

## Lecture 6 - Semiclassical transport & the Boltzmann equation

(1)

With our knowledge of the master equation and transition rates we now want to start writing down a slightly more microscopic description of systems with many particles, and we will derive the Boltzmann equation that describes the statistical properties of the motion and collisions in such a collection of particles. Originally, the Boltzmann equation comes from kinetic theory, which studied a classical system of  $N$  particles described by a classical Hamiltonian

$$H = \sum_{i=1}^N \left( \frac{p_i^2}{2m} + v(x_i) \right) + \sum_{i < j} u(x_i - x_j)$$

### Analytical mechanics refresher

$$H = H(q, p) \text{ Hamiltonian (total energy)}$$

Hamilton's equations of motion

$$\begin{cases} \dot{\vec{q}} = \frac{\partial H}{\partial \vec{p}} \\ \dot{\vec{p}} = -\frac{\partial H}{\partial \vec{q}} \end{cases}$$

$$\underline{\text{Example:}} \quad H = \frac{p^2}{2m} + v(\vec{r})$$

$$\text{then } \vec{v} \equiv \dot{\vec{r}} = \frac{\partial H}{\partial \vec{p}} = \frac{\vec{p}}{m}$$

$$m\vec{a} \equiv \ddot{\vec{p}} = -\frac{\partial H}{\partial \vec{r}} = -\frac{\partial v}{\partial \vec{r}} = \vec{F}$$

### Time evolution

$O(q, p)$  some observable. Then

$$\begin{aligned} \frac{dO}{dt} &= \frac{\partial O}{\partial t} + \frac{\partial O}{\partial q} \cdot \dot{q} + \frac{\partial O}{\partial p} \cdot \dot{p} = \frac{\partial O}{\partial t} + \frac{\partial O}{\partial q} \frac{\partial H}{\partial p} - \frac{\partial O}{\partial p} \frac{\partial H}{\partial q} \\ &= \frac{\partial O}{\partial t} + \{O, H\} \end{aligned} \quad (\text{compare quantum mechanics})$$

with the Poisson bracket defined as

$$\{A, B\} = \frac{\partial A}{\partial \bar{q}} \cdot \frac{\partial B}{\partial \bar{p}} - \frac{\partial A}{\partial \bar{p}} \frac{\partial B}{\partial \bar{q}}$$


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In the first lecture we discussed the probability density of finding particle  $i$  within  $d\mathbf{x}_i$  of  $\mathbf{x}_i$  with momentum  $\mathbf{p}_i$  within  $d\mathbf{p}_i$ , i.e.

$$g(x_1, \dots, x_N; p_1, \dots, p_N) \frac{dx_1 dp_1}{h^d} \dots \frac{dx_N dp_N}{h^d}$$

while we could in principle try to follow how  $g$  evolves in time under the influence of  $H$ , in practice this is not possible.  $g$  also contains way more information than we generally need. For many observables, it is sufficient to know the one-body density in phase space,  $f(\bar{r}, \bar{p}; t)$  that gives the number of particles in a volume  $d\bar{r}$  around  $\bar{r}$  and with momentum range  $d\bar{p}$  around  $\bar{p}$  as  $f(\bar{r}, \bar{p}; t) d\bar{r} d\bar{p}$ . In principle,  $f$  can be obtained from  $g$  as follows:

$$f(\bar{r}, \bar{p}; t) = \sum_i \langle \delta(\bar{x}_i(t) - \bar{r}) \delta(\bar{p}_i(t) - \bar{p}) \rangle \\ = N \int \prod_{i=2}^N d\bar{x}_i d\bar{p}_i g(\bar{r}, \bar{x}_2, \dots, \bar{x}_N; \bar{p}, \bar{p}_2, \dots, \bar{p}_N; t)$$

This can be formally useful in order to understand where  $f$  comes from, but since we in practice never calculate  $g$ , we should rather think in terms of  $f$ . The one-body distribution function  $f$  satisfies:

$$\int d^3p f(\bar{r}, \bar{p}; t) = n(\bar{r}, t) \quad \text{density of particles}$$

$$\int d^3r n(\bar{r}, t) = N \quad \text{total number of particles.}$$

In the absence of an external potential  $V$ , translation symmetry is recovered and the equilibrium distribution is

$$f^*(\vec{r}, \vec{p}) = \frac{n}{(2\pi m k_B T)^{3/2}} e^{-\vec{p}^2/2mk_B T} \quad \text{with } n = \frac{N}{V}$$

If we know  $f$  we can compute expectation values of observables that only depend on  $\vec{r}$  and  $\vec{p}$ , such as particle current

$$\vec{j}(\vec{r}, t) = \int d\vec{p} f(\vec{r}, \vec{p}; t) \frac{\vec{p}}{m}$$

and energy current

$$\vec{j}_e(\vec{r}, t) = \int d\vec{p} f(\vec{r}, \vec{p}; t) E(p) \frac{\vec{p}}{m}$$

etc. We now want to obtain an equation that allows us to calculate  $f$  systematically.

