Lecture 2: The Boltzmann equation

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Outline

The Boltzmann equation

Collision transformation

Collision operator

Maxwellian

Conservation laws

Symmetry of the Boltzmann equation
Today, I will talk about

Inner beauty of the Boltzmann equation

Outer beauty attracts, but inner beauty captivates.

Kate Angell
The Boltzmann equation

- **Velocity Distribution function:**

\[ F = F(x, \xi, t) \]: velocity distribution function (number density function) of monatomic particles (e.g. Ar, He, ...).

\[ F(x, \xi, t) \Delta x \Delta \xi \approx \text{number of particles inside } \Delta x \Delta \xi. \]
• **Particle trajectory** (bi-characteristics) in phase space:

\[
\begin{align*}
\frac{dx}{dt} & = \xi, \\
\frac{d\xi}{dt} & = E(x, t), \\
x(0) & = x, \\
\xi(0) & = \xi.
\end{align*}
\]

In the absence of collisions between particles, \( F = F(x, \xi, t) \) is preserved (conserved) along the particle path:

\[
\frac{dF}{dt} = \frac{d}{dt} F(x(t), \xi(t), t) \\
= \partial_t F + \dot{x} \cdot \nabla_x F + \dot{\xi} \cdot \nabla_\xi F \bigg|_{(x(t), \xi(t), t)} \\
= \partial_t F + \xi \cdot \nabla_x F \\
= 0.
\]

This is a transport equation in phase space.
However, when there are collisions,

\[
\frac{dF}{dt} = \text{Jump in } F \text{ due to collisions} \bigg|_{\text{collision time}}.
\]

We denote \( Q(F, F) \) by the jump in \( F \) and call it "collision operator".
• Assumptions in the derivation of the collision operator.

1. Due to the rarefaction, multiple collisions other than binary are neglected.
2. Collisions are **LOCAL** and **INSTANTANEOUS**

\[ Q(F, F) \text{ operates only in the velocity variable } \xi \text{ in } F. \]
The Boltzmann equation (1872)

\[ \partial_t F + \xi \cdot \nabla_x F = \frac{1}{Kn} Q(F, F), \]

Rate of change in \( F \) along particle trajectory

where

\[ Q(F, F)(x, \xi, t) = \int_{R^3 \times S^2} q(\xi - \xi^*, \omega) (F' F' - FF^*) d\omega d\xi^*. \]

Difficulty of the Boltzmann equation comes from the collision operator
• Between collisions (free transport)

\[
\frac{dx_i}{dt} = \xi_i, \quad \frac{d\xi_i}{dt} = 0, \quad i = 1, \ldots, N.
\]

• The linear transport equation:

\[
\partial_t F + \xi \cdot \nabla_x F = 0, \quad x, \xi \in \mathbb{R}^3, \quad t > 0,
\]

\[
F(x, \xi, 0) = F_0(x, \xi).
\]

Then, it is easy to see that

\[
F(x, \xi, t) = F_0(x - t\xi, \xi).
\]

Next, we study the collision operator \( Q(F, F) \).
Collisions between particle-particle

For a monatomic gas e.g. Ar, H, i.e., Molecule = atom

- Micro-reversibility $(\xi, \xi_*) \iff (\xi', \xi'_*)$:

\[
1 + 1 = 1 + 1, \quad \xi + \xi_* = \xi' + \xi'_*, \quad \frac{|\xi|^2}{2} + \frac{|\xi_*|^2}{2} = \frac{|\xi'|^2}{2} + \frac{|\xi'_*|^2}{2}.
\]

cf. Hard sphere, reversible, translational energy, elastic collisions
Recall the **elastic collision relation**:

\[ \xi + \xi^* = \xi' + \xi'_* , \quad |\xi|^2 + |\xi^*|^2 = |\xi'|^2 + |\xi'_*|^2. \]

