Monday, 19 October 2020 16:00

Last time: marginal s-particle PDFs ρ_s and distributions f_s.

Liouville's equation $\frac{\partial \rho}{\partial t} + \{\rho, H\} = 0$

BBGKY hierarchy

Bogoliubov – Born – Green – Kirkwood – Yvon 1935 – 1949

Specialise the N-particle Hamiltonian for 2-body interactions:

$$\mathcal{H} = \sum_{i=1}^{N} \frac{|\mathbf{p}_i|^2}{2m} + \sum_{1 \le i < j \le N} \phi(|\mathbf{q}_i - \mathbf{q}_j|)$$

The ordered sum over $1 \le i < j \le N$ counts each pair once, and exclude self-interactions.

To find evolution equations for ρ_s and f_s it's convenient to split

$$\mathcal{H} = \mathcal{H}_s + \mathcal{H}_{N-s} + \mathcal{H}'$$

where $\mathcal{H}_s$ and $\mathcal{H}_{N-s}$ involve particles $1, \dots, s$ and $s+1, \dots, N$ only

$$\mathcal{H}_s = \sum_{i=1}^{s} \frac{|\mathbf{p}_i|^2}{2m} + \sum_{1 \le i < j \le s} \phi(|\mathbf{q}_i - \mathbf{q}_j|)$$

$$\mathcal{H}_{N-s} = \sum_{i=s+1}^{N} \frac{|\mathbf{p}_i|^2}{2m} + \sum_{s+1 \le i < j \le N} \phi(|\mathbf{q}_i - \mathbf{q}_j|)$$

The two groups of particles $1, \dots, s$ and $s+1, \dots, N$ only interact through $\mathcal{H}' = \sum_{i=1}^{s} \sum_{j=s+1}^{N} \phi(|\mathbf{q}_i - \mathbf{q}_j|)$

To save writing, define

$$\mathbf{F}_{ij} = \frac{\partial}{\partial \mathbf{q}_i} \phi(|\mathbf{q}_i - \mathbf{q}_j|) = -\mathbf{F}_{ji}$$

Differentiating the definition of ρ_s with respect to time gives

$$\frac{\partial \rho_s}{\partial t} = \int dV_{s+1} \dots dV_N \frac{\partial \rho}{\partial t}$$

$$= -\int dV_{s+1} \dots dV_N \{\rho, \mathcal{H}_s + \mathcal{H}_{N-s} + \mathcal{H}'\}$$

Think about each term separately.

$\mathcal{H}_s$ doesn't depend on $\mathbf{p}_{s+1}, \mathbf{q}_{s+1}, \dots \mathbf{p}_N, \mathbf{q}_N$ so we can take $\int dV_{s+1} \dots dV_N$ inside the derivatives defining the Poisson bracket to get

$$\int dV_{s+1} \dots dV_N \{\rho, \mathcal{H}_s\}$$
$$= \left\{ \int dV_{s+1} \dots dV_N \, \rho, \mathcal{H}_s \right\}$$
$$= \{\rho_s, \mathcal{H}_s\}$$

The $\mathcal{H}_{N-s}$ contribution vanishes because the integrand is an exact divergence:

$$\int dV_{s+1} \dots dV_N \{\rho, \mathcal{H}_{N-s}\}$$
$$= \int dV_{s+1} \dots dV_N \sum_{k=1}^{N} \left[\frac{\partial \rho}{\partial \mathbf{q}_k} \cdot \frac{\partial \mathcal{H}_{N-s}}{\partial \mathbf{p}_k} - \frac{\partial \rho}{\partial \mathbf{p}_k} \cdot \frac{\partial \mathcal{H}_{N-s}}{\partial \mathbf{q}_k} \right]$$

$$= \int dV_{s+1} \dots dV_N \sum_{i=s+1}^{N} \left[\frac{\partial \rho}{\partial \mathbf{q}_i} \cdot \frac{\mathbf{p}_i}{m} - \frac{\partial \rho}{\partial \mathbf{p}_i} \cdot \underbrace{\sum_{j=i+1}^{N} \frac{\partial \phi(|\mathbf{q}_i - \mathbf{q}_j|)}{\partial \mathbf{q}_i}}_{= \mathbf{F}_{ij}} \right]$$

$$= \int dV_{s+1} \dots dV_N \sum_{i=s+1}^{N} \left[\frac{\partial}{\partial \mathbf{q}_i} \cdot \left(\frac{\rho \mathbf{p}_i}{m} \right) - \frac{\partial}{\partial \mathbf{p}_i} \cdot \left(\rho \sum_{j=i+1}^{N} \mathbf{F}_{ij} \right) \right]$$