### One-particle distribution function in quantum mechanics

So far, our discussion has been classical, but most of it still applies in some sense in quantum mechanics. Of course, the equilibrium distribution would be, for fermions, the Fermi-Dirac

$$f^*(\vec{r}, \vec{k}; t) = \frac{1}{\exp\left(\frac{\epsilon(\vec{k}) - \mu}{k_B T}\right) + 1}$$

But, what does it mean to say that a quantum mechanical particle has momentum  $\vec{p}$  and position  $\vec{r}$ ? Doesn't the uncertainty principle explicitly tell us that it is not possible to specify both at the same time? Yes, but... First, we are talking about probability density. In a metal, for example, the relevant momentum scale is the Fermi momentum  $\bar{p}_F = \hbar \bar{k}_F$ ;  $|\bar{k}_F| = k_F$

If the function  $f(\vec{r}, \vec{p})$  varies slowly in space compared with  $\Delta x \sim \frac{\hbar}{m p} = k_F^{-1}$  then we don't need to worry too much about the uncertainty principle. We can also appeal to Ehrenfest's theorem, which states that the expectation values of the position and momentum of a wave packet follow the classical equations of motion

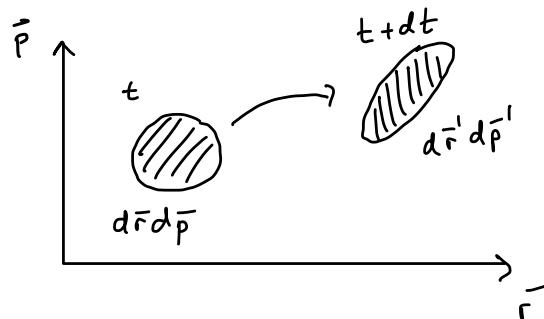
$$\frac{d}{dt} \langle \hat{r} \rangle = \frac{1}{m} \langle \hat{p} \rangle$$

$$\frac{d}{dt} \langle \hat{p} \rangle = - \langle \nabla \cdot \mathbf{v}(\hat{r}) \rangle.$$

So, we will think of the electrons in a metal, say, as wave packets. Interactions between particles can then lead to scattering of one wave packet from another, and impurities lead to scattering of the wave packets. But on a longer scale and in between such scattering events the wave packets will simply evolve smoothly and this evolution can readily be captured by the evolution of the probability distribution function  $f(\vec{r}, \vec{p}; t)$ . Note that this means that we can generally include the influence of external perturbations, such as an electric or magnetic field in this flow of  $f$ .

### The Boltzmann equation

Consider, then, the flow of  $f(\vec{r}, \vec{p}; t)$  in phase space in the absence of collisions and impurity scattering:



Remember from the first lecture that  $g$  satisfies Liouville's theorem,

stating that the flow of  $g$  in phase space is incompressible.

In this context this means that phase space volume is invariant  $d\bar{r}d\bar{p} = d\bar{r}'d\bar{p}'$ . Therefore,

$$f(\bar{r} + \dot{\bar{r}}dt, \bar{p} + \dot{\bar{p}}dt, t + dt) d\bar{r}'d\bar{p}' = f(\bar{r}, \bar{p}; t) d\bar{r}d\bar{p}$$

Taylor expanding we then obtain

$$\frac{\partial f}{\partial t} + \frac{\partial f}{\partial \bar{r}} \cdot \dot{\bar{r}} + \frac{\partial f}{\partial \bar{p}} \cdot \dot{\bar{p}} = 0$$

Keeping in mind that we are assuming there are no collisions, that is  $H = \epsilon(p) + U_{\text{ext}}(r)$ , we have

$$\dot{\bar{r}} = \frac{d\bar{r}}{dt} = \frac{\partial H}{\partial p} = \frac{\partial \epsilon}{\partial p} = \vec{v}(p)$$

$$\dot{\bar{p}} = -\frac{\partial H}{\partial \bar{r}} = -\frac{\partial U}{\partial \bar{r}} = \vec{F}_{\text{ext}}$$

Therefore

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \frac{\partial f}{\partial \bar{r}} + \vec{F} \cdot \frac{\partial f}{\partial \bar{p}} = 0$$

By introducing the Liouville operator

$$L = \frac{\partial}{\partial t} + \vec{v} \cdot \frac{\partial}{\partial \bar{r}} + \vec{F} \cdot \frac{\partial}{\partial \bar{p}}$$

This takes the simple form

$$Lf = 0$$

This only describes the effect of the motion without any collision. To describe the motion realistically we need to take into account the effects of collisions.