Note that we have *six* unknown \((\xi', \xi'_*)\) and *four* scalar equations. Therefore, for a given initial velocities \((\xi, \xi^*)\), we will have a *two parameter family of final velocities*. 
Theorem: (Collision transformation)

\[
\begin{align*}
\xi' &= \xi - ((\xi - \xi_*) \cdot \omega) \omega, \\
\xi_*' &= \xi_* + ((\xi - \xi_*) \cdot \omega) \omega, \quad \omega \in S^2.
\end{align*}
\]
Proof. We introduce a unit vector $\omega \in S^2$ having the direction of the change in velocity of the first molecule.

$$\xi' - \xi = A\omega, \quad A: \text{scalar}.$$  

Note that $\omega$ is well-defined unless $\xi' - \xi = 0$.

Then, conservation of momentum yields

$$\xi'_* - \xi_* = -A\omega.$$ 

On the other hand, conservation of energy implies

$$A = \omega \cdot (\xi_* - \xi).$$
• **Theorem:**

Collision transformation is an isometry from $\mathbb{R}^6$ to $\mathbb{R}^6$,
i.e., $\frac{\partial (\xi', \xi_*)}{\partial (\xi, \xi_*)} = 1$.

◊ Properties of collision transformation

1. Interchange of pre collisional velocities $\xi$ and $\xi_*$ produces
   an interchange of post collisional velocities $\xi'$ and $\xi'_*$.

2. Angles are unchanged by the collision, i.e.,

   $$|(\xi'_* - \xi'_) \cdot \omega| = |(\xi_* - \xi) \cdot \omega|.$$
Definition: Collision invariant

\( \varphi = \varphi(\xi, \xi^*) \) is a collision invariant if and only if it is invariant under the collision transformation (map), i.e.,

\[
\varphi(\xi', \xi'^*) = \varphi(\xi, \xi^*), \quad \xi, \xi^* \in \mathbb{R}^3.
\]

Remark. 1. Every collision invariant \( \varphi \) is a function of \( \xi + \xi^* \) and \( |\xi|^2 + |\xi^*|^2 \), i.e.,

\[
\varphi(\xi, \xi^*) = \Phi(\xi + \xi^*, |\xi|^2 + |\xi^*|^2).
\]

2. Summational invariant = a collision invariant which splits into a sum of functions \( \xi \) and \( \xi^* \):

\[
\varphi(\xi, \xi^*) = \psi(\xi) + \psi(\xi^*).\]
- **Theorem**: Boltzmann, Carlemann, Grad

Suppose that a $C^2$ function $\varphi$ satisfies

$$\varphi(\xi) + \varphi(\xi^*) = \varphi(\xi') + \varphi(\xi^*').$$

Then,

$$\varphi(\xi) = a + b \cdot \xi + c|\xi|^2.$$  

Every summational invariant is spanned by $1, \xi_1, \xi_2, \xi_3, |\xi|^2$.  

By physical argument in scattering process, the collision kernel $q$ can be shown to be a function of $\xi_* - \xi$ and $\omega$.

- **Boltzmann’s collision integral:**

$$Q(F, F)(x, \xi, t) = \iiint_{\mathbb{R}^3 \times S^2} q(\xi_* - \xi, \omega) \left(F' F_* - FF_*\right) d\xi_*.$$  

where

$$F_* = F(\xi_*), \quad F' = F(\xi').$$

For a gas of hard spheres with radius $r$,

$$q(\xi_* - \xi, \omega) = r^2 |(\xi_* - \xi) \cdot \omega|.$$
For an inversely proportional intermolecular potential, i.e.,

\[ F \approx \frac{1}{r^s}, \]

the collision kernel \( q \) takes the form

\[ q(\xi_* - \xi, \omega) = C|\xi_* - \xi|^\gamma \beta_\gamma(\theta), \quad -3 < \gamma \leq 1. \]

- Grad cut-off assumption: Replace a singular part of \( \beta_\gamma(\theta) \) by a smoother part so that \( q \) is integrable in \( \theta \)-variable.

