Classical Iransport Menomena

1. Nzive Kinetic Theory (Clausius, Maxwell, Boltzmann

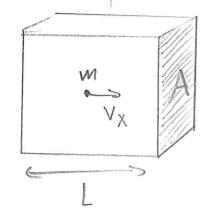
The general postulates are the following:

· Very large number of molecules, but large separation compared to size;

· Particles more around randomly with a certain velocity distribution;

· Collisions between particles and with walls are perfectly elastic, and there are no other interactions.
· Particles obey New ton's Laws.

1.1. The particle in a box



$$\Delta p_x = 2mv_x$$
, $\Delta f = \frac{2L}{v_x}$

$$F = \frac{mv_x^2}{L} \Rightarrow p = \frac{mv_x^2}{LA} = \frac{mv_x^2}{V}$$

$$\Rightarrow pV = mv_x^2$$

For N)>1 perficles we expect pV=nRT=NkBT and there fore

$$\langle V_X^2 \rangle = \langle V_Y^2 \rangle = \langle V_Z^2 \rangle = \frac{k_B T}{m}$$

1.2. The Mexwell-Boltzmann distribution We impose 2 few constraints on the velocity distribution F(V).

* Spherical symmetry:

* Independent components:

$$F(\vec{v}) = f_{x}(v_{x})f_{y}(v_{y})f_{z}(v_{z})$$

These considerations together with differentiability

fix e gaussian
$$f_{x}(v_{x}) = f(v_{x}) = \frac{1}{\sqrt{2\pi\sigma^{2}}} e^{-\frac{v_{x}^{2}}{2\sigma^{2}}}.$$

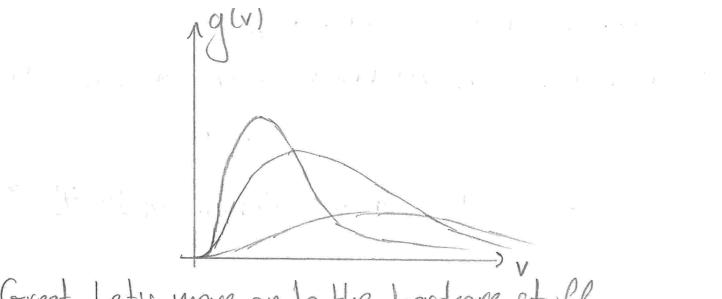
From the particle in a box we conclude or = KBT

$$\Rightarrow f(v_x) = \sqrt{\frac{m}{2\pi k_B T}} e^{-\frac{m v_x^2}{2k_B T}}$$

2nd therefore

$$F(\vec{v}) = \left(\frac{M}{2TK_BT}\right)^{3/2} e^{-\frac{Mv^2}{2K_BT}}$$

2nd the speed distribution is just
$$q(v) = \left(\frac{m}{2\pi k_B T}\right)^{3/2} 4\pi v^2 e^{-\frac{mv^2}{2k_B T}}$$



Great. Let's move on to the hardcore stuff.

2. Dynamics of classical densities

Suppose we have an N-body system of particles labele i with positions \(\tilde{q} \); and momenta \(\tilde{p} \). Any conservative dynamics can be described by a Hamiltonian H(\(\tilde{p} \), \(\tilde{q} \) i) Such that

$$\vec{q} = \frac{\partial H}{\partial \vec{p}}$$

$$\vec{p} = -\frac{\partial H}{\partial \vec{q}}$$

The point $\mu(t) = (\vec{q}_i(t), \vec{p}_i(t))$ is said to live in the system's 6N dimensional phase-space, and flows around as time goes by.

If we know exactly the point $\mu(0)$, we can in principle integrate the equations of motion to get $\mu(t)$.

