Recap: BBGKY Hierarchie

$$\partial_t f_1 + v_1 \nabla_{r_1} f_1 + \vec{F} \nabla_{p_1} f_1 = - \int dR_2\, \vec{K}_{12} \nabla_{p_1} f_2$$

$$\left[\partial_t + v_1 \nabla_{r_1} + v_2 \nabla_{r_2} + \vec{F}_1 \nabla_{p_1} + \vec{F}_2 \nabla_{p_2} + K_{12} (\nabla_{p_1} - \nabla_{p_2})\right] f_2$$
$$= - \int dR_3 \left(\vec{K}_{13} \vec{\nabla}_{p_1} + \vec{K}_{23} \nabla_{p_2} \right) f_3$$

coupled set of evolution equations for reduced k-body distributions

→ need for truncations

① Long range interactions

mean-field approximation

$$f_2 \approx f_1 f_1$$

$$\int dR_2 \vec{K}_{12} \vec{\nabla}_{p_1} f_2 = \underbrace{\left[\int dR_2\, \vec{K}_{12}\, f_1(t, \vec{r}_2, \vec{p}_2) \right]}_{\vec{F}_{int}(\vec{r}_1)} \nabla_{p_1} f_1$$

closed at one-body level

② Scales in BBGKY hierarchy

Spatial variation $\tau_S \sim \left(v \, \frac{\nabla_r f}{f}\right)^{-1}$

external forces $\tau_e \sim \left(\frac{v}{k_B T} \nabla_r V\right)^{-1}$

$$\tau_S \approx \tau_e$$

more importantly

$$\tau_c \sim \left(\frac{v}{k_B T} \nabla_r W\right)^{-1}$$

Since for short range interactions $\frac{\nabla_r W}{W} \gg \frac{\nabla_r f}{f}$

we have hierarchy of scales

$$\tau_c \ll \tau_s, \tau_e$$

Now collisions (τ_c) enters in two different ways on LHS (for $N \geq 2$) and on the RHS of BBGKY

Need to relate f_N and f_{N+1} to estimate importance of RHS terms

Generally
$$f_2 = \frac{1}{N-2} \int \frac{d^3 r_3 \, d^3 p_3}{(2\pi\hbar)^3} f_3 \approx \frac{V}{N} \int \frac{d^3 p_3}{(2\pi\hbar)^3} f_3$$

Hence for RHS terms spatial integral is cut-off by range of interaction

$$\int d\Omega_3 \, \vec{K}_{13} \, \vec{\nabla}_{p_1} f_3 \sim r_0^3 \, K_{13}(r_0) \int \frac{d^3 p_3}{(2\pi\hbar)^3} f_3$$

So
$$\frac{\int d\Omega_3 \, \vec{K}_{13} \vec{\nabla}_{p_1} f_3}{\vec{K}_{12} \vec{\nabla}_{p_1} f_2} \sim \frac{r_0^3}{d^3} \ll 1$$

where $d^3 \sim \frac{V}{N}$ is interparticle distance

Naturally RHS is small compared to LHS in dilute gas

$\boxed{\text{IV.}}$ Kinetic theory / Boltzmann equation

Specify assumptions

Dilute gas $\frac{N}{V} = d^3$ where d is interparticle distance

of

Classical particles meaning that the de Broglie wave-length (typical size of QM wave package) $\lambda_{\text{DeBroglie}} \sim \frac{2\pi\hbar}{\sqrt{2\pi m k_B T}}$ is small compared to interparticle distance

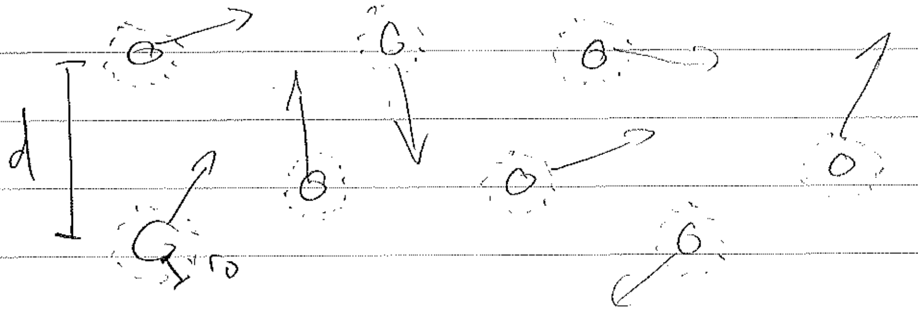
$$\boxed{\lambda_{\text{DeBroglie}} \ll d}$$