- Hard sphere, hard, Maxwellian and soft potential

\[
\begin{align*}
\gamma &= 1 \quad \text{hard sphere,} \quad 0 < \gamma < 1 \quad \text{hard potential} \\
\gamma &= 0 \quad \text{Maxwellian molecule,} \quad -3 < \gamma < 0 \quad \text{soft potential.}
\end{align*}
\]
Symmetry of $Q(F, F)$

- Using the property of collision map,

\[
\int Q(F, F) \varphi(\xi) d\xi \\
= \int \int \int (F' F_* - F F_*) \varphi |(\xi - \xi) \cdot \omega| d\omega d\xi_* d\xi \\
= \int \int \int (F' F_* - F F_*) \varphi_* |(\xi_* - \xi) \cdot \omega| d\omega d\xi_* d\xi \\
= \int \int \int (F' F_* - F F_*) \frac{\varphi + \varphi_*}{2} |(\xi_* - \xi) \cdot \omega| d\omega d\xi_* d\xi.
\]
• **Theorem:** Suppose that $F \in L^1(R^3)$ satisfies

$$F(\xi) = O(|\xi|^{-n}) \quad \text{as} \quad |\xi| \to \infty \quad \text{for all} \quad n \geq 0.$$  

Then, for any test function $\varphi = \varphi(\xi)$ with at most polynomial growth at infinity

$$\varphi(\xi) = O(1 + |\xi|^m) \quad \text{as} \quad |\xi| \to \infty \quad \text{for some} \quad m \geq 0,$$

we have

$$\int Q(F, F)\varphi(\xi)d\xi$$

$$= \int\int\int (F' F_* - FF_*) \frac{\varphi + \varphi_* - \varphi' - \varphi_*'}{4} |(\xi_* - \xi) \cdot \omega| d\omega d\xi_* d\xi.$$
Suppose that $0 < F \in L^1(R^3)$ is rapidly decaying and such that
$\ln F$ has polynomial growth at infinity.

- **Boltzmann’s inequality**

$$\int Q(F, F) \ln F(\xi) d\xi$$
$$= -\frac{1}{4} \iiint (F' F' - FF_*) \ln \left( \frac{F' F'}{FF_*} \right) |(\xi_* - \xi) \cdot \omega| d\omega d\xi_* d\xi \leq 0.$$  

Note that

$$\int Q(F, F) \varphi(\xi) d\xi = 0 \iff \ln F' + \ln F_* = \ln F + \ln F_*$$
$$\iff \ln F \text{ is a collision invariant.}$$
By previous theorem

\[
\ln \varphi \text{ is a collision invariant} \quad \iff \quad \ln \varphi = a + b \cdot \xi + c|\xi|^2, \quad a, c \in \mathbb{R}, \quad b \in \mathbb{R}^3
\]

\[
\iff \quad \varphi(x, \xi, t) = \frac{\rho(x, t)}{(2\pi R\theta)^{3/2}} e^{-\frac{|\xi - u(x, t)|^2}{2R\theta(x, t)}},
\]

where \( \rho, \theta > 0 \) and \( u \in \mathbb{R}^3 \).
• **Definition:** (Maxwellian)

\[ F \text{ is a Maxwellian } \iff F = M_{[\rho,u,\theta]}(\xi) = \frac{\rho(x,t)}{(2\pi R\theta)^{\frac{3}{2}}} e^{-\frac{|\xi - u(x,t)|^2}{2R\theta(x,t)}} \]

cf. Local and global (absolute) Maxwellians.

