We introduced reduced distributions

$$f_k = \int d^{(N-k)}V \, f$$

to capture k-body observables in systems of charge neutral particles

$$H_N = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i=1}^{N} V(\vec{r}_i) + \sum_{\substack{i=1 \\ j>i}}^{N} W(|\vec{r}_i - \vec{r}_j|)$$

BBGKY hierarchy of evolution equations for reduced distribution functions f_k

$$\frac{\partial}{\partial t} f_k + \underbrace{\overbrace{\sum_{i=1}^{k} \Big(\frac{\vec{p}_i}{m} \vec{\nabla}_{\vec{r}_i}}^{\text{free streaming}} + \overbrace{\vec{F}(\vec{r}_i)\, \vec{\nabla}_{\vec{p}_i} \Big) f_k}^{\text{external forces}}} + \overbrace{\sum_{\substack{i,j=1 \\ j>i}}^{k} \vec{K}_{ij}(\vec{r}_i - \vec{r}_j) \left(\vec{\nabla}_{\vec{p}_i} - \vec{\nabla}_{\vec{p}_j} \right) f_k}^{\text{two-body interactions between identified particles}}$$

$$= \underbrace{- \int d\Omega_{k+1} \sum_{i=1}^{k} \vec{K}_{i,k+1}(\vec{r}_i - \vec{r}_{k+1})\, \vec{\nabla}_{\vec{p}_i} f_{k+1}}_{\text{two body interactions with other particles in the system}}$$

so far exact reformulation of Liouville equation, will now consider truncations

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Systems of electrically charged particles in the presence of electromagnetic potentials $(\phi, \vec{A})$ which give rise to the following external electromagnetic fields

<u>electric field</u> $\vec{E}(t,\vec{r}) = -\vec{\nabla}\phi(t,\vec{r}) - \frac{\partial \vec{A}(t,\vec{r})}{\partial t}$

<u>magnetic field</u> $\vec{B}(t,\vec{r}) = \vec{\nabla}_{\vec{r}} \times \vec{A}(t,\vec{r})$

Hamiltonian is now given by

$$H_N = \sum_{i=1}^{N} \frac{\left(\vec{p}_i - q\vec{A}(t,\vec{r}_i)\right)^2}{2m} + \sum_{i=1}^{N} q\,\phi(t,\vec{r}_i) + \sum_{\substack{i=1 \\ j>i}}^{N} W(|\vec{r}_i - \vec{r}_j|)$$

change in classical EOMs

kinetic momentum

$$\dot{\vec{r}}_i = \frac{\partial H}{\partial \vec{p}_i} = \frac{\vec{p}_i - q\vec{A}(t,\vec{r}_i)}{m} \equiv \frac{\vec{p}_i^{\,(\mathrm{kin})}}{m}$$

$$\dot{\vec{p}}_i = -\frac{\partial H}{\partial \vec{r}_i} = -q\vec{\nabla}_{\vec{r}_i}\phi(t,\vec{r}_i) - \sum_{\substack{j=1 \\ j\neq i}}^{N} \vec{\nabla}_{\vec{r}_i} W(|\vec{r}_i - \vec{r}_j|)$$

$$- \vec{\nabla}_{\vec{r}_i} \frac{\left(\vec{p}_i - q\vec{A}(t,\vec{r}_i)\right)^2}{2m}$$

Now we evaluate the new terms component wise for particle i, with j,k spatial indices

$$\frac{\partial}{\partial r_j} - \frac{(p_n - qA_n(t,\vec{r}))(p_n - qA_n(t,\vec{r}))}{2m}$$

$$= q\dot{r}_n \, \partial_{r_j} A_n$$

$$= q\dot{r}_n \left(\partial_{r_j} A_n - \partial_{r_n} A_j\right) + q\dot{r}_n \partial_{r_n} A_j$$

Now comparing with

$$\vec{B} = \vec{\nabla} \times \vec{A} \Rightarrow B_m = \varepsilon^{lnm} \partial_{r_l} A_n$$

we find

$$(\dot{\vec{r}} \times \vec{B})_j = \varepsilon^{jkm} \dot{r}_k B_m$$

$$= \varepsilon^{jkm} \dot{r}_k \varepsilon^{lnm} \partial_{r_l} A_n$$

$$= \dot{r}_n \left(\partial_{r_j} A_n - \partial_{r_n} A_j\right)$$

Such that

$$\dot{\vec{p}}_i = -q \vec{\nabla}_{\vec{r}_i} \phi(t,\vec{r}_i) + q\dot{\vec{r}}_i \times \vec{B}(t,\vec{r}) + q\,(\dot{\vec{r}}_i \cdot \vec{\nabla}_{\vec{r}_i}) \vec{A}(t,\vec{r}) + \sum_{j\neq i} \vec{K}_{ij}(\vec{r}_i - \vec{r}_j)$$

