

LECTURE II

SCATTERING

RANDOM SCATTERING

$f(p, t)$: density of particles with a state p at time t .

Particles undergo a random change in state (a 'collision') with a certain frequency.

$$S(p, p') dp = d\mathcal{P}\{p' \rightarrow p\}$$

p' : pre-collision state, p : post-collision state

BOLTZMANN VS. BROWN

At each infinitesimal time interval Δt flip a coin.

$$\mathcal{P}[\text{scatter}] = \omega(p'), \quad \mathcal{P}[\text{not scatter}] = 1 - \omega(p'),$$

if *scatter*, choose a new state p from the distribution $S(p, p') dp$

This gives

$$f(p, t + \Delta t) = \int S(p, p') \omega(p') f(p', t) dp' + \int \delta(p - p') (1 - \omega(p')) f(p', t) dp'$$

The Boltzmann model :

$\omega(p') = \gamma(p')\Delta t$ with $\gamma(p')$ collision frequency

\Rightarrow Boltzmann equation for $\Delta t \rightarrow 0$

$$\partial_t f(p, t) = \int S(p, p') \gamma(p') f(p', t) dp' - \gamma(p) f(p, t)$$

$f(x, p, t)$ density of particles with momentum p

Brownian motion:

$\omega = 1$ scatter each time (producing a random walk according to a Wiener process)

But scatter 'only a little bit' $S(p, p') \approx \delta(p - p')$

$$S(p, p') = (A\Delta t)^{-dim(p)/2} R\left(\frac{p - p'(1 + \Delta t B)}{\sqrt{A\Delta t}}, p'\right), \quad \int \begin{pmatrix} 1 \\ q \\ |q|^2 \end{pmatrix} R(q, p') dq =$$

weak formulation:

$$\int \psi(p) f(p, t + \Delta t) dp = \int \psi(p'(1 + \Delta t B) + \sqrt{\Delta t A q}) R(q, p') f(p', t) dq p'$$

gives for $\Delta t \rightarrow 0$

$$\int \psi(p) \partial_t f(p, t) dp = \int f(p') [B p' \cdot \nabla \psi(p') + A \Delta t (p')] dp'$$

or the Fokker - Planck equation

$$\partial_t f = \nabla_p \cdot [A \nabla_p f - B p \cdot \nabla_p f]$$

Boltzmann:

$$\partial_t f(p, t) = \int S(p, p') \gamma(p') f(p', t) dp' - \gamma(p) f(p, t)$$

Brownian motion:

$$\partial_t f = \nabla_p \cdot [A \nabla_p f - B p \cdot \nabla_p f]$$

A remark on Markov processes

- ▶ The frequency ω is independent of the last time the scattering event has occurred.
- ▶ For 'intelligent' particles (traffic, production systems) this is often unrealistic.

$$\mathcal{P}[\Delta T_{scat}] = \gamma e^{-\gamma \Delta T_{scat}}$$

ΔT_{scat} : time between scattering events.

Non - Markov processes:

Enlarge the state space: $p \rightarrow (p, \tau)$

τ : time elapsed since the last scattering event

$$p' \rightarrow p, \tau = 0 \text{ with } \mathcal{P} = \gamma(\tau) \Delta t,$$

$$p' \rightarrow p, \tau \rightarrow \tau + \Delta t \text{ with } \mathcal{P} = 1 - \gamma(\tau) \Delta t,$$

$$\mathcal{P}[\Delta T] = c \exp\left[-\int_0^{\Delta T} \gamma(\tau) d\tau\right]$$

Gives the Boltzmann equation

$$\partial_t f + \partial_\tau f = Q[f](p, \tau, t)$$

The Boltzmann equation

$$\partial_t f(p, t) + C[\mathcal{E}, f] = Q[f] = \int S(p, p') \gamma(p') f(p') dp' - \gamma(p) f(p) \int S(p', p) dp'$$

$$C[\mathcal{E}, f] = \nabla_p \mathcal{E} \nabla_x \cdot f - \nabla_x \mathcal{E} \cdot \nabla_p f, \quad \mathcal{E} = \frac{|p|^2}{2} + \phi(x)$$

The mean free path $\gamma(p')$: scattering frequency of particle with momentum p' .

