

Kinetic theory of gases

Toan T. Nguyen
Penn State University
<http://toannguyen.org>
<http://blog.toannguyen.org>

Graduate Student seminar, PSU
Jan 19th, 2017

Fall 2017, I teach a graduate topics course: **same topics !**

Solid



Example
Ice



Liquid



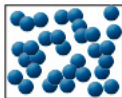
Example
Water



Gas



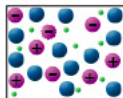
Example
Steam



Plasma



Example
Ionised Gas



● Molecules

● ● Ions

● Electrons

Figure : 4 states of matter, plus Bose-Einstein condensate!

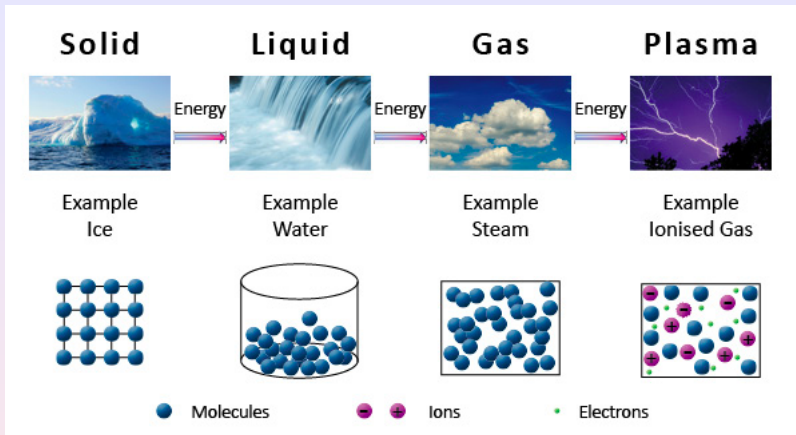


Figure : 4 states of matter, plus Bose-Einstein condensate!

- James Clerk Maxwell, in 1859, gave birth to kinetic theory: use the **statistical approach** to describe the dynamics of a (rarefied) gas.

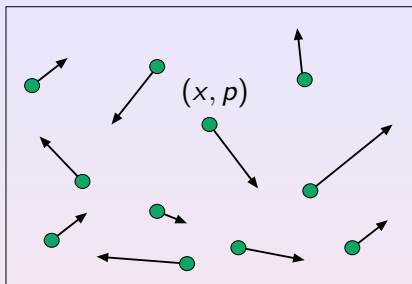


Figure : Kinetic theory of gases: phase space!

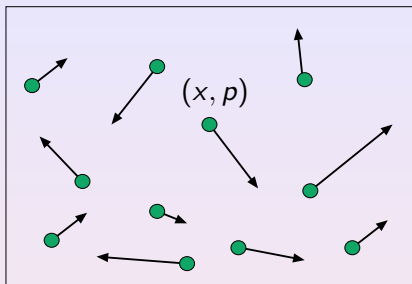


Figure : Kinetic theory of gases: phase space!

- Gas molecules are identical.
- One-particle phase space: position $x \in \Omega \subset \mathbb{R}^d$, momentum $p \in \mathbb{R}^d$

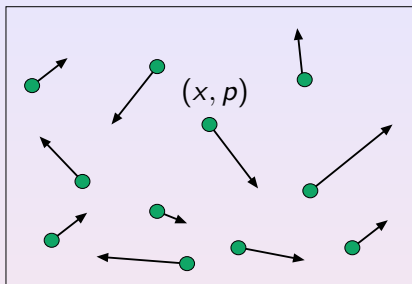


Figure : Kinetic theory of gases: phase space!

- Gas molecules are identical.
- One-particle phase space: position $x \in \Omega \subset \mathbb{R}^d$, momentum $p \in \mathbb{R}^d$
- $f(t, x, p)$ the probability density distribution. Mass: $f(t, x, p) dx dp$.
- **Interest:** the dynamics of $f(t, x, p)$? Non-equilibrium theory.