2.1. Liouville's theorem Determining $\mu(0)$ for large systems, however, is an experimentally downting task. We therefore resort to 2 probabilistic treatment. Define the phase space density p(u, t) such that the probability to find the system in 2 small neigh borhood dr = Td3q; d3p; of µ is P(µ, +) dT. Then there are a few ways to realize that of behaves like a fluid moving through phase space, $\frac{d\rho}{dt} = \frac{\partial\rho}{\partial t} + \frac{\partial\rho}{\partial q} \cdot \dot{q}i + \frac{\partial\rho}{\partial p} \cdot \dot{p}i = \frac{\partial\rho}{\partial t} + \frac{1}{2}\rho_1 + \frac{1}{2} = 0.$ The expectation value for time-independent observables $O(\mu)$ is given by <0)(+)= \drp(\mu,+) with time evolution

 $\frac{d\langle 0\rangle}{dt} = \langle \{0, H\} \rangle.$

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2.2. Statistical equilibrium Equilibrium thermodynamics is concerned with a few macroscopic observables such as total energy 0, tempera-How can we devise a distribution peg such that these observables don't depend on time? An obvious way to do this is to set apeq = 0. Given 2 set of conserved quantities {La] for our system, this can easily be done by writing geg(µ)=p(H(µ), La(µ)). The dependence on H can be simply understood as the fundamental postulate of statistical mechanics. 2.3. Reversibility Our present formalism cannot deal with the approach to equilibrium. Classical mechanics is reversible. It we take $\mu(0) = (\vec{q};(0), \vec{p};(0))$ >> Tu(0)=(9,(0),-p,(0)), then we have $\mu(t) = (\vec{q}_{i}(t), \vec{p}_{i}(t))$ $T\mu(t) = (\vec{q}_i(-t), -\vec{p}_i(-t))$

So for any state converging to peg, there's an equally good state diverging from it. We need 2 bit more depth in this description. Or may be not? Let's think about it for a bit.

3. The BBGKY hierarchy

When we did baby kinetic theory, we interred some macros copic properties from the distribution of a single particle. Why exactly are we trying to describe the motion of 1023 of them?

Thatis a great question, and it's at the heart of what comes n'ext. How many particles should we describe to be able to understand what's happening?

Suppose we have N in distinguishable particles in our system. Define the s-particle density

 $f(\vec{p}_1, \vec{q}_1, ..., \vec{q}_{s,t}) = \frac{N!}{(N-s)!} \int_{i=s+1}^{N} d\vec{p}_i \vec{p}_i \vec{p}_i ..., \vec{q}_{s,t} \vec{p}_{s+1} ..., \vec{q}_{N,t})$

2s the expected number of s-tuplets of particles around a region of phase space.

The ideal gas Hamiltonian is

$$H = \sum_{i=1}^{N} \left[\frac{\vec{p}_{i}^{2}}{2m} + U(\vec{q}_{i}^{2}) \right] + \sum_{(i,j)=1}^{N} V(|\vec{q}_{i}^{2} - \vec{q}_{j}^{2}|)$$

To describe the evolution of fs, it's convenient to brezk Hinto three parts

$$H_{S} = \sum_{n=1}^{S} \left[\frac{\vec{p}_{n}^{2}}{2m} + U(\vec{q}_{n}) \right] + \sum_{(n,m)=1}^{S} V(|\vec{q}_{n} - \vec{q}_{m}|)$$

$$H_{N-S} = \sum_{i=s+1}^{N} \left[\frac{\vec{p}_{i}^{2}}{2m} + U(\vec{q}_{i}^{2}) \right] + \sum_{(i,j)=s+1}^{N} V(|\vec{q}_{i}^{2} - \vec{q}_{i}^{2}|)$$

$$H' = \sum_{n=1}^{S} \sum_{i=s+1}^{N} V(|\vec{q}_{n} - \vec{q}_{i}^{2}|)$$

$$N = 1 = s+1$$

and we have

We now have by Liouville's theorem

the first bracket is trivial,

the second one gives O,

$$\frac{0fs}{0t} + \{fs, Hs\} = -\frac{N!}{(N-s)!} \int_{i=s+1}^{N} dT_{i} \{g, H'\}$$