Subject to

short range interactions such that $W(r) \sim 0$ for $r \gg r_0$ where r_0 is the range of interaction which is assumed to be much smaller than the typical inter-particle distance

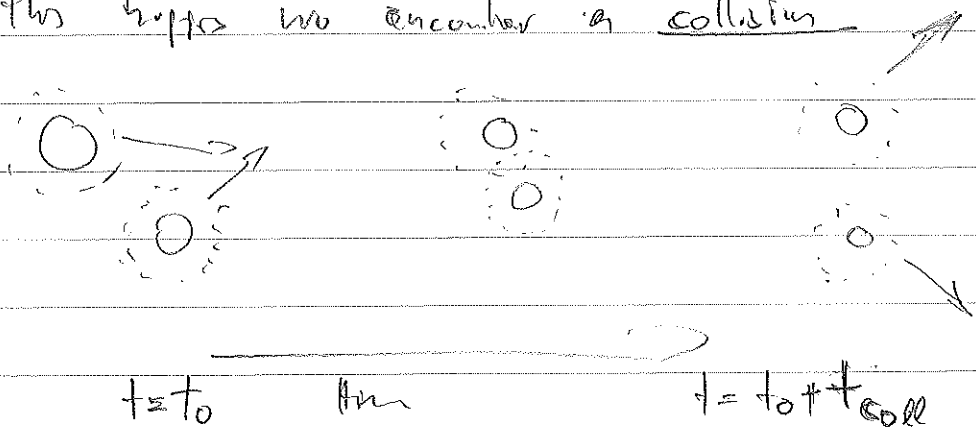
We require $\boxed{r_0 \ll d}$ such that particles in the gas move freely most of the time except for the rare instances where they interact with each other

So the generic picture is as follows



Individual particles fly for a long distance $l_{mfp} \sim V_i t_{mfp}$ before they interact with another particle

When this happens we encounter a collision



which occurs on a time scale

$$\boxed{t_{coll} \ll t_{mfp}}$$

Subsequently the particles again travel for a long distance $\sim l_{mfp}$ before encountering a new collision event with a different particle, very far away

Ultimately, we are interested in describing dynamics which leads to equilibration of the system

$\Rightarrow$ will require many collisions

$t_{eq} \gg t_{mfp}$

Hence we are not necessarily interested in details on very short time scales of single collision t_{coll} or very short distance scale $\sim r_0$

<u>Idea:</u> Consider <u>coarse grained description</u> on time scales $\Delta t \gg t_{coll}$ and length scale $\Delta l \gg r_0$

Except for the effect of collisions particles free-stream on these two scales -

Coarse grained evolution of one body density governed by

$$\frac{\partial}{\partial t} f_1 + \vec{v}_1 \vec{\nabla}_{\vec{r}_1} f_1 + \vec{F} \vec{\nabla}_{\vec{p}_1} f_1 = \left(\left.\frac{\partial f_1}{\partial t}\right|_{coll} \right)$$

where on scales $\Delta t \gg t_{coll}$ and $\Delta l \gg r_0$

collisions described by

$\left.\frac{\partial f_1}{\partial t}\right|_{coll}$ appear as local & instantaneous events

Now what is $\left.\frac{\partial f_1}{\partial t}\right|_{coll}$? We know from BBGKY that this corresponds to effect of two-body correlations

$$\left.\frac{\partial f_1}{\partial t}\right|_{coll} = - \int d\Omega_2 \, \vec{K}_{12} \, \vec{\nabla}_{p_1} \, f_2(t, \vec{r}_1, \vec{p}_1, \vec{r}_2, \vec{p}_2)$$