I. Collisionless Kinetic Theory

Hamilton 1830's classical mechanics¹: one-particle Hamiltonian $H(x, p)$
(induced from Lagrangian):

$$\dot{x} = \nabla_p H, \quad \dot{p} = -\nabla_x H$$

¹In truth, it should be an N-particle Hamiltonian dynamics, then mean field limit or BBGKY hierarchy to kinetic theory. [S1: Presentation on its formal derivation?](#)

Hamilton 1830's classical mechanics¹: **one-particle Hamiltonian** $H(x, p)$
(induced from Lagrangian):

$$\dot{x} = \nabla_p H, \quad \dot{p} = -\nabla_x H$$

Examples:

- Free particles:

$$H(x, p) = \frac{1}{2m}|p|^2$$

¹In truth, it should be an N-particle Hamiltonian dynamics, then mean field limit or BBGKY hierarchy to kinetic theory. **S1**: Presentation on its formal derivation?

Hamilton 1830's classical mechanics¹: **one-particle Hamiltonian** $H(x, p)$
(induced from Lagrangian):

$$\dot{x} = \nabla_p H, \quad \dot{p} = -\nabla_x H$$


Examples:

- Free particles:

$$H(x, p) = \frac{1}{2m}|p|^2$$

- Particles in a potential:

$$H(x, p) = \frac{1}{2m}|p|^2 + V_{pot}(x)$$

¹In truth, it should be an N-particle Hamiltonian dynamics, then mean field limit or BBGKY hierarchy to kinetic theory. **S1**: Presentation on its formal derivation? 

- Also for plasmas: charged particles in electromagnetic fields

$$H(x, p) = \frac{1}{2m} |p - qA(x)|^2 + \phi(x)$$

with electric and magnetic potentials ϕ, A .

- Also for plasmas: charged particles in electromagnetic fields

$$H(x, p) = \frac{1}{2m} |p - qA(x)|^2 + \phi(x)$$

with electric and magnetic potentials ϕ, A .

- Force acting on particles:

$$F = -\nabla_x H = E + \frac{q}{m} (p \times B)$$

which is the Lorentz force, with $E = -\nabla_x \phi$ and $B = \nabla_x \times A$.

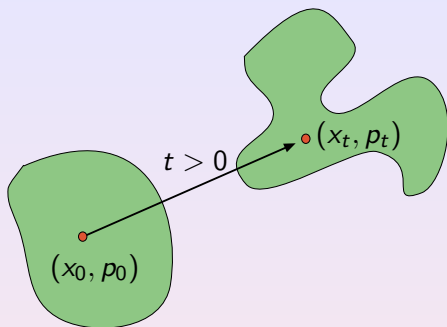


Figure : **Liouville's Theorem**: volume in phase space remains constant (Exercise: prove this).

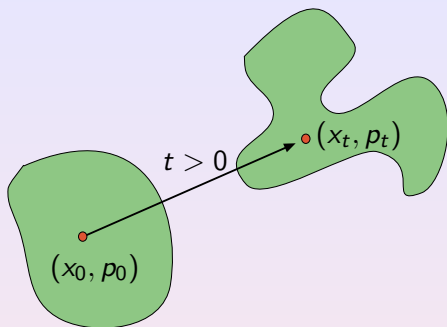


Figure : **Liouville's Theorem**: volume in phase space remains constant (Exercise: prove this).

This yields the kinetic equation: $\partial_t f = \{H, f\}$ (Poisson bracket), explicitly

$$\begin{aligned}
 0 &= \frac{d}{dt} f(t, x(t), p(t)) = \partial_t f + \nabla_p H \cdot \nabla_x f - \nabla_x H \cdot \nabla_p f \\
 &= \partial_t f + v \cdot \nabla_x f + F_{\text{force}} \cdot \nabla_v f
 \end{aligned}$$

Three examples of **kinetic equations** (remain very active):

Three examples of **kinetic equations** (remain very active):

