cdot v<0}|n(x)\cdot v|^3 M(v;T_W)\,\mathrm{d}v-(d-1)T_W \\ =& |v'|^2-(d+1)T_W. \end{aligned} \tag{3.180}$$

By (3.169), we find that, for every $x \in \partial\Omega|_D$,

$$\begin{aligned} n(x)\cdot\langle v\otimes vf\rangle =& \int_{n(x)\cdot v'>0}\left[v'+\left(\frac{2\pi}{T_W}\right)^{\frac{1}{2}} n(x)\right][n(x)\cdot v']f(t,x,v')\,\mathrm{d}v', \\ n(x)\cdot\left\langle vf,\frac{1}{2}|v|^2\right\rangle =& \int_{n(x)\cdot v'>0}\left(\frac{1}{2}|v'|^2-\frac{d+1}{2}T_W\right)[n(x)\cdot v']f(t,x,v')\,\mathrm{d}v', \end{aligned} \tag{3.181}$$

which implies that the diffuse (thermal) reflection boundary condition thereby globally conserves only mass, instead of momentum and energy.

3.8 Properties and Estimates of the Collision Operator

In this subsection, we present some properties and estimates on $Q = Q^+ - Q^-$ in Lebesgue and Sobolev spaces, including the following two different types of estimates:

- For the **bilinear** form $Q(g,f) = Q^+(g,f) - Q^-(g,f)$:
  To establish the bilinear estimates, we shall impose an additional assumption on the angular kernel: *no frontal collision should occur*, i.e., $b(\cos\theta)$ should vanish for θ close to π:
  $$\exists \theta_b > 0, \quad \text{supp } b(\cos\theta) \subset \{\theta \mid 0 \le \theta \le \pi - \theta_b\}. \tag{3.182}$$
- For the **quadratic** form $Q(f,f) = Q^+(f,f) - Q^-(f,f)$:
  The assumption (3.182) is not necessary, indeed, $Q^+(f,g) = \tilde{Q}^+(g,f)$ if $\tilde{Q}^+$ is the Boltzmann gain operator associated with the kernel $\tilde{b}(\cos\theta) = b(\cos(\pi-\theta))$.
  In particular,
  $$b(\cos\theta) \quad \text{and} \quad [b(\cos\theta) + b(\cos(\pi-\theta))]\,\mathbf{1}_{0\le\theta\le\frac{\pi}{2}} \tag{3.183}$$
  define the same quadratic operator Q^+, and the latter satisfies the assumption (3.182) automatically.

Note that $Q^+(g,f)$ and $Q^+(f,g)$ will not necessarily satisfy the same estimates, since the assumption (3.182) is not symmetric. To exchange the roles of f and g, we will therefore be led to introduce the assumption: *no grazing collision should occur*, i.e.,

$$\exists \theta_b > 0, \quad \text{supp } b(\cos\theta) \subset \{\theta \mid \theta_b \le \theta \le \pi\}. \tag{3.184}$$

Theorem 3.17. *let $k, \eta \in \mathbb{R}, s \in \mathbb{R}_+, p \in [1,\infty]$, and let B be a collision kernel of the form* (3.26)*, satisfying the assumption* (3.182)*. Then, the following estimates hold:*

$$\|Q^+(g,f)\|_{L^p_\eta(\mathbb{R}^d)} \le C_{k,\eta,p}(B)\|g\|_{L^1_{|k+\eta|+|\eta|}(\mathbb{R}^d)}\|f\|_{L^p_{k+\eta}(\mathbb{R}^d)}, \tag{3.185}$$

$$\|Q^+(g,f)\|_{W^{s,p}_\eta(\mathbb{R}^d)} \le C_{k,\eta,p}(B)\|g\|_{W^{\lceil s\rceil,1}_{|k+\eta|+|\eta|}(\mathbb{R}^d)}\|f\|_{W^{s,p}_{k+\eta}(\mathbb{R}^d)}, \tag{3.186}$$

where $C_{k,\eta,p}(B) = cst\left[\sin\left(\frac{\theta_b}{2}\right)\right]^{\min(\eta,0)-\frac{2}{p'}}\|b\|_{L^1(\mathbb{S}^{d-1})}\|\Psi\|_{L^\infty_{-k}}$, and "cst" denotes various constants which does not depend on the collision kernel B.