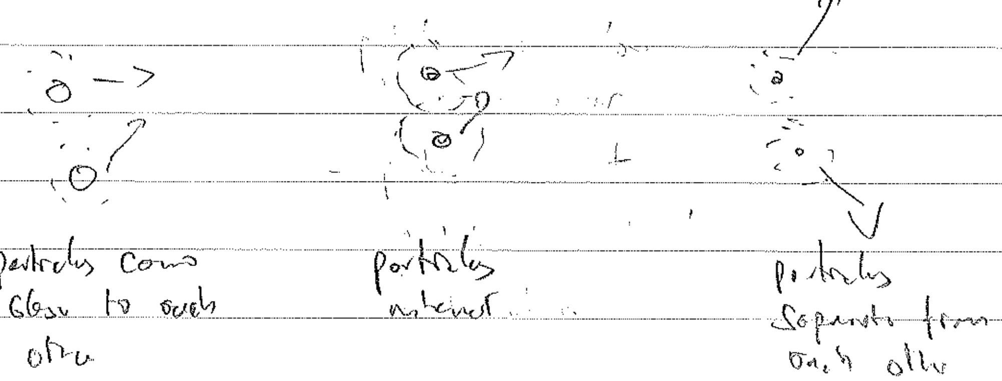
and we will employ this shortly to derive collision kernel macroscopically

However before doing so, it is useful first to consider hommuter derivations

Heuristic derivation of Boltzmann equation

What is effect of collisions, i.e. short range interactions in dilute gas on time scales $\Delta t \gg t_{coll}$ and length scales $\Delta l \gg r_0$

Starting from two uncorrelated particles



even though interaction induces correlation between two particles, the two particles will separate far in space before they interact again with another particle

molecular chaos: can assume that interacting particles are uncorrelated with each other before every interaction

Can estimate number of collisions per unit time by Stosszahl ansatz

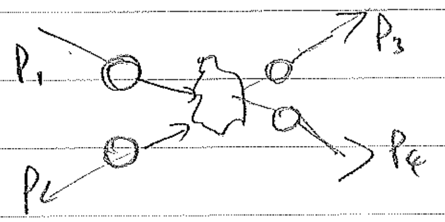
Namely in coarse grained approach particles have to be at same point $\vec{r}_1 \simeq \vec{r}_2$ for collision to take place

Since particles are assumed to be uncorrelated

$$\frac{dN_{coll}}{dt} \propto f_1(t, \vec{r}_1, \vec{p}_1)\, f(t, \vec{r}_1, \vec{p}_2)$$

~~Since we have coarse grained description we no longer know exact details of individual scattering, e.g. impact parameter etc.~~

~~→ Outcome of scattering event will be statistically distributed~~



Need to integrate Distribution of possible outcomes

$$\tilde{W}(p_1 p_2 \rightarrow p_3 p_4)$$

Of course $\tilde{w}(p_1 p_2 \rightarrow p_3 p_4)$ should satisfy basic principles of energy & momentum conservation

$$\tilde{w}(p_1 p_2 \rightarrow p_3 p_4) = w(p_1 p_2 \rightarrow p_3 p_4)\left(\frac{2\pi}{\hbar}\right)\delta\left(\frac{p_1^2}{2m}+\frac{p_2^2}{2m}-\frac{p_3^2}{2m}-\frac{p_4^2}{2m}\right)$$

$$(2\pi\hbar)^3\,\delta^{(3)}\left(\vec{p}_1+\vec{p}_2-\vec{p}_3-\vec{p}_4\right)$$

as well as usual symmetry relations eg under parity $(\vec{p}_i \rightarrow -\vec{p}_i)$ and time reversal $(\vec{p}_1, \vec{p}_2, \vec{p}_3, \vec{p}_4 \rightarrow -\vec{p}_3, -\vec{p}_4, -\vec{p}_1, -\vec{p}_2)$

Combining these two

$$\tilde{W}(\vec{p}_1, \vec{p}_2 \rightarrow \vec{p}_3 \vec{p}_4) = \tilde{W}(\vec{p}_3, \vec{p}_4 \rightarrow \vec{p}_1 \vec{p}_2)$$

i.e. probability of inverse process is identical

Now how do individual collisions affect one-body distribution

$\frac{\partial}{\partial t} f(t, \vec{x}_1, \vec{p}_1)$

need to consider two effects

particle with $\vec{p}_1$ interacts with other particle $\vec{p}_2$

→ **loss** of particles with momentum $\vec{p}_1$

interactions of $\vec{p}_3$ and $\vec{p}_4$ produce particle $\vec{p}_1$ and $\vec{p}_2$