This is written in terms of a collision integral, which <sup>(6)</sup>  
at this point we simply write as

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \frac{\partial f}{\partial \vec{r}} + \vec{F} \cdot \frac{\partial f}{\partial \vec{p}} = \left( \frac{\partial f}{\partial t} \right)_{\text{coll}}$$

or

$$\frac{\partial f}{\partial t} = \left( \frac{\partial f}{\partial t} \right)_{\text{coll}}$$

Note: Sometimes people write

$$\left( \frac{\partial f}{\partial t} \right)_{\text{str}} = - \vec{j} \cdot \frac{\partial f}{\partial \vec{r}} - \vec{F} \cdot \frac{\partial f}{\partial \vec{p}}$$

for a streaming term, and then

$$\frac{\partial f}{\partial t} = \left( \frac{\partial f}{\partial t} \right)_{\text{str}} + \left( \frac{\partial f}{\partial t} \right)_{\text{coll}}$$

making explicit that there are two distinct contributions to  
the time evolution of  $f$ , streaming motion and collisions.

### Scattering processes

What processes contribute to the collision integral?

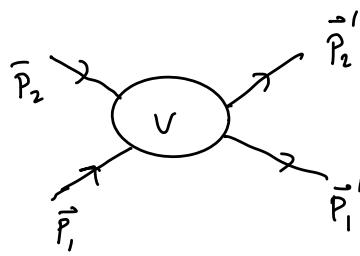
i) Single particle scattering



Example: disorder potential  $w(\vec{r})$

ii) Two-particle scattering

- interactions  $v(\vec{r}, \vec{r}')$



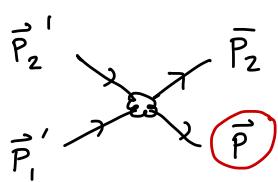
For now let us focus on the second type.

A collision takes place over a typical time scale  $\tau_c$  ⑦ and length scale  $d$ . Let us coarse grain over this length scale such that we can assume the collision takes place in a single point  $\bar{r}$ . This requires  $\tau_c$  to be the smallest time scale in the problem.

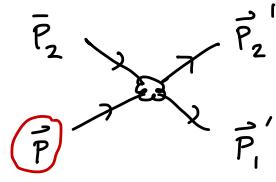
In particular,  $\tau_c \ll \tau$

where  $\tau$  is the mean free time, the average time a particle travels between collisions. In practice, this means that the density of particles should be small, such as in a gas or electrons in a semiconductor.

There are two types of contributions to  $(\frac{\partial f}{\partial t})_{\text{coll}}$ , those that increase  $f(\bar{p}, \bar{r})$  and those that decrease it:



gain



loss

To make further progress we need to know two quantities:

- i) The scattering rate  $\omega(\vec{p}_1, \vec{p}_2 \rightarrow \vec{p}'_1, \vec{p}'_2)$

This is calculated from the microscopic theory, which could be quantum, using scattering theory.

- ii) The probability of finding two particles at  $\bar{r}$  with momenta  $\bar{p}$  and  $\bar{p}'$ . This is the two-particle distribution function  $f_2(\bar{r}, \bar{p}; \bar{r}', \bar{p}'; t)$

$$f_2(\vec{r}\vec{p}; \vec{r}'\vec{p}'; t) = \sum_{ij} \langle \delta(\vec{x}_i(t) - \vec{r}) \delta(\vec{p}_i(t) - \vec{p}) \delta(\vec{x}_j(t) - \vec{r}') \delta(\vec{p}_j(t) - \vec{p}') \rangle$$

$$= N(N-1) \int_{i=3}^N d\vec{r}_i d\vec{p}_i \rho(\vec{r}, \vec{r}', \vec{r}_3, \dots, \vec{r}_N; \vec{p}, \vec{p}', \vec{p}_3, \dots, \vec{p}_N)$$

With these functions and our knowledge of gain-loss rate equations, we can simply write down

$$\left( \frac{\partial f}{\partial t} \right)_{\text{coll}} = \int d\vec{p}_2 d\vec{p}'_2 d\vec{p}_2' \left[ w(p'_1 p'_2 \rightarrow \vec{p} \vec{p}_2) f_2(\vec{r} \vec{p}_1; \vec{r} \vec{p}_2; t) - w(\vec{p} \vec{p}_2 \rightarrow \vec{p}'_1 \vec{p}'_2) f_2(\vec{r} \vec{p}_1; \vec{r} \vec{p}_2; t) \right]$$

Note that this depends on  $f_2$  and not only  $f$ . The differential equation for  $f$  therefore does not close. For an exact solution we would need to know  $f_2$ . We could follow a similar procedure to derive an equation for  $f_3$ , which would be of the form

$$h_2 f_2 = \left( \frac{\partial f_2}{\partial t} \right)_{\text{coll}}$$

but  $\left( \frac{\partial f_2}{\partial t} \right)_{\text{coll}}$  would depend on  $f_3$ . The equation for  $f_3$  depends on  $f_4$  etc. Impossible to solve, and also not our goal as that would amount to solving the exact full dynamics. Instead we need an approximation that truncates this series.