Remark 3.18. *Note that if the assumption* (3.182) *is replaced by assumption* (3.184)*, then the same estimates hold with $Q^+(g,f)$ replaced by $Q^+(f,g)$.*

Proof. The proof is cited from [**?**, Theorem 2.1] with some refinements, and still based on duality that

$$\|Q^+(g,f)\|_{L^p_\eta(\mathbb{R}^d)} = \sup_{\|\phi\|_{L^{p'}_{-\eta}(\mathbb{R}^d)}\le 1}\left\{\int_{\mathbb{R}^d} Q^+(g,f)(v)\phi(v)\,\mathrm{d}v\right\}. \tag{3.187}$$

We apply the pre-post collisional change of variables, namely$(v, v_*, \sigma) \to (v', v'_*, \hat{q})$ as in (3.39), to obtain

$$\int_{\mathbb{R}^d} Q^+(g,f)\phi(v)\,\mathrm{d}v = \int_{\mathbb{R}^d\times\mathbb{R}^d}\left(\int_{\mathbb{S}^{d-1}} B(v-v_*,\sigma)\phi(v')\,\mathrm{d}\sigma\right) g(v_*)f(v)\,\mathrm{d}v_*\,\mathrm{d}v \tag{3.188}$$

for all $\|\phi\|_{L^{p'}_{-\eta}(\mathbb{R}^d)} \leq 1$. Let us define the linear operator by

$$S\phi(v) = \int_{\mathbb{S}^{d-1}} B(v - v_*, \sigma)\phi\left(\frac{v + |v|\sigma}{2}\right) \mathrm{d}\sigma. \tag{3.189}$$

Then,

$$\int_{\mathbb{R}^d} Q^+(g, f)\phi(v)\,\mathrm{d}v = \int_{\mathbb{R}^d} g(v_*)\left(\int_{\mathbb{R}^d} f(v)\left[\tau_{v_*} S\left(\tau_{-v_*}\phi\right)(v)\,\mathrm{d}v\right]\right) \mathrm{d}v_*. \tag{3.190}$$

We shall delve into the operator S in the weighted L^1 and L^∞ norms. For brevity, we denote $v^+ = \left(\frac{v+|v|\sigma}{2}\right)$.

By the use of inequality:

$$\sin\left(\frac{\theta_b}{2}\right)|v| \leq |v^+| \leq |v| \tag{3.191}$$

which is a consequence of (3.182), we find

$$\|S\phi\|_{L^\infty_{-k-\eta}} \leq \mathrm{cst}\left[\sin\left(\frac{\theta_b}{2}\right)\right]^{\min(\eta,0)} \|b\|_{L^1(\mathbb{S}^{d-1})}\|\Psi\|_{L^\infty_{-k}}\|\phi\|_{L^\infty_{-\eta}}. \tag{3.192}$$

Next, we turn to the L^1-estimate. First,

$$\begin{aligned}\|S\phi\|_{L^1_{-k-\eta}} &= \int_{\mathbb{R}^d}\int_{\mathbb{S}^{d-1}} \Psi(|v|)\left\langle v\right\rangle^{-k-\eta} b(\cos\theta)|\psi(v^+)|\,\mathrm{d}\sigma\,\mathrm{d}v \\ &\leq \left[\sin\left(\frac{\theta_b}{2}\right)\right]^{\min(\eta,0)} \|\Psi\|_{L^\infty_{-k}}\int_{\mathbb{R}^d}\int_{\mathbb{S}^{d-1}} b(\cos\theta)|\psi(v^+)|\left\langle v^+\right\rangle^{-\eta}\,\mathrm{d}\sigma\,\mathrm{d}v\end{aligned} \tag{3.193}$$

The change of variable $v \longmapsto v^+$ is allowed because b has compact support in $[0, \pi - \theta_b]$, and its Jacobian is $\frac{2^{d-1}}{\cos^2\left(\frac{\theta}{2}\right)}$. By applying it, we find