$|\nabla \mathcal{E}(p')| \gamma(p')$: mean free path.

Bosons and Fermions:

$$\gamma(p') = \frac{L_{MFP}}{|\nabla \mathcal{E}(p')|}$$

Maxwellian Molecules:

$$\gamma(p') = \gamma_0, \quad L_{MFP} = \gamma_0 |\nabla \mathcal{E}(p')|$$

CONSERVATION

There are certain quantities which remain unchanged in this process $\kappa(p) = \kappa(p')$

$$\partial_t \int \kappa(p) f(p, t) dp = 0$$

Weak formulation:

$$\int \psi(p) Q[f](x, p) dp = \int [\psi(p) - \psi(p')] S(p, p') \gamma(p') f(p') dp p'$$

$\kappa(p)$ conserved in scattering $\kappa(p) = \kappa(p')$

$$S(p, p') \rightarrow \delta(\kappa(p) - \kappa(p')) S(p, p')$$

$$\int \kappa(p) Q[f](p) dp = \int [\kappa(p) - \kappa(p')] \delta(\kappa - \kappa') S(p, p') \omega(p') f(p') dp p' = 0$$

$$\Rightarrow \partial_t \int \kappa(p) f(p) dp = 0$$

BINARY PARTICLE INTERACTIONS

$$x = (x_1, x_2), \quad p = (p_1, p_2),$$

f : particle of type 1 is at position x_1 with momentum p_1 and particle of type 2 is at position x_2 with momentum p_2 .

$$\mathcal{E} = \mathcal{E}_1(x_1, p_1) + \mathcal{E}_2(x_2, p_2).$$

- ▶ statistical independence: $f(x_1, x_2, p_1, p_2) = f_1(x_1, p_1)f_2(x_2, p_2)$
- ▶ Integrate out the other density functions gives two Boltzmann equations for the two density functions f_1, f_2

$$\partial_t f_1(x_1, p_1, t) + [\mathcal{E}, f_1] =$$

$$\int S(p, p') \gamma(p') f_1(p'_1) f_2(p'_2) dp'_1 p'_2 p_2 - f_1(p_1) \int \gamma(p) f_2(p_2) S(p', p) dp'_1 p'_2 p_2$$

$$\partial_t f_2(x_2, p_2, t) + [\mathcal{E}, f_2] =$$

$$\int S(p, p') \gamma(p') f_1(p'_1) f_2(p'_2) dp'_1 p'_2 p_1 - f_2(p_2) \int \gamma(p) f_1(p_1) dp'_1 p'_2 p_1$$

- ▶ Scattering of particles of the same type: (gas dynamics)
 $f_1 = f_2$, $Q[f, f]$ quadratic integral operator. Electron - electron scattering.
- ▶ Scattering of particles of different type. (Two different gases, electron - phonon interaction). Either two BTEs or assume an ansatz for f_2

MICRO - REVERSIBILITY AND MAXWELLIAN KERNELS

The transition $p' \rightarrow p$ is as likely as the transition $p \rightarrow p'$, meaning the scattering cross section $S\gamma$ is symmetric.

$$S(p, p')\gamma(p') = S(p', p)\gamma(p)$$

This, together with the conservation properties, determines the kernel elements of Q

$$\int \psi(p)Q[f](x, p) dp = \frac{1}{2} \int [\psi(p) - \psi(p')]S(p, p')\gamma(p')[f(x, p') - f(x, p)] dp p'$$

$$S \approx \delta(\kappa(p) - \kappa(p')) \Rightarrow Q[f(x, \kappa(p))] = 0$$

For the binary interaction operator we have

$$\kappa(p_1, p_2) = \kappa_1(p_1) + \kappa_2(p_2) \Rightarrow f_1 f_2 = G(x_1, x_2, \kappa_1 + \kappa_2)$$

