

Recap: Discussed Boltzmann equation in limit of $k_B \ll 1$, where (in the far evolution) is governed by Hilbert expansion

By organizing terms in powers of k_B we find that LHS suppressed compared to RHS collisions

$$\text{Expanding } f = f^{(0)} + f^{(1)} + \dots$$

$$\underline{LO:} \quad C[f^{(0)}] = 0$$

$\Rightarrow f^{(0)}$ is local equilibrium solution determined by collision invariants

$$\underline{NLO:} \quad \left(\frac{\partial}{\partial t} + \vec{v} \cdot \vec{\nabla}_r + \frac{\vec{v}}{T} \cdot \vec{\nabla}_p \right) f^{(0)} = \underbrace{SC[f^{(0)}, f^{(1)}]}_{\text{linearized collision operator}}$$

\Rightarrow formally $f^{(1)}$ determined by inversion of collision operator $SC[f^{(0)}, f^{(1)}]$

Difficult in practice and subtle since

$SC[f^{(0)}, f^{(1)}]$ has zero eigenvalues associated with conserved quantities

\Rightarrow Corrections $f^{(1)}$ to local equilibrium distributions $f^{(0)}$ should not carry conserved quantities

Since all other modes not associated with conserved quantities relax away, can model effect by relaxation time approximation

$$\left(\frac{\partial}{\partial t} + \vec{v} \cdot \nabla_r + \vec{F} \cdot \nabla_p \right) f = C[f] \stackrel{RTA}{=} - \frac{f - f^{(0)}}{\tau_2(\vec{r}, \vec{p})}$$

where $f^{(0)}$ is the local equilibrium solution, with parameters T, μ, \vec{v} obtained by matching the conserved quantities, e, n, \vec{p} for mono-atomic gas

If we demand that perturbation $f^{(1)}$ does not carry conserved quantity

$$\int_{\vec{p}} f^{(1)} = 0 \quad \int_{\vec{p}} \vec{p} f^{(1)} = 0 \quad \int_{\vec{p}} \frac{3}{2} f^{(1)} = 0$$

then (normalized collision operator in RTA) obeys the form

$$\therefore \delta C[f^{(0)}, f^{(1)}] = - \frac{f^{(1)}}{\tau_2(\vec{r}, \vec{p})}$$

Calculation of transport coefficients

→ Basic idea is to exploit microscopic Boltzmann framework, to calculate non-equilibrium corrections to fluxes of conserved quantities which appear in macroscopic description of non-equilibrium systems (as discussed in Chapter 1)

Electrical conductivity (σ)

Which depends static response to external electric field, i.e. for isotropic materials

$$\vec{J}_{el} = \sigma \vec{E}$$

Mistake in previous lecture
→ Chance to discuss again and see what went wrong

We have a force $\vec{F}_L = q\vec{E}$ acting on all charged particles in the system

Balance equation for number:

for each species i :

$$\frac{d}{dt} \int d^3r n_i \vec{v}_i = \int d^3r \vec{p}_i f_i(t; \vec{r}, \vec{p}_i)$$

So for homogeneous systems

$$\frac{d}{dt} f_i = -q_i \vec{E} \cdot \vec{v}_p f_i + \sum_j C_{ij} [f_i, f_j]$$

Now if we look at total number of all particles

$$\frac{d}{dt} \left(\sum_i \vec{p}_i \right) = \frac{d}{dt} \sum_i \int d^3r n_i \vec{v}_i = \left(\sum_i q_i n_i \right) \vec{E} + \sum_{i,j} \int d^3r \vec{p}_i C_{ij} [f_i, f_j]$$

So if on various copic level all interactions are unambiguously conserved

$$\frac{d}{dt} \sum_i m_i \vec{v}_i = q_i v_i \vec{E}$$

such that in particular for a single component

$$\frac{d}{dt} m_i \vec{v}_i = q_i v_i \vec{E}$$

we get $(q=0)$ velocities or $(q \neq 0)$ constant accelerations

So for the system to be not accelerated as a whole
we need charge neutrality

$$\sum_i q_i n_i = 0$$

e.g. change of electron number by change of nuclei

only in this situation can we seek for stationary solutions

In this limit $\frac{qE}{m \omega_{ce}} \ll V_{th}$ we can then expand

$$f_i = f_i^{(0)} + f_i^{(1)} + \dots$$

for each species

So if all species are interacting electrically with each other

$$\sum_j C_{ij} [f_i^{(0)}, f_j^{(0)}] = 0$$

$\Rightarrow f_i^{(0)}$ is local equilibrium distribution with same T, \vec{v} for all species

$$q_i \vec{E} \cdot \vec{p} f_i^{(0)} = -q_i \vec{E} \cdot \frac{\vec{p}}{m_i} f_i^{(0)} = \underbrace{\sum_j C_{ij} [f_i^{(0)}, f_j^{(0)}]}_{\text{interactions between same species}}$$

$$\underbrace{\sum_{j \neq i} C_{ij} [f_i^{(0)}, f_j^{(0)}] + C_{ij} [f_i^{(0)}, f_i^{(0)}]}_{\text{interacts with other particles}}$$