Now if instead of looking at the canonical momentum $\vec{p}_i$ we look at the kinetic momentum $\vec{p}_i^{\,(kin)}$

$$\vec{p}_i^{\,(kin)} = \vec{p}_i - q\vec{A}(t,\vec{r}_i)$$

such that

$$\dot{\vec{p}}_i^{\,(kin)} = \dot{\vec{p}}_i - q\left(\frac{\partial \vec{A}(t,\vec{r}_i)}{\partial t} + \left(\dot{\vec{r}}_i \cdot \vec{\nabla}_{\vec{r}_i}\right)\vec{A}(t,\vec{r}_i)\right)$$

$$= \underbrace{-q\left(\vec{\nabla}_{r_i}\phi(t,\vec{r}_i) + \frac{\partial \vec{A}(t,\vec{r}_i)}{\partial t}\right)}_{\equiv\, q\vec{E}(t,\vec{r}_i)}$$

$$+ q\,\dot{\vec{r}}_i \times \vec{B}(t,\vec{r}_i)$$

$$+ \sum_{j\neq i} \vec{U}_{ij}(\vec{r}_i - \vec{r}_j)$$

So in terms of $\vec{r}_i$ and $\vec{p}_i^{(kin)}$

the classical EOMs take the form

$$\dot{\vec{r}}_i = \frac{\vec{p}_i^{(kin)}}{m}$$

$$\dot{\vec{p}}_i^{(kin)} = \underbrace{q\vec{E}(t,\vec{r}_i) + q\frac{\vec{p}_i^{(kin)}}{m}\times\vec{B}(t,\vec{r}_i)}_{\text{Lorentz force } \vec{F}_L(\vec{r}_i,\vec{p}_i^{(kin)})} + \underbrace{\sum_{j\neq i}\vec{V}_{ij}(\vec{r}_i-\vec{r}_j)}_{\text{two body interactions}}$$

Now the formulation in terms of

$p_i^{(kin)}$ has another advantage, namely

that in contrast to p_i it is gauge invariant.

If we consider a gauge transformation

$\vec{A}(t,\vec{r})$, p_i will change, yet

the physical quantities $\vec{E}(t,\vec{r})$, $\vec{B}(t,\vec{r})$, $\vec{r}_i$, $\vec{p}_i^{(kin)}$

will remain the same

$\Rightarrow$ Beneficial to switch to a description in

terms of $\vec{r}_i$, $\vec{p}_i^{(kin)}$

Now the rest of the derivation of the BBGKY hierarchy proceeds essentially along the same lines yielding e.g. for the one body density

$$\boxed{\begin{aligned}&\left(\frac{\partial}{\partial t} + \frac{\vec{p}_1^{\,(\mathrm{kin})}}{m}\vec{\nabla}_{r_1} + \vec{F}_L(\vec{r}_1, \vec{p}_1^{\,(\mathrm{kin})})\,\vec{\nabla}_{p_1^{(\mathrm{kin})}}\right) f_1(t, \vec{r}_1, \vec{p}_1^{\,(\mathrm{kin})}) \\ &= -\int \frac{d^3 r_2\, d^3 p_2^{(\mathrm{kin})}}{(2\pi\hbar)^3}\, \vec{K}_{12}(\vec{r}_1 - \vec{r}_2)\,\vec{\nabla}_{p_1^{\mathrm{kin}}}\, f_2(t, \vec{r}_1, \vec{p}_1^{\,(\mathrm{kin})}, \vec{r}_2, \vec{p}_2^{\,(\mathrm{kin})})\end{aligned}}$$

where

$$\vec{F}_L(\vec{r}_1, \vec{p}_1^{\,(\mathrm{kin})}) = q\,\vec{E}_{\mathrm{ext}}(t, \vec{r}_1) + q\,\frac{\vec{p}_1^{\,(\mathrm{kin})}}{m} \times \vec{B}_{\mathrm{ext}}(t, \vec{r}_1)$$

is the Lorentz force due to external $\vec{E}$ and $\vec{B}$ fields applied to the system

Note that instead of $p_1^{(\mathrm{kin})}$ one can equivalently use the velocity $v_1 = \frac{p_1^{(\mathrm{kin})}}{m}$ as done e.g. in Bonitz's lecture notes