For particle - particle scattering $f_1 = f_2$ this gives the Maxwellian

$$f_1(x_1, p_1) = \rho(x_1) \exp(\mu(x_1) \cdot \kappa(p_1))$$

For particle - background scattering we assume the ansatz

$f_2(x_2, p_2) = \exp(-\mu \cdot \kappa_2(p_2))$ this gives

$$f_1(x_1, p_1) = \rho(x) \exp[-\mu \cdot \kappa_1(p_1)]$$

ENTROPY AND INFORMATION LOSS

$S(f)$ convex functional that is decreased by $Q[f]$.

$$\partial_t f = Q[f], \quad DS(f)(Q[f]) \leq 0, \quad \forall f$$

$$\partial_t S(f) = DS(f)(\partial_t f) = DS(f)(Q[f])$$

$S(f)$ acts like the nonlinear version of a norm and guarantees stability. It also drives the solution towards the kernel f_{eq} in the long time limit.

A PROBABILISTIC DEFINITION OF ENTROPY

Differential amount of information gained by observing an experiment.

An argument for the logarithm: **The Von Neumann entropy**

- ▶ Consider N balls in a bag, either black (b) with probability p or white (w) with probability $1 - p$.

$$\Delta I(\mathcal{E}) = \phi(\mathcal{P}(\mathcal{E}))$$

$$\Delta I(\mathcal{E}_1 \cup \mathcal{E}_2) = \Delta I(\mathcal{E}_1) + \Delta I(\mathcal{E}_2)$$

$$\mathcal{P}(\mathcal{E}_1 \cup \mathcal{E}_2) = \mathcal{P}(\mathcal{E}_1)\mathcal{P}(\mathcal{E}_2)$$

$$\Rightarrow \phi(P_1 P_2) = \phi(P_1) + \phi(P_2) \Rightarrow \phi(P) = -K \ln(P)$$

Entropies of the Boltzmann equation

I. Particle - particle scattering:

For electron - electron scattering $f_1 = f_2$ we have to have

$$S(p_1, p_2, p'_1, p'_2)\gamma(p'_1, p'_2) = S(p_2, p_1, p'_2, p'_1)\gamma(p'_2, p'_1)$$

and therefore in the weak formulation

$$\begin{aligned} & \int \psi(p_1)Q[f](p_1) dp_1 = \\ & \frac{1}{2}[\psi(p_1) - \psi(p'_1)]S(p, p')\gamma(p') [f(p'_1)f(p'_2) - f(p_1)f(p_2)] dp_1 p_2 p'_1 p'_2 \\ & = \frac{1}{4}[\psi_1 + \psi_2 - \psi'_1 - \psi'_2]S(p, p')\gamma(p') [f'_1 f'_2 - f_1 f_2] dp_1 p_2 p'_1 p'_2 \end{aligned}$$

Setting $\psi = \ln(f)$ implies

$$DS(f)(Q[f]) = \int \ln(f)Q[f] dp_1$$

$$= \frac{1}{4}[\ln(f_1 f_2) - \ln(f'_1 f'_2)]S(p, p')\gamma(p')[f'_1 f'_2 - f_1 f_2] dp_1 p_2 p'_1 p'_2 \leq 0$$

Therefore the entropy functional S is given by

$$S(f) = \int f(\ln f - 1) dp$$

II. Particle - background scattering:

The Boltzmann operator can be written in weak form as

$$\int \psi_1 Q[f_1] dp_1 =$$

$$\int (\psi_1 - \psi'_1) S(p, p') \gamma(p') e^{-\mu(\kappa_1 + \kappa_2)} (f'_1 e^{\mu\kappa'_1} - f_1 e^{\mu\kappa_1}) dp p'$$

Therefore

$$\int g'(f_1 e^{\mu\kappa_1}) Q[f_1] dp_1 \leq 0$$

holds for any convex function g and monotone function g' and

$$DS(f)\delta f = \int g'(f e^{\mu\kappa_1}) \delta f dp$$

for any convex g .

THE RELATIVE ENTROPY

$$\int g'(f_1 e^{\kappa_1}) Q[f_1] dp_1 \leq 0$$

$S(f)$ = has to be conserved by the transport operator (the Poisson bracket).

$$\int g'(f e^{\mu \kappa_1}) [\mathcal{E}, f] dxp = 0$$