$$= 0$$

The remaining interaction term is

$$\int dV_{s+1} \dots dV_N \sum_{k=1}^{N} \left[\frac{\partial \rho}{\partial \mathbf{p}_k} \cdot \frac{\partial \mathcal{H}'}{\partial \mathbf{q}_k} - \frac{\partial \rho}{\partial \mathbf{q}_k} \cdot \frac{\partial \mathcal{H}'}{\partial \mathbf{p}_k} \right]$$

$$= \int dV_{s+1} \dots dV_N \left(\sum_{i=1}^{s} \frac{\partial \rho}{\partial \mathbf{p}_i} \cdot \sum_{j=s+1}^{N} \mathbf{F}_{ij} + \underbrace{\sum_{j=s+1}^{N} \frac{\partial \rho}{\partial \mathbf{p}_j} \cdot \sum_{i=1}^{s} \mathbf{F}_{ji}}_{= \frac{\partial}{\partial \mathbf{p}_j} \cdot \left(\rho \sum_{i=1}^{N} \mathbf{F}_{ji} \right)} \right)$$

The second term is an exact divergence, that contributes zero.

$$= (N-s) \int dV_{s+1} \dots dV_N \sum_{i=1}^{s} \frac{\partial \rho}{\partial \mathbf{p}_i} \cdot \mathbf{F}_{i,s+1}$$

since the sum over $j = s+1, \dots, N$ contributes $N-s$ identical terms since ρ is symmetric under swapping particles.

$$= (N-s) \sum_{i=1}^{s} \int dV_{s+1} \, \mathbf{F}_{i,s+1} \cdot \frac{\partial}{\partial \mathbf{p}_i} \left(\int dV_{s+2} \dots dV_N \, \rho \right)$$

$$= (N-s) \sum_{i=1}^{s} \int dV_{s+1} \, \mathbf{F}_{i,s+1} \cdot \frac{\partial \rho_{s+1}}{\partial \mathbf{p}_i}$$

Assembling the 3 pieces gives the BBGKY hierarchy

$$\frac{\partial \rho_s}{\partial t} + \{\rho_s, \mathcal{H}_s\} = (N-s) \sum_{i=1}^{s} \int dV_{s+1} \frac{\partial \phi(|\mathbf{q}_i - \mathbf{q}_j|)}{\partial \mathbf{q}_i} \cdot \frac{\partial \rho_{s+1}}{\partial \mathbf{p}_i}$$

or

$$\frac{\partial f_s}{\partial t} + \{f_s, \mathcal{H}_s\} = \sum_{i=1}^{s} \int dV_{s+1} \frac{\partial \phi(|\mathbf{q}_i - \mathbf{q}_j|)}{\partial \mathbf{q}_i} \cdot \frac{\partial f_{s+1}}{\partial \mathbf{p}_i}.$$

The LHS describes how the s particles evolve independently of the others. All the coupling is through the RHS.

This hierarchy is still exact, assuming all the boundary terms from $\int$ing by parts vanish, and describes time-reversible evolution.

$\frac{\partial f_1}{\partial t}$ depends on f_2

$\frac{\partial f_2}{\partial t}$ depends on f_3

and so on until we get to f_N.

There's a parallel line of development for hard spheres. No potentials, but the integrations must be over configurations such that the spheres do not overlap, bringing in boundary terms.

Exercise: use the f_1 and f_2 equations to show that $\langle \mathcal{H} \rangle$ is conserved.

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VI The Boltzmann equation

We need an argument based on separation of timescales to justify truncating the BBGKY hierarchy in the Boltzmann – Grad limit $nd^3 \to 0$ with $nd^2 = O\left(\frac{1}{\lambda_{mfp}}\right)$ fixed.

