

2.2) The Boltzmann Equation

(1)

2.2.1) The relevant time scales

$$\frac{\partial f_1(\vec{q}_1, \vec{p}_1, t)}{\partial t} + \{f_1, H\} = \int d\vec{q}_2 d\vec{p}_2 \frac{\partial V(\vec{q}_1, \vec{q}_2)}{\partial \vec{q}_1} \cdot \frac{\partial f_2(\vec{q}_1, \vec{p}_1, \vec{q}_2, \vec{p}_2)}{\partial \vec{p}_1} \quad (F_1)$$

free evolution

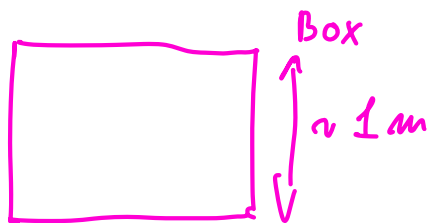
interaction term

Comment: $V=0 \Rightarrow \frac{\partial f_1}{\partial t} + \{f_1, H\} = 0$ is a closed equation.

"Collision free Boltzmann equation" studied in Part 2.

\Rightarrow The difficulty is to deal with the right-hand side.

Involved time-scales:



All time and length scales of $V(\vec{q})$ are macroscopic.

The solution of $\frac{\partial f}{\partial t} = -\frac{1}{\tau} f$ is $f(t) = f(0) e^{-\frac{t}{\tau}} \Rightarrow \tau$ is a relaxation time

$[\{f_1, H\}] = \left[\frac{f_1}{\tau_F} \right] \Rightarrow \tau_F$ is the relaxation time scale of the gas without interaction.

$\tau_F \sim$ time to cross the box $\approx \frac{L}{v} \Rightarrow v = ?$

$$m_{N_2} = \frac{2 \times 14 \times 10^{-3}}{N_A} \quad ; \quad \frac{1}{2} m_{N_2} \langle \vec{v}^2 \rangle = \frac{3}{2} k_B T \Rightarrow v = \sqrt{\langle \vec{v}^2 \rangle} \approx \sqrt{\frac{3 k_B T}{m_{N_2}}}$$

$\Rightarrow v \approx 500 \text{ m/s} \Rightarrow \tau_F \approx 10^{-2} \text{ s} \Rightarrow$ time scale over which $\{f_1, H\}$ makes f_1 relax

(2)

$$\left[\int d\vec{q}_2 d\vec{p}_2 \frac{\partial f_2}{\partial \vec{p}_1} \cdot \frac{\partial v}{\partial \vec{q}_1} \right] = \left[\frac{f_1}{\tau_{int}} \right] ; \tau_{int} \text{ the time it takes for interaction to make } f_1 \text{ relax}$$

$\tau_{int} = ?$

① duration of a collision $\tau_{col} \simeq \frac{d}{v}$; with d the particle size

$d \sim 3 \text{ \AA} \Rightarrow \tau_{col} \simeq 6 \cdot 10^{-13} \text{ s} = 0.6 \text{ ps}$.

But, most of the time, there are no collisions !

② time between collisions τ_{int}

Every τ_{col} , the particle travels its size. If there is a particle ahead, there is a collision, otherwise, there is no collision.

probab. of collision: $P_c = d^3 \times n$, where n is the gas number density.

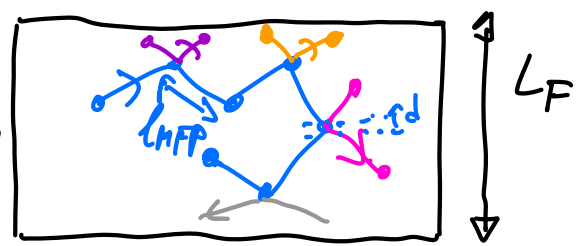
$$PV = NkT \Rightarrow n = \frac{N}{V} = \frac{P}{kT} \simeq 2.4 \times 10^{25} \text{ m}^{-3} \Rightarrow P_c = \frac{d^3 P}{kT} \simeq 6.5 \times 10^{-4}$$