The final one evaluates to $\frac{\partial f_s}{\partial t} + \{f_s, H_s\} = \frac{s}{2} \int d\Gamma_{s+1} \frac{\partial V(|\vec{q_n} - \vec{q_{s+1}}|)}{\partial \vec{q_n}} \frac{\partial f_{s+1}}{\partial \vec{p_n}}$

this is a hierarchy of Neguations. We need to trun-cate it somewhere. But where?

4. The Boltzmann equation

Take the first two equations in the hierarchy.

$$\begin{bmatrix}
 \frac{\partial}{\partial t} - \frac{\partial U}{\partial q_1} \cdot \frac{\partial}{\partial p_1} + \vec{p_1} \cdot \frac{\partial}{\partial q_1} \end{bmatrix} f_1 = \int d\Gamma_2 \frac{\partial V(|\vec{q_1} - \vec{q_2}|)}{\partial \vec{q_1}} \cdot \frac{\partial f_2}{\partial p_1}$$

$$\begin{bmatrix}
\frac{\partial}{\partial t} - \frac{\partial U}{\partial \vec{q}_1} \cdot \frac{\partial}{\partial \vec{p}_1} & \frac{\partial U}{\partial \vec{q}_2} \cdot \frac{\partial}{\partial \vec{p}_2} + \frac{\vec{p}_1}{\vec{p}_1} \cdot \frac{\partial}{\partial \vec{q}_1} + \frac{\vec{p}_2}{\vec{p}_2} \cdot \frac{\partial}{\partial \vec{q}_2} \\
\frac{\partial}{\partial V} \left(\vec{Q} \cdot \vec{q}_1 \cdot \vec{q}_2 \cdot \vec{p}_1 \cdot \vec{q}_2 \cdot$$

$$-\frac{9V(|\vec{q_1}-\vec{q_2}|)}{9\vec{q_1}}\cdot\left(\frac{9}{9\vec{p_1}}-\frac{9}{9\vec{p_2}}\right)\right]\vec{f_2}=$$

$$= \int dT_3 \left[\frac{\partial V(1\vec{q_1} - \vec{q_3}1)}{\partial \vec{q_1}} \frac{\partial}{\partial \vec{p_1}} + \frac{\partial V(1\vec{q_2} - \vec{q_3}1)}{\partial \vec{q_2}} \frac{\partial}{\partial \vec{p_2}} \right] f_3$$

We have three relevant time scales.

It the particles have number density in and a characteristic volume of, we can write

1 ~ nd3
Zx Zc

So if the particles are very dilute, the right hand sides grow smaller and smaller!

Letis Gruncate the hierarchy setting the second r.h.s.

Now note that the eguation for fz has collision terms.

It should evolve much faster than for, so we can approximate it to a "steady state". Also, the external terms are not at all relevant during a collision.

With these considerations, the Egustion for fa is

for similar reasons, f_2 should be much more sensitive to variations of the relative coordinate $\vec{q} = \vec{q_2} - \vec{q_3}$ than of the C.M. $\vec{Q} = \vec{q_1} + \vec{q_2}$. We then write

$$\frac{\partial V(|\vec{q}_1 - \vec{q}_2|)}{\partial \vec{q}_1} \cdot \left(\frac{\partial}{\partial \vec{p}_1} - \frac{\partial}{\partial \vec{p}_2} \right) f_2 \approx - \left(\frac{\vec{p}_1 - \vec{p}_2}{m} \right) \cdot \frac{\partial f_2}{\partial \vec{q}}.$$

