Non-equilibrium physics WS 20/21 - Exercise Sheet 7:

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1 Discussion:

- i) What are the differences between the collisions integral of the Boltzmann equation for classical and quantum systems?
- ii) What is the physical meaning of balance equations, and how can the fluxes of particle number and momentum be understood from a microscopic perspective?

2 In-class problems:

2.1 Energy balance in the Boltzmann equation

i) Derive the balance equation for the kinetic energy density

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

and show that the energy flux J_E is given by

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

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

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

3 Homework problems:

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3.1 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

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

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

$$\mathcal{I}_{\text{coll}}[h](t, \vec{r}, \vec{p_1}) = \int_{\vec{p_2}} \int_{\vec{p_3}} \int_{\vec{p_4}} \tilde{w}(\vec{p_1}\vec{p_2} \to \vec{p_3}\vec{p_4}) f^{(0)}(\vec{p_2}) \left[h(t, \vec{r}, \vec{p_3}) + h(t, \vec{r}, \vec{p_4}) - h(t, \vec{r}, \vec{p_1}) - h(t, \vec{r}, \vec{p_2}) \right]$$

(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

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

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

$$\int_{\vec{p_1}} f^{(0)}(\vec{p_1}) \Big[h_i(\vec{p_1}) \Big]^2 = 1$$

- 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 $\tilde{w}(\vec{p}_1\vec{p}_2 \to \vec{p}_3\vec{p}_4)$ 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 $t \to \infty$.

3 Homework problems:

3.2 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

$$S_{\rm cl}(t) = -k_B \int d^{6N} \mathcal{V} \ f(t, \{\vec{r_i}\}, \{\vec{p_i}\}) \ \log \Big(f(t, \{\vec{r_i}\}, \{\vec{p_i}\}) \Big)$$

is conserved under Hamiltonian time evolution.

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