It takes n_ϵ time intervals for a collision to occur where $P n_\epsilon \simeq 1$

$$\Rightarrow n_\epsilon = \frac{kT}{d^3 P} \simeq 1500$$

$$\tau_{int} = n_\epsilon \tau_{col} = \frac{kT}{d^3 P} \simeq 9 \cdot 10^{-10} \text{ s}$$

Mean free path: $\ell_{MFP} = v \tau_{int} \sim 460 \text{ nm}$



Three well separated time scales in the system: $\tau_F \gg \tau_{int} \gg \tau_{col}$
 $10^{-2} \quad 10^{-9} \quad 10^{-12}$

$$\tau_F \sim 10^{-2} \text{ s} \gg \tau_{int} \sim 10^{-9} \text{ s} \gg \tau_{col} \sim 10^{-12} \text{ s}$$

$$L_F \sim 1 \text{ m} \gg \ell_{MFP} \sim 460 \text{ nm} \gg d \sim 0.5 \text{ nm}$$

Boltzmann equation:

Describe the evolution over τ such that: $\tau_{int} \gg \tau \gg \tau_{col}$

→ collisions look instantaneous

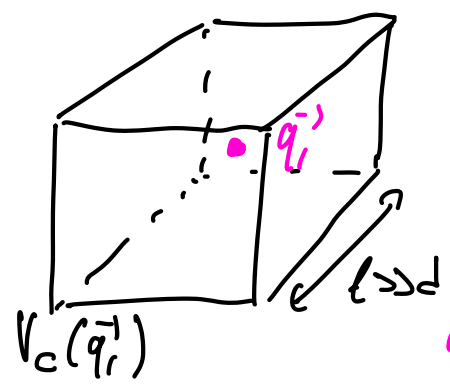
→ — are still rare and somewhat random events.

2.2.2) The coarse graining

Start from $\{f_1, f_2, H_1\} = \int d\vec{q}_2 d\vec{p}_2 \frac{\partial V(\vec{q}_1, \vec{q}_2)}{\partial \vec{q}_1} \cdot \frac{\partial}{\partial \vec{p}_1} f_2(\vec{q}_1, \vec{p}_1, \vec{q}_2, \vec{p}_2)$

Build a coarse grained dynamics over scales τ, ℓ such that

$$\tau_{int} \gg \tau \gg \tau_{col} \quad \text{and} \quad \ell_{MFP} \gg \ell \gg d$$



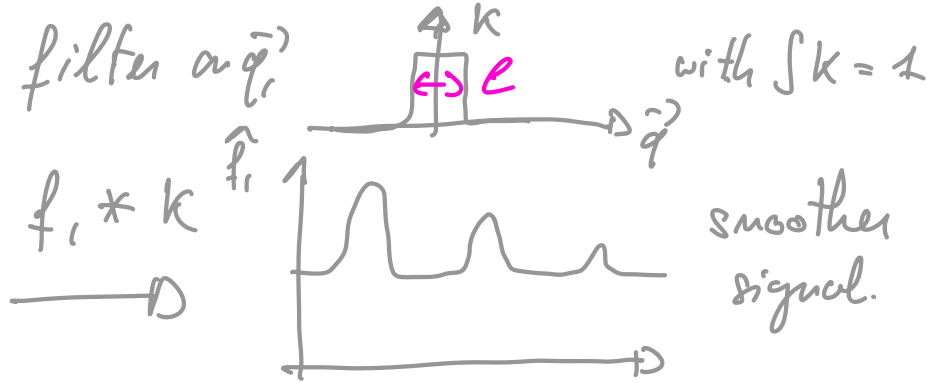
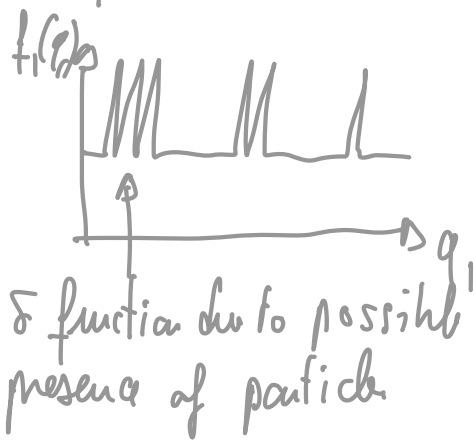
Local number density in phase space

$$\hat{f}_i(\vec{q}_i, \vec{p}_i, t) \simeq \frac{1}{V_C} \int_{V_C(\vec{q}_i)} d\vec{q}_i' f_i(\vec{q}_i', \vec{p}_i, t) \quad (c\&)$$

average density within a finite volume near \vec{q}_i .

