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Kinetic theory lecture 1

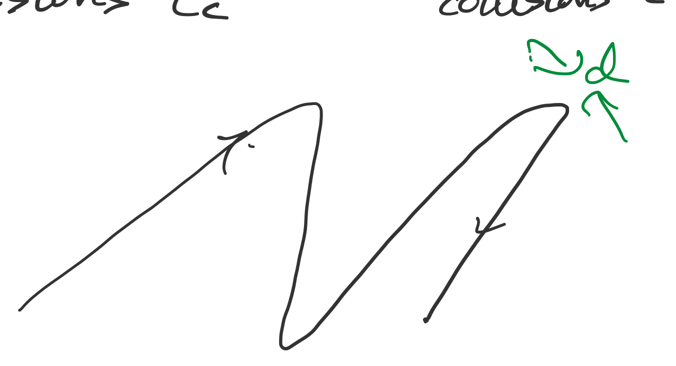
Reduced probabilistic description of $N \gg 1$ interacting particles.

Avogadro's number: 6×10^{23} particles per mole.

In principle $6N$ ODEs, but not practice.

To do better, we rely on a separation of scales.

Timescale of collisions τ_c $\ll$ Timescale between collisions τ $\ll$ Hydrodynamic timescale T



Typical particle speed is the sound speed c_s.

Interaction diameter $d = c_s \tau_c$ $\ll$ mean free path $\lambda_{mfp} = c_s \tau$ $\ll$ hydrodynamic length scale L

Picture: free flight for distance λ_{mfp}, sharp bends of diameter d.
Boltzmann regime

Opposite Coulomb/Vlasov picture has gently swerving trajectories from weak long-range interactions.

Boltzmann equation describes systems in the Boltzmann-Grad limit:

number density $n \to \infty$
interaction diameter $d \to 0$
with $\lambda_{mfp} = O\left(\frac{1}{nd^2}\right)$ is finite & nonzero

Think of "hard spheres" of diameter d.
In one mean free path, each sweeps out a cylinder of volume
$\frac{\pi}{4} d^2 \lambda_{mfp}$
n particles must fill a unit volume
$\frac{\pi}{4} n d^2 \lambda_{mfp} = 1$

The Boltzmann-Grad limit
$\Rightarrow nd^3 \to 0$
so the system is dilute

We start with Newton's laws for N particles, a reversible Hamiltonian system, and derive the irreversible Boltzmann and Navier-Stokes equations.

Three levels of description:

N-particle Hamiltonian system
$6N$ ODEs for p_i, q_i $\quad i = 1, \ldots, N$

Boltzmann equation for the 1-particle distribution $f_1(\underline{x}, \underline{v}, t)$, one integro-differential equation.

Navier-Stokes, five PDEs in 3D for $\rho(\underline{x}, t)$, $\underline{u}(\underline{x}, t)$, $T(\underline{x}, t)$.

II N-particle Hamiltonian mechanics

system of N particles, positions $\underline{x}_i$ and velocities $\underline{v}_i$, mass m.

Canonical coordinates $\underline{p}_i = m \underline{v}_i$
$\underline{q}_i = \underline{x}_i$

Potential $\Phi(\underline{x}_1, \ldots, \underline{x}_N)$

Hamiltonian $$\mathcal{H} = \sum_{i=1}^{N} \frac{|\underline{p}_i|^2}{2m} + \Phi(\underline{q}_1, \ldots, \underline{q}_N)$$

Hamilton's equations $$\dot{\underline{q}}_i = \frac{\partial \mathcal{H}}{\partial \underline{p}_i}$$
$$\dot{\underline{p}}_i = -\frac{\partial \mathcal{H}}{\partial \underline{q}_i}$$