$$\Big[\underbrace{\frac{\partial}{\partial t} + \frac{\underline{p}_1}{m}\cdot\frac{\partial}{\partial \underline{q}_1} + \frac{\underline{p}_2}{m}\cdot\frac{\partial}{\partial \underline{p}_2}}_{1/T} \underbrace{- \underline{F}_{12}\cdot\left(\frac{\partial}{\partial \underline{p}_1} - \frac{\partial}{\partial \underline{p}_2}\right)}_{1/\tau_c}\Big] f_2$$

$$= \underbrace{\int dV_3 \Big[\underbrace{\underline{F}_{13}\cdot\frac{\partial}{\partial \underline{p}_1} + \underline{F}_{23}\cdot\frac{\partial}{\partial \underline{p}_2}}_{1/\tau_c \text{ before } \int}\Big] f_3}_{1/\tau}$$

and

$$\Big[\underbrace{\frac{\partial}{\partial t} + \frac{\underline{p}_1}{m}\cdot\frac{\partial}{\partial \underline{q}_1}}_{1/T}\Big] f_1 = \underbrace{\int dV_2 \Big[\underline{F}_{12}\cdot\left(\frac{\partial}{\partial \underline{p}_1} - \frac{\partial}{\partial \underline{p}_2}\right)\Big] f_2}_{1/\tau}$$

An extra exact divergence that does nothing. The RHS of the f_1 equation now matches a term in the LHS of the f_2 equation.

Every expression in [...] has dimensions of frequency (1/time).

$\frac{\underline{p}_i}{m}\cdot\frac{\partial}{\partial \underline{q}_i}$ is a hydrodynamic advection time equivalent to $c_s\nabla$.

$\frac{\partial \phi}{\partial \underline{q}_i}\cdot\frac{\partial}{\partial \underline{p}_i} \sim \frac{1}{\tau_c}$ is the inverse duration of a collision during which pairs of particles are close to each other.

The ϕ terms on the RHS scale differently as they involve f_{s+1}, not f_s, with an $\int dV_{s+1}$.

$\frac{f_{s+1}}{f_s} \sim n$, the probability of finding one more particle per unit volume.

However $\int dV_{s+1}$ is only appreciable over an $O(d^3)$ volume where the integrand is non-zero.

The timescale of each RHS is $\tau = \frac{\tau_c}{n d^3} \gg \tau_c$.

We can drop the $O(1/\tau)$ RHS of the f_2 equation, leaving the $O(1/\tau_c)$ term on the LHS.

The f_1 equation is special. Particles can't collide with themselves so there's no $O(1/\tau_c)$ term on the LHS. We need to keep the $O(1/\tau)$ RHS.

f_2 evolves as though no other particles were present, equivalent to ignoring ternary & higher collisions.

It's tempting to try
$$f_2(\underline{q}_1, \underline{p}_1, \underline{q}_2, \underline{p}_2, t) = f_1(\underline{q}_1, \underline{p}_1, t)\, f_1(\underline{q}_2, \underline{p}_2, t).$$
This leads to the Vlasov equation, but it's only valid for weak long-range interactions.

This approximation says particles are uncorrelated. How can particles interact while staying uncorrelated?

The simplified f_2 equation has 2 different timescales:

$$0 = \Big[\underbrace{\frac{\partial}{\partial t} + \frac{\underline{p}_1}{m}\cdot\frac{\partial}{\partial \underline{p}_1} + \frac{\underline{p}_2}{m}\cdot\frac{\partial}{\partial \underline{p}_2}}_{O(1/T)} \underbrace{- \underline{F}_{12}\cdot\left(\frac{\partial}{\partial \underline{p}_1} - \frac{\partial}{\partial \underline{p}_2}\right)}_{O(1/\tau_c)}\Big] f_2$$

There's a faster timescale hidden in the $O(1/T)$ terms that we can isolate by writing
$$\underline{q}_1 = \underline{Q} - \tfrac{1}{2}\underline{q}, \quad \underline{q}_2 = \underline{Q} + \tfrac{1}{2}\underline{q}$$
in terms of a mean position
$$\underbrace{\underline{Q} = \tfrac{1}{2}(\underline{q}_1 + \underline{q}_2)}_{O(L)} \ \& \text{ separation } \underbrace{\underline{q} = \underline{q}_2 - \underline{q}_1}_{O(d)}$$

$$\Big[\underbrace{\frac{\partial}{\partial t} + \frac{1}{2}\frac{\underline{p}_1 + \underline{p}_2}{m}\cdot\frac{\partial}{\partial \underline{Q}}}_{O(1/T)} + \underbrace{\frac{\underline{p}_2 - \underline{p}_1}{m}\cdot\frac{\partial}{\partial \underline{q}}}\ \underbrace{- \underline{F}_{12}\cdot\left(\frac{\partial}{\partial \underline{p}_1} - \frac{\partial}{\partial \underline{p}_2}\right)}\Big] f_2 = 0 \quad \text{both } O(1/\tau_c)$$

We can understand a collision by treating f_2 as steady on the τ_c timescale (like a Lagrangian in fluid dynamics. Particles are moving, but f_2 is steady)

Bogoliubov did this more formally by seeking a particular functional form for f_2.

