BASICS OF THE KINETIC THEORY

References:

- Physical kinetics – Landau / Lifshitz
- P. Lipavsky lecture notes on Condensed Matter physics
- T. Schäfer arXiv: 0808.0734

Plan:
a) Validity of the hydrodynamics and the kinetic theory
b) Boltzmann equation
c) H-theorem
d) Macroscopic quantities from the Boltzmann eq.

a) Hydrodynamics describes the evolution of fluids in terms of macroscopic densities and currents. No microscopic description needed.

Validity: (*) $\frac{L}{\ell_{mfp}} \gg 1$

L – length scale over which densities and currents vary considerably

ℓ_{mfp} – mean free path distance of the microconstituents between the collisions

(**) no quasiparticle description needed

Kinetic theory of gases describes the evolution of gases in terms of the microscopic constituents, which evolve freely with occasional collisions

Validity: (*) Diluteness condition $n^{1/3} d \ll 1$

n – gas density ; d – range of the molecular forces

(**) quasiparticle description is necessary

(***) $T \gg \frac{d}{\bar{v}}$

T – evolution time of interest ; $\bar{v}$ – average velocity

6) The central quantity in the kinetic theory is the Boltzmann distribution $f(\vec{k}, \vec{r}, t)$. It is the density of the particles in the one-particle phase space $\{\vec{r}, \vec{k}\}$

$$\Delta N = f(\vec{k}, \vec{r}, t)\, d\vec{k}\, d\vec{r}$$

Free evolution

Consider an ensemble of particles, which evolves without collisions, in the external force field $\vec{F}$. According to the Liouville's theorem:

$$\frac{df}{dt} = 0 = \frac{\partial f}{\partial t} + \frac{\vec{k}}{m} \cdot \frac{\partial f}{\partial \vec{r}} + \vec{F} \cdot \frac{\partial f}{\partial \vec{k}} \rightarrow \text{PDE of free evolution}$$

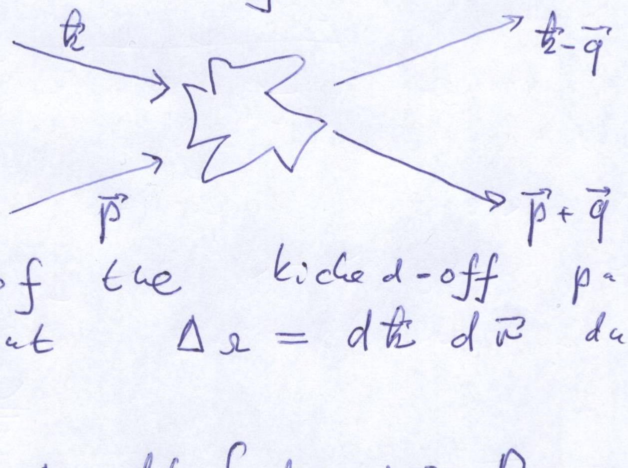
Boltzmann equation

In a dilute gas there are occasional collisions. These collisions can kick off the particles from the phase space volume element. During the collision the position is almost unchanged, but the momentum changes discontinuosly. We take into account of this:

$$\frac{df}{dt} = C[f]$$

$C[f]$ - collision integral → some functional of f.

Consider a two-body collision:



$\vec{q}$ - momentum transfer

The number of the kicked-off particles from the volume element $\Delta \Omega = d\vec{k}\, d\vec{r}$ during the time interval dt:

$$d_- \Delta N = \Delta N\, dt \int d\vec{p}\, d\vec{q}\, \underbrace{P_{\vec{k},\vec{p} \rightarrow \vec{k}-\vec{q}, \vec{p}+\vec{q}}}_{\text{probability of the direct collision}} f_{\vec{p}}$$

$$\Delta N = d\vec{k}\, d\vec{r}\, f_{\vec{k}}\,; \quad f_{\vec{k}} \equiv f(\vec{k}, \vec{r}, t);$$