$$\begin{aligned}\|S\phi\|_{L^1_{-k-\eta}} &\leq \left[\sin\left(\frac{\theta_b}{2}\right)\right]^{\min(\eta,0)} \|\Psi\|_{L^\infty_{-k}}\int_{\mathbb{R}^d}\int_{\mathbb{S}^{d-1}} b(\cos\theta)|\psi(v^+)|\left\langle v^+\right\rangle^{-\eta}\,\mathrm{d}\sigma\,\mathrm{d}v \\ &\leq \left[\sin\left(\frac{\theta_b}{2}\right)\right]^{\min(\eta,0)} \|\Psi\|_{L^\infty_{-k}}\int_{\mathbb{R}^d}\int_{\mathbb{S}^{d-1}} b(\cos\theta)|\phi(v^+)|\left\langle v^+\right\rangle^{-\eta}\frac{2^{d-1}}{\cos^2\left(\frac{\theta}{2}\right)}\,\mathrm{d}v^+\,\mathrm{d}\sigma \\ &\leq \mathrm{cst}\left[\sin\left(\frac{\theta_b}{2}\right)\right]^{\min(\eta,0)-2} \|b\|_{L^1(\mathbb{S}^{d-1})}\|\Psi\|_{L^\infty_{-k}}\|\phi\|_{L^1_{-\eta}}\end{aligned} \tag{3.194}$$

By the Riesz-Thorin Interpolation Theorem, from inequalities (3.193)-(3.194), we deduce that

$$\|S\phi\|_{L^p_{-k-\eta}} \leq C_{k,\eta,\varphi'}(B)\|\phi\|_{L^p_{-\eta}}, \quad 1 \leq p \leq \infty, \tag{3.195}$$

where

$$C_{k,\eta,\varphi'}(B) = \mathrm{cst}\left[\sin\left(\frac{\theta_b}{2}\right)\right]^{\min(\eta,0)-\frac{p}{2}} \|b\|_{L^1(\mathbb{S}^{d-1})}\|\Psi\|_{L^\infty_{-k}}. \tag{3.196}$$

Plugging this inequality (3.195) into (3.190), we find

$$\begin{aligned}
\left|\int_{\mathbb{R}^d} Q^+(g,f)\phi(v)\,\mathrm{d}v\right| \leq & \int_{\mathbb{R}^d}\left(\int_{\mathbb{R}^d}|f(v)|\left|\left[\tau_{-v_*}S\left(\tau_{v_*}\phi\right)\right](v)\,\mathrm{d}v\right|\right)|g(v_*)|\,\mathrm{d}v_* \\
\leq & \int_{\mathbb{R}^d}\|f\|_{L^p_{k+\eta}}\|\tau_{-v_*}S\left(\tau_{v_*}\phi\right)\|_{L^{p'}_{-k-\eta}}|g(v_*)|\,\mathrm{d}v_* \\
\leq & \|f\|_{L^p_{k+\eta}}\int_{\mathbb{R}^d}|g(v_*)|\left\langle v_*\right\rangle^{|k+\eta|}\|S(\tau_{v_*})\|_{L^{p'}_{-\eta}}\,\mathrm{d}v_* \\
\leq & C_{k,\eta,\varphi'}(B)\|f\|_{L^p_{k+\eta}}\int_{\mathbb{R}^d}|g(v_*)|\left\langle v\right\rangle^{|k+\eta|}\|\tau_{v_*}\phi\|_{L^{p'}_{-\eta}}\,\mathrm{d}v_* \\
\leq & C_{k,\eta,\varphi'}(B)\|f\|_{L^p_{k+\eta}}\|\phi\|_{L^{p'}_{-\eta}}\int_{\mathbb{R}^d}|g(v_*)|\left\langle v_*\right\rangle^{|k+\eta|+|\eta|}\,\mathrm{d}v_* \\
\leq & C_{k,\eta,\varphi'}(B)\|f\|_{L^p_{k+\eta}}\int_{\mathbb{R}^d}|g(v_*)|\left\langle v_*\right\rangle^{|k+\eta|+|\eta|}\,\mathrm{d}v_* \\
\leq & C_{k,\eta,\varphi'}(B)\|f\|_{L^p_{k+\eta}}\|g\|_{L^1_{|k+\eta|+|\eta|}}
\end{aligned} \tag{3.197}$$

This concludes the proof of the estimate (3.185).

