Derivation of Boltzmann equation from BBGKY

Start from evolution equations for f_1, f_2

$$\Big(\frac{\partial}{\partial t} + \underbrace{\vec{v}\,\vec{\nabla}_r} + \underbrace{\vec{F}\,\vec{\nabla}_p}\Big) f_1 = -\int_{\Omega_2} \underbrace{\vec{K}_{12}\,\vec{\nabla}_{p_1} f_2}$$

$$\Big(\frac{\partial}{\partial t} + \underbrace{\vec{v}_1\vec{\nabla}_{r_1} + \vec{v}_2\vec{\nabla}_{r_2}}_{\text{free streaming}} + \underbrace{\vec{F}_1\vec{\nabla}_{p_1} + \vec{F}_2\vec{\nabla}_{p_2}}_{\text{external forces}} + \underbrace{\vec{K}_{12}(\vec{\nabla}_{p_1} - \vec{\nabla}_{p_2})}_{\text{two-body}}\Big) f_2 = -\underbrace{\int_{\Omega_3} (\vec{K}_{13}\vec{\nabla}_{p_1} + \vec{K}_{23}\vec{\nabla}_{p_2}) f_3}_{\text{interactions}}$$

and realize that in a dilute gas ($r_0 \ll d$) terms on the RHS are suppressed by powers of the diluteness parameter $\frac{r_0^3}{d^3}$. Specifically the term containing f_3 represents a higher-order correction and will be neglected at leading order

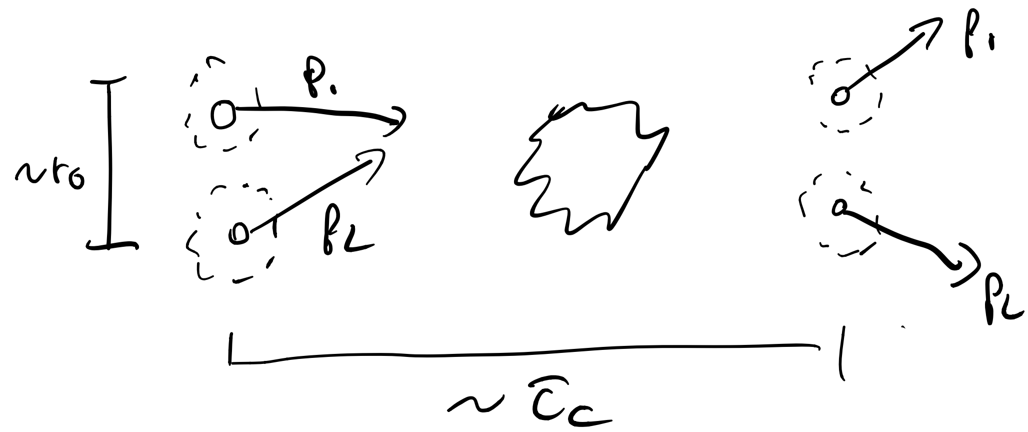
$\Rightarrow$ closed set of evolution equations at the two-body level (f_1, f_2)

Strategy of derivation will be to find an approximate solution for f_2 and use it to close evolution equation for f_1, which will account for the effect of collisions

$$\left(\frac{\partial}{\partial t} + \underbrace{\vec{v}_1\vec{\partial}_{r_1} + \vec{v}_2\vec{\partial}_{r_2}}_{\text{motion of particles 1,2}} + \underbrace{\vec{F}_1\vec{\partial}_{p_1} + \vec{F}_2\vec{\partial}_{p_2}}_{\text{forces on particles 1,2}} + \underbrace{\vec{K}_{12}(\vec{\partial}_{p_1} - \vec{\partial}_{p_2})}_{\text{interaction of particles 1,2}}\right) f_2 \simeq 0$$

Now most of the time effect of f_2 on f_1 is negligible, due to suppression by diluteness. However, when two particles get close to each other f_2 will change rapidly over a time scale $\sim \tau_c$, which is the effect that we want to capture

Now consider such a collision event



which takes place on a microscopic distance scale $\sim r_0$ over a microscopic time scale $\sim \tau_c$.