particles "infinitely close to \vec{q}_i "

Comment: (CG) can be seen as a convolution between $f_1(\vec{q}_1, \vec{p}_1, t)$ and a filter $\propto \vec{q}_1$ with $\int k = 1$



Time evolution of $\hat{f}_1(\vec{q}_1, \vec{p}_1, t)$:

$$\frac{1}{V_c} \int_{V_c} d\vec{q}_1' \partial_\epsilon f_1(\vec{q}_1', \vec{p}_1, t) = \partial_\epsilon \hat{f}_1(\vec{q}_1, \vec{p}_1, t)$$

$$= -\frac{1}{V_c} \int_{V_c} d\vec{q}_1' \{f_1(\vec{q}_1', \vec{p}_1, t), H_1\} + \frac{1}{V_c} \int_{V_c} d\vec{q}_1' \int d\vec{q}_2 d\vec{p}_2 \frac{\partial V(\vec{q}_1' \cdot \vec{q}_2)}{\partial \vec{q}_1'} \frac{\partial f_2}{\partial \vec{p}_1}$$

①, the free evolution

② the interaction term
 $\equiv \frac{\partial \hat{f}_1}{\partial t} \Big|_{\text{col}}$

2.2.2.1] The free evolution

Since nothing happens on scale l due to H_1 , we expect that

$$\partial_\epsilon \hat{f}_1 + \{ \hat{f}_1, H_1 \} = [\text{evolution due to collisions}] \equiv \frac{\partial \hat{f}_1}{\partial t} \Big|_{\text{col.}}$$

Comput ①:

$$\textcircled{*} \frac{1}{V_c} \int_{V_c} d\vec{q}_1' \frac{\partial H}{\partial \vec{q}_1'} \cdot \frac{\partial}{\partial \vec{p}_1} f_1 \approx \frac{\partial H}{\partial \vec{q}_1'} \Big|_{\vec{q}_1} \cdot \frac{\partial}{\partial \vec{p}_1} \underbrace{\frac{1}{V_c} \int_{V_c} d\vec{q}_1' f_1}_{= \hat{f}_1} = \frac{\partial H}{\partial \vec{q}_1'} \cdot \frac{\partial \hat{f}_1}{\partial \vec{p}_1}$$

\propto constant in V_c

$$\textcircled{*} -\frac{1}{V_c} \int d\vec{q}_1' \frac{\partial H}{\partial \vec{p}_1'} \cdot \frac{\partial f_1(\vec{q}_1', \vec{p}_1, t)}{\partial \vec{q}_1'} = -\frac{\partial H}{\partial \vec{p}_1} \cdot \left[\frac{1}{V_c} \int d\vec{q}_1' \frac{\partial f_1(\vec{q}_1', \vec{p}_1, t)}{\partial \vec{q}_1'} \right]$$

By linearity, the spatial average of the gradient is the gradient of the spatial average (5)

$$\int_{V(\vec{q}_i)} d\vec{q}_i' \frac{\partial f}{\partial \vec{q}_i'}(\vec{q}_i', \vec{p}_i', t) = \frac{\partial}{\partial \vec{p}_i'} \int_{V(\vec{q}_i)} d\vec{q}_i' f(\vec{q}_i', \vec{p}_i', t) = \frac{\partial}{\partial \vec{p}_i'} \hat{f}_i(\vec{q}_i, \vec{p}_i, t)$$

$$\Rightarrow -\frac{1}{V_c} \int d\vec{q}_i' \frac{\partial H}{\partial \vec{p}_i'} \cdot \frac{\partial f_i}{\partial \vec{q}_i'}(\vec{q}_i', \vec{p}_i', t) = -\frac{\partial H}{\partial \vec{p}_i'} \cdot \frac{\partial \hat{f}_i}{\partial \vec{q}_i'}$$