Since number can be transferred between different particle species (+, -, neutrals) can approximate RHS by RTA

and calculate $\mathcal{J}_{el} = \sum_j q_j \int \frac{\vec{p}}{m_j} f_j^{(0)}$

Similarly for Lorentz gas, one neglects interaction between same particles $C_{ii} = 0$ and considers interaction with static scattering centers

weight $\delta = \text{heavy}$ $C_{ij} = n_s \int \frac{d\vec{p}'}{m_s} \frac{d\sigma}{d\Omega} [f_i(\vec{p}') + f_i(\vec{p})]$

Since this allows for momentum transfer to heavy particles, can again be approximated by RTA

Conversely, if only single species of charged particles Δ considered, and interaction conserves momentum

$$q_i \frac{\vec{E} \cdot \vec{p}}{m_i k_B T} \psi_i^{(0)}(\vec{p}) = \delta C [\psi_i^{(0)}, \psi_i^{(0)}]$$

has no solution for $q \neq 0$ because $\int_{\vec{p}} \vec{p} \cdot \psi_i^{(0)} \neq 0$

$$\int_{\vec{p}} \vec{p} \cdot \psi_i^{(0)} = 0$$

However in the case our models for stationary solution Δ does not physical because system subject to constant accelerations

Need to account for macroscopic motion by velocity $\vec{v}(t)$ for homogeneous system

$$\psi_i^{(0)}(\vec{p}, t) = n \left(\frac{2\pi k_B T}{m_i} \right)^{3/2} \exp\left(-\frac{(\vec{p} - m_i \vec{v}(t))^2}{2m_i k_B T}\right)$$

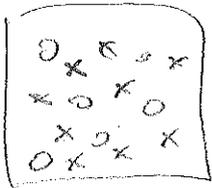
$$\text{where } \vec{v}(t) = \frac{q \vec{E}}{m} t + \vec{v}(0) \text{ such that } \left(\frac{\partial}{\partial t} + q \vec{E} \cdot \vec{\nabla}_p \right) \psi_i^{(0)} = -\frac{(\vec{p} - m_i \vec{v}(t))}{m_i k_B T} \left(-m_i \dot{\vec{v}}(t) + q \vec{E} \right) \psi_i^{(0)} = 0$$

Since in this case effect of \vec{E} field is not small needs to be accounted for directly at the level of $\psi_i^{(0)}$

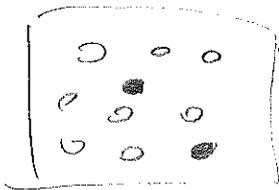
Diffusion and heat conduction

Now with these subtleties in mind we can look at diffusion and heat conduction which are phenomena associated with spatial gradients of the density/chemical potential and/or temperature

We can consider two physical situations where our calculations will be applicable



Lorentz gas: Collection of light particles moving interacting with heavy particles treated as static scattering centers



Self-diffusion of a tracer:

Interaction of a retroactively marked atom in dilute gas dominated by interaction with unmarked particles

Note that in both cases we allow for minimal exchange with the environment

Conversely if we were to look at the effects of temperature/density gradients in a nonequilibrium gas this would lead to macroscopic motion which is well described by deserted-hydrodynamically in the limit $\lambda \ll l$

We will consider that the local equilibrium conditions $T(\vec{r}, \vec{p})$ and $n(\vec{r}, \vec{p})$ are equivalently $\mu(\vec{r}, \vec{p})$ are determined externally, e.g. by controlling temperature of rest of the system and radioactive excitation such that

$$T(\vec{r}, \vec{p}) = T(\vec{r}) \quad \mu(\vec{r}, \vec{p}) = \mu(\vec{r})$$

and both have independent

So we have for the expansion around local equilibrium background

$$f^{(0)}(\vec{r}, \vec{p}) = \exp\left(\frac{-\vec{p}^2/2m - \mu(\vec{r})}{k_B T(\vec{r})}\right)$$

where instead of usual formulation with density $n(\vec{r})$ we have chosen $\mu(\vec{r})$ to describe variations in density to make contact with approaches introduced in various other descriptions