Rewrite in Poisson bracket form as
$\dot{\underline{q}}_i = \{\underline{q}_i, \mathcal{H}\}$ and $\dot{\underline{p}}_i = \{\underline{p}_i, \mathcal{H}\}$,

and more generally for any $F(\underline{q}, \underline{p}, t)$ with $\underline{q} = (\underline{q}_1, \ldots, \underline{q}_N)$
$\underline{p} = (\underline{p}_1, \ldots, \underline{p}_N)$

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \{F, \mathcal{H}\}$$

where $$\{A, B\} = \sum_{i=1}^{N} \frac{\partial A}{\partial \underline{q}_i} \cdot \frac{\partial B}{\partial \underline{p}_i} - \frac{\partial B}{\partial \underline{q}_i} \cdot \frac{\partial A}{\partial \underline{p}_i}$$

Accounts for any explicit time-dependence, such as $F = t$.

IV Reduced s-particle distribution functions

The N-particle distribution
$$\rho(\underline{q}_1, \dots, \underline{q}_N, \underline{p}_1, \dots, \underline{p}_N, t)$$
offers no simplification over the 6N ODEs, rather the reverse...

We can recover the ODE system by taking ρ to be a product of δ-functions corresponding to the initial conditions:
$$\rho(\underline{q}, \underline{p}, t=0) = \delta^3(\underline{q}_1 - \underline{q}_1^{(0)})\,\delta^3(\underline{p}_1 - \underline{p}_1^{(0)}) \dots \delta^3(\underline{q}_N - \underline{q}_N^{(0)})\,\delta^3(\underline{p}_N - \underline{p}_N^{(0)})$$
where δ^3 is the 3D δ-function.

Assuming ρ is normalized to be a probability density function (PDF)
$$\int dV_1 \dots dV_N \, \rho(\underline{q}, \underline{p}, t) = 1,$$
we can define normalised reduced or marginal PDFs as
$$\rho_1(\underline{q}_1, \underline{p}_1, t) = \int dV_2 \dots dV_N \, \rho(\underline{q}, \underline{p}, t).$$
$$\rho_2(\underline{q}_1, \underline{q}_2, \underline{p}_1, \underline{p}_2, t) = \int dV_3 \dots dV_N \, \rho(\underline{q}, \underline{p}, t),$$
$$\rho_s(\underline{q}_1, \dots \underline{q}_s, \underline{p}_1, \dots, \underline{p}_s, t) = \int dV_{s+1} \dots dV_N \, \rho(\underline{q}, \underline{p}, t)$$

If the particles are indistinguishable, these functions are all symmetric under permutations of their arguments, e.g.
$$\rho_2(\underline{q}_1, \underline{q}_2, \underline{p}_1, \underline{p}_2, t) = \rho_2(\underline{q}_2, \underline{q}_1, \underline{p}_2, \underline{p}_1, t)$$
on swapping particle 1 and particle 2.

In kinetic theory it's more common to use the s-particle distribution function f_s. The first of these is
$$\underbrace{f_1(\underline{p}', \underline{q}', t)}_{\text{each in 3D}} = \left\langle \sum_{i=1}^{N} \delta^3(\underline{p}' - \underline{p}_i)\,\delta^3(\underline{q}' - \underline{q}_i) \right\rangle$$
$$= N \int dV_2 \dots dV_N \, \rho(\underline{q}', \underline{q}_2, \dots, \underline{q}_N, \underline{p}', \underline{p}_2, \dots, \underline{p}_N, t)$$
where the N comes from the particles being indistinguishable, so it doesn't matter which is "particle 1".

In a plasma, one would define an f_1 for each species and sum over just the particles of a particular species.

More generally
$$f_s(\underline{q}_1, \underline{q}_2, \dots, \underline{q}_s, \underline{p}_1, \underline{p}_2, \dots \underline{p}_s, t) = \frac{N!}{(N-s)!} \rho_s(\underline{q}_1, \dots, \underline{q}_s, \underline{p}_1, \dots, \underline{p}_s, t),$$
We can choose "particle 1" in N ways, in the first slots of f_s, then "particle 2" in $N-1$ ways etc, giving
$$\frac{N!}{(N-s)!} = N(N-1)\dots(N-s+1)$$
ways to choose s particles from N.