The number of the kicked-in particles:

$$d_+ \Delta N = d\vec{k}\, d\vec{r}\, dt \int d\vec{p}\, d\vec{q}\, \underbrace{P_{\vec{k}-\vec{q},\vec{p}+\vec{q}\to\vec{k},\vec{p}}}_{\text{inverse collision probability}}\, f_{\vec{p}+\vec{q}}\, f_{\vec{k}-\vec{q}}$$

$$C[f] = \frac{d_+\Delta N - d_-\Delta N}{d\vec{k}\, d\vec{r}\, dt} = \int d\vec{p}\, d\vec{q}\; P\left(f_{\vec{p}+\vec{q}}\, f_{\vec{k}-\vec{q}} - f_{\vec{p}}\, f_{\vec{k}}\right)$$

where we assumed: $P = P_{k-q,p+q\to k,p} = P_{\vec{k},\vec{p}\to k-q,p+q}$ (*)

We arrive to the Boltzmann kinetic equation:

$$\boxed{\frac{\partial f}{\partial t} + \frac{\vec{k}}{m}\cdot\frac{\partial f}{\partial \vec{r}} + \vec{F}\cdot\frac{\partial f}{\partial \vec{k}} = \int d\vec{p}\, d\vec{q}\; P\left(f_{\vec{p}+\vec{q}}\, f_{\vec{k}-\vec{q}} - f_{\vec{p}}\, f_{\vec{k}}\right)}$$

integro-differential equation

Remarks:

α) The probability P is related to the differential cross-section $d\sigma$:

$$P \sim \frac{d\sigma}{dq}\,\frac{|\vec{k}-\vec{p}|}{m}$$

β) Our assumption (*) about the probability P can be relaxed. We will still arrive at the B. equation employing the unitarity of the S-matrix

$$\sum_n{}' |S_{ni}|^2 = \sum_n{}' |S_{in}|^2$$

details in Landau / Lifshitz

γ) If $\vec{F}=0$, the B. equation can be rewritten in the relativistically invariant form

$$p^\mu \partial_\mu f = C[f]$$

c) H-theorem (eta-theorem) – 1872 – Boltzmann

We can show from the B equation that the entropy of the system grows with time.

$$\boxed{S = -k_B \int d\vec{k}\; f_{\vec{k}} \ln f_{\vec{k}}}$$

entropy density

Consider a simplified set up: (*) $\vec{F} = 0$

(**) homogeneous gas $n = \text{const}$

For general derivation see Landau/Lifshitz

$$\frac{\partial S}{\partial t} = -k_B \int d\vec{k}\, \frac{\partial f_{\vec{k}}}{\partial t}\left(\ln f_{\vec{k}} + 1\right) = -k_B \int d\vec{k}\, \frac{\partial f_{\vec{k}}}{\partial t} \ln f_{\vec{k}}$$

where we used $\dfrac{\partial n}{\partial t} = \int d\vec{k}\, \dfrac{\partial f_k}{\partial t} = 0$

From the Boltzmann equation:

$$\frac{\partial S}{\partial t} = k_B \int d\vec{k}\, d\vec{p}\, d\vec{q}\;\; P\left(f_{\vec{k}} f_{\vec{p}} - f_{\vec{p}+\vec{q}} f_{\vec{k}-\vec{q}}\right) \ln f_{\vec{k}} \qquad (**)$$

In order to determine the sign of $\frac{\partial S}{\partial t}$ we must symmetrize the last relation: four possibilities

$k' = k \qquad p' = p \qquad q' = q$ (original)