→ **gain** of particles with momentum $\vec{p}_1$

Combining the two possibilities, averaging over all possible outcomes weighted by statistical distribution $\tilde{W}$ and Stoßzahl we get the Boltzmann equation

$$\left(\frac{\partial}{\partial t} + \vec{v}_1 \vec{\nabla}_{r_1} + \vec{F} \vec{\nabla}_{p_1}\right) f_1(t, \vec{r}_1, \vec{p}_1) = \underbrace{C[f_1](t, \vec{r}_1, \vec{p}_1)}_{\text{collision integral}}$$

correct for double counting of identical pairs 1,2 and 3,4

$$C[f_1](t, \vec{r}_1, \vec{p}_1) = -\frac{1}{2} \int \frac{d^3p_2}{(2\pi\hbar)^3} \frac{d^3p_3}{(2\pi\hbar)^3} \frac{d^3p_4}{(2\pi\hbar)^3} \tilde{W}(\vec{p}_1 \vec{p}_2 \to \vec{p}_3 \vec{p}_4)$$

$$\times \left[\underbrace{f(t, \vec{r}, \vec{p}_1) f(t, \vec{r}_1, \vec{p}_2)}_{\text{loss}} - \underbrace{f(t, \vec{r}_1, \vec{p}_3) f(t, \vec{r}_1, \vec{p}_4)}_{\text{gain}}\right]$$

Comments: Boltzmann equation closed at one-body level

→ molecular chaos assumption / Stoßzahlansatz effectively truncates the BBGKY hierarchy

Coarse graining in space & time make the equation local in space and time

→ all single particle distributions evaluated at the same position $\vec{r}_1$ and time t

One often denotes

$$f_1(t, \vec{r}_1, \vec{p}_1) = f(t, \vec{r}, \vec{p}) = f$$

$$f(t, \vec{r}, \vec{p}_2) = f_2$$

$$f(t, \vec{r}, \vec{p}_3) = f_3$$

$$\vdots$$

$$\left(\partial_t + \vec{v}\nabla_r + \vec{F}\nabla_p\right) f = -\frac{1}{2}\int_{p_2, p_3, p_4} \tilde{W}(p\,p_2 \to p_3 p_4)\left[f f_2 - f_3 f_4\right]$$

where $\int_{p_i} = \int \frac{d^3 p_i}{(2\pi\hbar)^3}$

Besides classical particles as considered in our example can also derive Boltzmann equation in quantum theory ($\rightsquigarrow$ QFT)

bosons: Bose enhancement

$$C[f] = -\frac{1}{2}\int_{p_2p_3p_4} \tilde{w}(pp_2 \to p_3p_4)\left[ff_2(1+f_3)(1+f_4) - f_3f_4(1+f)(1+f_2)\right]$$

fermions: Pauli blocking

$$C[f] = -\frac{1}{2}\int_{p_2p_3p_4} \tilde{w}(pp_2 \to p_3p_4)\left[ff_2(1-f_3)(1-f_4) - f_3f_4(1-f)(1-f_2)\right]$$

where classical particle limit is recovered for $f \ll 1$

Besides classical particles, the Boltzmann equation for bosons has an interesting limit $f \gg 1$ where only Bose enhanced processes are allowed

classical fields/waves:

$$C[f] = -\frac{1}{2}\int_{p_2p_3p_4} \tilde{w}(pp_2 \to p_3p_4)\left[ff_2(f_3+f_4) - f_3f_4(f+f_2)\right]$$

which plays an important role e.g. in studying acoustic turbulence

Derivation of collision term from BBGKY hierarchy

We start from evolution equation for f_2

$$\left[\frac{\partial}{\partial t} + v_1 \vec{\nabla}_{r_1} + v_2 \vec{\nabla}_{r_2} + \vec{F}_1 \vec{\nabla}_{p_1} + \vec{F}_2 \vec{\nabla}_{p_2} + \vec{K}_{12}\left(\vec{\nabla}_{p_1} - \vec{\nabla}_{p_2}\right)\right] f_2$$

$$= - \int \left(K_{13} \nabla_{p_1} + K_{23} \nabla_{p_2}\right) f_3 \, d\Omega_3$$

