

Non-equilibrium physics WS 18/19 – Exercise Sheet 7:

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1 Discussion:

- i) Discuss the concept of entropy and its relevance for equilibrium and non-equilibrium systems.

2 In-class problems:

2.1 Energy balance in the Boltzmann equation

- i) Derive the balance equation for the kinetic energy density

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

and show that the energy flux J_E is given by

$$J_{E_{\text{kin}}}(t, \vec{r}) = \int \frac{d^3\vec{p}}{(2\pi\hbar)^3} \frac{p^2}{2m} \frac{\vec{p}}{m} f(t, \vec{r}, \vec{p}),$$

- ii) Calculate the particle number flux $J_N(t, \vec{r})$, the kinetic energy flux $J_{E_{\text{kin}}}(t, \vec{r})$ and the momentum flux $J_{\vec{p}}(t, \vec{r})$ for an ideal gas in local thermal equilibrium, where

$$f(t, \vec{r}, \vec{p}) = f^{(0)}(t, \vec{r}, \vec{p}) = n(t, \vec{r}) \left(\frac{2\pi\hbar^2}{mk_B T(t, \vec{r})} \right)^{3/2} \exp \left[-\frac{(\vec{p} - m\vec{v}(t, \vec{r}))^2}{2mk_B T(t, \vec{r})} \right].$$

3 Homework problems:

3.1 Entropy conservation in classical dynamics

- i) Starting from the Liouville equation for the evolution of the phase-space density $f(t, \{\vec{r}_i\}, \{\vec{p}_i\})$ of a classical systems of N particles with two-body interactions

$$\left[\frac{\partial}{\partial t} + \sum_{i=1}^N \frac{\vec{p}_i}{m} \vec{\nabla}_{\vec{r}_i} + \sum_{i=1}^N \frac{\vec{F}(\vec{r}_i)}{m} \vec{\nabla}_{\vec{p}_i} + \sum_{i=1}^N \sum_{j \neq i} \vec{K}_{ij}(|\vec{r}_i - \vec{r}_j|) \vec{\nabla}_{\vec{p}_i} \right] f(t, \{\vec{r}_i\}, \{\vec{p}_i\}) = 0$$

show that the classical entropy

$$S_{\text{cl}}(t) = -k_B \int d^{6N} \mathcal{V} f(t, \{\vec{r}_i\}, \{\vec{p}_i\}) \log \left(f(t, \{\vec{r}_i\}, \{\vec{p}_i\}) \right)$$

is conserved under Hamiltonian time evolution.

(Hint: What is time derivative of the classical entropy $S_{\text{cl}}(t)$?)

3.2 Linearized Boltzmann equation

Consider the Boltzmann equation for neutral particles with mass m in absence of external forces.

- i) Show that the Maxwell–Boltzmann distribution

$$f^{(0)}(\vec{p}) = n \left(\frac{2\pi\hbar^2}{mk_B T} \right)^{3/2} \exp \left[-\frac{\vec{p}^2}{2mk_B T} \right]$$

with constant temperature T and density n is a stationary solution of the Boltzmann equation.

Next we will consider small perturbations away from the equilibrium solution, which will be characterized by a function $h(t, \vec{r}, \vec{p})$ according to

$$f(t, \vec{r}, \vec{p}) = f^{(0)}(\vec{p}) [1 + h(t, \vec{r}, \vec{p})] .$$

and we will neglect terms of $\mathcal{O}(h^2)$ and higher in the following.

- ii) Show that that the linearized evolution equation for h is given by

$$\left(\frac{\partial}{\partial t} + \frac{\vec{p}_1}{m} \vec{\nabla}_{\vec{r}} \right) h(t, \vec{r}, \vec{p}_1) = \mathcal{I}_{\text{coll}}[h](t, \vec{r}, \vec{p}_1)$$

where $\mathcal{I}_{\text{coll}}[h](t, \vec{r}, \vec{p}_1)$ denotes (linear) collisions operator

$$\mathcal{I}_{\text{coll}}[h](t, \vec{r}, \vec{p}_1) = \int_{\vec{p}_2} \int_{\vec{p}_3} \int_{\vec{p}_4} \tilde{w}(\vec{p}_1 \vec{p}_2 \rightarrow \vec{p}_3 \vec{p}_4) f^{(0)}(\vec{p}_2) [h(t, \vec{r}, \vec{p}_3) + h(t, \vec{r}, \vec{p}_4) - h(t, \vec{r}, \vec{p}_1) - h(t, \vec{r}, \vec{p}_2)]$$

(Hint: Detailed balance in equilibrium guarantees $f^{(0)}(\vec{p}_1) f^{(0)}(\vec{p}_2) = f^{(0)}(\vec{p}_3) f^{(0)}(\vec{p}_4)$ for all combinations of momenta allowed by energy conservation.)

We now specialize on homogenous perturbations, where $h(t, \vec{r}, \vec{p}_1) = h(t, \vec{p}_1)$ is independent of the spatial coordinate \vec{r} . In order to investigate their behavior, we follow the usual strategy and search for eigenfunctions $h_i(\vec{p}_1)$ of the collisions operator $\mathcal{I}_{\text{coll}}$, defined by the condition

$$\mathcal{I}_{\text{coll}}[h_i](\vec{p}_1) = \lambda_i h_i(\vec{p}_1) \quad (1)$$

where i labels the different eigenfunctions. We will assume that all eigenfunctions can be normalized according to

$$\int_{\vec{p}_1} f^{(0)}(\vec{p}_1) [h_i(\vec{p}_1)]^2 = 1$$

- iii) Show that $\lambda = 0$ is a five fold degenerate eigenvalue and write down the corresponding unnormalized eigenfunctions $h_1(\vec{p}_1), \dots, h_5(\vec{p}_1)$.
(Hint: Detailed properties of the transition rates $\tilde{w}(\vec{p}_1\vec{p}_2 \rightarrow \vec{p}_3\vec{p}_4)$ are irrelevant to answer this questions – instead the eigenfunctions are determined by basic fundamental properties of two-body collisions.)
- iv) Show that all other eigenvalues λ_i are negative $\lambda_i \leq 0$.
(Hint: Exploit the normalization condition to express the eigenvalue λ_i as an integral moment of the collisions operator $\int_{\vec{p}_1} f^{(0)}(\vec{p}_1) h_i(\vec{p}_1) \mathcal{I}_{\text{coll}}[h_i](\vec{p}_1)$. Exploit the symmetries of the integrand to show that it is negative definite.)
- v) Based on the assumption that the eigenfunctions $h_i(\vec{p}_1)$ form a complete set, discuss the qualitative properties of the general solution $h(t, \vec{p}_1)$ for a homogenous perturbation in the long time limit $t \rightarrow \infty$.