We therefore make the assumption of molecular chaos  
(or Stosszahl-Ausatz) that

$$f_2(\vec{r}, \vec{p}_1; \vec{r}, \vec{p}_2) \approx f(\vec{r}, \vec{p}_1) f(\vec{r}, \vec{p}_2).$$

Note that when we use this approximation in the expression for  $\left(\frac{\partial f}{\partial t}\right)_{\text{coll}}$  it is used for the two particles just before the collision takes place. If the motion of all the particles in the long time between the collisions is chaotic (hence the name) we can safely assume that the particles are not correlated before the collision.

To make further progress, we use time-reversal invariance and parity symmetry of the microscopic motion which together imply

$$w(\vec{p}_1, \vec{p}_2 \rightarrow \vec{p}'_1, \vec{p}'_2) = w(-\vec{p}'_1, -\vec{p}'_2 \rightarrow -\vec{p}_1, -\vec{p}_2) = w(\vec{p}'_1, \vec{p}'_2 \rightarrow \vec{p}, \vec{p}_2)$$

Using this we obtain (suppressing  $\vec{r}$  in the notation)

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = \int d\vec{p}_2 d\vec{p}'_1 d\vec{p}'_2 w(\vec{p} \vec{p}_2 \rightarrow \vec{p}'_1 \vec{p}'_2) \left[ f(\vec{p}'_1) f(\vec{p}'_2) - f(\vec{p}) f(\vec{p}_2) \right]$$

One can use symmetries to constrain the transition probability further.

$$\vec{p}_1 + \vec{p}_2 = \vec{p}'_1 + \vec{p}'_2 \quad \text{conservation of momentum}$$

$$\frac{p_1^2}{2m} + \frac{p_2^2}{2m} = \frac{(p'_1)^2}{2m} + \frac{(p'_2)^2}{2m} \quad \text{conservation of energy}$$

This means that the length of the relative momentum

$$|\vec{q}| = |\vec{p}_2 - \vec{p}_1| = p_2^2 + p_1^2 - 2\vec{p}_1 \cdot \vec{p}_2 = (p'_2)^2 + (p'_1)^2 - 2\vec{p}'_1 \cdot \vec{p}'_2 = |\vec{p}'_2 - \vec{p}'_1|$$

is conserved. It can however be rotated by a solid angle  $\hat{\Omega}$   
i.e.

$$\vec{p}'_2 - \vec{p}'_1 = |\vec{p}_2 - \vec{p}_1| \hat{\Omega} \quad \text{where } |\hat{\Omega}| = 1.$$

Thus, knowing  $\vec{P}_1, \vec{P}_2$  and  $\hat{\Omega}$  gives  $\vec{P}'_1$  and  $\vec{P}'_2$  via

$$\vec{P}'_1 = \frac{1}{2} (\vec{P}_1 + \vec{P}_2 - |\vec{P}_2 - \vec{P}_1| \hat{\Omega})$$

$$\vec{P}'_2 = \frac{1}{2} (\vec{P}_1 + \vec{P}_2 + |\vec{P}_2 - \vec{P}_1| \hat{\Omega})$$

Taken together this means that

$$\int d\vec{P}'_1 \int d\vec{P}'_2 w(\vec{P}_1, \vec{P}_2 \rightarrow \vec{P}'_1, \vec{P}'_2) [f(\vec{P}'_1) f(\vec{P}'_2) - f(\vec{P}_1) f(\vec{P}_2)]$$

$$= \int d^2\Omega \frac{\partial \sigma}{\partial \Omega} |\vec{v} - \vec{v}_2| [f(\vec{P}'_1) f(\vec{P}'_2) - f(\vec{P}_1) f(\vec{P}_2)]$$

where we used the definition of the differential cross section.

Altogether we get the Boltzmann equation:

$$\begin{aligned} \frac{\partial f}{\partial t} + \vec{v} \cdot \frac{\partial f}{\partial \vec{r}} + \vec{F} \cdot \frac{\partial f}{\partial \vec{p}} &= \int d\vec{P}_2 d\vec{P}'_1 d\vec{P}'_2 w(\vec{P}, \vec{P}_2 \rightarrow \vec{P}'_1, \vec{P}'_2) [f(\vec{P}'_1) f(\vec{P}'_2) - f(\vec{P}_1) f(\vec{P}_2)] \\ &= \int d\vec{P}_2 \int d^2\Omega \frac{\partial \sigma}{\partial \Omega} |\vec{v} - \vec{v}_2| [f(\vec{P}'_1) f(\vec{P}'_2) - f(\vec{P}_1) f(\vec{P}_2)] \end{aligned}$$

### Boltzmann's H-theorem

Define

$$H(t) = \int d\vec{r} d\vec{p} f(\vec{r}, \vec{p}, t) \ln f(\vec{r}, \vec{p}, t)$$

If  $f$  satisfies the Boltzmann equation, then

$$\frac{dH}{dt} \leq 0$$

↗

Proof:

$$\frac{dH}{dt} = \int d\vec{r} d\vec{p} \frac{\partial f}{\partial t} (\ln f + 1) = \int d\vec{r} d\vec{p} \frac{\partial f}{\partial t} \ln f$$

