Boltzmann equation

Effective description of non-equilibrium dynamics on coarse grained scales

$$\left(\frac{\partial}{\partial t} + \frac{\vec{p}}{m}\vec{\nabla}_r + \vec{F}(\vec{r})\vec{\nabla}_p\right) f(t,\vec{r},\vec{p}) = C[f](t,\vec{r},\vec{p})$$

with collision integral coupling the effect of interactions between particles in a dilute gas

$$C[f](t,\vec{r},\vec{p}) = \frac{1}{2}\int_{p_2}\int_{p_3}\int_{p_4} \tilde{w}(p_1 p_2 \to p_3 p_4)\left[f_3 f_4 - f_1 f_2\right]$$

Shorthand notation: $\int_{p_2} = \int \frac{d^3 p_2}{(2\pi\hbar)^3}$

$$f_2 = f(t,\vec{r},\vec{p}_2), \quad f_3 = f(t,\vec{r},p_3), \quad \ldots$$

Due to assumption of molecular chaos, the equation is closed at the level of single particle distribution f, effectively truncating the BBGKY hierarchy

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Similar to our discussion of classical particles we can also derive a Boltzmann equation or kinetic equation for other physical systems (see. e.g QFT course)

Classical fields / waves:

$$C[f] = \frac{1}{2}\int_{p_2p_3p_4} \tilde{w}(p_1p_2 \to p_3p_4)\left[f_3 f_4 (f_1+f_2) - f_1 f_2 (f_3+f_4)\right]$$

allows only for interactions where one of the final states is already occupied

Quantum theory:

Bosons: Bose enhancement

$$C[f] = \frac{1}{2}\int_{p_2p_3p_4} \tilde{w}(p_1p_2 \to p_3p_4)\left[f_3 f_4 (1+f_1)(1+f_2) - f_1 f_2 (1+f_3)(1+f_4)\right]$$

reduces to classical particles for $f \ll 1$
classical fields for $f \gg 1$

Famous: Pauli blocking

$$C[f] = \frac{1}{2}\int_{p_2p_3p_4} \tilde{w}(p_1p_2 \to p_3p_4)\left[f_3 f_4 (1-f_1)(1-f_2) - f_1 f_2 (1-f_3)(1-f_4)\right]$$

reduces to classical particles for $f \ll 1$ and restricts phase space distribution to be $f \leq 1$ to comply with the Pauli exclusion principle

Based on this discussion we see that a lot of interesting physics can be described by kinetic equations; we will now proceed to study important formal properties and subsequently consider applications to near- and far-from equilibrium systems

Balance equations

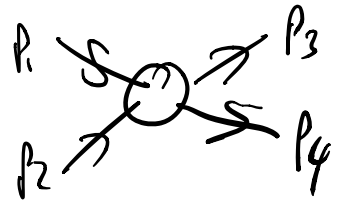
Express conservation laws at the level of a macroscopic description

Based on derivation of the Boltzmann equation the microscopic conservation laws enter at the level of the cross-section/ transition rate

$$C[f](\vec{r}, \vec{p}) = \int_{p_2 p_3 p_4} I(p, p_2, p_3, p_4)$$

$$I(p, p_2, p_3, p_4) = \tilde{W}(p, p_2 \to p_3 p_4) \left[f_3 f_4 - f f_2 \right]$$

characterizing a scattering process



Now the integrand I will have the following symmetries

1) Simple relabeling of momenta

$$((1,2),(3,4)) \hookrightarrow ((2,1),(3,4)) \hookrightarrow ((2,1),(4,3)) \hookrightarrow ((1,2),(4,3))$$

$$I(p_1,p_2,p_3,p_4) = I(p_2,p_1,p_3,p_4) \dots$$

2) microreversibility (consequence of P&T)

$$((1,2),(3,4)) \hookrightarrow ((3,4),(1,2))$$

$$I(p_1,p_2,p_3,p_4) = -I(p_3,p_4,p_1,p_2)$$

due to sign change in statistical factor

Now to derive balance equations, we will make use of these symmetries and consider a characteristic function $\chi(\vec{p})$ which describes a property that is conserved in a micro scale interaction