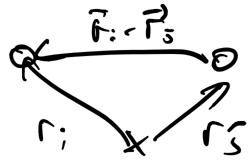
Mean-field approximation

Now one of the reasons that this is interesting is that the two-body forces between charged particles are of a very particular nature that allows us to explore different truncations of the BBGKY hierarchy

Specifically for non-relativistic charged particles ($|\vec{v}| \ll c$) interactions are dominated by the static Coulomb force

interaction potential $$W(|\vec{r}_i - \vec{r}_j|) = \frac{-q^2}{4\pi\varepsilon_0} \frac{1}{|\vec{r}_i - \vec{r}_j|}$$

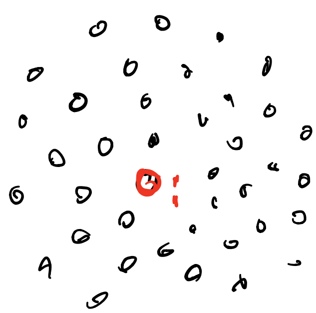
two-body forces $$\vec{K}_{ij}(\vec{r}_i - \vec{r}_j) = \frac{q^2}{4\pi\varepsilon_0} \frac{\vec{r}_i - \vec{r}_j}{|\vec{r}_i - \vec{r}_j|^3}$$



Now in contrast to other molecular forces there is no natural scale suppressing the interaction at large distances

So the force is <u>long range</u> in the sense that

$$|\vec{h}_{ij}| \propto \frac{1}{|\vec{r}_i - \vec{r}_j|^2}$$



Such that if we consider the force on particle (i) this will originate from the sum of the forces of many particles which are far away from the particle

Since many distant particles contribute to the force, it is reasonable to neglect genuine two particle correlations

Vlasov approximation:

$$f_2(t,\vec{r}_1,\vec{p}_1^{(kin)},\vec{r}_2,\vec{p}_2^{(kin)}) \simeq f_1(t,\vec{r}_1,\vec{p}_1^{(kin)})\, f_1(t,\vec{r}_2,\vec{p}_2^{(kin)}) + \text{correlations}$$

probability to find pair of particles 1&2

independent probability to find particles 1 and 2

neglect

Now evaluating the effect of two-body interactions in this approximation we get

$$\int \frac{d^3r_2\, d^3p_2^{(kin)}}{(2\pi\hbar)^3} \vec{K}_{12}(\vec{r}_1-\vec{r}_2)\, \vec{\nabla}_{p_1^{(kin)}} f_2(t,\vec{r}_1,\vec{p}_1^{(kin)},\vec{r}_2,\vec{p}_2^{(kin)})$$

$$= q \underbrace{\left[\frac{q}{4\pi\varepsilon_0}\int \frac{d^3r_2\, d^3p_2^{(kin)}}{(2\pi\hbar)^3} \frac{\vec{r}_1-\vec{r}_2}{|\vec{r}_1-\vec{r}_2|^3} f_1(t,\vec{r}_2,\vec{p}_2^{(kin)})\right]} \vec{\nabla}_{p_1^{(kin)}} f_1(t,\vec{r}_1,\vec{p}_1^{(kin)})$$

mean internal electric field $\vec{E}_{int}(t,\vec{r}_1)$ induced by all particles in the system

such that with Vlasov/mean-field approximation the BBGKY hierarchy is closed at the level of the one-body density

Vlasov equation:

$$\left[\frac{\partial}{\partial t} + \frac{\vec{p}_1^{(kin)}}{m}\vec{\nabla}_{\vec{r}_1} + q\left(\vec{E}_{ext} + \vec{E}_{int} + \frac{\vec{p}_1^{(kin)}}{m}\times\vec{B}_{ext}\right)\vec{\nabla}_{\vec{p}_1}\right] f_1\left(t,\vec{r}_1,\vec{p}_1^{(kin)}\right)=0$$

with

$$\vec{E}_{int}(t,\vec{r}_1) = \frac{q}{4\pi\varepsilon_0}\int\frac{d^3r_2\, d^3p_2^{(kin)}}{(2\pi\hbar)^3}\,\frac{\vec{r}_1-\vec{r}_2}{|\vec{r}_1-\vec{r}_2|^3}\, f_1\left(t,\vec{r}_2,\vec{p}_2^{(kin)}\right)$$

Note that due to the back-reaction via the induced electric field the Vlasov equation is non-linear and must be solved self-consistently

Since we only considered static Coulomb interaction, there are no internal magnetic fields induced, as they are suppressed by powers of $\frac{|\vec{v}|}{c}$

If one wants to improve on this, then more generally one has to solve single particle evolution equation along with the Maxwell equations to describe $\vec{E}$ and $\vec{B}$ fields and include radiation effects