For the proof of the estimate (3.186), it is based on the formula

$$\nabla Q^{\pm}(g,f) = Q^{\pm}(\nabla g, f) + Q^{\pm}(g,\nabla f) \tag{3.198}$$

which is direct consequence of the bi-linearity and the Galilean Invariant property of the Boltzmann operator, namely $\tau_h Q(g,f) = Q(\tau_h g, \tau_h f)$. From Eq. (3.198), it is easy tp deduce a Leibniz formula for the derivatives of Q^+ at any order, and the Eq. (3.186) easily follows for any $s \in \mathbb{N}$. Indeed, whenever $s \in \mathbb{N}$ we can apply the estimate (3.185) to each term of the Leibniz formula for $\partial^\mu Q^+(g,f)$ and find

$$\begin{aligned}
\|Q^+(g,f)\|^p_{W^{s,p}_\eta} = & \sum_{|\nu|\leq s}\|\partial^\nu Q^+(g,f)\|^p_{L^p_\eta} \\
= & \sum_{|\nu|\leq s}\sum_{\mu\leq\nu}\binom{\nu}{\mu}\|Q^+\left(\partial^\mu g, \partial^{\nu-\mu} f\right)\|^p_{L^p_\eta} \\
\leq & C_{k,\eta,p}(B)\sum_{|\nu|\leq s}\sum_{\mu\leq\nu}\binom{\nu}{\mu}\|\partial^\mu g\|^p_{L^1_{|k+\eta|+|\eta|}}\|\partial^{\nu-\mu} f\|^p_{L^p_{k+\eta}} \\
\leq & C_{k,\eta,p}(B)\|g\|^p_{W^{s,1}_{|k+\eta|+|\eta|}}\|f\|^p_{W^{s,p}_{k+\eta}}
\end{aligned} \tag{3.199}$$

such that the general case of (3.186) is obtained by use of the Riesz-Thorin Interpolation Theorem, with respect to the variable f. □

Remark 3.19. *(i) The same estimate will hold for the quadratic form $Q^+(f,f)$ in the sense that: for $k,\eta \in \mathbb{R}, p \in [1,+\infty]$,*

$$\|Q^+(f,f)\|_{L^p_\eta(\mathbb{R}^d)} \leq C_k(B)\|f\|_{L^1_{|k+\eta|+|\eta|}(\mathbb{R}^d)}\|f\|_{L^p_{k+\eta}(\mathbb{R}^d)}, \tag{3.200}$$

$$\|Q^+(f,f)\|_{W^{s,p}_\eta(\mathbb{R}^d)} \leq C_k(B)\|f\|_{W^{\lceil s\rceil,1}_{|k+\eta|+|\eta|}(\mathbb{R}^d)}\|f\|_{W^{s,p}_{k+\eta}(\mathbb{R}^d)}, \tag{3.201}$$

where $C_{k,\eta,p}(B) = cst\|b\|_{L^1(\mathbb{S}^{d-1})}\|\Psi\|_{L^\infty_{-k}}$.

(ii) For the particular case $\eta \geq 0$, it is possible to obtain slightly better weight exponents in Theorem 3.17 above as well as the quadratic estimate: indeed, we can use the inequality

$$|v|^2 \leq |v'|^2 + |v'_*|^2 \tag{3.202}$$

to split the weight on the two arguments of Q^+ and get

$$\|Q^+(g,f)\|_{L^p_\eta} \leq cst \|Q^+(G,F)\|_{L^p} \tag{3.203}$$

where $F(v) = f(v)\langle v\rangle^\eta$ and $G(v) = g(v)\langle v\rangle^\eta$. When $\eta \geq 0$, the conclusion of Theorem 3.17 thus becomes

$$\|Q^+(g,f)\|_{L^p_\eta(\mathbb{R}^d)} \leq C_{k,\eta,p}(B)\|g\|_{L^1_{k+\eta}(\mathbb{R}^d)}\|f\|_{L^1_{k+\eta}(\mathbb{R}^d)}, \tag{3.204}$$

$$\|Q^+(g,f)\|_{W^{s,p}_\eta(\mathbb{R}^d)} \leq C_{k,\eta,p}(B)\|g\|_{W^{\lceil s\rceil,1}_{k+\eta}(\mathbb{R}^d)}\|f\|_{W^{s,p}_{k+\eta}(\mathbb{R}^d)}. \tag{3.205}$$

For the loss operator Q^-, we shall present the lower bound:

Proposition 3.20. *Assume that the collision kernel B has a lower bound in the integral sense that*

$$\int_{\mathbb{S}^{d-1}} B(v-v_*,\sigma)\,\mathrm{d}\sigma \geq K_B|v-v_*|^\gamma, \quad (K_B>0,\ \gamma>0) \tag{3.206}$$