$k' = p \qquad p' = k \qquad q' = -q$

$k' = k-q \qquad p' = p+q \qquad q' = -q$

$k' = p+q \qquad p' = k-q \qquad q' = q$

P and the first bracket in (**) are not affected by the substitutions, only the ln terms change:

$$\boxed{\frac{\partial S}{\partial t}} = k_B \int d\vec{k}\, d\vec{p}\, d\vec{q}\;\; P\left(f_{\vec{k}} f_{\vec{p}} - f_{\vec{p}+\vec{q}} f_{\vec{k}-\vec{q}}\right) \times \frac{1}{4}\left(\ln f_{\vec{k}} + \ln f_{\vec{p}} - \ln f_{\vec{k}-\vec{q}} - \ln_{\vec{p}+\vec{q}}\right) = k_B \int d\vec{k}\, d\vec{p}\, d\vec{q}\;\; P$$

$$\left(f_{\vec{k}} f_{\vec{p}} - f_{\vec{p}+\vec{q}} f_{\vec{k}-\vec{q}}\right) \frac{1}{4}\left(\ln\left(f_{\vec{k}} f_{\vec{p}}\right) - \ln\left(f_{\vec{k}-\vec{q}} f_{\vec{p}+\vec{q}}\right)\right) \boxed{\geq 0}$$

because $(x-y)(\ln x - \ln y) \geq 0$ for $x, y \in \mathbb{R}_+$

Equilibrium destribution

In equilibrium $\frac{\partial S}{\partial t} = 0$ and hence

$$\ln f_{\vec{k}} + \ln f_{\vec{p}} - \ln f_{\vec{k}-\vec{q}} - \ln f_{\vec{p}+\vec{q}} = 0$$

Thus $\ln f_{\vec{k}}$ is a linear combination of the integrals of motion. For $\vec{F}=0$:

$$\ln f_{k} = a\frac{\vec{k}^2}{2m} + \vec{b}\cdot\vec{k} + c$$

This leads to the Maxwell distribution:

$$f_0 = f_k = \frac{n}{(2\pi m k_B T)^{3/2}} e^{-\frac{(\vec{k}-\vec{\bar{k}})^2}{2m k_B T}}$$

where $a, \vec{b}, c$ determine $T, \vec{\bar{k}}$ and n.

Near-equilibrium treatment – relaxation time approximation

We can find a corresponding locally equilibrium distribution f_0 to every B. distribution f.

If the difference $\delta f = f - f_0$ is small we can approximate the collision integral $C[f]$:

(Chapman–Enskog) $C[f] = - \frac{f - f_0}{\tau}$ → because $C[f_0] = 0$

→ relaxation time

tends the system to equilibrium

The relaxation time τ is given by:

$$\tau = \frac{l_{mfp}}{v}$$

The mean free path distance can be expressed as:

$$l_{mfp} \triangleq \frac{1}{n\sigma} \sim \bar{r}\left(\frac{\bar{r}}{d}\right)^2 \sim d\left(\frac{\bar{r}}{d}\right)^3$$

where $\sigma \sim d^2$ $\quad n \sim (\bar{r})^{-3}$

In the kinetic theory $\frac{\bar{r}}{d} \gg 1 \Rightarrow l_{mfp} \gg \bar{r}$

d) Macroscopic quantities from the B. equation

We can derive the hydrodynamic equations from the Boltzmann kinetic equation.

Continuity equation in the coordinate space:

Integrate the B. equation $\int d\vec{k}$:

First recall:

$$\underbrace{n}_{\text{density}} = \int d\vec{k}\, f_{\vec{k}} \qquad \underbrace{\vec{j}}_{\text{particle current}} = \int d\vec{k}\, \frac{\vec{k}}{m} f_{\vec{k}}$$

First term: $\int d\vec{k}\, \frac{\partial f_{\vec{k}}}{\partial t} = \frac{\partial}{\partial t} \int d\vec{k}\, f_{\vec{k}} = \frac{\partial}{\partial t} n$

Second term: $\int d\vec{k}\, \frac{\vec{k}}{m} \cdot \frac{\partial f}{\partial \vec{r}} = \frac{\partial}{\partial \vec{r}} \cdot \int d\vec{k}\, \frac{\vec{k}}{m} f = \frac{\partial \vec{j}}{\partial \vec{r}}$

Third term: $\int d\vec{k}\, \vec{F} \cdot \frac{\partial f}{\partial \vec{k}} = \vec{F} \cdot \int d\vec{k}\, \frac{\partial f}{\partial \vec{k}} = 0$ (integration by parts)