$\Downarrow$

Scales in BBGKY hierarchy

Generally physically meaningful approximations are based on expansions in small parameters, e.g determined by a separation of scales

e.g in the previous discussion we assumed that

$$|\vec{u}| \ll c \quad \text{and} \quad r_0 \gg d$$

velocity — speed of light — range of interaction — interparticle distance

Now in order to derive meaningful truncations of the BBGKY hierarchy, we need to identify the relevant time and distance scales

Start by considering system of non-interacting particles

Single particle Liouville / collisionless Boltzmann equation

$$\left(\frac{\partial}{\partial t} + \underbrace{\vec{v}\,\vec{\nabla}_r}_{\sim 1/\tau_s} + \underbrace{\vec{F}(t,\vec{r})\,\vec{\nabla}_p}_{\sim 1/\tau_e}\right) f_1(t,\vec{r},\vec{p}) = 0$$

from which we can identify two different time scales

τ_s describes the time scale over which spatial gradients of f relax

τ_e describes the time scale on which f responds to external forces

If we estimate these two scales e.g. for a near equilibrium system

$$\left(\tfrac{1}{2}mv^2\right) \sim k_B T \qquad v \sim \sqrt{\frac{k_B T}{m}} \sim \frac{k_B T}{\sqrt{m k_B T}}$$

$$1/\tau_s \sim \frac{\vec{v}\,\vec{\nabla}_r f}{f} \sim \frac{k_B T}{\sqrt{m k_B T}} \left|\frac{\nabla_r f}{f}\right|$$

$$\nabla_p f \sim \nabla_p f_{eq} \sim \frac{f}{\sqrt{m k_B T}}$$

$$1/\tau_e \sim \frac{\vec{F}\,\vec{\nabla}_p f}{f} \overset{\vec{F} = -\vec{\nabla} V}{\sim} \frac{|\vec{\nabla}_r V|}{\sqrt{m k_B T}} \sim \frac{V}{\sqrt{m k_B T}} \left|\frac{\vec{\nabla}_r V}{V}\right|$$

Now typically the thermal energy $k_B T \gtrsim V$ is large compared to external potentials (except ultra-cold gases) and the length scales of potential V vary on larger distance scales

$$\left|\frac{\vec{\nabla}_r f}{f}\right| \gtrsim \left|\frac{\vec{\nabla}_r V}{V}\right| \gtrsim \left|\frac{\vec{\nabla}_r V}{k_B T}\right|$$

So typically

$$1/\tau_s \gtrsim 1/\tau_e \Rightarrow \tau_e \gtrsim \tau_s$$

means that typically individual particles move around quite a bit before reacting to an external influence

although this is not strictly speaking necessary for the following derivations

Next we consider the two scale associated with two-body interactions. which appear in two different ways

If we look at evolution equations for f_1, f_2

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

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

$$= -\int_{\Omega_3} (\vec{K}_{13}\vec{\partial}_{p_1} + \vec{K}_{23}\,\vec{\partial}_{p_2}) f_3$$

we find that the evolution equation for f_1 is special in the sense that it does not include two-body interactions on the left-hand side

If we look at evolution equation for f_2, we can identify a new time scale

$$\frac{1}{\tau_c} \sim \frac{\vec{K}_{12}\left(\vec{\nabla}_{p_1} - \vec{\nabla}_{p_2}\right) f_2}{f_2} \overset{\vec{K}_{12} \sim -\vec{\nabla} W}{\sim} \frac{|\vec{\nabla}_r W|}{\sqrt{m k_B T}} \sim \frac{W}{\sqrt{m k_B T}} \left| \frac{\vec{\nabla}_r W}{W} \right|$$

Now the interaction energy $W \sim k_B T$, however for typical gases of neutral constituents the interaction is <u>short range</u> meaning that W varies on microscopic distance scales

$$\frac{\nabla_r W}{W} \sim 1/r_0 \quad \text{range of interaction}$$

$$\frac{\nabla_r f}{f} \sim 1/L \quad \text{macroscopic length scale associated with gradients}$$

So if we compare the two scales

$$1/\tau_c \sim \sqrt{\frac{k_B T}{m}}\ 1/r_0$$

$$1/\tau_s \sim \sqrt{\frac{k_B T}{m}}\ 1/L$$

we find a clear separation of scales

$$\frac{\tau_c}{\tau_s} \sim \frac{r_0}{L} \ll 1$$

Such that the collision time τ_c is typically much smaller than the time scale τ_s characterizing the response to spatial gradients

$\Rightarrow$ many collisions will occur during the time that the system responds to spatial gradients