• **Theorem:** Boltzmann

The space of collision invariants is 5-dimensional and spanned by

\[ \varphi_0 = 1, \quad \varphi_i = \xi_i, \quad i = 1, 2, 3, \quad \varphi_4 := |\xi|^2. \]
**H-Theorem (irreversibility)**

We set

\[ H := \int F \log F d\xi, \quad \mathcal{H} = \int \xi F \log F d\xi. \]

Then, \( H \) satisfies

\[
\partial_t H + \nabla_x \cdot \mathcal{H} = \frac{1}{4Kn} \iint \log \frac{FF^*}{F'F_*'} \left( F'F_*' - FF_*' \right) q(\xi_* - \xi, \omega) d\omega d\xi_1 d\xi_2 \leq 0.
\]

The Boltzmann equation is a dissipative equation

cf. physical entropy = -H.
Note that equality holds if and only if $F$ is in thermo-equilibrium

$$Q(F, F) = 0$$

if and only if $F$ belong to the 5-dimensional thermo-equilibrium manifold

$$\{F : F = M[ρ, u, θ], \quad ρ > 0, θ > 0, u ∈ R^3\}.$$  

The H-Theorem says that there is a tendency for the solution $F$ of the Boltzmann equation to approach the equilibrium manifold.
Recall the identity

\[
\int Q(F, F)\varphi(\xi) d\xi = \int\int\int (F' F'_{\ast} - FF_{\ast}) \frac{\varphi + \varphi_{\ast} - \varphi' - \varphi'_{\ast}}{4} |(\xi_{\ast} - \xi) \cdot \omega| d\omega d\xi_{\ast} d\xi.
\]

We substitute \(\varphi(\xi) = 1, \xi, |\xi|^2\) into the above relation and obtain

\[
\int \begin{pmatrix}
1 \\
\xi \\
|\xi|^2 \\
\frac{2}{2}
\end{pmatrix} Q(F, F) d\xi = 0.
\]
Local conservation laws

Integrate the Boltzmann equation times $\varphi_i$, $i = 0, 4$, we get

$$\int \left( \frac{1}{|\xi|^2} \right) \left[ \partial_t F + \xi \cdot \nabla_x F \right] d\xi = \int \left( \frac{1}{|\xi|^2} \right) Q(F, F) d\xi$$

$$= 0.$$
Macroscopic observables

For a given kinetic density $F = F(x, \xi, t)$, we set

$$\rho(x, t) := \int F d\xi \quad \text{local mass density}$$

$$\rho u(x, t) := \int \xi F d\xi \quad \text{local momentum density}$$

$$\rho E(x, t) := \int \frac{|\xi|^2}{2} F d\xi \quad \text{local energy density}$$

$$\rho e(x, t) := \int \frac{|\xi - u|^2}{2} F d\xi \quad \text{local internal energy density}$$

$$\rho E = \rho e + \frac{1}{2} \rho |u|^2.$$
We can further simply by introducing stress tensor and heat flux

\[ p_{ij} := \int (\xi_i - u_i)(\xi_j - u_j) F d\xi, \quad p = \frac{1}{3} \text{tr} P, \]
\[ q_i := \int (\xi_i - u_i) |\xi - u|^2 F d\xi. \]

For a local maxwellian \( F = M \),

\[ p_{ij} = 0, \quad i \neq j, \quad q_i = 0, \quad i = 1, 2, 3. \]
\[
\int \left( \frac{1}{\xi} \right) \left[ \frac{\xi}{|\xi|^2} \right] \left[ \partial_t F + \xi \cdot \nabla_x F \right] d\xi = 0.
\]

\[\iff\]

- **Conservation laws** (Parts of moment system)

\[
\begin{align*}
\partial_t \rho + \nabla_x \cdot (\rho u) &= 0, \quad \text{mass}, \\
\partial_t (\rho u) + \nabla_x \cdot (\rho u \otimes u + P) &= 0, \quad \text{momentum}, \\
\partial_t (\rho E) + \nabla_x \cdot (\rho u E + Pu + q) &= 0 \quad \text{energy}.
\end{align*}
\]

These are 5 scalar equations for the 14 macroscopic variables:
1 for density, 3 for gas velocity \(u\), 1 for total energy \(E = e + \frac{|u|^2}{2}\), 6 for stress tensor \(P\), and 3 for heat flux \(q\). underdetermined system.
In classical fluid dynamics the conservation laws is closed under some constitutive relations for a stress tensor $P$ and heat flux $q$ to close the local conservation laws.