Due to energy & momentum conservation the COM momentum $\vec{p}_1 + \vec{p}_2$ will be unchanged during the collision, whereas $\vec{p}_1 - \vec{p}_2$ varies rapidly

Similarly the position $\vec{r}_1 - \vec{r}_2$ which dictates the force $\vec{K}_{12}(\vec{r}_1 - \vec{r}_2)$ varies on the scale $\sim r_0$, which is significant in describing the two-body interaction. However, the fact that $\vec{r}_1 + \vec{r}_2$ changes by $\sim r_0$ is negligible if we consider particle densities and external forces to vary on scales $L \gg r_0$

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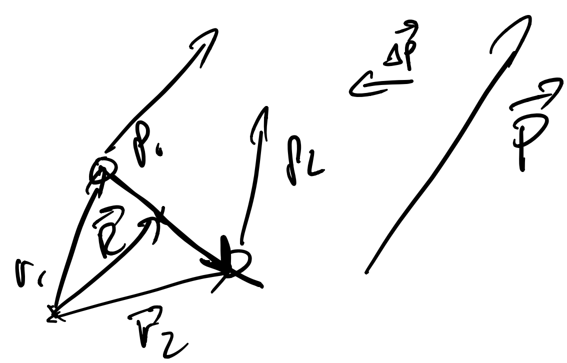

Now to take advantage of these simplifications we introduce new coordinates

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

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

such that

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

$$\vec{\nabla}_{\vec{p}_2} = \frac{\partial \vec{P}}{\partial \vec{p}_2} \vec{\nabla}_{\vec{P}} + \frac{\partial \Delta\vec{p}}{\partial \vec{p}_2} \vec{\nabla}_{\Delta\vec{p}} = \vec{\nabla}_{\vec{P}} - \frac{1}{2} \vec{\nabla}_{\Delta\vec{p}}$$

$$\vec{\nabla}_{\vec{r}_1} = \frac{1}{2} \vec{\nabla}_R - \vec{\nabla}_{\Delta\vec{r}}$$

$$\vec{\nabla}_{\vec{r}_2} = \frac{1}{2} \vec{\nabla}_R + \vec{\nabla}_{\Delta\vec{r}}$$

Evaluating the various forms in the evolution equation for f_2, we have

$$\frac{\vec{p}_1}{m}\vec{\nabla}_{r_1} + \frac{\vec{p}_2}{m}\vec{\nabla}_{r_2} = \frac{1}{2}\frac{\vec{p}_1+\vec{p}_2}{m}\vec{\nabla}_R - \frac{\vec{p}_1-\vec{p}_2}{m}\vec{\nabla}_{\Delta\vec{r}}$$

$$\vec{F}_1\vec{\nabla}_{p_1} + \vec{F}_2\vec{\nabla}_{p_2} = \left(\vec{F}_1+\vec{F}_2\right)\vec{\nabla}_{\vec{p}} + \frac{1}{2}\left(\vec{F}_1-\vec{F}_2\right)\vec{\nabla}_{\Delta\vec{p}}$$

and the evolution equation for f_2 takes the form

$$\left[\frac{\partial}{\partial t} + \frac{1}{2}\frac{\vec{P}}{m}\vec{\nabla}_R - 2\frac{\Delta\vec{p}}{m}\vec{\nabla}_{\Delta r} + \left(\vec{F}_1+\vec{F}_2\right)\vec{\nabla}_p + \frac{1}{2}\left(\vec{F}_1-\vec{F}_2\right)\vec{\nabla}_{\Delta\vec{p}} + \vec{K}_{12}(\Delta\vec{r})\vec{\nabla}_{\Delta\vec{p}}\right]f_2 = 0$$

Now since the separation $|\Delta\vec{r}|$ has to be of order r_0 for collision to take place, we have $\vec{r}_1 \simeq \vec{r}_2$ and thus $\vec{F}_1 \simeq \vec{F}_2$ and we can neglect this term