Going back to the f_1 equation:
$$\Big[\frac{\partial}{\partial t} + \frac{\underline{p}_1}{m}\cdot\frac{\partial}{\partial \underline{q}_1}\Big] f_1 = \int dV_2\, \underline{F}_{12}\cdot\left(\frac{\partial}{\partial \underline{p}_1} - \frac{\partial}{\partial \underline{p}_2}\right) f_2$$
$$= \left.\frac{df_1}{dt}\right|_{coll} \quad \text{collision term}$$
$$= \int d\underline{p}_2 \int d\underline{q}_2\, \frac{\underline{p}_2 - \underline{p}_1}{m}\cdot\frac{\partial}{\partial \underline{q}} f_2$$
$$= \int d\underline{p}_2 \int d\underline{q}_2\, \frac{\partial}{\partial \underline{q}}\cdot\left(\frac{\underline{p}_2 - \underline{p}_1}{m} f_2\right)$$

Integrating over a sphere S of radius 2ℓ where $d \ll \ell \ll \lambda_{mfp}$ in $\underline{q}$ gives
$$\left.\frac{df_1}{dt}\right|_{coll} = \int d\underline{p}_2 \int dS\, \underline{n}_s\cdot\underline{V}\, f_2$$
where $\underline{n}_s$ is the outward normal on S and $\underline{V} = \frac{\underline{p}_2 - \underline{p}_1}{m}$.

$$\underline{q} = 2\ell\underline{n}_s, \quad \underline{q}_1 = \underline{Q} - \ell\underline{n}_s, \quad \underline{q}_2 = \underline{Q} + \ell\underline{n}_s.$$

Later we will assume that f_1 doesn't vary on lengthscales much smaller than λ_{mfp} so $\underline{Q}$, $\underline{q}_1$, $\underline{q}_2$ are interchangeable.

Now decompose the integration over the sphere S into integrations over 2 hemispheres:

S_+ with $\underline{n}_s\cdot\underline{V} > 0$, particles moving apart after a collision

S_- with $\underline{n}_s\cdot\underline{V} < 0$, particles moving together before a collision

$$\left.\frac{df_1}{dt}\right|_{coll} = \int d\underline{p}_2 \int_{S_+} dS\, |\underline{n}_s\cdot\underline{V}|\, f_2 \quad G$$
$$- \int d\underline{p}_2 \int_{S_-} dS\, |\underline{n}_s\cdot\underline{V}|\, f_2 \quad L$$
$$= \text{gain term } G - \text{loss term } L$$

The LHS is a function of $\underline{p}_1$, $\underline{q}_1$, t.

The loss term L describes particles with momentum $\underline{p}_1$ colliding with particles with some other momentum $\underline{p}_2$ to emerge from the collision with new momenta $\underline{p}_1'$ and $\underline{p}_2'$.

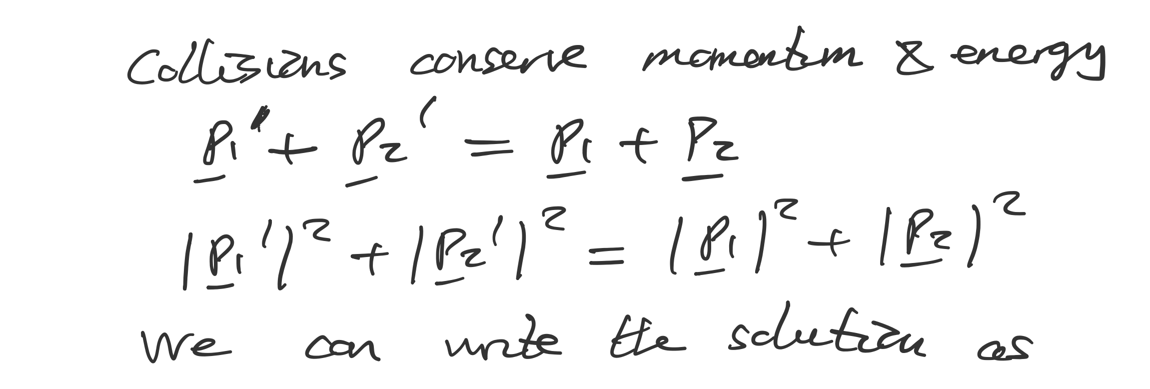
The gain term G describes particles with pre-collision momenta $\underline{p}_1'$ & $\underline{p}_2'$ colliding to emerge with momenta $\underline{p}_1$ & $\underline{p}_2$.