We again look for stationary solutions in the limit $k_B \ll 1$ when $\epsilon_{\text{eff}} \ll L$

Especially $f = f^{(0)} + f^{(1)}$ we allow for $O(k_B)$

$$\vec{\nabla} \cdot \vec{\nabla}_r f^{(0)}(r, p) = \delta \left(\frac{p^2}{2m}, f^{(0)} \right)_{\text{PFL}} = - \frac{f^{(1)}(r, p)}{\epsilon_{\text{eff}}(T(r), \mu(r), \vec{p})}$$

So using

$$\vec{\nabla}_r f^{(0)}(r, p) = - \frac{1}{k_B} \left[\frac{\partial^2}{\partial m} \vec{\nabla}_r \left(\frac{1}{T(r)} \right) + \vec{\nabla}_r \left(- \frac{\mu(r)}{T(r)} \right) \right] f^{(0)}(r, p)$$

we have

$$f^{(1)}(r, p) = \frac{\epsilon_{\text{eff}}(r, p)}{m k_B} \vec{\nabla}_r \left[\frac{\partial^2}{\partial m} \vec{\nabla}_r \left(\frac{1}{T(r)} \right) + \vec{\nabla}_r \left(- \frac{\mu(r)}{T(r)} \right) \right] f^{(0)}(r, p)$$

Now we can compute the current, e.g.:

$$\begin{aligned} \vec{J}_N^r &= \int_p \frac{p_i}{m} f = - \int_p \frac{p_i}{m} p_j \nabla_j X \\ &= \frac{1}{3} \int_p \frac{\partial^2}{\partial m} \nabla_i X \end{aligned}$$

So again we do not need to consider tensor response but are left with simple scalar response coefficients, as expected from Curie principle

Sum for

$$\vec{J}_E^r = \int \frac{p_i}{m} \frac{\partial^2}{\partial m}$$

So we got

$$\vec{J}_N = \frac{1}{3\mu_0 k_B} \int_{\vec{p}} \epsilon_p(\vec{r}|\vec{p}) \vec{p}^2 \left[\begin{matrix} (0) \\ \vec{r}|\vec{p} \end{matrix} \right] \left[\begin{matrix} -2 \\ \frac{p}{2m} \left(\vec{\nabla}_r \frac{1}{r} \right) + \vec{\nabla}_r \left(\frac{-M}{r} \right) \end{matrix} \right]$$

$$\vec{J}_E = \frac{1}{6\mu_0 k_B} \int_{\vec{p}} \epsilon_p(\vec{r}|\vec{p}) \vec{p}^2 \left[\begin{matrix} (0) \\ \vec{r}|\vec{p} \end{matrix} \right] \left[\begin{matrix} -2 \\ \frac{p}{2m} \left(\vec{\nabla}_r \frac{1}{r} \right) + \vec{\nabla}_r \left(\frac{-M}{r} \right) \end{matrix} \right]$$

Comparing this with our linear response ansatz

$$\vec{J}_N = L_{NN} \vec{\nabla} \left(\frac{-M}{r} \right) + L_{NE} \vec{\nabla} \left(\frac{1}{r} \right)$$

$$\vec{J}_E = L_{EE} \vec{\nabla} \left(\frac{1}{r} \right) + L_{EN} \vec{\nabla} \left(\frac{-M}{r} \right)$$

we obtain the various Kohn coefficients by comparison

Specifically for $\tau_R = \text{const}$ we can easily compute the various integrals

$$\int_{\vec{p}} \frac{\vec{p}^2}{2m} f^{(0)} = e = \frac{3}{2} n k_B T$$

$$\int_{\vec{p}} \vec{p} \frac{\vec{p}^2}{2m} f^{(0)} = 5 n k_B T e$$

$$\int_{\vec{p}} \vec{p} \frac{\vec{p}^2}{2m} f^{(0)} = 35 (n k_B T)^2 e$$

$$L_{NN} = \frac{\tau_R}{3 m^2 k_B} \times 2m \times \frac{3}{2} n k_B T = \frac{n \tau_R T}{m}$$

$$L_{NE} = \frac{\tau_R}{3 m^2 k_B} \times 5 n k_B T \times \frac{3}{2} n k_B T = \frac{5}{2} \frac{n \tau_R T}{m} k_B T$$

$$L_{EN} = L_{NE} \quad \text{via Onsager relations}$$

$$L_{EE} = \frac{\tau_R}{6 m^3 k_B} 35 (n k_B T)^2 \frac{3}{2} n k_B T = \frac{35}{4} \frac{n \tau_R T}{m} (k_B T)^2$$