- **Vlasov** dynamics (transport in phase space):

$$\partial_t f + v \cdot \nabla_x f + F \cdot \nabla_v f = 0$$

Three examples of **kinetic equations** (remain very active):

- **Vlasov** dynamics (transport in phase space):

$$\partial_t f + v \cdot \nabla_x f + F \cdot \nabla_v f = 0$$

- **Vlasov-Poisson**:

$$F = -\nabla_x \phi, \quad -\Delta_x \phi = \sigma \int_{\mathbb{R}^3} f(t, x, v) dv,$$

with $\sigma = 1$ (plasma physics: charged particles) or $\sigma = -1$ (gravitational case: stars in a galaxy).

Three examples of **kinetic equations** (remain very active):

- **Vlasov** dynamics (transport in phase space):

$$\partial_t f + v \cdot \nabla_x f + F \cdot \nabla_v f = 0$$

- **Vlasov-Poisson**:

$$F = -\nabla_x \phi, \quad -\Delta_x \phi = \sigma \int_{\mathbb{R}^3} f(t, x, v) dv,$$

with $\sigma = 1$ (plasma physics: charged particles) or $\sigma = -1$ (gravitational case: stars in a galaxy).

- **Vlasov-Maxwell** (plasma): Lorentz force $F = E + v \times B$ with the electromagnetic fields E, B solving **Maxwell** (generated by charge and current density).

- Can you solve Vlasov, the Cauchy problem?

- Can you solve Vlasov, the Cauchy problem? In fact, it's simply ODEs:

$$\dot{x} = v, \quad \dot{v} = F(t, x, v)$$

Then, Vlasov $f(t, x, v) = f_0(x_{-t}, v_{-t})$.

- Can you solve Vlasov, the Cauchy problem? In fact, it's simply ODEs:

$$\dot{x} = v, \quad \dot{v} = F(t, x, v)$$

Then, Vlasov $f(t, x, v) = f_0(x_{-t}, v_{-t})$.

- One needs Lipschitz bounds on $F(t, x, v)$.

- Can you solve Vlasov, the Cauchy problem? In fact, it's simply ODEs:

$$\dot{x} = v, \quad \dot{v} = F(t, x, v)$$

Then, Vlasov $f(t, x, v) = f_0(x_{-t}, v_{-t})$.

- One needs Lipschitz bounds on $F(t, x, v)$.
- **Vlasov-Poisson:** $F = -\nabla_x \phi$ and $-\Delta \phi = \pm \int f(t, x, v) dv$. Roughly speaking: $\nabla_x F = \nabla_x^2 (-\Delta_x)^{-1} \rho \approx \rho$, up to a **log** of derivatives of f .

- Can you solve Vlasov, the Cauchy problem? In fact, it's simply ODEs:

$$\dot{x} = v, \quad \dot{v} = F(t, x, v)$$

Then, Vlasov $f(t, x, v) = f_0(x_{-t}, v_{-t})$.

- One needs Lipschitz bounds on $F(t, x, v)$.
- **Vlasov-Poisson:** $F = -\nabla_x \phi$ and $-\Delta \phi = \pm \int f(t, x, v) dv$. Roughly speaking: $\nabla_x F = \nabla_x^2 (-\Delta_x)^{-1} \rho \approx \rho$, up to a **log** of derivatives of f .
- Global unique solutions (1991): Pfaffelmoser, Lions-Perthame, Schaeffer, Glassey's book.

- Can you solve Vlasov, the Cauchy problem? In fact, it's simply ODEs:

$$\dot{x} = v, \quad \dot{v} = F(t, x, v)$$

Then, Vlasov $f(t, x, v) = f_0(x_{-t}, v_{-t})$.

- One needs Lipschitz bounds on $F(t, x, v)$.
- **Vlasov-Poisson:** $F = -\nabla_x \phi$ and $-\Delta \phi = \pm \int f(t, x, v) dv$. Roughly speaking: $\nabla_x F = \nabla_x^2 (-\Delta_x)^{-1} \rho \approx \rho$, up to a **log** of derivatives of f .
- Global unique solutions (1991): Pfaffelmoser, Lions-Perthame, Schaeffer, Glassey's book.
- **Vlasov-Maxwell:** **Outstanding open problem!** Glassey Strauss's theorem.