Then, for all $f \in L^1_2(\mathbb{R}^d)$ with finite entropy $H(f) = \int_{\mathbb{R}^d} f\log f < C_H$, there exists a constant K_f (only depending on a lower bound on the mass $\int_{\mathbb{R}^d} f\mathrm{d}v$ and upper bounds on the energy $\int_{\mathbb{R}^d} f|v|^2\mathrm{d}v$ and entropy $H(f)$) such that

$$Q^-(f,f)(v) := f(v)L[f](v) \geq K_f f(v)\left(1+|v|\right)^\gamma. \tag{3.207}$$

Similarly, if in the right-hand side of (3.206)*, the term $|v-v_*|^\gamma$ is replaced by $\min\{|v-v_*|^\gamma, 1\}$, then the conclusion* (3.207) *should be replaced by*

$$Q^-(f,f)(v) \geq K_f f(v). \tag{3.208}$$

Proof. Start from the estimate that, for $j>1$,

$$\int_{|v-v_*|<r} f(v_*)\,\mathrm{d}v_* \leq \int_{|v-v_*|<r, f(v_*)<j} f(v_*)\,\mathrm{d}v_* + \frac{1}{\log j}\int_{f(v_*)>j} f(v_*)\log f(v_*)\,\mathrm{d}v_* \tag{3.209}$$

For a suitable choice of r and j only depending on the mass $\int_{\mathbb{R}^d} f(v)\mathrm{d}v$ and upper bound entropy C_H, we get

$$\int_{|v-v_*|<r} f(v_*)\,\mathrm{d}v_* < \frac{1}{2}\int_{\mathbb{R}^d} f(v)\,\mathrm{d}v \tag{3.210}$$

Furthermore, on the one hand,

$$\begin{aligned} L[f](v) =& \int_{\mathbb{R}^d}\left(\int_{\mathbb{S}^{d-1}} b(\cos\theta)\,\mathrm{d}\sigma\right)|v-v_*|^\gamma f(v_*)\,\mathrm{d}v_* \\ >& K_B\left[\int_{|v-v_*|>r} f(v_*)\,\mathrm{d}v_*\right] r^\gamma \\ >& K_B\left[\frac{1}{2}\int_{\mathbb{R}^d} f(v)\,\mathrm{d}v\right] r^\gamma \\ :=& \frac{K_B}{2}\|f\|_{L^1} r^\gamma \end{aligned} \tag{3.211}$$

on the other hand, to get another estimate of $L[f]$, we notice that

$$|v - v_*|^\gamma \geq |v|^\gamma - |v_*|^\gamma, \quad \text{for } 0 < \gamma \leq 1, \tag{3.212}$$

Then, we obtain

$$\begin{aligned} L[f](v) \geq K_B \int_{\mathbb{R}^d} f(v_*)|v - v_*|^\gamma \, \mathrm{d}v_* \geq & K_B \int_{\mathbb{R}^d} f(v_*) \left(|v|^\gamma - |v_*|^\gamma\right) \, \mathrm{d}v_* \\ \geq & \left(\int_{\mathbb{R}^d} f(v_*) \, \mathrm{d}v_* \right) |v|^\gamma - \int_{\mathbb{R}^d} f(v_*)|v_*|^\gamma \, \mathrm{d}v_* \\ \geq & \left(\int_{\mathbb{R}^d} f(v_*) \, \mathrm{d}v_* \right) |v|^\gamma - \int_{\mathbb{R}^d} f(v_*)|v_*|^2 \, \mathrm{d}v_* \\ := & \|f\|_{L^1} |v|^\gamma - \|f\|_{L^1_2} \end{aligned} \tag{3.213}$$

Combine the estimates (3.211)-(3.213), we finally conclude that

$$L[f](v) \geq K_f (1 + |v|)^\gamma. \tag{3.214}$$

□

Remark 3.21. *For $1 < \gamma \leq 2$, we can apply the following estimate with the help of convexity of the hard potential kernel, if the mass $\int_{\mathbb{R}^d} f \mathrm{d}v$ is normalized as one as well as the momentum $\int_{\mathbb{R}^d} f v \mathrm{d}v$ is kept as zero:*

$$\begin{aligned} L[f](v) = & \int_{\mathbb{R}^d} B(v - v_*, \sigma) f(v_*) \, \mathrm{d}\sigma \, \mathrm{d}v_* \\ \geq & K_B \int_{\mathbb{R}^d} |v - v_*|^\gamma f(v_*) \, \mathrm{d}\sigma \, \mathrm{d}v_* \\ \geq & K_B \left| \int_{\mathbb{R}^d} (v - v_*) f(v_*) \, \mathrm{d}v_* \right|^\gamma \\ \geq & K_B |v|^\gamma \end{aligned} \tag{3.215}$$

where the Jensen's inequality is utilized in the second inequality above.

