III Reduced distribution functions

So far discussed microscopic dynamics fully
i.e. by considering all d.o.f. explicitly

classically: $f(t, \{q_i\}, \{p_i\})$ phase space distribution

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \sum_i \dot{q}_i \frac{\partial f}{\partial q_i} + \sum_i \dot{p}_i \frac{\partial f}{\partial p_i} = 0$$ Liouville equation

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}$$

quantum: $\hat{\rho}$ or ρ_W density operator / Wigner function

$$i\hbar \frac{\partial \hat{\rho}}{\partial t} = [\hat{H}, \hat{\rho}]$$ Liouville-von Neumann equation

We discussed at the beginning that in many cases keeping track of full N-body distribution
▷ impractical / impossible

-> will now discuss how to reduce information content

We will limit ourselves to classical case
for simplicity, quantum case ▷ analogous
but more cumbersome

So far we have described system by

$$f(t, \{\vec{r}_i\}, \{\vec{p}_i\})$$

which for identical particles is symmetric under ordering:

$$(\vec{r}_i, \vec{p}_i) \Leftrightarrow (\vec{r}_j, \vec{p}_j)$$

and normalized such that

$$\int d^{6N}V \; f(t, \{\vec{r}_i\}, \{\vec{p}_i\}) = 1$$

with $d^{6N}V = \frac{1}{N!} \prod_{i=1}^{N} \frac{d^3r_i \, d^3p_i}{(2\pi\hbar)^3}$

Hence if we compute expectation values of observables

$$\langle O(t, \{r_i\}, \{p_i\}) \rangle = \int d^{6N}V \; O(t, \{r_i\}, \{p_i\}) \, f(t, \{r_i\}, \{p_i\})$$

Now typically the observables we are interested in do not involve all $\{r_i\}$ and all $\{p_i\}$.

In order to characterize d.o.f. first specify system we are interested in and see what information can be accessed

We are typically interested in systems of $N \gg 1$ indistinguishable particles with general form of Hamiltonian

$$H_N = \underbrace{\sum_{i=1}^{N} H_i^{kin}}_{\text{kinetic energy}} + \underbrace{\sum_{i=1}^{N} H_i^{pot}}_{\text{potential energy}} + \underbrace{\sum_{\substack{i=1 \\ j>i}}^{N} H_{ij}^{int}}_{\substack{\text{interaction energy for} \\ \text{2-particle interactions}}}$$

Specifically for a system of neutral particles with 2-body interactions

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

if particles are charged, there is also a vector potential $\vec{A}_i(t, \vec{r})$ resulting in a replacement of canonical momentum $\vec{p} \to \vec{p} - q\vec{A}$

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

Note that dependence of 2-body force $|\vec{r}_i - \vec{r}_j|$ is not most general form. e.g. spin-orbit couplings are counterexample. However what we will learn remains applicable with suitable extensions.

Consider e.g. $\langle E_{kin} \rangle$ as typical observable

$$E_{kin}(\{r_i\},\{p_i\}) = \sum_{i=1}^{N} \frac{p_i^2}{2m}$$

$$\langle E_{kin} \rangle = \int d^{6N}V \left(\sum_{i=1}^{N} \frac{p_i^2}{2m} \right) f(t,\{r_i\},\{p_i\})$$

Now since we are dealing with N indistinguishable particles f is symmetric for all (r_i, p_i)

$$= \int d^{6N}V \left(N \frac{p_1^2}{2m} \right) f(t,\{r_i\},\{p_i\})$$

Since observable no-longer depends on $p_2, \dots p_N$ can integrate them out

$$d^{6N}V = \frac{1}{N} \frac{d^3\vec{r}_1 \, d^3p_1}{(2\pi\hbar)^3} \, d^{6(N-1)}V$$

$$= \int \frac{d^3r_1 \, d^3p_1}{(2\pi\hbar)^3} \frac{p_1^2}{2m} \underbrace{\int d^{6(N-1)}V \, f(t,\{r_i\},\{p_i\})}$$

We find that E_{kin} (or any other one body observable) can be obtained from a reduced distribution

$$\underset{\text{one-body distribution}}{f_1(t,\vec{r}_1,\vec{p}_1)} = \int d^{6(N-1)}V \underbrace{f(t,\{r_i\},\{p_i\})}_{N\text{-body distribution}}$$

by marginalizing over $N-1$ positions & momenta

Note that one-body distribution is normalized as

$$\int \frac{d^3\vec{r}_1\, d^3\vec{p}_1}{(2\pi\hbar)^3}\; f_1(t,\vec{r}_1,\vec{p}_1) = N \qquad \text{(number of particles)}$$

where appearance of $(2\pi\hbar)^3$ depends on convention

Should be thought of as unnormalized probability distribution

Now H_N also involves 2-body interactions
→ What about interaction energy?

$$E_{int} = \sum_{\substack{i\geq 1\\ j>1}}^{N} W(|\vec{r}_i - \vec{r}_j|)$$

$$\langle E_{int} \rangle = \int d^{6N}V \left(\sum_{\substack{i\geq 1\\ j>1}}^{N} W(|\vec{r}_i - \vec{r}_j|) \right) f(t,\{\vec{r}_i\},\{\vec{p}_i\})$$