Several mathematical issues: $\partial_t f = \{H, f\}$ (focus on previous examples).

Several mathematical issues: $\partial_t f = \{H, f\}$ (focus on previous examples).

- Infinitely many conserved quantities, and infinitely many equilibria:

$$\frac{D}{dt}\varphi(f) = 0, \quad f_* = \varphi(H(x, p))$$

for arbitrary $\varphi(\cdot)$. Which one is dynamically stable? and shouldn't it be just Gaussian? Maxwell-Boltzmann distribution (next section)?

Several mathematical issues: $\partial_t f = \{H, f\}$ (focus on previous examples).

- Infinitely many conserved quantities, and infinitely many equilibria:

$$\frac{D}{dt}\varphi(f) = 0, \quad f_* = \varphi(H(x, p))$$

for arbitrary $\varphi(\cdot)$. Which one is dynamically stable? and shouldn't it be just Gaussian? Maxwell-Boltzmann distribution (next section)?

- Hence, large time dynamics and stability of equilibria are very delicate!

$$\text{VP:} \quad \partial_t f + v \cdot \nabla_x f - \nabla_x \phi \cdot \nabla_v f = 0, \quad -\Delta \phi = \rho - 1.$$

- For instance, homogenous equilibria

$$\mu = \mu(e), \quad e := \frac{1}{2}|v|^2, \quad \phi_0 = 0.$$

$$\text{VP: } \quad \partial_t f + v \cdot \nabla_x f - \nabla_x \phi \cdot \nabla_v f = 0, \quad -\Delta \phi = \rho - 1.$$

- For instance, homogenous equilibria

$$\mu = \mu(e), \quad e := \frac{1}{2}|v|^2, \quad \phi_0 = 0.$$

- **Arnold:** Look at casimir's invariant

$$\mathcal{A}[f] = \iint \left[\frac{1}{2}|v|^2 f + \varphi(f) \right] dv dx + \frac{1}{2} \int |\nabla \phi|^2 dx.$$

$$\text{VP: } \quad \partial_t f + v \cdot \nabla_x f - \nabla_x \phi \cdot \nabla_v f = 0, \quad -\Delta \phi = \rho - 1.$$

- For instance, homogenous equilibria

$$\mu = \mu(e), \quad e := \frac{1}{2}|v|^2, \quad \phi_0 = 0.$$

- **Arnold:** Look at casimir's invariant

$$\mathcal{A}[f] = \iint \left[\frac{1}{2}|v|^2 f + \varphi(f) \right] dv dx + \frac{1}{2} \int |\nabla \phi|^2 dx.$$

- μ is a critical point iff $\varphi'(\mu) = -\frac{1}{2}|v|^2$ or $\varphi' = -\mu^{-1}$. Convexity of $\mathcal{A}[f]$ requires

$$\mu_e < 0.$$

$$\text{VP: } \quad \partial_t f + v \cdot \nabla_x f - \nabla_x \phi \cdot \nabla_v f = 0, \quad -\Delta \phi = \rho - 1.$$

- For instance, homogenous equilibria

$$\mu = \mu(e), \quad e := \frac{1}{2}|v|^2, \quad \phi_0 = 0.$$

- **Arnold:** Look at casimir's invariant

$$\mathcal{A}[f] = \iint \left[\frac{1}{2}|v|^2 f + \varphi(f) \right] dv dx + \frac{1}{2} \int |\nabla \phi|^2 dx.$$

- μ is a critical point iff $\varphi'(\mu) = -\frac{1}{2}|v|^2$ or $\varphi' = -\mu^{-1}$. Convexity of $\mathcal{A}[f]$ requires

$$\mu_e < 0.$$

- $\mu_e < 0$ implies Arnold's nonlinear stability. But, **what's long-time dynamics?**