Proof: $\underline{1d}$: $F(x) = \frac{1}{2\ell} \int_{x-\ell}^{x+\ell} f(y) dy$

$\Rightarrow F'(x) \stackrel{\text{ Leibniz } \circ}{=} \frac{1}{2\ell} (f(x+\ell) - f(x-\ell)) = \frac{1}{2\ell} \int_{x-\ell}^{x+\ell} f'(y) dy$

\underline{nd} : $F(\vec{n}) = \frac{1}{V} \int_{V(\vec{n})} d^m \vec{y} f(\vec{y})$

For any $d\vec{\ell}$, $F(\vec{n} + d\vec{\ell}) - F(\vec{n}) \simeq \vec{\nabla} F \cdot d\vec{\ell}$

$$= \frac{1}{V} \left[\int_{V(\vec{n} + d\vec{\ell})} f(\vec{y}) d^m \vec{y} - \int_{V(\vec{n})} f(\vec{y}') d^m \vec{y}' \right]$$

$\int_{\vec{y} \rightarrow \vec{y}' + d\vec{\ell}}$

$$= \frac{1}{V} \left[\int_{V(\vec{n})} [f(\vec{y}' + d\vec{\ell}) - f(\vec{y}')] d^m \vec{y}' \right]$$

$$= \frac{1}{V} \left[\int_{V(\vec{n})} \vec{\nabla} f(\vec{y}') \cdot d\vec{\ell} d^m \vec{y}' \right]$$

$$= \left[\frac{1}{V} \int_{V(\vec{n})} \vec{\nabla} f(\vec{y}') d^m \vec{y}' \right] d\vec{\ell} \Rightarrow \vec{\nabla} F = \frac{1}{V} \int_{V(\vec{n})} \vec{\nabla} f(\vec{y}) d^m \vec{y}$$

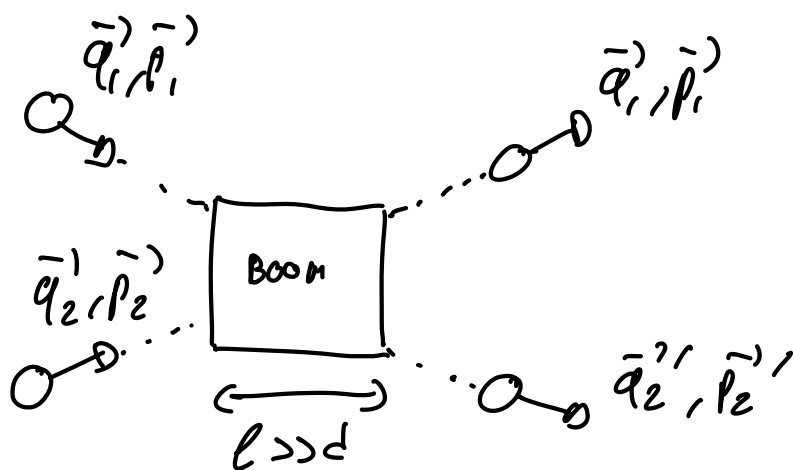
All in all, upon spatial coarse graining,

⑥

$$\partial_t f_i + \{f_i, H_i\} \xrightarrow{\frac{1}{V_c} \int d\vec{q}_i} \partial_t \hat{f}_i + \{\hat{f}_i, H_i\}$$

This entirely accounts for transport and we now need to account for how the collisions, i.e. compute $\frac{\partial \hat{f}_i}{\partial t} \Big|_{\text{col}}$

2.2.2.2] The collisions



Resolving precisely what happens during collisions is very difficult.

\Rightarrow Can we build directly the resulting dynamics for \hat{f}_i ?

Time-scale

* On time $\sim \tau_{\text{col}}$, very rare collisions, the average phase space density barely evolves

* On time $\sim \tau_{\text{HFP}}$, frequent collisions $\Rightarrow \hat{f}_i$ evolves $\Rightarrow \tau_{\text{HFP}}$ is a natural evolution time of $\hat{f}_i \Rightarrow \hat{f}_i = \hat{f}_i(\frac{t}{\tau_{\text{HFP}}})$

* Consider $\tau_{\text{HFP}} \gg \tau \gg \tau_{\text{col}}$, few collisions here and there so that the average phase space density does not evolve much and