So performing the same tricks but now keeping two phase space variables

$$= \underbrace{\frac{1}{N(N-1)}}_{\text{measure}} \int \frac{d^3r_1 d^3p_1}{(2\pi\hbar)^3} \frac{d^3r_2 d^3p_2}{(2\pi\hbar)^3} \left(\underbrace{\frac{N(N-1)}{2}}_{\#\text{ pairs}} W(|r_1 - r_2|) \right.$$

$$\left. \int d^{6N-2}V\, f(t,\{\vec{r}_i\},\{\vec{p}_i\}) \right)$$

$$= \frac{1}{2} \int \frac{d^3r_1\, d^3p_1}{(2\pi\hbar)^3} \frac{d^3r_2\, d^3p_2}{(2\pi\hbar)^3}\; W(|\vec{r}_1 - \vec{r}_2|)\; f_2(t,\vec{r}_1,\vec{p}_1,\vec{r}_2,\vec{p}_2)$$

where the two body phase density is again a reduced distribution function obtained by marginalizing over $(N-2)$ phase space variables, normalized such that

$$\int \frac{d^3r_1\, d^3p_1}{(2\pi\hbar)^3}\,\frac{d^3r_2\, d^3p_2}{(2\pi\hbar)^3}\, f_2(t, \vec{r}_1, \vec{p}_1, \vec{r}_2, \vec{p}_2) = \underbrace{N(N-1)}_{\text{number of pairs}}$$

Again any two-body observable can be calculated from f_2

Same for k-body with $f_k = \int d^{6(N-k)}_{V}\, f$

We see that typical observables of interest only involve reduced distribution functions

⇒ Derive evolution equations directly reduced distribution functions

BBGKY Hierarchy

Generally for the N-particle system the dynamics is fully described by the Liouville equation

$$\frac{\partial f}{\partial t} + \sum_{i=1}^{N} \dot{\vec{r}}_i \vec{\nabla}_{r_i} f + \sum_{i=1}^{N} \dot{\vec{p}}_i \vec{\nabla}_{p_i} f = 0$$

Where $\dot{\vec{r}}_i$ and $\dot{\vec{p}}_i$ are obtained from classical EOMs

We will focus on system of uncharged particles, i.e. no vector potential

$$\dot{\vec{r}}_i = \vec{\nabla}_{p_i} H = \frac{\vec{p}_i}{m} = \vec{v}_i$$

whereas for conserved energy

$$\dot{\vec{p}}_i = -\vec{\nabla}_{r_i} H = -\vec{\nabla}_{r_i} V(\vec{r}_i) - \sum_{j\neq i} \vec{\nabla}_{r_i} W(|\vec{r}_i - \vec{r}_j|)$$

$$= \underbrace{\vec{F}_i(\vec{r}_i)}_{\text{external forces}} + \underbrace{\sum_{j\neq i} \vec{K}_{ij}(\vec{r}_i - \vec{r}_j)}_{\text{two body forces}}$$

with vector potential things get a little more involved → will discuss later

Now with this Liouville equation takes the form

$$\frac{\partial f}{\partial t} + \sum_{i=1}^{N} \vec{v}_i \vec{\nabla}_{r_i} f + \sum_{i=1}^{N} F_i(\vec{r}_i) \vec{\nabla}_{p_i} f + \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} \vec{K}_{ij}(\vec{r}_i - \vec{r}_j) \vec{\nabla}_{p_i} f = 0$$

can then obtain evolution for reduced densities f_k by integrating out N-k degrees of freedom

1) $$\frac{\partial}{\partial t} f_1 = \frac{\partial}{\partial t} \int d^{6(N-1)}V \, f_N(t, \{\vec{r}_i\}, \{\vec{p}_i\}) = \int d^{6(N-1)}V \, \frac{\partial f_N}{\partial t}$$

where we denote $f_1 = f_1(t, \vec{r}_1, \vec{p}_1)$ (one-body)
and $f_N = f(t, \{\vec{r}_i\}, \{\vec{p}_i\})$ (full phase space dist)

2) $$\int d^{6(N-1)}V \left(\sum_{i=1}^{N} \frac{\vec{p}_i}{m} \vec{\nabla}_{r_i} \right) f_N$$

$$= \frac{p_1}{m} \vec{\nabla}_{r_1} f_1 + \underbrace{\int d^{6(N-1)}V \left(\sum_{i=2}^{N} \frac{\vec{p}_i}{m} \vec{\nabla}_{r_i} \right) f_N}_{= \sum_{i=2}^{N} \frac{\vec{p}_i}{m} \underbrace{\int d^{6(N-1)}V \, \vec{\nabla}_{r_i} f_N}_{\text{boundary terms vanish since } f \text{ is normalized}} = 0}$$

$$= \frac{p_1}{m} \vec{\nabla}_{r_1} f_1$$

Same procedure applies to

3) $$\int d^{6(N-1)}V \sum_{i=1}^{N} \vec{F}(\vec{r}_i)\, \vec{\nabla}_{p_i} f_N$$

$$= \vec{F}(r_1)\, \nabla_{p_1} f_1 \quad + \text{ vanishing boundary terms}$$

Now the most interesting term is the one related to two-body interactions

4) $$\int d^{6(N-1)}V \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} \vec{K}_{ij}(\vec{r}_i - \vec{r}_j)\, \vec{\nabla}_{p_i} f$$

again if $\vec{\nabla}_{p_i}$ is not w.r.t. p_1 we create vanishing boundary terms so

$$= \int d^{6(N-1)}V \sum_{j=2}^{N} \vec{K}_{1j}(\vec{r}_1 - \vec{r}_j)\, \vec{\nabla}_{p_1} f$$