Since we are interested in describing effects of collisions on time scales $\sim\tau_c$ where effects of COM motion and external forces are negligible, we can further drop the associated terms

So we get

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

describing the relative motion of two particles during a collision event

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Now to obtain the collision integral of the Boltzmann equation, we need

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

subject to coarse graining on time scales $\Delta t \gg \tau_{coll}$ and $\Delta r \gg r_0$

During a collision f_2 can change rapidly, unless

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

which is a stationary solution $\left(\frac{\partial}{\partial t} f_2 \simeq 0\right)$ of the evolution equation for relative motion

Since we are interested in averages over long time scales, we will approximate the evolution of f_2 by its quasi-stationary solution where using

$$\vec{\nabla}_{\Delta p} = \vec{\nabla}_{p_1} - \vec{\nabla}_{p_2} \quad \Big\| \quad 2\,\frac{\Delta\vec{p}}{m} = \vec{v}_1 - \vec{v}_2$$

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

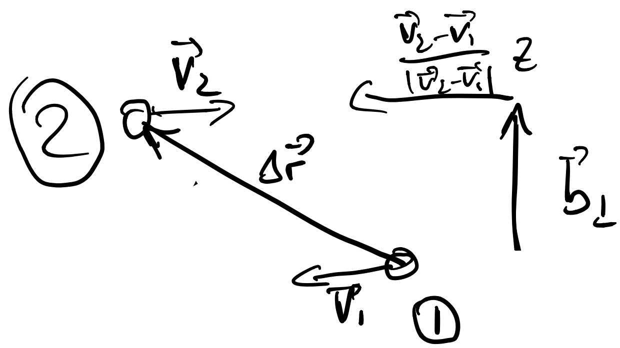
such that by evaluating $\left.\frac{\partial f_1}{\partial t}\right|_{coll}$ and realizing that $\vec{\nabla}_{\vec{p}_2}$ gives rise to a vanishing boundary term, we obtain

$$\left.\frac{\partial f_1}{\partial t}\right|_{coll} = \int \frac{d^3 r_2 \, d^3 p_2}{(2\pi\hbar)^3} \left(\vec{v}_2 - \vec{v}_1\right) \vec{\nabla}_{\Delta \vec{r}} f_2\left(t, \vec{r}_1, \vec{p}_1, \vec{r}_2, \vec{p}_2\right)$$

Now to evaluate this, we first realize that we can change integration variables

$$\int d^3 \vec{r}_2 = \int d^3(\vec{r}_2 - \vec{r}_1) = \int d^3 \Delta\vec{r}$$

which we can further decompose with respect to its components, parallel and perpendicular to the relative velocity e.g



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

such that evaluating

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

$$\int d^3\Delta\vec{r} = \int d^2\vec{b}_\perp \int dz$$

we got

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

$$\int dz\, \frac{\partial}{\partial z} f_2\left(t, \vec{r}_1, \vec{p}_1, \vec{r}_1+\vec{b}_\perp+z\frac{\vec{v}_2-\vec{v}_1}{|\vec{v}_2-\vec{v}_1|}, \vec{p}_2\right)$$