3.9 Fourier Transform of the Collision Operator (Bobylev Identity)

The Fourier transformation has been widely used in the analysis of various kind of partial differential equations. However, it used to be very painful to find an elegant representation of the Boltzmann equation in the Fourier space, even though the Boltzmann operator possesses a nice weak formulation. Thanks to A. V. Bobylev, this problem turned out not as intricate as one may imagine, at least for the Maxwellian molecules. Since then, the so-called "Bobylev Identity" has become an extremely powerful technique in the study of the Boltzmann equation, especially in the case of spatially homogeneous theory.

Proposition 3.22. *Consider the Boltzmann collision operator $Q(g, f)$ with its collision kernel B being the Maxwellian molecule b, i.e., B does not depend on $|v - v_*|$,*

$$Q(g, f)(v) = \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} b \left(\frac{v - v_*}{|v - v_*|} \cdot \sigma \right) \left[g(v'_*) f(v') - g(v_*) f(v) \right] \, \mathrm{d}\sigma \, \mathrm{d}v_*. \tag{3.216}$$

Then, the following formulas hold,

$$\begin{aligned}\mathcal{F}\left[Q^+(g,f)\right](\xi) &= \int_{\mathbb{S}^2} b\left(\frac{\xi}{|\xi|\cdot\sigma}\right)\hat{g}(\xi^-)\hat{f}(\xi^+)\,\mathrm{d}\sigma,\\ \mathcal{F}\left[Q^-(g,f)\right](\xi) &= \int_{\mathbb{S}^2} b\left(\frac{\xi}{|\xi|\cdot\sigma}\right)\hat{g}(0)\hat{f}(\xi)\,\mathrm{d}\sigma,\end{aligned} \tag{3.217}$$

where,

$$\xi^+ = \frac{\xi}{2} + \frac{|\xi|}{2}\sigma, \qquad \xi^- = \frac{\xi}{2} - \frac{|\xi|}{2}\sigma. \tag{3.218}$$

Proof. By performing the weak formulation, for any test function ϕ, we have,

$$\int_{\mathbb{R}^3} Q^+(g,f)(v)\phi(v)\mathrm{d}v = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} b\left(\frac{v-v_*}{|v-v_*|}\cdot\sigma\right) g(v_*)f(v)\phi(v')\,\mathrm{d}\sigma\,\mathrm{d}v_*\,\mathrm{d}v. \tag{3.219}$$

Selecting $\phi(v) = \mathrm{e}^{-\mathrm{i}v\cdot\xi}$ in the identity above, we have

$$\begin{aligned}&\mathcal{F}\left[Q^+(g,f)\right](\xi)\\ &= \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} b\left(\frac{v-v_*}{|v-v_*|}\cdot\sigma\right) g(v_*)f(v)\,\mathrm{e}^{-\mathrm{i}\left(\frac{v+v_*}{2}+\frac{|v-v_*|}{2}\sigma\right)\cdot\xi}\,\mathrm{d}\sigma\,\mathrm{d}v_*\,\mathrm{d}v\\ &= \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} b\left(\frac{v-v_*}{|v-v_*|}\cdot\sigma\right) g(v_*)f(v)\,\mathrm{e}^{-\mathrm{i}\frac{v+v_*}{2}\cdot\xi}\,\mathrm{e}^{-\mathrm{i}\frac{|v-v_*|}{2}\sigma\cdot\xi}\,\mathrm{d}\sigma\,\mathrm{d}v_*\,\mathrm{d}v,\end{aligned} \tag{3.220}$$

according to the general change of variable,

$$\int_{\mathbb{S}^2} F(k\cdot\sigma, l\cdot\sigma)\,\mathrm{d}\sigma = \int_{\mathbb{S}^2} F(l\cdot\sigma, k\cdot\sigma)\,\mathrm{d}\sigma, \quad |l| = |k| = 1, \tag{3.221}$$