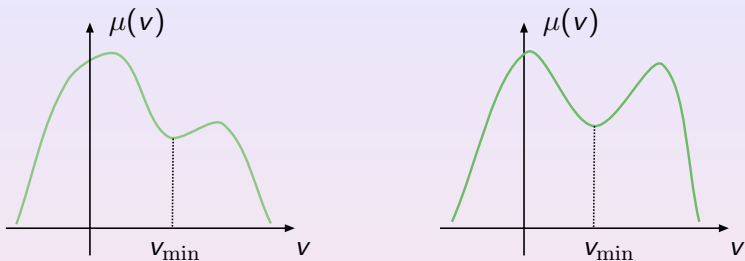


Figure : Stable vs unstable equilibria. Beautiful Penrose's iff criteria:

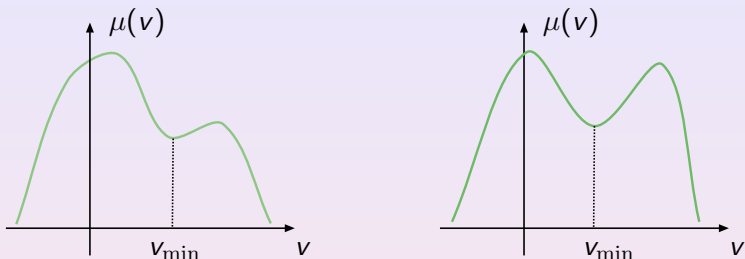


Figure : Stable vs unstable equilibria. Beautiful Penrose's iff criteria: **linearly unstable** iff v_{\min} exists and

$$\text{P.V.} \int_{\mathbb{R}} \frac{\mu'(v) dv}{v - v_{\min}} > 0.$$

S2: Presentation on Penrose's criteria?

- Mouhot-Villani: **nonlinear** Landau damping of Penrose stable homogenous equilibria of VP (earning Villani a Fields medal).
- **S3**: presentation on linearized case?

- Mouhot-Villani: **nonlinear** Landau damping of Penrose stable homogenous equilibria of VP (earning Villani a Fields medal).
- **S3**: presentation on linearized case?
- **Open**: Are there stable inhomogenous equilibria (VP)? $f_* = \varphi(H(x, p))$.

- Mouhot-Villani: **nonlinear** Landau damping of Penrose stable homogenous equilibria of VP (earning Villani a Fields medal).
- **S3**: presentation on linearized case?
- **Open**: Are there stable inhomogenous equilibria (VP)? $f_* = \varphi(H(x, p))$.
- Some of my works (available on my homepage):
 - Stability of inhomogenous equilibria of VM (w/ Strauss).
 - Various asymptotic limits of Vlasov (w/ Han-Kwan).
 - Non-relativistic limits of VM (w/ Han-Kwan and Rousset).

II. Collisional Kinetic Theory

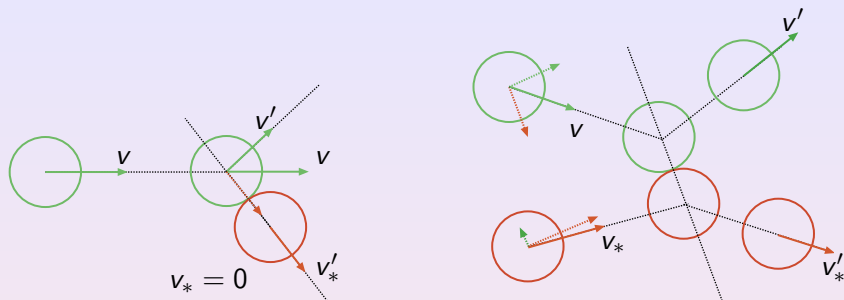


Figure : Elastic collisions: momentum and energy are exchanged between particles, however conserved, after collision:

