

Non-equilibrium physics WS 20/21 – Exercise Sheet 2:

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1 Discussion:

- i) What are *Markovian* out-of-equilibrium processes? What is the general form of *linear constitutive relations* and what are *direct and indirect* transport phenomena? What symmetry principles and constraints apply to the linear kinetic coefficients?

2 In-class problems:

2.1 Constitutive relations for heat and particle transfer between containers

Consider again the heat and particle transfer between two containers A and B (c.f. problem 3.1 sheet 1). We found that the net energy and particle fluxes were determined by

$$J^N = J_N^{B \rightarrow A} - J_N^{A \rightarrow B}, \quad J^E = J_E^{B \rightarrow A} - J_E^{A \rightarrow B},$$

with

$$J_N^{A \rightarrow B} = \frac{1}{\sqrt{2\pi m k_B T_A}} S p_A, \quad J_E^{A \rightarrow B} = \sqrt{\frac{2k_B T_A}{\pi m}} S p_A$$

and similarly for $J_{N/E}^{B \rightarrow A}$.

- i) Express the fluxes J^N and J^E in terms of the affinities

$$F_N = \Delta\left(-\frac{\mu}{T}\right) = -\frac{\mu_A}{T_A} + \frac{\mu_B}{T_B} \quad F_E = \Delta\left(\frac{1}{T}\right) = \frac{1}{T_A} - \frac{1}{T_B}.$$

to linear order for small F_N and F_E . If necessary, you can use that the following identity for the pressure of an ideal gas $\frac{p_A}{p_B} = \left(\frac{T_A}{T_B}\right)^{5/2} e^{\frac{\mu_A}{k_B T_A} - \frac{\mu_B}{k_B T_B}}$.

- ii) Determine the kinetic coefficients $L_{EE}, L_{EN}, L_{NE}, L_{NN}$. What symmetries do you recognize?
- iii) Calculate the entropy production rate dS/dt in the linear transport regime and show that $dS/dt \geq 0$.

3 Homework problems:

3.1 Stokes-Einstein relation

Consider a rare species of heavy particles of mass m suspended in a fluid in thermal equilibrium at a const. temperature T and subject to the gravitational force $\vec{F}_g(\vec{x}) = -\vec{\nabla}V(\vec{x})$, where $V(\vec{x}) = mgz$ denotes the gravitational potential.

- i) Determine the form of the linear constitutive relation for the current \vec{J}_n in the presence of the gravitational potential. Express the result in terms of a diffusion and drift contribution $\vec{J}_n = \vec{J}_n^{Diffusion} + \vec{J}_n^{Drift}$ analogous to the discussion of a charged particle in an electric field.
- ii) Show that the general form of the equilibrium density distribution $n(z)$ (as a function of the height z) is of the form $n(z) = n_0 e^{-\lambda z}$ and determine λ as a function of m, g, k_B, T .

We will now consider a microscopic description of the particles inside the fluid, which in addition to the gravitational force \vec{F}_g are subject to a damping force $\vec{F}_s = -6\pi R\eta\vec{x}$, where R and \vec{x} denote the radius and velocity of the particle and η is the shear viscosity.

- iii) Determine the terminal drift velocity v_{Drift} of particles in the gravitational field and calculate the the associated drift current \vec{J}_n^{Drift} in terms of n, m, g, R, η . By comparing your result of the microscopic calculation of \vec{J}_n^{Drift} , with the corresponding expression obtained from the linear constitutive relation obtained in (i), determine the kinetic coefficient L_{nn} as a function of m, g, k_B, T, η, R .
- iv) Establish the Stokes-Einstein relation between the diffusion constant D and the shear viscosity η .

3.2 Causal diffusion

Consider a modification of the diffusion equation, where instead of the usual constitutive relation $\vec{J}_n = -D\vec{\nabla}n$ the continuity equation

$$\frac{\partial}{\partial t}n + \vec{\nabla}\vec{J}_n = 0,$$

is supplemented by an additional relaxation type equation

$$\frac{\partial}{\partial t}\vec{J}_n + \frac{1}{\tau}(\vec{J}_n + D\vec{\nabla}n) = 0,$$

for the particle flux density \vec{J}_n .

- i) Decouple the evolution equations for \vec{J}_n and n to derive the Cattaneo equation for the evolution particle number density $n(t, \vec{x})$, assuming a constant relaxation time τ and diffusion coefficient D .
- ii) Expressing the solution of the d -dimensional Cattaneo equation

$$\left[\tau \frac{\partial^2}{\partial t^2} + \frac{\partial}{\partial t} - D\Delta \right] n(t, \vec{x}) = 0$$

in the form $n(t, \vec{x}) = \int \frac{d^d k}{(2\pi)^d} \frac{d\omega}{(2\pi)} \int \tilde{n}(\omega, k) e^{-i\omega t} e^{i\vec{k}\vec{x}}$, determine the dispersion relation $\omega(k)$.

- iii) Determine the group velocity $v_g(k) = Re \frac{\partial \omega(k)}{\partial k}$ and the phase velocity $v_{ph}(k) = Re \frac{\omega(k)}{k}$

iv) Show that the retarded Greens function

$$G_R(t, \vec{k}) = \frac{i}{2\pi\tau} \frac{e^{-i\omega_+(k)t} - e^{-i\omega_-(k)t}}{\omega_+(k) - \omega_-(k)} \theta(t)$$

with $\omega_{\pm}(k) = \frac{-i}{2\tau} \pm \frac{1}{2\tau} \sqrt{4Dk^2\tau - 1}$, is the solution to the equation

$$\left[\tau \frac{\partial^2}{\partial t^2} + \frac{\partial}{\partial t} + Dk^2 \right] G_R(t, \vec{k}) = \frac{1}{(2\pi)} \delta(t),$$

which describes the time evolution of a density perturbation localized at the point $\vec{x} = 0$ and initial time $t = 0$

v) Now we will focus on the case of one-dimensional diffusion ($d = 1$). Determine the retarded propagator $G_R(t, x)$ in coordinate space, using that

$$\int_{-\infty}^{\infty} dk \frac{e^{-i\omega_+(k)t} - e^{-i\omega_-(k)t}}{\omega_+(k) - \omega_-(k)} e^{ikx} = \frac{-i\pi}{\sqrt{D/\tau}} e^{-t/2\tau} I_0(\xi) \theta(\sqrt{D/\tau} t - |x|).$$

where I_0 is the modified Bessel function and $\xi = \frac{1}{2} \sqrt{\frac{t^2}{\tau^2} - \frac{x^2}{D\tau}}$. Visualize the propagation of the wave-package. Which properties do the coefficients D, τ have to satisfy for the evolution to be causal?