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Integrating both sides of this equation gives the K.H.S of the egustion for fr, $\int d\Gamma_2 \frac{\partial V(|\vec{q_1} - \vec{q_2}|)}{\partial \vec{q_1}} \frac{\partial f_2}{\partial \vec{p_1}} \approx \int d^3\vec{p_2} d^3\vec{q} \left(\frac{\vec{p_2} - \vec{p_1}}{m}\right).$ 0 f2 [p1, q1, p2, q1+q, +). We integrate on of along the direction of $\vec{p} = \vec{p_1} - \vec{p_2}$, giving $\int d\Gamma_{2} \frac{\partial V(|\vec{q_{1}} - \vec{q_{2}}|)}{\partial \vec{q_{1}}} \cdot \frac{\partial f_{2}}{\partial \vec{p_{2}}} \approx \int d^{3}\vec{p_{2}} d^{2}\vec{b} |\vec{v_{1}} - \vec{v_{2}}|$ [f2(p1, q1, p2, b,+,+) -f2[P1,91,P2,6,-,+)] P1= P1+P2+ | P1-P2 | D2 $\vec{p}_{2}^{1} = \frac{\vec{p}_{1} + \vec{p}_{2} - |\vec{p}_{1} - \vec{p}_{2}|\hat{\Omega}}{2}$ $\sqrt{\vec{p}'} = \vec{p}_1 - \vec{p}_2$ by time-veversal symmetry, fz(p1, q1, p2, 6,+,+) = $f_2(\vec{p}_1, \vec{q}_1, \vec{p}_2, \vec{b}, -, +)$.

We substitute and get
$$\int d\Gamma_2 \frac{\partial V(|\vec{q}_1 - \vec{q}_2|)}{\partial \vec{q}_1} \frac{\partial f_2}{\partial \vec{p}_1} = \int d^3\vec{p}_2 d^2\vec{b} |\vec{v}_1 - \vec{v}_2|$$

$$\left[\int_{Z} (\vec{p}_1, \vec{q}_1, \vec{p}_2, \vec{b}_1 - 1 +) \right]$$

$$= \int_{Z} (\vec{p}_1, \vec{q}_1, \vec{p}_2, \vec{b}_1 - 1 +) \right]$$
we can also write this interms of the differential cross-section as
$$\int d\Gamma_2 \frac{\partial V(|\vec{q}_1 - \vec{q}_2|)}{\partial \vec{q}_1} \frac{\partial f_2}{\partial \vec{p}_1} \approx \int d^3\vec{p}_2 d^2\Omega \left| \frac{d\sigma}{d\Omega} \right| |\vec{v}_1 - \vec{v}_2|$$

$$\left[\int_{Z} (\vec{p}_1, \vec{q}_1, \vec{p}_2, \vec{b}_1 - 1 +) \right]$$
We now set the assumption of molecular chaos,
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We now set the assumption of molecular chaos,
$$\int_{Z} (\vec{p}_1, \vec{q}_1, \vec{p}_2, \vec{b}_1 - 1 +) \right]$$
and get the Boltzmann equation,
$$\left[\frac{\partial}{\partial t} - \frac{\partial V}{\partial \vec{q}_1}, \frac{\partial}{\partial \vec{p}_1} + \frac{\partial}{m}, \frac{\partial}{\partial \vec{q}_1} \right] f_1 = -\int_{Z} d^3\vec{p}_2 d^2\Omega \left| \frac{d\sigma}{d\Omega} \right| |\vec{v}_1 - \vec{v}_2|$$

and get the Boltzmann equation,

$$\left[f_{1}(\vec{p}_{1},\vec{q}_{1},+) f_{1}(\vec{p}_{2},\vec{q}_{1},+) - f_{1}(\vec{p}_{1},\vec{q}_{1},+) f_{1}(\vec{p}_{2},\vec{q}_{1},+) \right] .$$