Now can again use symmetry to rewrite

$$= \frac{1}{N-1} \int d^{6(N-2)}V \int \frac{d^3r_2\, d^3p_2}{(2\pi\hbar)^3} (N-1)\, \vec{K}_{12}(\vec{r}_1 - \vec{r}_2)\, \vec{\nabla}_{p_1} f$$

can then perform integration over $d^{6(N-2)}V$

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

So collecting all the terms and dividing $\int d\Gamma_2 = \int \frac{d^3r_2\, d^3p_2}{(2\pi\hbar)^3}$

$$(*) \quad \frac{\partial f_1}{\partial t} + \vec{v}_1 \vec{\nabla}_{r_1} f_1 + \vec{F}(r_1) \vec{\nabla}_{p_1} f_1 = - \int d\Gamma_2 \, \vec{K}_{12} \vec{\nabla}_{p_1} f_2$$

$\Rightarrow$ Evolution equation for one-body f_1
density involves two-body den f_2
due to pair wise interactions

Note: If no pair-wise interactions
are present RHS of $(*)$
vanishes

$\Rightarrow$ closed evolution equation for
one body density f_1

Now how does evolution equation for two-body density f_2 look like?

terms 1)-3) are trivial
just pick up derivatives w.r.t to both $\nabla_{r_1}, \nabla_{p_1}$ and $\nabla_{r_2}, \nabla_{p_2}$ (everything else gives vanishing boundary terms)

What about term 4)

$$\int d^{6(N-2)}V \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} K_{ij}(\vec{r}_i-\vec{r}_j)\, \vec{\nabla}_{p_i} f$$

Now ∇_{p_1} and ∇_{p_2} give rise to non-vanishing terms. We therefore get three types of terms

$$= \left(K_{12}\nabla_{p_1} + K_{21}\nabla_{p_2}\right) f_2$$
$$+ \int d^{6(N-2)}V \sum_{j=3}^{N} K_{1j}(\vec{r}_1-\vec{r}_j)\nabla_{p_1} f$$
$$+ \int d^{6(N-2)}V \sum_{j=3}^{N} K_{2j}(\vec{r}_2-\vec{r}_j)\nabla_{p_2} f$$

using $K_{21} = -K_{12}$ (actio = re-actio)

$$= K_{12}(\nabla_{p_1} - \nabla_{p_2}) f_2$$
$$+ \frac{1}{N-2}\int dR_3 \int d^{6(N-3)}V\, (N-2)\left(K_{13}\nabla_{p_1} + K_{23}\nabla_{p_2}\right) f$$
$$= K_{12}(\nabla_{p_1} - \nabla_{p_2}) + \int dR^3 \left(K_{13}\nabla_{p_1} + K_{23}\nabla_{p_2}\right) f_3$$

So collecting everything

$$\frac{\partial}{\partial t} f_2 + (v_1 \nabla_{r_1} + v_2 \nabla_{r_2}) f_2$$
$$+ (F_1 \nabla_{p_1} + F_2 \nabla_{p_2}) f_2$$
$$+ K_{12} (\nabla_{p_1} - \nabla_{p_2}) f_2$$
$$= - \int d\Omega_3 \, (K_{13} \nabla_{p_1} + K_{23} \nabla_{p_2}) \, f_3$$

So again we find that evolution equation for 2 body density f_2 involves three body density f_3

Indeed we can immediately generalize this for $1 \leq k < N$

$$\frac{\partial}{\partial t} f_k + \sum_{i=1}^{k} (v_k \nabla_{r_k} + F_k \nabla_{p_k}) f_k$$
$$\sum_{\substack{i,j=1 \\ j>i}}^{k} K_{ij} (\nabla_{p_i} - \nabla_{p_j}) f_k$$
$$= - \int d\Omega_{k+1} \sum_{i=1}^{k} K_{i,k+1} \nabla_{p_i} \, f_{k+1}$$

for $k = N$ we simply have Liouville Eqn for $f = f_N$

We have derived a set of coupled evolution equations for k-body distributions

→ BBGKY Hierarchy

Bogoliubov, Born, Green, Kirkwood, Yvon

Up to this point this represents an exact representation of the Liouville equation

However the real use of BBGKY comes from the fact that the hierarchy can be truncated under many physical circumstances

When / How to truncate depends on the system at hand

e.g. range of interactions
interparticle distance
. . .

Different truncations useful in different contexts

→ Subject of next few lectures