Boltzmann's collision number assumption or "stosszahlansatz" assumes that pairs of particles moving towards each other (not yet collided) are uncorrelated.

The loss term becomes

$$L = \int d\underline{p}_2 \int_{S_-} dS\, |\underline{n}_s\cdot\underline{V}|\, f_1(\underline{p}_1, \underline{q}_1, t)\, f_1(\underline{p}_2, \underline{q}_2, t)$$

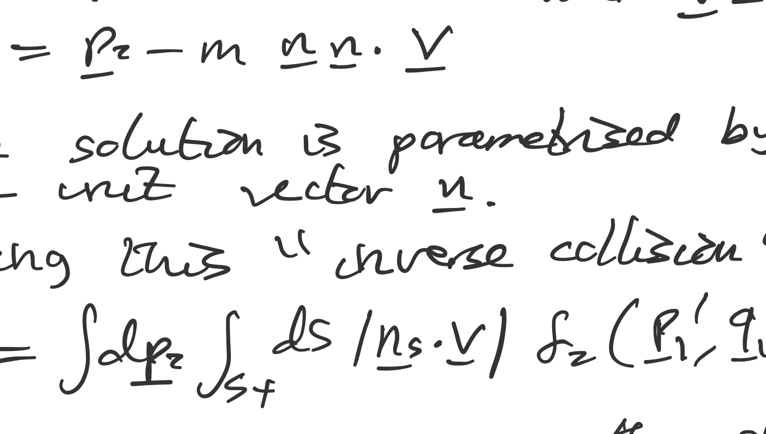
We still have a problem with the gain term, involving pairs of particles moving away from each other, having become correlated in a collision.



We need to find pairs of momenta $\underline{p}_1'$ and $\underline{p}_2'$ that emerge as pairs of momenta $\underline{p}_1$ and $\underline{p}_2$ after collisions.

Collisions conserve momentum & energy
$$\underline{p}_1' + \underline{p}_2' = \underline{p}_1 + \underline{p}_2$$
$$|\underline{p}_1'|^2 + |\underline{p}_2'|^2 = |\underline{p}_1|^2 + |\underline{p}_2|^2$$
We can write the solution as
$$\underline{p}_1 = \underline{p}_1' + m\,\underline{n}\,\underline{n}\cdot\underline{V}'$$
$$\underline{p}_2 = \underline{p}_2' - m\,\underline{n}\,\underline{n}\cdot\underline{V}'$$
where $\underline{V}' = \frac{1}{m}(\underline{p}_2' - \underline{p}_1')$ and $\underline{n}$ is a unit vector.

We can calculate that
$$\underline{p}_2 - \underline{p}_1 = (\underline{\underline{I}} - 2\underline{n}\,\underline{n})\cdot(\underline{p}_2' - \underline{p}_1')$$
so the relative velocity reflects in the plane perpendicular to $\underline{n}$,
so $|\underline{p}_2 - \underline{p}_1| = |\underline{p}_2' - \underline{p}_1'|$.



This reflection defines an invertible transformation with unit Jacobian (up to sign) that we can invert to get
$$\underline{p}_1' = \underline{p}_1 + m\,\underline{n}\,\underline{n}\cdot\underline{V} \quad \text{where } \underline{V} = \frac{\underline{p}_2 - \underline{p}_1}{m}$$
$$\underline{p}_2' = \underline{p}_2 - m\,\underline{n}\,\underline{n}\cdot\underline{V}$$
The solution is parametrised by the unit vector $\underline{n}$.

Using this "inverse collision"
$$G = \int d\underline{p}_2 \int_{S_+} dS\, |\underline{n}_s\cdot\underline{V}|\, f_2(\underline{p}_1', \underline{q}_1', \underline{p}_2', \underline{q}_2', t)$$

Now we can use the stosszahl-ansatz for $\underline{p}_1'$ & $\underline{p}_2'$, giving
$$G = \int d\underline{p}_2 \int_{S_+} dS\, |\underline{n}_s\cdot\underline{V}|\, f_1(\underline{p}_1', \underline{q}_1', t) \times f_1(\underline{p}_2', \underline{q}_2', t)$$

$$\left(\frac{\partial}{\partial t} + \frac{\underline{p}_1}{m}\cdot\frac{\partial}{\partial \underline{q}_1}\right) f_1 = G - L$$
a closed integro-differential equation for f_1 – the Boltzmann equation.