Coming up: specialise to 2-particle potentials so
$$H = \sum_{i=1}^{N} \frac{|\underline{p}_i|^2}{2m} + \sum_{1 \le i < j \le N} \phi(|\underline{q}_i - \underline{q}_j|)$$
Consistent with only 2-particle interactions being significant in a dilute gas under the Boltzmann-Grad scaling.

A good conceptual model is the Lennard-Jones potential, $1/r^6$ attraction and a $1/r^{12}$ repulsion.

$1/r^6$ comes from fluctuating partial charges (van der Waals)

$1/r^{12}$ models the Pauli exclusion principle repulsion.

$1/r^5$ repulsion, called "Maxwell molecules". Nice theoretical simplification, but a bit too soft.

Hard spheres

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III Liouville's theorem: N-particle distributions

Properties we can measure for a system are some limited set of observables $O(\underline{q}, \underline{p})$, e.g. fluid density or velocity averaged over little regions of space & time.

The ergodic hypothesis says that a finite time average is the same as taking an average over an ensemble of many such N-particle systems, reproducing the same observables but differing in fine details.

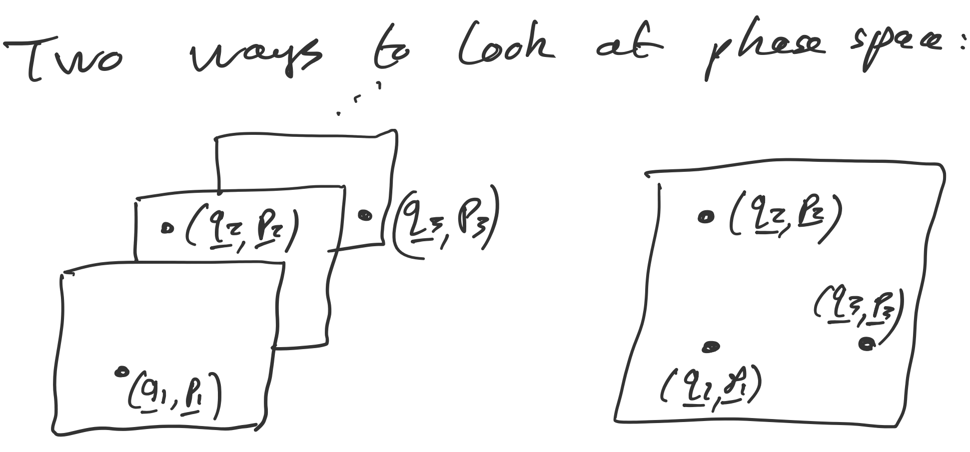
We can represent this ensemble by a density $\rho(\underline{q}_1, \dots, \underline{q}_N, \underline{p}_1, \dots \underline{p}_N, t)$ in 6N-dimensional phase space.

We can use ρ to define ensemble averages for any function $O(\underline{q}, \underline{p})$:

$$\langle O \rangle = \int dV_1 \dots dV_N \, \rho(\underline{q}, \underline{p}, t) \, O(\underline{q}, \underline{p})$$

where $dV_i = d\underline{q}_i \, d\underline{p}_i$ is the 6D volume element associated with particle i.

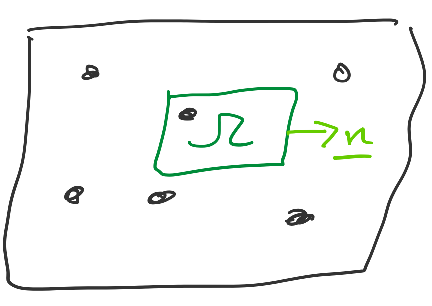
Two ways to look at phase space:



(natural for ρ) (natural for f, see later)

Liouville's theorem says that the evolution of ρ corresponds to a volume-preserving flow in phase space.