Q: Which ones can you guess?

e.g. $\chi(\vec{p}) = 1$ particle number

$\chi(\vec{p}) = \vec{p}$ momentum

$\chi(\vec{p}) = \frac{\vec{p}^2}{2m}$ energy

Now we know that at the level of each micro scale interaction we have

$$\chi(\vec{p}_1) + \chi(\vec{p}_2) = \chi(\vec{p}_3) + \chi(\vec{p}_4)$$

i.e. χ is a <u>collisional invariant</u>

which in the Boltzmann equation is reflected by the fact that the transition probability

$$\tilde{W}(p_1 p_2 \to p_3 p_4) = (2\pi\hbar)^3 \delta(\vec{p}_1 + \vec{p}_2 - \vec{p}_3 - \vec{p}_4) \left(\frac{2\pi}{\hbar}\right) \delta\left(\frac{\vec{p}_1^{\,2}}{2m} + \frac{\vec{p}_2^{\,2}}{2m} - \frac{\vec{p}_3^{\,2}}{2m} - \frac{\vec{p}_4^{\,2}}{2m}\right)$$

$$W(p_1 p_2 \to p_3 p_4)$$

is non-zero if and only if this condition is satisfied

Ψ

Now to establish the balance equations for a collisional invariant, we can look at its changes due to collisions

$$\left(\frac{\partial \chi}{\partial t}\right)_{coll}^{(t,\vec{r}_1)} = \int_{p_1} \chi(\vec{p}_1)\; C[f](t,\vec{r},\vec{p}_1)$$

$$= \int_{p_1 p_2 p_3 p_4} \chi(p_1)\; I(p_1,p_2,p_3,p_4)$$

By relabeling the integration variables

$$= \frac{1}{4} \int_{p_1 p_2 p_3 p_4} \chi(p_1)\; I(p_1,p_2,p_3,p_4)$$

$(1 \leftrightarrow 2)$ $\quad + \frac{1}{4} \int_{p_1 p_2 p_3 p_4} \chi(p_2)\; I(p_2,p_1,p_3,p_4)$

$(1,2) \leftrightarrow (3,4)$ $\quad + \frac{1}{4} \int_{p_1 p_2 p_3 p_4} \chi(p_3)\; I(p_3,p_4,p_1,p_2)$

$(3 \leftrightarrow 4)$ $\quad + \frac{1}{4} \int_{p_1 p_2 p_3 p_4} \chi(p_4)\; I(p_4,p_3,p_1,p_2)$

Now making use of the symmetries we can express everything in terms of $I(p_1 p_2 p_3 p_4)$

$$= \frac{1}{4} \int_{p_1 p_2 p_3 p_4} \left[\chi(p_1) + \chi(p_2) - \chi(p_3) - \chi(p_4) \right] I(p_1 p_2 p_3 p_4)$$

$= 0$ since χ is a collisional invariant

Physically this means that collisions do not change the local density of

$$\chi(t, \vec{r}) = \int_{\vec{p}} \chi(\vec{p}) f(t, \vec{r}, \vec{p})$$

any conserved quantity, so we can derive "simple" evolution equations for the density $\chi(t, \vec{r})$

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Particle number:

We consider $\chi(\vec{p}) = 1$ such that

$$n(t,\vec{r}) = \int_{\vec{p}} f(t,\vec{r},\vec{p})$$ particle number density

we then get

$$\frac{\partial}{\partial t} n(t,\vec{r}) = \int_{\vec{p}} \frac{\partial}{\partial t} f(t,\vec{r},\vec{p})$$

$$\overset{\text{BTE}}{=} \int_{\vec{p}} \left(-\frac{\vec{p}}{m} \vec{\nabla}_r f(t,\vec{r},\vec{p}) - \vec{F}(\vec{r}) \vec{\nabla}_p f(t,\vec{r},\vec{p}) + C[f](t,\vec{r},\vec{p}) \right]$$

$$= -\vec{\nabla}_r \int_{\vec{p}} \frac{\vec{p}}{m} f(t,\vec{r},\vec{p})$$

boundary term $\to 0$

collisional invariant $= 0$

So we obtain

$$\frac{\partial}{\partial t} n(t,\vec{r}) + \vec{\nabla}_{\vec{r}} \int \frac{d^3\vec{p}}{(2\pi\hbar)^3} \frac{\vec{p}}{m} f(t,\vec{r},\vec{p}) = 0$$