due to the existence of an isometry on $\mathbb{S}^2$ exchanging l and k, we have, by exchanging the rule of $\frac{\xi}{|\xi|}$ and $\frac{v-v_*}{|v-v_*|}$,

$$\begin{aligned}&\int_{\mathbb{S}^2} g(v_*)f(v)b\left(\frac{v-v_*}{|v-v_*|}\cdot\sigma\right)\mathrm{e}^{-\mathrm{i}\frac{|v-v_*|}{2}\sigma\cdot\xi}\,\mathrm{d}\sigma\\ &= \int_{\mathbb{S}^2} g(v_*)f(v)b\left(\frac{\xi}{|\xi|}\cdot\sigma\right)\mathrm{e}^{-\mathrm{i}\frac{|\xi|}{2}\sigma\cdot(v-v_*)}\,\mathrm{d}\sigma\end{aligned} \tag{3.222}$$

Thus,

$$\begin{aligned}&\mathcal{F}\left[Q^+(g,f)\right](\xi)\\ &= \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} g(v_*)f(v)b\left(\frac{v-v_*}{|v-v_*|}\cdot\sigma\right)\mathrm{e}^{-\mathrm{i}\frac{v+v_*}{2}\cdot\xi}\,\mathrm{e}^{-\mathrm{i}\frac{|v-v_*|}{2}\sigma\cdot\xi}\,\mathrm{d}\sigma\,\mathrm{d}v_*\,\mathrm{d}v\\ &= \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} g(v_*)f(v)b\left(\frac{\xi}{|\xi|}\cdot\sigma\right)\mathrm{e}^{-\mathrm{i}\frac{v+v_*}{2}\cdot\xi}\,\mathrm{e}^{-\mathrm{i}\frac{|\xi|}{2}\sigma\cdot(v-v_*)}\,\mathrm{d}\sigma\,\mathrm{d}v_*\,\mathrm{d}v\\ &= \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} g(v_*)f(v)b\left(\frac{\xi}{|\xi|}\cdot\sigma\right)\mathrm{e}^{-\mathrm{i}v\cdot\left(\frac{\xi}{2}+\frac{|\xi|}{2}\sigma\right)}\,\mathrm{e}^{-\mathrm{i}v_*\cdot\left(\frac{\xi}{2}-\frac{|\xi|}{2}\sigma\right)}\,\mathrm{d}\sigma\,\mathrm{d}v_*\,\mathrm{d}v\\ &= \int_{\mathbb{S}^2} b\left(\frac{\xi}{|\xi|}\cdot\sigma\right)\hat{f}(\xi^+)\hat{g}(\xi^-)\,\mathrm{d}\sigma,\end{aligned} \tag{3.223}$$

where, unlike the elastic case, the ξ^+ and ξ^- are defined as

$$\xi^+ = \frac{\xi}{2} + \frac{|\xi|}{2}\sigma, \qquad \xi^- = \frac{\xi}{2} - \frac{|\xi|}{2}\sigma. \tag{3.224}$$

And the formula for $\mathcal{F}\left[Q^{-}(g,f)\right](\xi)$ is then easily obtained by the same kind of but more simpler computations. $\square$

For a given probability measure F or its density function f, we define the corresponding characteristic function $\varphi(\xi)$ by the Fourier transform:

$$\varphi(\xi) = \hat{f}(\xi) := \int_{\mathbb{R}^3} \mathrm{e}^{-\,\mathrm{i}v\cdot\xi} f(v)\,\mathrm{d}v = \int_{\mathbb{R}^3} \mathrm{e}^{-\,\mathrm{i}v\cdot\xi}\,\mathrm{d}F(v), \tag{3.225}$$

where the f is regarded as the distribution density function of the cumulative distribution function F in the sense of Radon-Nikodym derivative.

And its inversion formula by normalization writes

$$f(v) = \int_{\mathbb{R}^3} \mathrm{e}^{\mathrm{i}v\cdot\xi} \hat{f}(\xi)\,\mathrm{d}\xi = \int_{\mathbb{R}^3} \mathrm{e}^{\mathrm{i}v\cdot\xi} \varphi(\xi)\,\mathrm{d}\xi. \tag{3.226}$$

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.

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