↑ since  $\int d\vec{r} d\vec{p} f = N$  independent of time.

$$= \int d\vec{r}_1 d\vec{p}_1 \left\{ \left[ -\vec{v} \cdot \frac{\partial f_1}{\partial \vec{r}} - \vec{F} \cdot \frac{\partial f_1}{\partial \vec{p}} \right] \ln f_1 + \int d\vec{p}_2 d^2 \Omega \frac{\partial \sigma}{\partial \Omega} |\vec{v}_1 - \vec{v}_2| [f_1 f_2' - f_1' f_2] \ln f_1 \right\}$$

$\hat{f}_1 = f(\vec{P}_1)$   
 $\hat{f}_2 = f(\vec{P}_2)$  etc.

The first part with the streaming terms is zero, as can be checked by repeated partial integration (check!)

Since we are integrating over  $\vec{p}_1$  and  $\vec{p}_2$  we can change the labels without changing the integral. Using (schematically)

$$I = \frac{1}{2} \left( \int d\vec{p}_1 d\vec{p}_2 (I(p_1, p_2) + I(p_2, p_1)) \right) \text{ and } \ln f_1 + \ln f_2 = \ln(f_1 f_2)$$

we then get

$$\frac{dH}{dt} = \frac{1}{2} \int d\vec{r}_1 d\vec{p}_1 d\vec{p}_2 d^2 \Omega \frac{\partial \sigma}{\partial \Omega} |\vec{v}_1 - \vec{v}_2| [f_1 f_2' - f_1' f_2] \ln(f_1 f_2)$$

Finally, using the symmetry of the cross section under time reversal and parity we can take  $\vec{p}_1 \vec{p}_2 \leftrightarrow \vec{p}'_1 \vec{p}'_2$  without changing the value of the integral. Again averaging over the two we get

$$\frac{dH}{dt} = \frac{1}{4} \int d\vec{r}_1 d\vec{p}_1 d\vec{p}_2 d^2 \Omega \frac{\partial \sigma}{\partial \Omega} |\vec{v}_1 - \vec{v}_2| [f_1 f_2' - f_1' f_2] [\ln(f_1 f_2) - \ln(f_1' f_2')]$$

$$\leq 0$$

since  $(y-x)(\ln y - \ln x) \geq 0$

In equilibrium  $S = -k_B H$  gives thermal entropy. It is a generalization to non equilibrium and reflects irreversibility.

Q: At which point in our derivation did irreversibility sneak in?

A: when we took  $f_2(\vec{r}, \vec{p}_1; \vec{r}, \vec{p}_2) = f(\vec{r}, \vec{p}_1) f(\vec{r}, \vec{p}_2)$

Note that  $\frac{dt}{dt} = 0$  if  $f(\vec{p}_1) f(\vec{p}_2) = f(\vec{p}'_1) f(\vec{p}'_2)$  which is a version of detailed balance which is satisfied in equilibrium. One can in fact use this necessary condition to derive a functional form for the equilibrium distribution  $f_{eq}$ .

### Conservation laws

Suppose we have some local observable  $\chi(\vec{r}, \vec{p})$ .

The local density corresponding to this observable is

$$n_\chi(\vec{r}) = \int d\vec{p} \chi(\vec{r}, \vec{p}) f(\vec{r}, \vec{p})$$

If  $n_\chi$  corresponds to a conserved quantity, it should be conserved in collisions, that is

$$\left( \frac{\partial n_\chi}{\partial t} \right)_{coll} = \int d\vec{p} \chi(\vec{r}, \vec{p}) \left( \frac{\partial f}{\partial t} \right)_{coll} = 0$$

Let's check this.

The derivation is the same as for the H-theorem, but since it was a bit quick, let's do it again:

$$\begin{aligned} \left( \frac{\partial n_\chi}{\partial t} \right)_{coll} &= \int d\vec{p}_1 d\vec{p}_2 d^3 \Omega \frac{\partial \sigma}{\partial \Omega} |\vec{v}_1 - \vec{v}_2| [f_1 f_2' - f_1' f_2] \chi(\vec{r}, \vec{p}_1) \\ &= \int Dx [f_1' f_2' - f_1 f_2] \chi(\vec{p}_1) = (*) \end{aligned}$$

where we introduced  $Dx = d\vec{p}_1 d\vec{p}_2 d^3 \Omega \frac{\partial \sigma}{\partial \Omega} |\vec{v}_1 - \vec{v}_2|$  to simplify notation, and suppress  $\vec{r}$  in the notation (as it is always the same).

$$(*) = \frac{1}{2} \int Dx [f_1' f_2' - f_1 f_2] [\chi(p_1) + \chi(p_2)]$$

↑ using  $\int dp_1 dp_2 I(p_1, p_2) = \frac{1}{2} \int dp_1 dp_2 (I(p_1, p_2) + I(p_2, p_1))$

$$= \frac{1}{4} \int Dx [f_1' f_2' - f_1 f_2] [\chi(p_1) + \chi(p_2) - \chi(p_1') - \chi(p_2')]$$