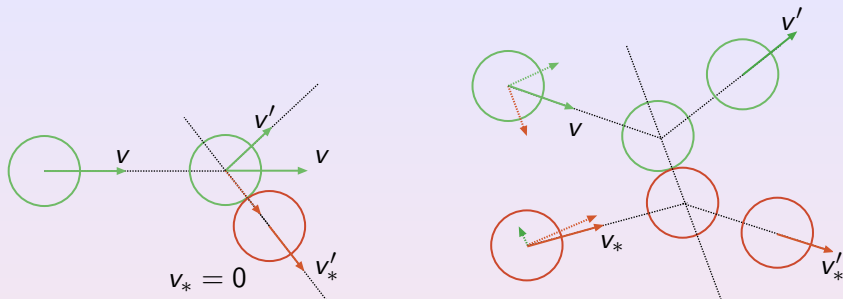
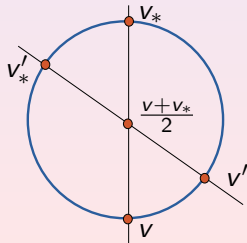


Figure : Elastic collisions: momentum and energy are exchanged between particles, however conserved, after collision:

- $v + v_* = v' + v'_*$
- $|v|^2 + |v_*|^2 = |v'|^2 + |v'_*|^2$

Sphere S_{vv_*} :



One has the Boltzmann equation:

$$\partial_t f - \{H, f\} = Q[f]$$

in which collision operator $Q[f]$:

One has the **Boltzmann equation**:

$$\partial_t f - \{H, f\} = Q[f]$$

in which collision operator $Q[f]$:

$$Q[f](x, v) = \iiint_{\mathbb{R}^9} \underbrace{\omega(v, v_* | v', v'_*)}_{\text{Scattering}} \left[\underbrace{f_2(x, v', v'_*)}_{\text{Gain}} - \underbrace{f_2(x, v, v_*)}_{\text{Loss}} \right] dv_* dv' dv'_*$$

with $f_2(x, v, v_*)$ the probability distribution of finding two particles with respective momenta.

One has the **Boltzmann equation**:

$$\partial_t f - \{H, f\} = Q[f]$$

in which collision operator $Q[f]$:

$$Q[f](x, v) = \iiint_{\mathbb{R}^9} \underbrace{\omega(v, v_* | v', v'_*)}_{\text{Scattering}} \left[\underbrace{f_2(x, v', v'_*)}_{\text{Gain}} - \underbrace{f_2(x, v, v_*)}_{\text{Loss}} \right] dv_* dv' dv'_*$$

with $f_2(x, v, v_*)$ the probability distribution of finding two particles with respective momenta.

- **Molecular chaos assumption**:

$$f_2(x, v, v_*) = f(x, v)f(x, v_*)$$

asserting velocities are uncorrelated **before** the collision (unlike Hamiltonian, here it introduces a notion of **time** arrow!).

- Conservation laws: $v', v'_* \in S_{v v_*}$ and hence

$$dv' dv'_* = d\sigma(S_{v v_*}) = |v - v_*| d\sigma(n), \quad n \in S_2.$$

- Conservation laws: $v', v'_* \in S_{vv_*}$ and hence

$$dv' dv'_* = d\sigma(S_{vv_*}) = |v - v_*| d\sigma(n), \quad n \in S_2.$$

- (symmetric) **Scattering**: Elastic hard-sphere collisions:

$$\omega(v, v_* | v', v'_*) = \frac{|n \cdot (v - v_*)|}{|v - v_*|} \quad (\text{angle of collision})$$

- Conservation laws: $v', v'_* \in S_{v v_*}$ and hence

$$dv' dv'_* = d\sigma(S_{v v_*}) = |v - v_*| d\sigma(n), \quad n \in S_2.$$

- (symmetric) **Scattering**: Elastic hard-sphere collisions:

$$\omega(v, v_* | v', v'_*) = \frac{|n \cdot (v - v_*)|}{|v - v_*|} \quad (\text{angle of collision})$$