Now performing the z-integration of the derivative, we get

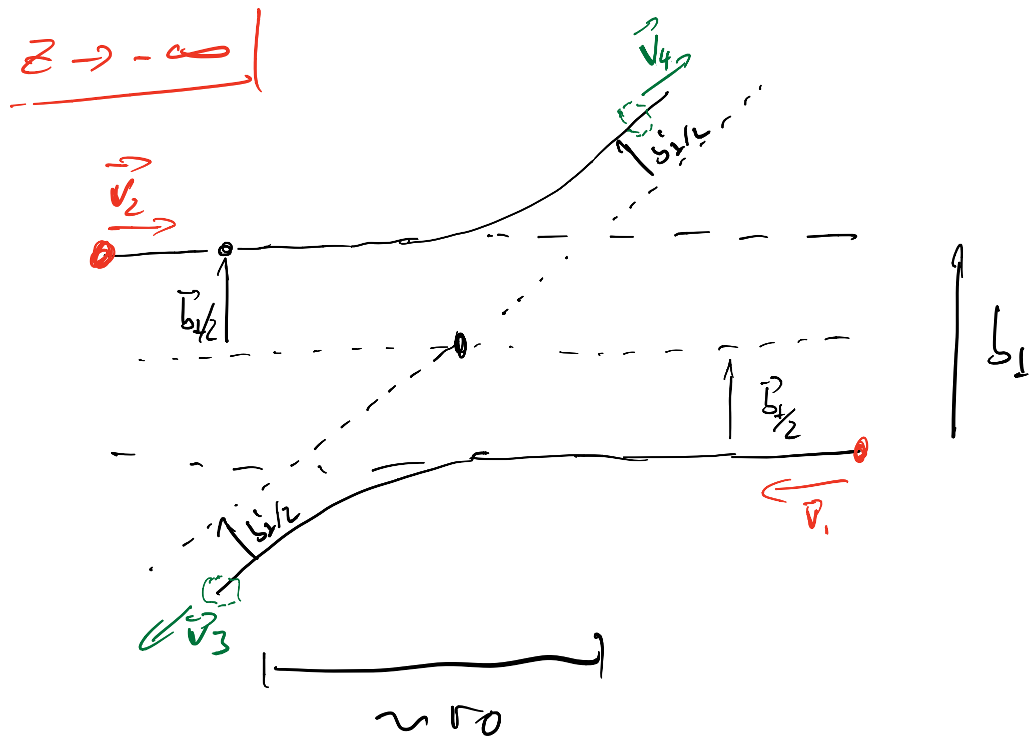
$$= \int \frac{d^3 p_2}{(2\pi\hbar)^3} \int d^2\vec{b}_\perp \, |\vec{V}_2 - \vec{V}_1| \left[\bar{f}_2\left(t, \vec{r}_1, \vec{p}_1, \vec{r}_1 + \vec{b}_\perp + z\frac{\vec{V}_2 - \vec{V}_1}{|\vec{V}_2 - \vec{V}_1|}, \vec{p}_2\right) \right]_{z=-\infty}^{z=+\infty}$$

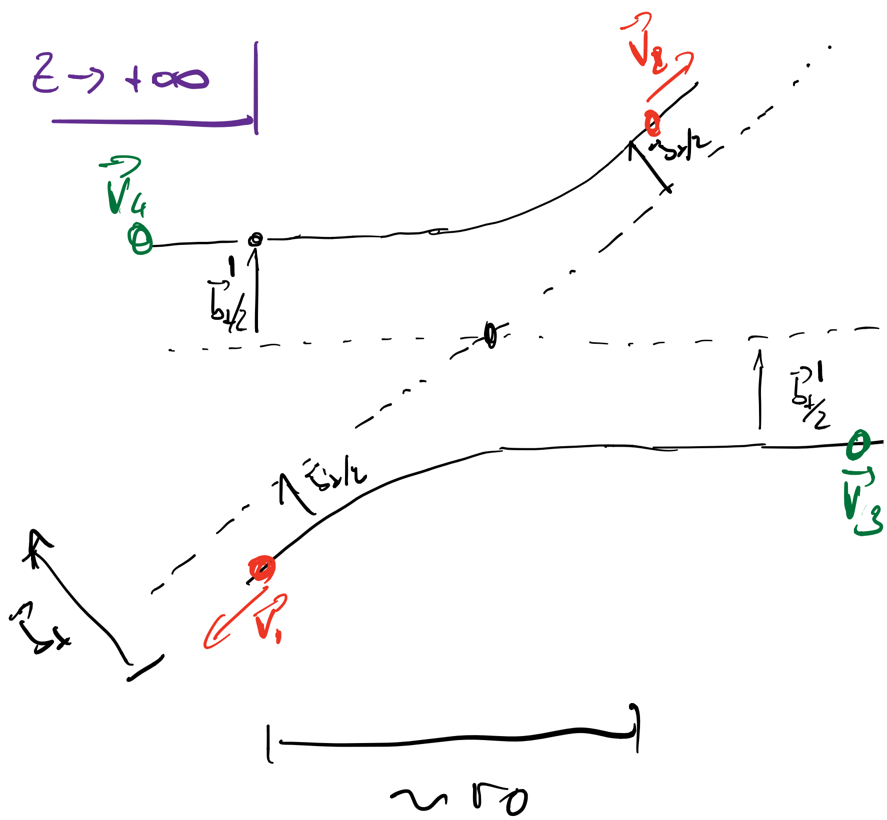
which describes the two particle correlation function before ($z \to -\infty$) and after ($z \to +\infty$) the collision has taken place