5. The H- theorem

$$H(t) = \int d^{3}\vec{p} d^{3}\vec{q} \int_{1}^{1} \log f_{1}$$

$$H = \int d^{3}\vec{p} d^{3}\vec{q} \log f_{1} \frac{\partial f_{1}}{\partial t}$$

$$= \int d^{3}\vec{p} d^{3}\vec{q} \log f_{1} \left(\frac{\partial U}{\partial \vec{q}} \cdot \frac{\partial f_{1}}{\partial \vec{p}} - \vec{p} \cdot \frac{\partial f_{1}}{\partial \vec{q}} \right)$$

$$- \int d^{3}\vec{p}_{1} d^{3}\vec{p}_{2}^{2} d^{3}\vec{q} d^{2}\vec{b} |\vec{V}_{1} - \vec{V}_{2}| \log f_{1}(\vec{p}_{1}, \vec{q})$$

$$= \int f_{1}(\vec{p}_{1}, \vec{q}) f_{1}(\vec{p}_{2}, \vec{q}) - f_{1}(\vec{p}_{1}, \vec{q}) f_{1}(\vec{p}_{2}, \vec{q})$$

$$= \int f_{1}(\vec{p}_{1}, \vec{q}) f_{1}(\vec{p}_{2}, \vec{q}) - f_{1}(\vec{p}_{1}, \vec{q}) f_{1}(\vec{p}_{2}, \vec{q})$$

The first term vanishes, and in the second we can swap $\vec{p_1} \leftrightarrow \vec{p_2}$

$$\dot{H} = -\frac{1}{2} \int_{0}^{3} \vec{p}_{1} d^{3} \vec{p}_{2} d^{3} \vec{q} d^{2} \vec{b} | \vec{v}_{1} - \vec{v}_{2}| \log f_{1}(\vec{p}_{1}, \vec{q}) f_{1}(\vec{p}_{2}, \vec{q})$$

$$[f_{1}(\vec{p}_{1}, \vec{q}) f_{1}(\vec{p}_{2}, \vec{q}) - f_{1}(\vec{p}_{1}, \vec{q}) f_{1}(\vec{p}_{2}, \vec{q})]$$

Doing something similar for popi,

$$\dot{H} = -\frac{7}{4} \left[d^3 \vec{p_1} d^3 \vec{p_2} d^3 \vec{q} d^2 \vec{b} | \vec{V_1} - \vec{V_2} | \right]$$

$$\left[f_1(\vec{p_1}) f_1(\vec{p_2}) - f_1(\vec{p_1}) f_2(\vec{p_2}) \right]$$

[log fr(pi)fr(pi)-log fr[pi)fr(pi)] <0.

6. Local equilibrium Setting the integrand to zero,

 $f_1(\vec{p_1})f_1(\vec{p_2}) = f_1(\vec{p_1})f_1(\vec{p_2})$

so log for is 2 linear combination of any additive conserved quantity for a collision, and by comparison with the M-B distribution, we write the local equilibrium distribution

$$f_{1}^{(0)}(\vec{p},\vec{q},t) = \frac{N(\vec{q},t)}{(2TTm k_{B}T(\vec{q},t))^{3/2}} exp\left[\frac{(\vec{p}-m\vec{v}(\vec{q},t))^{2}}{2m k_{B}T(\vec{q},t)}\right]$$

where n is the local particle number density,

and we have local expectation values for any single particle operator O(p,q)

7. Conservation Laws Let's abovess how exactly for can approach an equilibrium distribution.

(i) f2(q1,q2) relzxes to f1(q1)f1(q2) et times ~ Zc (ii) forelexes to local equilibrium locally maximizing H 2+ every point, 2+ time scales Zx

Civil for releases to global equilibrium at time scales Zu.

Consider now a single particle quantity of that is additively conserved in a collision,

X(p, q, +) + X(p2, q, +) = X(p1, q, +) + X(p2, q, +).