Since in a dilute gas the
RHS is suppressed by diluteness parameter

$$\frac{\int K_{12} \nabla_{p_1} f_3 \, d\Omega_3}{K_{12} \nabla_{p_1} f_2} \sim \frac{r_0^3}{d^3} \ll 1$$

this represents a higher order correlation
and will be neglected

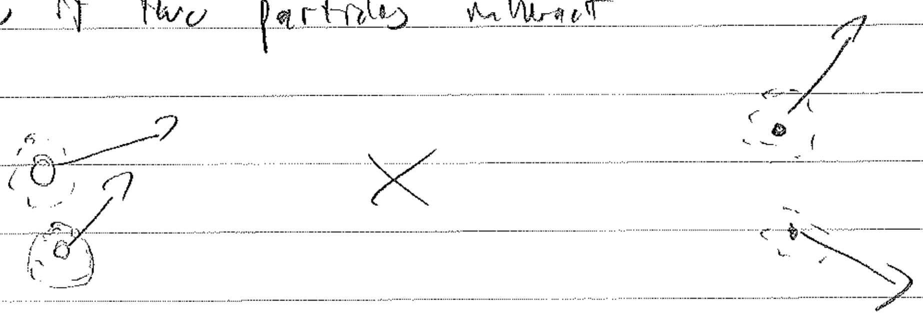
Note: On the level of heuristic derivation neglecting three body correlations
of the arguments for molecular chaos

We have then closed the BBGKY
hierarchy at the two-body level

Next we consider the evolution of two body Density,

$$\left[\frac{\partial}{\partial t} + \vec{v}_1 \vec{r}_1 + \vec{v}_2 \vec{r}_2 + \vec{F}_1 \vec{\nabla}_{p_1} + \vec{F}_2 \vec{\nabla}_{p_2} + \vec{K}_{12}(\vec{\nabla}_{p_1} - \vec{\nabla}_{p_2})\right] f_2 = 0$$

Now if two particles interact



the COM momentum $\vec{p}_1 + \vec{p}_2$ will not change whereas the relative momentum $\vec{p}_1 - \vec{p}_2$ changes quite dramatically over the time scale of the collision.

Likewise, the COM coordinate $\vec{r}_1 + \vec{r}_2$ changes slowly whereas the relative coordinate changes appreciably

Choice of coordinates

$$\vec{P} = \vec{p}_1 + \vec{p}_2 \qquad \Delta\vec{p} = \frac{1}{2}(\vec{p}_1 - \vec{p}_2)$$

$$\vec{R} = \frac{1}{2}(\vec{r}_1 + \vec{r}_2) \qquad \Delta\vec{r} = \vec{r}_2 - \vec{r}_1$$

$$\vec{\nabla}_{p_1} = \frac{\partial \vec{P}}{\partial \vec{p}_1} \vec{\nabla}_{\vec{P}} + \frac{\partial \Delta\vec{p}}{\partial \vec{p}_1} \vec{\nabla}_{\Delta\vec{p}} = \vec{\nabla}_{\vec{P}} + \frac{1}{2}\vec{\nabla}_{\Delta\vec{p}}$$

$$\vec{\nabla}_{p_2} = \quad '' \qquad '' \quad = \vec{\nabla}_{\vec{P}} - \frac{1}{2}\vec{\nabla}_{\Delta\vec{p}}$$

$$\vec{\nabla}_{r_1} = \frac{1}{2}\vec{\nabla}_R - \vec{\nabla}_{\Delta\vec{r}}$$

$$\vec{\nabla}_{r_2} = \frac{1}{2}\vec{\nabla}_R + \vec{\nabla}_{\Delta\vec{r}}$$

$$\Big[\frac{\partial}{\partial t} + (\vec{F}_1 + \vec{F}_2)\vec{\nabla}_P + \frac{1}{2}(\vec{F}_1 - \vec{F}_2)\vec{\nabla}_{\Delta p}$$

$$+ \frac{1}{2}\frac{\vec{P}}{m}\vec{\nabla}_R - 2\frac{\Delta\vec{p}}{m}\vec{\nabla}_{\Delta\vec{r}} + K_{12}(|\Delta\vec{r}|)\vec{\nabla}_{\Delta\vec{p}}\Big] f_2 = 0$$