↑ using  $p_1' = \frac{1}{2} (\bar{p}_1 + \bar{p}_2 - |\bar{p}_2 - \bar{p}_1| \hat{\Omega})$  + Jacobian unity and  
 $p_2' = \frac{1}{2} (\bar{p}_1 + \bar{p}_2 + |\bar{p}_2 - \bar{p}_1| \hat{\Omega})$  time reversal

$$= 0 \quad \text{if}$$

$$\boxed{\chi(p_1) + \chi(p_2) = \chi(p_1') + \chi(p_2')}$$

i.e. if  $\chi$  is a conserved quantity, such as

$$\chi = 1 \quad \text{particle number}$$

$$= \vec{P} \quad \text{momentum}$$

$$= \epsilon(\vec{p}) \quad \text{energy.}$$

### Equilibrium

In equilibrium  $\frac{dH}{dt} = 0$  and

$$f^0(\bar{p}_1) f^0(\bar{p}_2) = f^0(\bar{p}_1') f^0(\bar{p}_2')$$

Here the superscript zero refers to equilibrium. We then have

$$\ln f^0(\bar{p}_1) + \ln f^0(\bar{p}_2) = \ln f^0(\bar{p}_1') + \ln f^0(\bar{p}_2')$$

That is  $\ln f^0$  is invariant under collisions. If  $\mu$ ,  $\vec{p}$  and  $\epsilon$  are the only invariants, we must have

$$\ln f^0 = \beta(\mu + \vec{v} \cdot \vec{p} - \epsilon)$$

with  $\beta = \frac{1}{kT}$ ,  $\mu$  and  $\vec{v}$  constants. Writing them like this (14) is a convention. This means

$$f^0 = c \exp \left[ \beta (\mu - \varepsilon + \vec{v} \cdot \vec{p}) \right]$$

If  $\varepsilon = \frac{p^2}{2m}$  we can write this

$$f^0 = c \exp \left[ -\frac{1}{2mkT} (\vec{p} - m\vec{v})^2 \right]$$

where we have absorbed  $\mu$  and  $v^2$  into the coefficient  $c$ , which in turn is determined by normalization.

### Local equilibrium

The coefficients in the equilibrium function can depend on position

$$f^0(\vec{r}, p) = c \exp \left[ -\beta (\varepsilon - \mu - \vec{v} \cdot \vec{p}) \right]$$

with  $\beta = \beta(\vec{r}, t)$ ,  $\mu = \mu(\vec{r}, t)$  and  $\vec{v} = \vec{v}(\vec{r}, t)$ .

This is what is called local equilibrium.

Because of the locality of the collision term, the local equilibrium function is not affected by it, i.e.

$$\left( \frac{\partial f^0}{\partial t} \right)_{\text{coll}} = 0$$

Local equilibrium is however not equilibrium, and therefore not a solution to the Boltzmann equation. This means that it is affected by the streaming terms.

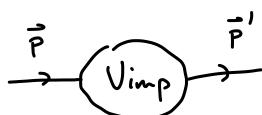
Note that if this gives rise to dynamics that are slow on the scale of the collision time, we have a separation of time scales: collisions quickly establish a local equilibrium, followed by streaming terms giving rise to slower dynamics of hydrodynamic variables.

One can in fact derive the equations of hydrodynamics when combined with conservation laws. Depending on the quantities looked at one obtains the diffusion eq., heat eq., Navier-Stokes etc.

### One-particle scattering

In a metal the electrons form a liquid called a Fermi liquid. Often one can just think of this as a dense gas of electrons that do not interact. Instead the effect of Coulomb interaction is incorporated into an effective mass, sometimes denoted  $m^*$  but more often simply as  $m$ . The value of this mass depends on the material and can be significantly different from the electron mass. Often we call these electrons with the effective mass quasi-particles, since they are not really the original electrons but lets not worry about these details and just think of them and call electrons.

Since these electrons do not interact, the single particle scattering contribution to the collision integral is important. This is the effect of an impurity potential  $V_{\text{imp}}(\vec{r})$  that scatters an electron with momentum  $\vec{p}$  into momentum  $\vec{p}'$



In general there will be a large number of impurities in a sample, with impurity density  $n_{\text{imp}}$ . If this impurity density is low enough, we can assume that the scattering takes place of only one impurity and ignore multiple scattering. This is often called the Born approximation.