• (Compressible Euler equations): For a monatomic gas,

$$p_{ij}^E = p \delta_{ij}, \quad p = \rho R \theta = \frac{2}{3} \rho e, \quad q^E = 0.$$

$$\partial_t \rho + \sum_{i=1}^{3} \partial_{x_i} (\rho u) = 0,$$

$$\partial_t (\rho u_j) + \sum_{i=1}^{3} \partial_{x_i} \left( \rho u_i u_j + \frac{2}{3} \rho e \right) = 0, \quad j = 1, 2, 3,$$

$$\partial_t \left( \rho \frac{|u|^2}{2} + \rho e \right) + \sum_{i=1}^{3} \partial_{x_i} \left[ \rho u_i \left( \frac{|u|^2}{2} + \frac{5}{3} e \right) \right] = 0.$$

5 equations and 5 unknown $\rho, u, \theta$
• (Compressible Navier-Stokes equations):

\[ p_{ij}^{NS} = p\delta_{ij} - \mu \left( \partial_{x_j} u_i + \partial_{x_i} u_j - \frac{2}{3} \sum_{k=1}^{3} \partial_{x_k} u^k \delta_{ij} \right) \]

\[ - \mu_B \sum_{k=1}^{3} \partial_{x_k} u^k \delta_{ij}, \]

\[ q^{NS} = -\kappa \nabla_x \theta, \]

where

\( \mu \): viscosity, \( \mu_B \): bulk viscosity, \( \kappa \): heat conductivity.
The pressure $p$, the internal energy $e$ together with the viscosity coefficients $\mu, \mu_B$ and the heat conductivity $k$ are functions of $\rho$ and $\theta$.

From the kinetic theory, we have

$$2\rho e = 3\rho, \quad \mu_B = 0.$$
Symmetry

Recall the Boltzmann equation:

$$\partial_t F + \xi \cdot \nabla_x F = \int_{bbr^3 \times S^2} |(\xi_* - \xi) \cdot \omega|(F'F_* - FF_*) d\omega d\xi_*.$$

Let $F = F(x, \xi, t)$ be a solution. Then, we have

• **Translation invariance**

  $$F(x, \xi, t - \bar{t}), \quad F(x - \bar{x}, \xi, t) : \text{solutions.}$$

• **Rotation invariance**

  $$F(Ux, U\xi, t) : \text{solution}, \quad UU^* = U^*U = I.$$
Consider a dilation

\[ \tilde{F} = \lambda^\alpha F, \quad \tilde{x} = \lambda^\beta x, \quad \tilde{\xi} = \lambda^\gamma \xi, \quad \tilde{t} = \lambda^\beta t. \]

Note that

\[ \tilde{F}(\tilde{x}, \tilde{\xi}, \tilde{t}) = \lambda^\alpha F(x, \xi, t) = \lambda^\alpha F(\lambda^{-\beta} \tilde{x}, \lambda^{-\gamma} \tilde{\xi}, \lambda^{-\delta} \tilde{t}). \]

Then, by direct calculation, we have

\[ \partial_t \tilde{F} = \lambda^{\alpha-\delta} \partial_t F, \]
\[ \tilde{\xi} \cdot \nabla \tilde{x} \tilde{F} = \lambda^{\alpha+\gamma-\beta} \xi \cdot \nabla x F, \]
\[ Q(\tilde{F}, \tilde{F}) = \int_{bbr^3 \times S^2} |(\tilde{\xi}_* - \tilde{\xi}) \cdot \omega| (\tilde{F}' \tilde{F}'_* - \tilde{F} \tilde{F}_*) d\omega d\tilde{\xi}_* \]
\[ = \lambda^{2\alpha+4\gamma} Q(F, F). \]
This leads two relations for four unknowns.

\[-\delta = \gamma - \beta = \alpha + 4\gamma.\]

Thus, we have a 2-parameter family of dilations.
Summary

- The Boltzmann equation describes the dynamics of dilute gases
- The Boltzmann equation is a dissipative system
- The compressible Euler equations can be formally derived from the Boltzmann equation.