Then we have

Using then the Boltzmann equation we get JX= Jd3p X(p,q,t)[3+ p. 3+ F. 3p] J, (p,q,t) where $\vec{F} = -\frac{\partial U}{\partial \vec{q}}$ is the external force. Using product rules we get

Let's substitute some N's and see what we get (a) Particle number:

where we've introduced $\vec{v} = \langle \vec{p}/m \rangle$ the local average velocity

(b) Momentum:

If
$$\chi = \vec{c} = \vec{p} - \vec{U}$$
, we get

nm(0++v; 0j)vi=-0; Pij-nFi where we've defined the pressure tensor Pij=nm<cicj>

Icl Kinetic energy

If $\chi = \frac{1}{2}mc^2$, using the continuity, we get

where we've introduced the everyge energy $\mathcal{E} = \langle \frac{1}{2} mc^2 \rangle$

the heat flux

$$\vec{h} = \frac{nm}{2} \langle \vec{c} c^2 \rangle$$

and the strain rate

So given expressions for Pij and h, these equations can imprinciple be solved. These are Navier-Stokes.

8. Zero-order hydrodynzmics

If we use finds an estimate for the density in a fluid, we get in particular

Pij=nksTSij, ho)=0, E0=3 ksT which leads to the fluid equations

$$Q_{\uparrow}N + \nabla \cdot (N\vec{\sigma}) = 0$$

$$NM(9++\vec{\sigma} \cdot \nabla)\vec{\sigma} = -\nabla (Nk_BT) + N\vec{F}$$

$$(9++\vec{\sigma} \cdot \nabla)T = -\frac{2}{3}T\nabla \cdot \vec{\sigma}.$$

2nd with the first and third equations we get $(9++\overrightarrow{O}\cdot\nabla)(\frac{n}{78/2})=0,$ nes, These egustions then describe adiabaticflow. 9. First-order hydrodynamics The local equilibrium solution sets the collision terms of the Bolfzmann equation to zero. The streaming terms, however, ren't zero. Acting on for with them we $[D_{+}+\vec{c}\cdot\nabla+\vec{F}\cdot\vec{Q}]\log f_{1}^{(0)}=\mathcal{I}[\log f_{1}^{(0)}]$ and if the fields satisfy the hydrodynamic equa-I [logfo] = m / (cicj - Sij c²) vij + (mc² - 5) ci git. We now estimate the r.h.s. of the Boltzmann eq. 25 follows. Expand for in a collision parameter q(p) as for for (1+g). Then we get $f_1 |_{coll} \approx - \int d^3p_2 d^2b |_{V_1} - V_2|_{f_1}^{(0)} (\vec{p_1})_{f_1}^{(0)} (\vec{p_2})$ $[g(\vec{p}_1) + g(\vec{p}_1) - g(\vec{p}_1) - g(\vec{p}_1)]$

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Then we get

$$g = -Z_{X} \times Z \left[\log \int_{1}^{\infty}\right]$$
So the correction to \int_{1}^{1} to leading order in Z_{X} is
$$\int_{1}^{(1)} \approx \int_{1}^{\infty} \left[1 - \frac{Z_{Y}M}{k_{BT}} \left(C_{1}C_{1} - \frac{S_{1}C^{2}}{3}\right) U_{1}^{2}\right]$$

$$-Z_{X} \left(\frac{MC^{2}}{2k_{BT}} - \frac{5}{2}\right) \frac{C_{1}}{T} \Im T \right].$$
In this scheme, we get
$$P_{1j}^{(1)} = nk_{BT} - 2nk_{BT}Z_{Y} \left(U_{1j} - \frac{S_{1j}}{3}U_{KK}\right)$$

$$\overline{h}^{(1)} = -\frac{5}{2} \frac{nk_{B}^{2}TZ_{X}}{m} \nabla T$$
(a) We get viscosity with (off-diagonal)
$$\mu = 2nk_{BT}Z_{Y}$$
(b) We get Fourier's Lzw with
$$K = \frac{5}{2} \frac{nk_{B}^{2}TZ_{X}}{M}$$