Using Fermi's golden rule, then, we have

$$w(\vec{p}' \rightarrow \vec{p}') = \frac{2\pi}{\hbar} n_{imp} |V_{imp}(\vec{p}' - \vec{p})|^2 \delta(E(p) - E(\vec{p}'))$$

with  $V_{imp}(\vec{q})$  the Fourier transform of  $V_{imp}(\vec{r})$ . Our collision integral is now

$$\left( \frac{\partial f}{\partial t} \right)_{coll} = \int \frac{d\vec{p}'}{(2\pi\hbar)^3} (w(\vec{p}' \rightarrow \vec{p}) f_{\vec{p}'} - w(\vec{p} \rightarrow \vec{p}') f_{\vec{p}})$$

If the size of the impurities is small compared with  $k_F^{-1}$ , we can write  $V_{imp}(\vec{r}) \propto \delta(\vec{r} - \vec{r}_0)$ , with  $\vec{r}_0$  the center of the impurity. In this case,  $|V_{imp}(\vec{q})|^2 = |V_{imp}|^2$  independent of  $\vec{q}$ . We then get

$$\left( \frac{\partial f}{\partial t} \right)_{coll} = \frac{\langle f \rangle_a - f}{\tau_p}$$

where  $\langle f \rangle_a$  is the average of  $f$  over all directions of  $\vec{p}$ , i.e.

$$\int \frac{d\vec{p}'}{(2\pi\hbar)^3} \delta(E(p) - E(\vec{p}')) f_{\vec{p}'} = \int \frac{p^2 d\vec{p}' d\omega_p}{(2\pi\hbar)^3} \underbrace{\frac{1}{|\partial \epsilon / \partial p|}}_{=v = P_m} \delta(p - p') f_{\vec{p}}$$

The momentum relaxation time

$$\tau_p^{-1} = \frac{2\pi}{\hbar} n_{imp} \cdot v |V_{imp}|^2$$

### Relaxation time approximation

This form of the collision integral is an example of a common approximation

$$\left( \frac{\partial f}{\partial t} \right)_{coll} = - \frac{f - f^o}{\tau}$$

where  $f^o = f^o(\vec{r}, \vec{p}, t)$  is a local equilibrium distribution function.

In the absence of streaming terms, and with  $\delta f = f - f_0$  (17)  
we have

$$\frac{\partial \delta f}{\partial t} = - \frac{\delta f}{\tilde{\tau}}$$

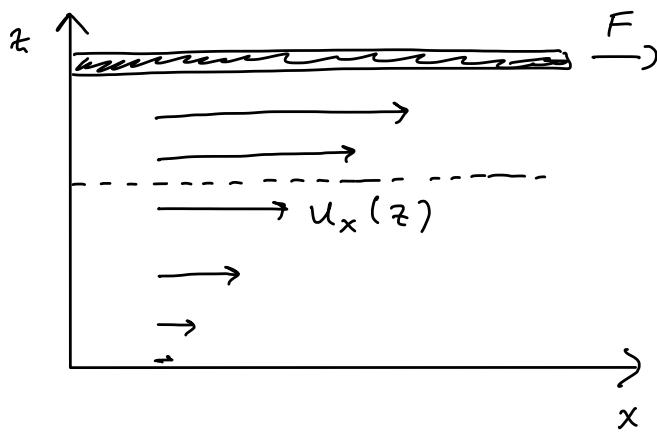
or  $\delta f(\vec{r}, \vec{p}, t) = \delta f(\vec{r}, \vec{p}, 0) e^{-t/\tilde{\tau}}$ ,

that is, the system relaxes exponentially everywhere towards the local equilibrium distribution on a time scale given by the relaxation time  $\tilde{\tau}$  (which in general is a function of  $\vec{p}$ , but we take it here to be constant).

Q: Which local equilibrium distribution function does one use in the relaxation time approximation?

## Viscosity

Let us now, as a way of demonstration, calculate the viscosity of a fluid. Imagine the following setup



A plate dragged with force  $F$  establishes a flow pattern in the fluid where the fluid at height  $z$  flows in the  $x$  direction with speed  $u_x(z)$ . As a consequence, there is a net flux of momentum in the  $x$  direction resulting in a drag force that counterbalances  $F$ .

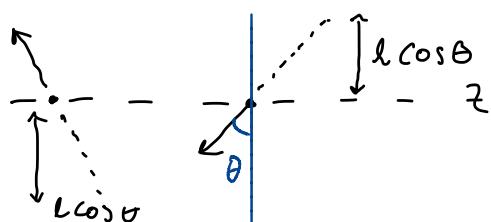
The momentum flux density  $P_{zx}$ , the drag force per area, is

given by

$$P_{zx} = -\eta \frac{\partial u_x}{\partial z}$$

where  $\eta$  is the viscosity.