Now inserting the expression

$$\vec{\jmath}_N(t,\vec{r}) = \int \frac{d^3p}{(2\pi\hbar)^3} \frac{\vec{p}}{m} f(t,\vec{r},\vec{p})$$ particle flux

number of particles x velocity

So we obtain back the transport

Continuity equation

$$\boxed{\frac{\partial}{\partial t} n(t,\vec{r}) + \vec{\nabla}_r \vec{\jmath}_N(t,\vec{r}) = 0}$$

Momentum balance:

We have $\chi(\vec{p}) = \vec{p}$ as collisional invariant which yields a balance equation for

$$P_i(t,\vec{r}) = \int_{\vec{p}} p_i \, f(t,\vec{r},\vec{p}) \quad \text{momentum density}$$

so performing the same steps

$$\frac{\partial}{\partial t} P_i(t,\vec{r}) \overset{\text{BTE}}{=} -\int_{\vec{p}} p_i \left[\underbrace{\frac{p_j}{m} \frac{\partial}{\partial r_j} f(t,\vec{r},\vec{p})}_{①} + \underbrace{\bar{f}_j(\vec{r}) \frac{\partial}{\partial p_j} f(t,\vec{r},\vec{p})}_{②} - \underbrace{C[f](t,\vec{r},\vec{p})}_{③} \right]$$

we can rewrite the terms as

① $$\frac{\partial}{\partial r_j} \int_{\vec{p}} p_i \frac{p_j}{m} f(t,\vec{r},\vec{p}) = \frac{\partial}{\partial r_j} \Im^{ij}_p(t,\vec{r})$$

momentum in i-direction; velocity in j-direction; momentum flux in j direction

② $\overline{F}_j(\vec{r}) \int_{\vec{p}} p_i \frac{\partial}{\partial p_j} f(t,\vec{r},\vec{p})$

integration by parts

$= -\overline{F}_j(\vec{r})\, \delta_{ij} \underbrace{\int_{\vec{p}} f(t,\vec{r},\vec{p})}_{= n(t,\vec{r})}$

$= -\overline{F}_i(\vec{r})\, n(t,\vec{r})$

which reflects Newtons law for each particle

③ vanishes as $\chi(\vec{p}) = p_i$ is a collisional invariant

So collecting everything we obtain

$$\frac{\partial}{\partial t} P_i(t,\vec{r}) + \frac{\partial}{\partial r_j} \Im_{\vec{p}}^{ij}(t,\vec{r}) = n(t,\vec{r})\, \overline{F}_i(\vec{r})$$

with the momentum flux determined by

$$\Im_{\vec{p}}^{ij}(t,\vec{r}) = \int \frac{d^3\vec{p}}{(2\pi\hbar)^3} \frac{p_i p_j}{m} f(t,\vec{r},\vec{p})$$

Energy balance

Similar manipulations (c.f. exercise 00) lead to a balance equation for the kinetic energy

$$\vec{e}_{kin}(t,\vec{r}) = \int_{\vec{p}} \frac{\vec{p}^2}{2m} f(t,\vec{r},\vec{p})$$

$$\boxed{\frac{\partial}{\partial t} e_{kin}(t,\vec{r}) + \vec{\nabla}_r \cdot \vec{J}_{e_{kin}}(t,\vec{r}) = \frac{\vec{F}(t,\vec{r}) \cdot \vec{P}(t,\vec{r})}{m}}$$

with $\vec{J}_{e_{kin}}(t,\vec{r}) = \int \frac{d^3p}{(2\pi\hbar)^3} \frac{\vec{p}}{m} \left(\frac{\vec{p}^2}{2m}\right) f(t,\vec{r},\vec{p})$

We obtain the microscopically derived analogues of balance equations in our macroscopic description, with fluxes expressed in terms of moments of the single particle distribution