Now since separation $|\Delta\vec{r}|$ has to be $\sim r_0$ (range of interaction) for collision to occur $\vec{r}_1 \simeq \vec{r}_2$ and therefore $\vec{F}_1 \simeq \vec{F}_2$ cancelling effects of external forces on relative motion

Since we consider $\Delta t \ll \tau_{ext}, \tau_s$ in coarse grained description effects of COM motion and forces will be negligible over this time scale

$\to$ can drop associated terms

So we have

$$\left[\frac{\partial}{\partial t} - 2\frac{\Delta\vec{p}}{m}\vec{\nabla}_{\Delta\vec{r}} + \vec{K}_{12}(|\Delta\vec{r}|)\vec{\nabla}_{\Delta\vec{p}}\right] f_2 \simeq 0$$

Now we have $\frac{\partial}{\partial t}$ can be very large on the scales t_{coll}

However what we need for coarse grained description of one body distribution

$$\left.\frac{\partial f_1}{\partial t}\right|_{coll} = -\int d\Omega_2\, \vec{K}_{12}\vec{\nabla}_{p_1} f_2$$

averaged over a time scale $\Delta t \gg t_{coll}$

Since rapid changes of f_2 do not contribute to long time average, can approximate f_2 by quasi-stationary solution $\left(\frac{\partial}{\partial t} f \simeq 0\right)$

So

$$\vec{K}_{12}(|\Delta\vec{r}|)\vec{\nabla}_{\Delta\vec{p}} f_2 = 2\frac{\Delta\vec{p}}{m}\vec{\nabla}_{\Delta\vec{r}} f_2$$

so we have

$$-\vec{K}_{12}(|\Delta\vec{r}|)\left(\vec{\nabla}_{p_1} - \vec{\nabla}_{p_2}\right) f_2 = -\left(\vec{V}_1 - \vec{V}_2\right)\vec{\nabla}_{\Delta\vec{r}} f_2$$

Now integrating over $\int d\Omega_2$ the $\vec{\nabla}_{p_2}$ contribution gives a vanishing boundary term

$$\left.\frac{\partial f_1}{\partial t}\right|_{coll} = \int d\Omega_2 (\vec{v}_2 - \vec{v}_1)\, \vec{\nabla}_{\Delta\vec{r}}\, f_2(t, \vec{r}_1, \vec{p}_1, \vec{r}_1 + \Delta\vec{r}, \vec{p}_2)$$

$$\text{where} \quad \int d\Omega_2 = \int \frac{d^3 r_2\, d^3 p_2}{(2\pi\hbar)^3} = \int \frac{d^3 p_2}{(2\pi\hbar)^3} \int d^3 \Delta r$$

Now for each $\vec{p}_1, \vec{p}_2$ we can decompose $\Delta\vec{r}$ into components parallel and perpendicular to $(\vec{v}_2 - \vec{v}_1)$

$$\Delta\vec{r} = \frac{(\vec{v}_2 - \vec{v}_1)}{|\vec{v}_2 - \vec{v}_1|} z + \vec{b}$$

$$\text{Then} \quad (\vec{v}_2 - \vec{v}_1)\, \vec{\nabla}_{\Delta\vec{r}} = |\vec{v}_2 - \vec{v}_1| \frac{\partial}{\partial z}$$