Let us first understand phenomenologically how this comes about. Consider a plane at a fixed  $z$ , and ask what is the momentum flow through this surface



Let us assume that all particles with negative velocity, came from  $z + l \cos\theta$  and therefore have average x speed  $u_x(z + l \cos\theta)$ . Similarly, the particles moving up have speed  $u_x(z - l \cos\theta)$ . The total flow of momentum in the z direction is then

$$\begin{aligned}\vec{j}_{P_x} &= \hat{n}_z \left[ \int_{v_z > 0} d\bar{v} P(\bar{v}) v_z m u_x(z - l \cos\theta) + \int_{v_z < 0} d\bar{v} P(\bar{v}) v_z m u_x(z + l \cos\theta) \right] \\ &= \hat{n}_z m \left[ \int_{v_z > 0} d\bar{v} P(\bar{v}) v_z u_x(z) - \int_{v_z < 0} d\bar{v} P(\bar{v}) v_z \frac{\partial u_x}{\partial z} l \cos\theta + \int_{v_z < 0} u_z \right]\end{aligned}$$

now, since  $\cos\theta = \frac{|v_z|}{v}$ , and the average of  $\langle v_z \rangle = 0$ , this gives

$$= -\hat{z} n m l \frac{\partial u_x}{\partial z} \int d\bar{v} P(\bar{v}) \frac{v_z^2}{v} = -\hat{z} n m l \frac{\partial u_x}{\partial z} \frac{1}{3} v_{av}$$

where  $v_{av}$  is the average particle speed

$$\begin{aligned}v_{av} &= \int d\bar{v} P(\bar{v}) v = \int_0^\infty 4\pi v^2 dr v \left( \frac{m}{2\pi k_B T} \right)^{3/2} \exp\left(-\frac{mv^2}{2k_B T}\right) \\ &\quad \uparrow \text{Maxwell velocity distribution} \\ P(v) &= \left( \frac{m}{2\pi k_B T} \right)^{3/2} \exp\left(-\frac{mv^2}{2k_B T}\right) \\ &= \sqrt{\frac{8}{\pi} \frac{k_B T}{m}}\end{aligned}$$

Altogether this gives us

$$j_z^x = P_{xz} = -\frac{1}{3} n m l v_{av} \frac{\partial u_x}{\partial z}$$

or

$$\eta = \frac{1}{3} n m l v_{av}$$

## Viscosity as a weakly inhomogeneous gas

Let's solve the same problem, illustrating on the way some general strategies towards solving the Boltzmann equation. First, if we only weakly perturb away from local equilibrium  $f^*(r, \vec{p})$ , we can write  $f = f^* + \delta f$

$$\left( \frac{\partial}{\partial t} + \frac{\vec{p}}{m} \cdot \frac{\partial}{\partial \vec{r}} + \vec{F} \cdot \frac{\partial}{\partial \vec{p}} \right) (f^* + \delta f) = \left( \frac{\partial f}{\partial t} \right)_{\text{coll}}$$

since the collision integral is zero for  $f^*$  the right hand side is of order  $\delta f$ . For the viscosity case  $\mu = \text{const}$ ,  $T = \text{const}$  and  $\vec{v} = u_x(z) \hat{x}$ . Also  $\vec{F} = 0$ , so the left hand side becomes simply

$$\frac{P_x}{m} \frac{\partial f^*}{\partial z}$$

The term  $\frac{\partial \delta f}{\partial z}$  is higher order in  $\delta f$  and we can therefore drop it. Generally, the constants  $\mu, T$  and  $\vec{v}$  can all depend on  $\vec{r}$  and  $t$ , giving a more complicated expression. (see e.g. Arrows)

Continuing

$$\frac{\partial f^*}{\partial t} = \frac{\partial f^*}{\partial u_x} \cdot \frac{\partial u_x}{\partial t} = + \frac{P_x}{k_B T} f^* \frac{\partial u_x}{\partial z}$$

since

$$f^* \sim e^{+ \frac{\vec{v} \cdot \vec{p}}{k_B T}}$$

In the relaxation time approximation, then

$$+ \frac{P_z P_x}{m} \frac{1}{k_B T} \frac{\partial u_x}{\partial z} f^0 = - \frac{\delta f}{\tau}$$

To calculate the momentum flux with this result

$$\begin{aligned} P_{xz} &= n \int d\bar{p} \, p_x v_z \delta f \\ &= -n \frac{\Sigma}{k_B T} \frac{\partial u_x}{\partial z} \int d\bar{p} \, p_x v_z \frac{P_z P_x}{m} f^0 \\ &= -n \frac{\Sigma}{k_B T} \frac{\partial u_x}{\partial z} \langle m v_x^2 m v_z^2 \rangle, \quad \underbrace{4 \langle \frac{1}{2} m v_x^2 \times \frac{1}{2} m v_z^2 \rangle} \\ &= -n \frac{\Sigma}{k_B T} \frac{\partial u_x}{\partial z} 4 \cdot (k_B T)^2 \\ &= -n \tau k_B T \frac{\partial u_x}{\partial z} \end{aligned}$$

and therefore

$$\begin{aligned} \gamma &= n k_B T \tau = n \left( \frac{\pi}{8} v_{av}^2 m \right) \cdot \frac{l}{v_{av}} \\ &= \frac{\pi}{8} n m l v_{av} \end{aligned}$$

i.e. a prefactor of  $\frac{\pi}{8}$  instead of  $\frac{1}{3}$  in our rough calculation. The difference is immaterial, since these are equally approximate calculations, but this second calculation contained important elements of a typical calculation.