Now lets have a look at the terms coupling f_1, f_2 and f_2, f_3 where in order to estimate their magnitude we need to relate the different distributions according to

$$f_k = \int d^{6(N-k)} V \, f = \frac{1}{N-k} \int d\Omega_{k+1} \, f_{k+1}$$

where $\int d\Omega_{k+1} = \int \frac{d^3 r_{k+1} \, d^3 p_{k+1}}{(2\pi\hbar)^3}$

$$f_1 = \frac{1}{N-1} \int d\Omega_2 \, f_2 \sim \frac{V}{N} \int d^3 p_2 \, f_2$$

$$f_2 = \frac{1}{N-2} \int d\Omega_3 \, f_3 \sim \frac{V}{N} \int d^3 p_3 \, f_3$$

Now if d is the typical distance between particles, then $\frac{N}{V} \sim \frac{1}{d^3}$

and we have

$$f_1 \sim d^3 \int d^3p_2 f_2$$

$$f_2 \sim d^3 \int d^3p_3 f_3$$

Now the time scales that appear in the evolution equations for f_1 and f_2 are

$$\frac{\int_{\Omega_2} \vec{K}_{12} \vec{\nabla}_{p_1} f_2}{f_1} \sim \frac{\int_{\Omega_2} \vec{K}_{12} \vec{\nabla}_{p_1} f_2}{\int_{\Omega_2} f_2} \sim \frac{r_0^3}{d^3} \frac{W}{r_0} \frac{1}{\sqrt{m k_B T}} \sim \frac{r_0^3}{d^3} \, 1/\tau_c$$

and similarly

$$\frac{\int_{\Omega_3} \left(\vec{K}_{13} \vec{\nabla}_{p_1} + \vec{K}_{23} \vec{\nabla}_{p_2} \right) f_3}{\int_{\Omega_3} f_3} \sim \frac{r_0^3}{d^3} \, 1/\tau_c$$

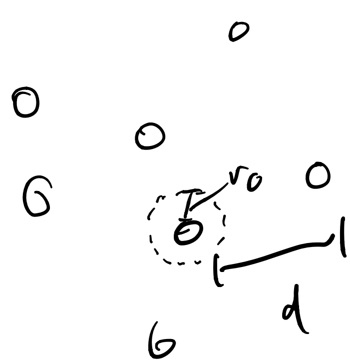
Clearly this introduces a new time scale related to τ_c in the evolution equation for f_1

However if we consider evolution equation for f_2, we should compare

$$\frac{1}{\tau_c} \quad , \quad \frac{r_0^3}{d^3}\frac{1}{\tau_c}$$

Now if we consider a <u>dilute gas</u> where the typical separation d between particles is large compared to the range of interactions r_0

$$d \gg r_0$$



then $1/\tau_c \gg \frac{r_0^3}{d^3} 1/\tau_c$ and

the terms originating from A_3

are negligible

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Now collecting all our results we got

$$\Big(\underbrace{\frac{\partial}{\partial t} + \vec{v}\cdot\vec{\nabla}_r}_{1/\tau_s} + \underbrace{\vec{F}\cdot\vec{\nabla}_p}_{1/\tau_e}\Big) f_1 = \underbrace{-\int dV_2\, \vec{K}_{12}\cdot\vec{\nabla}_{p_1} f_2}_{\frac{r_0^3}{d^3}\,\frac{1}{\tau_c}}$$

$$\Big(\underbrace{\frac{\partial}{\partial t} + \vec{v}_1\cdot\vec{\nabla}_{r_1} + \vec{v}_2\cdot\vec{\nabla}_{r_2}}_{1/\tau_s} + \underbrace{\vec{F}_1\cdot\vec{\nabla}_{p_1} + \vec{F}_2\cdot\vec{\nabla}_{p_2}}_{1/\tau_e} + \underbrace{\vec{K}_{12}\cdot(\vec{\nabla}_{p_1} - \vec{\nabla}_{p_2})}_{1/\tau_c}\Big) f_2 = \underbrace{-\int dV_3 \left(\vec{K}_{13}\cdot\vec{\nabla}_{p_1} + \vec{K}_{23}\cdot\vec{\nabla}_{p_2}\right) f_3}_{\frac{r_0^3}{d^3}\,\frac{1}{\tau_c}}$$

So for a dilute gas, $\frac{r_0^3}{d^3} \ll 1$

$\rightarrow$ Evolution of f_2 is much faster than evolution of f_1

$\rightarrow$ Effects of f_3 on f_2 are negligible

$\Rightarrow$ Exploit to obtain truncation of BBGKY hierarchy