$$\text{and} \quad \int d^3 \Delta r = \int dz \int d^2 \vec{b}$$

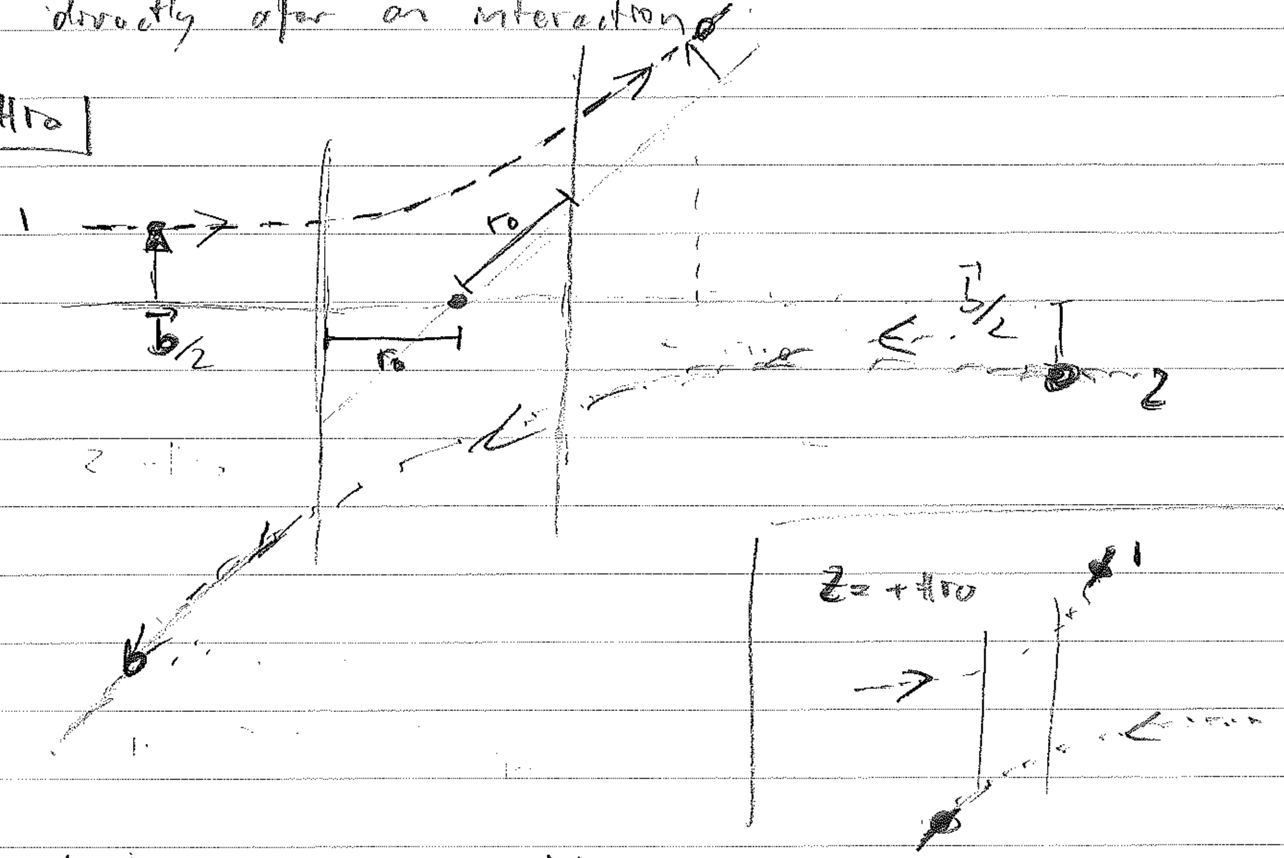
$$\left.\frac{\partial f_1}{\partial t}\right|_{coll} = \int \frac{d^2\vec{b}\, d^3 p_2}{(2\pi\hbar)^3} |\vec{v}_2 - \vec{v}_1|$$

$$\times \Big[f_2(t, \vec{r}_1, \vec{p}_1, \vec{r}_1 + \vec{b} + z\vec{e}_z, \vec{p}_2) \Big]_{z=-\#r_0}^{z=+\#r_0}$$

where # is a number of order unity

Now the key difference between upper and lower integration limit is that it describes ($z = -\# r_0$) a situation directly before an interaction or ($z = +\# r_0$) situation directly after an interaction

$z = -\# r_0$



Note that after interaction particles are correlated $\rightarrow$ non-trivial correlation can not employ Stoßzahl ansatz

