Lecture 2: The Boltzmann equation

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Outline

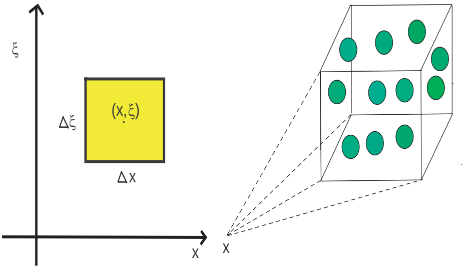
Today, I will talk about

Inner beauty of the Boltzmann equation

The Boltzmann equation

- Velocity Distribution function:

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



$F(x, \xi, t)\Delta x\Delta\xi \approx$ number of particles inside $\Delta x\Delta\xi$.

- Particle trajectory (bi-characteristics) in phase space:

$$\frac{dx}{dt} = \xi, \quad \frac{d\xi}{dt} = E(x,t),$$
$$x(0) = x, \quad \xi(0) = \xi.$$

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

$$\begin{aligned}
\frac{dF}{dt} &= \frac{d}{dt} F(x(t), \xi(t), t) \\
&= \partial_t F + \dot{x} \cdot \nabla_x F + \dot{\xi} \cdot \nabla_\xi F \Big|_{(x(t),\xi(t),t)} \\
&= \partial_t F + \xi \cdot \nabla_x F \\
&= 0.
\end{aligned}$$

This is a transport equation in phase space.

However, when there are collisions,

$$\frac{dF}{dt} = \text{Jump in } F \text{ due to collisions}\Big|_{\text{collision time}}.$$

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

     $Q(F, F)$ operates only in the velocity variable ξ in F.

- The Boltzmann equation (1872)

$$\underbrace{\partial_t F + \xi \cdot \nabla_x F}_{\text{Rate of change in } F \text{ along particle trajectory}} = \frac{1}{Kn} Q(F, F),$$

where

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

Difficulty of the Boltzmann equation comes from the collision operator

- Between collisions (free transport)

$$\frac{dx_i}{dt} = \xi_i, \quad \frac{d\xi_i}{dt} = 0, \quad i = 1, \cdots, N.$$

- The linear transport equation:

$$\partial_t F + \xi \cdot \nabla_x F = 0, \quad x, \xi \in \mathbb{R}^3, \quad t > 0,$$
$$F(x, \xi, 0) = F_0(x, \xi).$$

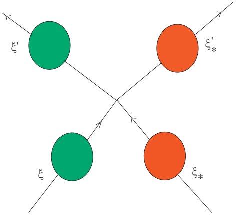
Then, it is easy to see that

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

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 $(\xi, \xi_*) \quad \Longleftrightarrow \quad (\xi', \xi'_*)$:

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

cf. Hard sphere, reversible, translational energy, elastic collisions

Collision transformation

Recall the elastic collision relation:

$$\xi + \xi_* = \xi' + \xi'_*, \quad |\xi|^2 + |\xi_*|^2 = |\xi'|^2 + |\xi'_*|^2.$$

Note that we have six unknown (ξ', ξ'_*) and four scalar equations. Therefore, for a given initial velocities (ξ, ξ_*), we will have a two parameter family of final velocities.

- **Theorem**: (Collision transformation)

$$\begin{aligned} \xi' &= \xi - ((\xi - \xi_*) \cdot \omega)\omega, \\ \xi'_* &= \xi_* + ((\xi - \xi_*) \cdot \omega)\omega, \quad \omega \in \mathbb{S}^2. \end{aligned}$$

Proof. We introduce a unit vector $\omega \in \mathbb{S}^2$ having the direction of the change in velocity of the first molecule.

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

Note that ω 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 ξ and ξ_* produces an interchange of post collisional velocities ξ' and ξ'_*.

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 φ 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 ξ and ξ:

$$\varphi(\xi, \xi_*) = \psi(\xi) + \psi(\xi_*).$$

- **Theorem**: Boltzmann, Carlemann, Grad

Suppose that a $\mathcal{C}^2$ function φ satisfies

$$\varphi(\xi) + \varphi(\xi_*) = \varphi(\xi') + \varphi(\xi'_*).$$

Then,

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

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 ω.

- Boltzmann's collision integral:

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

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 θ-variable.

• Hard sphere, hard, Maxwellian and soft potential

$$\begin{array}{llll} \gamma = 1 & \text{hard sphere,} & 0 < \gamma < 1 & \text{hard potential} \\ \gamma = 0 & \text{Maxwellian molecule,} & -3 < \gamma < 0 & \text{soft potential.} \end{array}$$

Symmetry of $Q(F, F)$

- Using the property of collision map,

$$\begin{aligned}
&\int Q(F,F)\varphi(\xi)d\xi \\
&= \iiint (F'F'_* - FF_*)\varphi|(\xi_* - \xi)\cdot\omega|d\omega d\xi_* d\xi \\
&= \iiint (F'F'_* - FF_*)\varphi_*|(\xi_* - \xi)\cdot\omega|d\omega d\xi_* d\xi \\
&= \iiint (F'F'_* - FF_*)\frac{\varphi + \varphi_*}{2}|(\xi_* - \xi)\cdot\omega|d\omega d\xi_* d\xi.
\end{aligned}$$

- **Theorem**: Suppose that $F \in L^1(R^3)$ satisfies

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

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

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

we have

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

Maxwellian

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

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

Note that

$$\int Q(F,F)\varphi(\xi)d\xi = 0 \quad \Longleftrightarrow \quad \ln F' + \ln F'_* = \ln F + \ln F_*$$

$$\Longleftrightarrow \quad \ln F \text{ is a collision invariant.}$$

By previous theorem

$$\begin{aligned}
&\ln\varphi \text{ is a collision invariant} \\
&\iff \quad \ln\varphi = a + \mathbf{b}\cdot\xi + c|\xi|^2, \quad a, c \in \mathbb{R}, \quad \mathbf{b} \in \mathbb{R}^3 \\
&\iff \varphi(x,\xi,t) = \frac{\rho(x,t)}{(2\pi R\theta)^{\frac{3}{2}}} e^{-\frac{|\xi - u(x,t)|^2}{2R\theta(x,t)}},
\end{aligned}$$

where $\rho, \theta > 0$ and $u \in R^3$.