Now if we investigate the two possibilities, we have

$\underline{z \to -\infty}$ | $\vec{V}_1, \vec{V}_2$ velocities of particles <u>before</u> the collision

$\underline{z \to +\infty}$ | $\vec{V}_1, \vec{V}_2$ velocities of particles <u>after</u> the collision


z → -∞
$\vec{v}_4$
$\vec{v}_2$
$\vec{b}_\perp/2$
$b_\perp$
$\vec{v}_1$
$\vec{v}_3$
~ r0


z → +∞
$\vec{v}_2$
$\vec{v}_4$
$\vec{b}'_\perp/2$
$\vec{v}_3$
$\vec{v}_1$
$\vec{b}_\perp$
~ r0

Since the microscopic scattering process is deterministic, there is a one-to-one mapping between the velocities $(\vec{v}_1, \vec{v}_2)$ and $(\vec{v}_3, \vec{v}_4)$ before and after the collision

$z \to +\infty$

$\Rightarrow$ probability to have $\vec{v}_1, \vec{v}_2$ after the collision is identical to probability of having $\vec{v}_3, \vec{v}_4$ before the collision

$$f_2\left(t, \vec{r}_1, \vec{p}_1, \vec{r}_1 + \vec{b}_\perp + z\frac{\vec{v}_2 - \vec{v}_1}{|\vec{v}_2 - \vec{v}_1|}, \vec{p}_2\right)$$

$$= f_2\left(t, \vec{r}_1, \vec{p}_3, \vec{r}_1 + \vec{b}_\perp' - z\frac{\vec{v}_4 - \vec{v}_3}{|\vec{v}_4 - \vec{v}_3|}, \vec{p}_4\right)$$

where $\vec{p}_{3,4} = \vec{p}_{3,4}(\vec{b}_\perp, \vec{p}_1, \vec{p}_2)$ is determined by solution to classical scattering problem

So we obtain

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

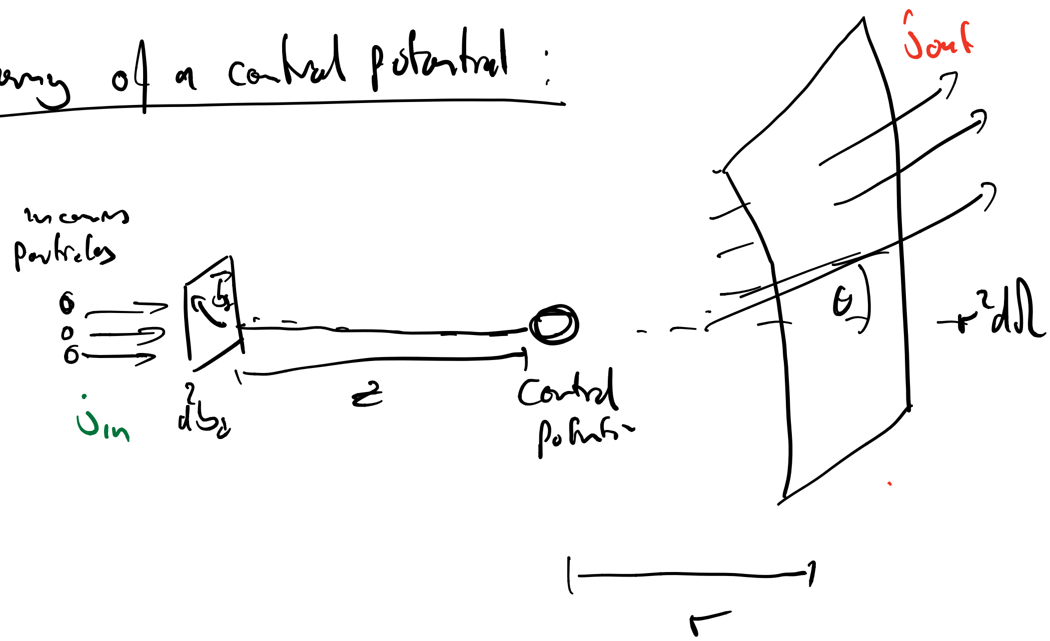
$$\Big[f_2\Big(t, \vec{r}_1, \vec{p}_3, \vec{r}_1 + \vec{b}_\perp' - \infty \frac{\vec{v}_4 - \vec{v}_3}{|\vec{v}_4 - \vec{v}_3|}, \vec{p}_4\Big) - f_2\Big(t, \vec{r}_1, \vec{p}_1, \vec{r}_1 + \vec{b}_\perp - \infty \frac{\vec{v}_2 - \vec{v}_1}{|\vec{v}_2 - \vec{v}_1|}, \vec{p}_2\Big) \Big]$$