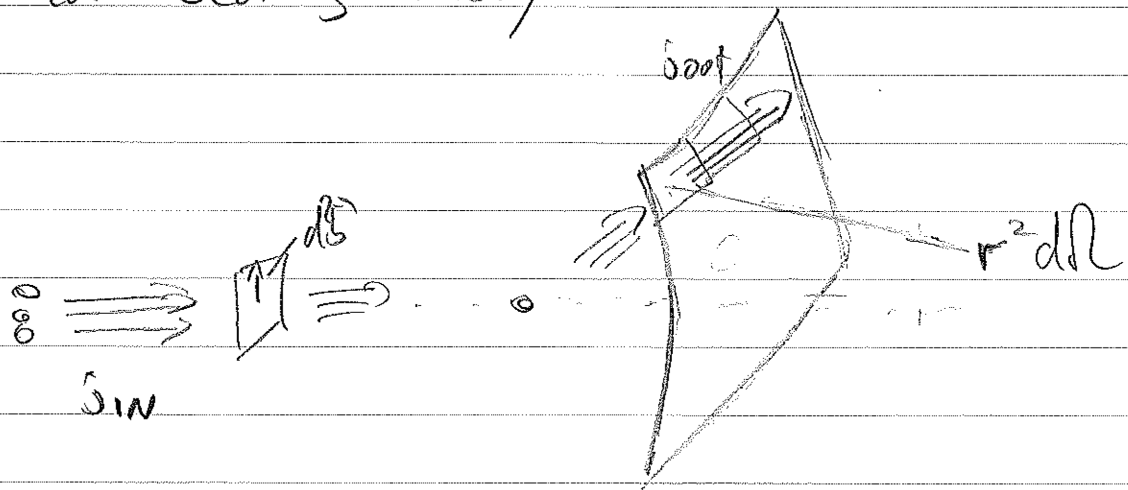
However since classical trajectories are deterministic can express probability to find 1,2 after collision terms of probability to find 3,4 before

$$f_2(t, \vec{r}_1, \vec{p}_1, \vec{r}_1 + b + \# z_0 \vec{e}_z, \vec{p}_2) = f_2(t, \vec{r}_1, \vec{p}_3, \vec{r}_1 + b - \# z_0 \vec{e}_z, \vec{p}_4)$$

where $p_{3/4} = p_{3/4}(b, \vec{p}_1, \vec{p}_2)$

Now to obtain Boltzmann equation in usual form still need to express $\int d^2b$ in terms of momentum integrals

Corresponding relation is given by classical scattering theory



$$\left|\frac{\vec{j}_{out}}{\vec{j}_{IN}}\right|(E_{com}, \theta, \varphi) = \frac{1}{r^2}\frac{d\sigma}{d\Omega}$$

Now if we integrate over all solid angles at some distance the total fluxes have to match

$$\int |\vec{j}_{IN}|\, d^2\vec{b} = \int |j_{out}|\, r^2 d\Omega$$

$$= \int \frac{d\sigma}{d\Omega}\, d\Omega\, |j_{IN}|$$

where Ω is the scattering angle between the outgoing particles

So collecting everything

$$\left.\frac{\partial f_1}{\partial t}\right|_{coll} = \int \frac{d^3p_2}{(2\pi\hbar)^3} \int \frac{d\sigma}{d\Omega}\, d\Omega\, |\vec{v}_2 - \vec{v}_1| \Big[f_2(t, \vec{r}_1, \vec{p}_3, \vec{r}_1 + \vec{b} - \# r_0 \vec{e}_z, \vec{p}_4)$$

$$- f_2(t, \vec{r}_1, \vec{p}_1, \vec{r}_1 + \vec{b} - \# r_0 \vec{e}_z, \vec{p}_2) \Big]$$

Due to coarse graining, we can neglect $\vec{b} - \# r_0 \vec{e}_z$ in the second argument of f_2 and employ the Stoßzahlansatz

$$f_2(t, \vec{r}_1, \vec{p}_3, \vec{r}_1, \vec{p}_4) = f_1(t, \vec{r}_1, \vec{p}_3)\, f_1(t, \vec{r}_1, \vec{p}_4)$$

etc.

to obtain the Boltzmann equation

We also learned that the transition rate is in fact given by

$$\tilde{W}(p_1 p_2 \to p_3 p_4)\, \frac{d^3p_3}{(2\pi\hbar)^3} \frac{d^3p_4}{(2\pi\hbar)^3} = \frac{d\sigma}{d\Omega}\, d\Omega\, |\vec{v}_2 - \vec{v}_1|$$