- **Defintion**: (Maxwellian)

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

cf. Local and global (absolute) Maxwellians.

- **Theorem**: Boltzmann

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

$$\varphi_0 = 1, \quad \varphi_i = \xi_i, \; i = 1,2,3, \quad \varphi_4 := |\xi|^2.$$

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

$$\partial_t H + \nabla_x \cdot \mathcal{H} = \frac{1}{4Kn} \iint \log \frac{FF_*}{F'F'_*} \left(F'F'_* - FF_* \right) q(\xi_* - \xi, \omega) d\omega d\xi_* d\xi \leq 0.$$

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 onl if F belong to the 5-dimensional thermo-equilbrium manifold

$$\{F \ : \ F = M_{[\rho,u,\theta]}, \quad \rho > 0, \theta > 0, u \in R^3\}.$$

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

Conservation laws

Recall the identity

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

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

$$\int \begin{pmatrix} 1 \\ \xi \\ \frac{|\xi|^2}{2} \end{pmatrix} Q(F,F)d\xi = 0.$$

- Local conservation laws

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

$$\begin{aligned}\int \begin{pmatrix} 1 \\ \xi \\ \frac{|\xi|^2}{2} \end{pmatrix} [\partial_t F + \xi \cdot \nabla_x F] d\xi &= \int \begin{pmatrix} 1 \\ \xi \\ \frac{|\xi|^2}{2} \end{pmatrix} Q(F, F) d\xi \\ &= 0.\end{aligned}$$

Macroscopic observables

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

$$\begin{aligned}
\rho(x,t) &:= \int F d\xi \quad \text{local mass density} \\
(\rho u)(x,t) &:= \int \xi F d\xi \quad \text{local momentum density} \\
(\rho E)(x,t) &:= \int \frac{|\xi|^2}{2} F d\xi \quad \text{local energy density} \\
(\rho e)(x,t) &:= \int \frac{|\xi - u|^2}{2} F d\xi \quad \text{local internal energy density} \\
\rho E &= \rho e + \frac{1}{2}\rho |u|^2.
\end{aligned}$$

We can further simply by introducing stress tensor and heat flux

$$
\begin{aligned}
p_{ij} &:= \int (\xi_i - u_i)(\xi_j - u_j) F d\xi, \quad p = \frac{1}{3}\mathrm{tr} P, \\
q_i &:= \int (\xi_i - u_i)|\xi - u|^2 F d\xi.
\end{aligned}
$$

For a local maxwellian $F = M$,

$$
p_{ij} = 0, \quad i \neq j, \qquad q_i = 0, \quad i = 1, 2, 3.
$$

$$\int \begin{pmatrix} 1 \\ \xi \\ \frac{|\xi|^2}{2} \end{pmatrix} [\partial_t F + \xi \cdot \nabla_x F] d\xi = 0.$$

$\Longleftrightarrow$

- Conservation laws (Parts of moment system)

$$\begin{aligned} &\partial_t \rho + \nabla_x \cdot (\rho u) = 0, \quad \text{mass}, \\ &\partial_t(\rho u) + \nabla_x \cdot (\rho u \otimes u + P) = 0, \quad \text{momentum}, \\ &\partial_t(\rho E) + \nabla_x \cdot (\rho u E + P u + q) = 0 \quad \text{energy}. \end{aligned}$$

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,

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

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

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

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

5 equations and 5 unknown ρ, u, θ

- (Compressible Navier-Stokes equations):

◇ Newton's law and Fourier's law

$$\begin{aligned} p_{ij}^{NS} &= p\delta_{ij} - \mu\Big(\partial_{x_j} u_i + \partial_{x_i} u_j - \frac{2}{3}\sum_{k=1}^{3} \partial_{x_k} u^k \delta_{ij}\Big) \\ &- \mu_B \sum_{k=1}^{3} \partial_{x_k} u^k \delta_{ij}, \\ q^{NS} &= -\kappa \nabla_x \theta, \end{aligned}$$

where

$$\mu: \text{ viscosity}, \quad \mu_B: \text{ bulk viscosity}, \quad \kappa: \text{ heat condcutivity.}$$

The pressure p, the internal energy e together with the viscosity coefficients μ, μ_B and the heat conductivity k are functions of ρ and θ.

From the kinetic theory, we have

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

Symmetry

Recall the Boltzmann equation:

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

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

$$\begin{aligned}
\partial_{\tilde{t}} \tilde{F} &= \lambda^{\alpha-\delta} \partial_t F, \\
\tilde{\xi} \cdot \nabla_{\tilde{x}} \tilde{F} &= \lambda^{\alpha+\gamma-\beta} \xi \cdot \nabla_x F, \\
Q(\tilde{F}, \tilde{F}) &= \int_{bbr^3 \times \mathbf{S}^2} |(\tilde{\xi}_* - \tilde{\xi}) \cdot \omega| (\tilde{F}' \tilde{F}'_* - \tilde{F} \tilde{F}_*) d\omega d\tilde{\xi}_* \\
&= \lambda^{2\alpha+4\gamma} Q(F, F).
\end{aligned}$$

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.