which starts to resemble the structure of gain and loss terms //

Now that we have expressed the all occurrences of f_2 in terms of f_2 <u>before the collision</u>, we can later make use of the molecular chaos assumption

However to obtain the collision integral in the Boltzmann equation in its usual form, we still have to express the result in terms of a number integral which is given by classical scattering theory (c.f. classical mechanics course)

Scattering of a central potential:



described in terms of differential cross-section

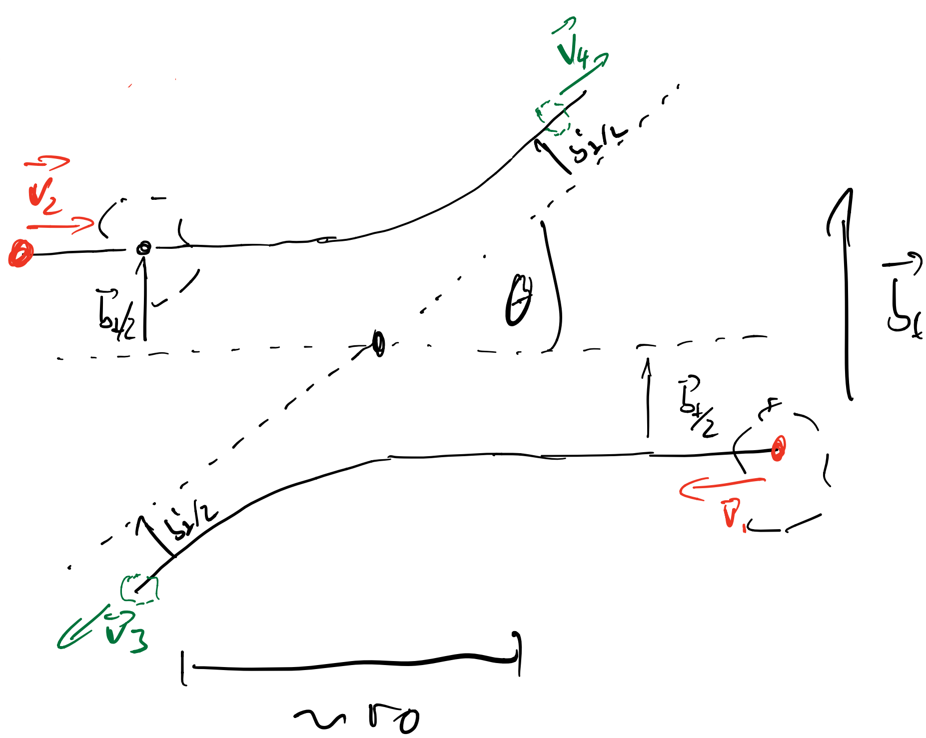
$$\left|\frac{\dot{J}_{out}}{\dot{J}_{in}}\right| (E_{com}, \theta, \phi) = \frac{1}{r^2} \frac{d\sigma}{d\Omega} (E_{com}, \theta, \phi)$$

where E_{com}, θ, φ are given in terms of momenta of incoming and outgoing particles