Collision term:

$$\int d\vec{k}\, d\vec{p}\, d\vec{q}\; P f_{\vec{k}} f_{\vec{p}} - \underbrace{\int d\vec{k}\, d\vec{p}\, d\vec{q}\; P f_{\vec{p}+\vec{q}} f_{\vec{k}-\vec{q}}}_{\substack{\text{substitution} \\ \vec{k}' = \vec{k}-\vec{q} \quad \vec{p}' = \vec{p}+\vec{q} \quad \vec{q}' = -\vec{q}}} = 0$$

We arrive at: $\boxed{\frac{\partial n}{\partial t} + \nabla \cdot \vec{j} = 0}$

Newton's equation

for simplicity $\vec{F} = 0$

Integrate the B. equation $\int d\vec{k}\, \vec{k}$:

$$\frac{\partial}{\partial t} \int d\vec{k}\, k_i f_{\vec{k}} + \frac{\partial}{\partial r_j} \int d\vec{k}\, \frac{k_i k_j}{m} f_{\vec{k}} = 0$$

as before the collision part does not contribute

$$Q_i = \int d\vec{k}\, k_i f_{\vec{k}} \qquad P_{ij} = \int d\vec{k}\, \frac{k_i k_j}{m} f_{\vec{k}}$$

$$\boxed{\frac{\partial}{\partial t} \underbrace{Q_i}_{\text{momentum current}} + \frac{\partial}{\partial r_j} \underbrace{P_{ij}}_{\text{momentum flux tensor}} = 0}$$

For the locally equilibrium distribution f_0:

$$P_{ij} = \underbrace{\rho}_{} n V_i V_j + \delta_{ij} P \qquad P = n k_B T$$

ideal fluid result

Transport coefficients – shear viscosity

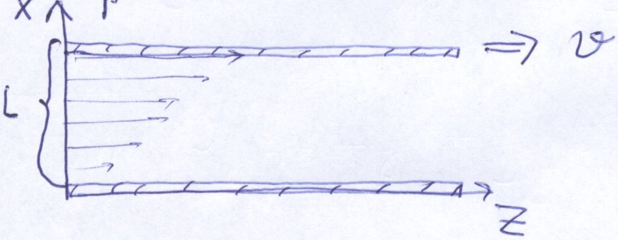
We can extract shear viscosity coefficient μ from the Boltzmann equation. To achieve this use the approximation of the relaxation time:

$$f = f_0 + \delta f \qquad C[f] = -\frac{\delta f}{\tau}$$

with locally equilibrium distribution f_0:

$$f_0 = \frac{n}{(2\pi m k_B T)^{3/2}} e^{-\frac{k_x^2 + k_y^2 + (k_z + \alpha x)^2}{2m k_B T}} \qquad \alpha = \frac{m v}{L}$$

which corresponds to the setting:



We are interested in the stationary solution $\frac{\partial f}{\partial t} = 0$ and assume $\vec{F} = 0$. The B. equation:

$$\frac{\vec{k}}{m} \cdot \frac{\partial f}{\partial \vec{r}} = -\frac{\delta f}{\tau}$$

neglect because α small

$$\delta f = -\tau \frac{\vec{k}}{m} \cdot \frac{\partial f}{\partial \vec{r}} \simeq -\tau \frac{k_x}{m} \frac{\partial f_0}{\partial x} = + \alpha \tau f_0 \frac{k_x (k_z + \alpha x)}{2 m k_B T}$$

$$P_{xz} = \int d\vec{k} \frac{k_x k_z}{m} f = \int d\vec{k} \frac{k_x k_z}{m} \delta f = \alpha \tau \int d\vec{k} f_0 \frac{k_x^2 k_z^2}{2 m^2 k_B T} =$$

$$= \alpha \tau \frac{n k_B T}{2m}$$

The shear viscosity is defined $\eta = \frac{P_{xz}}{v/L} = \frac{m P_{xz}}{\alpha}$

$$\eta = \frac{1}{2} \tau k_B T n$$

$\tau \sim l_{mfp}$

dynamical viscosity, Newton viscosity