- **The Boltzmann equation** (1872) for hard-sphere gases:

$$\partial_t f - \{H, f\} = \int_{\mathbb{R}^3} \int_{S_2} |n \cdot (v - v_*)| [f' f'_* - f f_*] dndv_*.$$

- Conservation laws: $v', v'_* \in S_{vv_*}$ and hence

$$dv' dv'_* = d\sigma(S_{vv_*}) = |v - v_*| d\sigma(n), \quad n \in S_2.$$

- (symmetric) **Scattering**: Elastic hard-sphere collisions:

$$\omega(v, v_* | v', v'_*) = \frac{|n \cdot (v - v_*)|}{|v - v_*|} \quad (\text{angle of collision})$$

- **The Boltzmann equation** (1872) for hard-sphere gases:

$$\partial_t f - \{H, f\} = \int_{\mathbb{R}^3} \int_{S_2} |n \cdot (v - v_*)| [f' f'_* - ff_*] dndv_*.$$

Is it solvable? Di Perna-Lions '89, Guo 2010. There remain many **outstanding open** problems.

- Boltzmann's H-Theorem: Look at the entropy:

$$\mathcal{H}(t) = \iint_{\mathbb{R}^6} f \log f \, dx dv.$$

- Boltzmann's H-Theorem: Look at the entropy:

$$\mathcal{H}(t) = \iint_{\mathbb{R}^6} f \log f \, dx dv.$$

- One has

$$\begin{aligned} \frac{d}{dt} \mathcal{H}(t) &= \int_{\mathbb{R}^3} \int_{S_2} |n \cdot (v - v_*)| \left[f' f'_* - f f_* \right] \log f \, dndxdvdv_* \\ &= \frac{1}{4} \int_{\mathbb{R}^3} \int_{S_2} |n \cdot (v - v_*)| \left[f' f'_* - f f_* \right] \log \frac{f f_*}{f' f'_*} \, dndxdvdv_* \\ &\leq 0. \end{aligned}$$

- Boltzmann's H-Theorem: Look at the entropy:

$$\mathcal{H}(t) = \iint_{\mathbb{R}^6} f \log f \, dx dv.$$

- One has

$$\begin{aligned} \frac{d}{dt} \mathcal{H}(t) &= \int_{\mathbb{R}^3} \int_{S_2} |n \cdot (v - v_*)| \left[f' f'_* - f f_* \right] \log f \, dndxdv dv_* \\ &= \frac{1}{4} \int_{\mathbb{R}^3} \int_{S_2} |n \cdot (v - v_*)| \left[f' f'_* - f f_* \right] \log \frac{f f_*}{f' f'_*} \, dndxdv dv_* \\ &\leq 0. \end{aligned}$$

- Entropy is decreasing ! (unlike Hamiltonian, there is a time arrow!).

- Boltzmann's H-Theorem: There is more: equilibria iff

$$ff_* = f'f'_*, \quad v', v'_* \in S_{vv_*}$$

and so iff (presentation?):

- **Boltzmann's H-Theorem:** There is more: equilibria iff

$$ff_* = f'f'_*, \quad v', v'_* \in S_{vv_*}$$

and so iff (presentation?): Maxwellian distribution

$$f(x, v) = Ce^{-\beta|v-u|^2} = \frac{\rho(x)}{(2\pi\theta(x))^{3/2}} e^{-\frac{|v-u(x)|^2}{2\theta(x)}}$$

in which (ρ, u, θ) denotes **macroscopic** density, velocity, and temperature of gases.

- Hydrodynamics limits (if time permits).

- Hydrodynamics limits (if time permits).
- Mathematical difficulty of the Cauchy problem and convergence to equilibrium.

- Hydrodynamics limits (if time permits).
- Mathematical difficulty of the Cauchy problem and convergence to equilibrium.
- Some of my works (available on my homepage):
 - On justification of Maxwell-Boltzmann distribution (w/ Bardos, Golse, Sentis)
 - on Quantum Boltzmann, interaction between fermions, bosons, and Bose-Einstein condensate (w/ Tran)