Now since all particles need to end up somewhere the total flux is conserved

$$\int |j_{in}|\, d^2\vec{b}_\perp = \int |j_{out}|\, r^2 d\Omega = \int \frac{d\sigma}{d\Omega} |j_{in}|\, d\Omega$$

Scattering of two particles:



can be mapped to scattering in a central potential by separating COM and relative motion of particles

So we can express

$$\int d^2b_\perp \, |\vec{v}_2 - \vec{v}_1| \, f_2\left(t, \vec{r}_1, \vec{p}_1, \vec{r}_1 + \vec{b}_\perp - \infty \frac{\vec{v}_2 - \vec{v}_1}{|\vec{v}_2 - \vec{v}_1|}, \vec{p}_2\right)$$

molecular chaos

$$\cong \int d^2b_\perp \, \underbrace{|\vec{v}_2 - \vec{v}_1| \, f_1(t, \vec{r}_1, \vec{p}_1) \, f_1\left(t, \vec{r}_1 + \vec{b}_\perp - \infty \frac{\vec{v}_2 - \vec{v}_1}{|\vec{v}_2 - \vec{v}_1|}, \vec{p}_2\right)}_{\text{incoming flux of particles}}$$

$$= \int d\Omega \, \frac{d\sigma}{d\Omega} \, |\vec{v}_2 - \vec{v}_1| \, f_1(t, \vec{r}_1, \vec{p}_1) \, f_1\left(t, \vec{r}_1 + \vec{b}_\perp - \infty \frac{\vec{v}_2 - \vec{v}_1}{|\vec{v}_2 - \vec{v}_1|}, \vec{p}_2\right)$$

Coarse graining
$\vec{b}_\perp \sim r_0 \ll \Delta r$

$$\simeq \int d\Omega \, \frac{d\sigma}{d\Omega} \, |\vec{v}_2 - \vec{v}_1| \, f_1(t, \vec{r}_1, \vec{p}_1) \, f_1(t, \vec{r}_1, \vec{p}_2)$$

Similarly for gain. term, we can use energy conservation $|\vec{v}_2 - \vec{v}_1| = |\vec{v}_3 - \vec{v}_4|$ and again relabel the fluxes

$$\int d^2 b_\perp \, |\vec{v}_2 - \vec{v}_1| \, f_2\left(t, \vec{r}_1, \vec{p}_3, \vec{r}_1 + \vec{b}_\perp' - \infty \frac{\vec{v}_4 - \vec{v}_3}{|\vec{v}_4 - \vec{v}_3|}, \vec{p}_4\right)$$

$$\simeq \int d\Omega \, \frac{d\sigma}{d\Omega} \, |\vec{v}_2 - \vec{v}_1| \, f_1(t, \vec{r}_1, \vec{p}_3) \, f_1(t, \vec{r}_1, \vec{p}_4)$$

So collecting everything, we get

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

$$\left[f_1(t, \vec{r}_1, \vec{p}_3) \, f_1(t, \vec{r}_1, \vec{p}_4) - f_1(t, \vec{r}_1, \vec{p}_1) \, f_1(t, \vec{r}_1, \vec{p}_2) \right]$$

which agrees with our heuristic derivation

We learn in addition, that the transition rates are determined by the scattering cross section

$$\int \frac{1}{2} \tilde{W}(p_1 p_2 \rightarrow p_3 p_4) \frac{d^3 p_3}{(2\pi\hbar)^3} \frac{d^3 p_4}{(2\pi\hbar)^3} = \int \frac{d\sigma}{d\Omega} (\vec{p}_1, \vec{p}_2, \vec{p}_3, \vec{p}_4) \left| \vec{v}_2 - \vec{v}_1 \right| d\Omega$$

where energy and momentum conservation are readily taken into account in the microscopic calculation, thus reducing the dimensionality of the integral