Consider a fixed volume Ω in phase space with boundary $\partial\Omega$.



The number of particles inside Ω is

$$n_\Omega = \int_\Omega dV \, \rho(\underline{q}, \underline{p}, t)$$

where $dV = dV_1 \dots dV_N$.

n_Ω is the expectation of an indicator function that's 1 for $(\underline{q}, \underline{p}) \in \Omega$, 0 otherwise.

As Ω is fixed,

$$\frac{dn_\Omega}{dt} = \int_\Omega dV \, \frac{\partial \rho}{\partial t}.$$

This must equal the change due to the flux of particles across $\partial\Omega$.

$$\frac{dn_\Omega}{dt} = -\int_{\partial\Omega} dS \, \underline{n} \cdot \dot{\underline{z}} \rho, \qquad \underline{z} = (\underline{q}, \underline{p})$$

where $\underline{n}$ is the outward unit normal on $\partial\Omega$ and $\dot{\underline{z}} = (\dot{\underline{q}}, \dot{\underline{p}})$.

Using the divergence theorem:

$$\frac{dn_\Omega}{dt} = -\int_\Omega dV \, \nabla_{\underline{z}} \cdot (\dot{\underline{z}} \rho)$$

This must coincide with the first expression for $\frac{dn_\Omega}{dt}$ for all fixed volumes Ω so

$$\frac{\partial \rho}{\partial t} + \nabla_{\underline{z}} \cdot (\dot{\underline{z}} \rho) = 0.$$

Unpacking the $\underline{z}$ notation:

$$\frac{\partial \rho}{\partial t} + \sum_{i=1}^{N} \left[\frac{\partial}{\partial \underline{q}_i} \cdot (\dot{\underline{q}}_i \rho) + \frac{\partial}{\partial \underline{p}_i} \cdot (\dot{\underline{p}}_i \rho) \right] = 0,$$

$$\frac{\partial \rho}{\partial t} + \sum_{i=1}^{N} \left[\frac{\partial}{\partial \underline{q}_i} \cdot \left(\frac{\partial H}{\partial \underline{p}_i} \rho \right) + \frac{\partial}{\partial \underline{p}_i} \cdot \left(-\frac{\partial H}{\partial \underline{q}_i} \rho \right) \right] = 0$$

$$\frac{\partial \rho}{\partial t} + \sum_{i=1}^{N} \left[\frac{\partial H}{\partial \underline{p}_i} \cdot \frac{\partial \rho}{\partial \underline{q}_i} - \frac{\partial H}{\partial \underline{q}_i} \cdot \frac{\partial \rho}{\partial \underline{p}_i} + \rho \underbrace{\left(\frac{\partial}{\partial \underline{q}_i} \cdot \frac{\partial H}{\partial \underline{p}_i} - \frac{\partial}{\partial \underline{p}_i} \cdot \frac{\partial H}{\partial \underline{q}_i} \right)}_{= 0 \text{ as } \frac{\partial^2 H}{\partial \underline{q}_i \partial \underline{p}_i} = \frac{\partial^2 H}{\partial \underline{p}_i \partial \underline{q}_i}} \right] = 0$$

$$\frac{\partial \rho}{\partial t} + \{\rho, H\} = 0.$$

Along trajectories in phase space

$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \{\rho, H\} = 0.$$

The particle trajectories define the characteristics for Liouville's equation as a PDE.

This is closely linked to reversibility: phase space volumes neither expand nor contract as they evolve.

More precisely, if $\rho(\underline{q}, \underline{p}, t)$ solves Liouville's equation, so does $\rho(\underline{q}, -\underline{p}, -t)$.

Exercise: show that

$$\frac{d}{dt} \langle O \rangle = \langle \{O, H\} \rangle$$

for any observable $O(\underline{q}, \underline{p})$.
Classical analogue of Ehrenfest's theorem in quantum mechanics.