Tutorial sheet 2

The exercises marked with a star are homework for next week.

Discussion topics:

What are "affinities" and "fluxes" in out-of-equilibrium systems? How do they relate to entropy production? What are "Markovian" "linear" out-of-equilibrium processes? Which properties obey the kinetic coefficients entering the fundamental relationships in such processes?

4. Equilibrium of particles in a fluid

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

i. Determine the form of the linear constitutive relation for the particle-number current $\vec{\mathcal{J}}_N$ in the presence of the gravitational potential. Express the result in terms of a diffusion and drift contribution $\vec{\mathcal{J}}_N = \vec{\mathcal{J}}_N^{\text{diffusion}} + \vec{\mathcal{J}}_N^{\text{drift}}$, where the diffusion term takes the same form as in Fick's law. You can assume $(\partial\mu/\partial n)_T = k_BT/n$, as holds in a classical ideal gas.

Hint: Check the discussion of charged particles in an electric field in the lectures. You may want to introduce a "gravito-chemical potential" μ_g.

ii. Show that the equilibrium density distribution $n(z)$ (as a function of the height z) is of the general form $n(z) = n_0\, \mathrm{e}^{-\lambda z}$ and determine λ as a function of m, g, k_B, T. If we want to have observable effects over distances of the order of a centimeter at $T = 300$ K, what should be the order of magnitude of the mass m?

iii. We shall now consider a microscopic description of the particles inside the fluid: in addition to the gravitational force $\vec{F}_g$, they are subject to a (Stokes') friction force $\vec{F}_S = -6\pi R\eta\vec{v}$, where R and $\vec{v}$ denote the radius and velocity of the particle (assumed to be spherical) and η is the shear viscosity.

a) Determine the terminal drift velocity $\vec{v}_{\text{lim}}$ of particles in the gravitational field and calculate the the associated drift current $\vec{\mathcal{J}}_N^{\text{drift}}$ in terms of the particle density n, m, g, R, and η. By comparing your result of the microscopic calculation of $\vec{\mathcal{J}}_N^{\text{drift}}$, with the corresponding expression obtained in **i**, determine the kinetic coefficient L_{NN} as a function of m, g, k_B, T, R, η.

b) Establish the (Stokes–Einstein) relation between the shear viscosity and the diffusion constant D.

*5. Heat transport in a rod

Consider a straight heat-conducting bar of length ℓ connecting two heat reservoirs at temperatures $T^{(A)}$ and $T^{(B)}$ with $T^{(A)} > T^{(B)}$. The entire system is thermally insulated from the outside world. We assume the heat flux to be small enough for the reservoirs to remain at constant temperatures and we consider the stationary (but not equilibrated!) situation $\partial T(t,\vec{r})/\partial t = 0$, where $T(t,\vec{r})$ denotes the temperature in the rod.

i. Recall the expression of Fourier's law for heat transport and deduce the equation satisfied by the local temperature in the rod. Give the solution to this equation fulfilling the boundary conditions of the problem.

ii. Entropy production

Let Q be the heat transferred per unit time from A to B, and $\mathcal{S}$ the cross-sectional area of the bar.

a) Give the energy flux density flowing along the rod, as well as the corresponding entropy flux density.

b) Consider a section $[x, x + \mathrm{d}x]$ of the rod. Write down the net entropy balance in the slice due to entropy flux entering and leaving it in the general case.

c) In the stationary regime considered here, the entropy in the slice remains by definition constant in time. Write down the local balance equation for entropy and deduce how much entropy is created at each point in the rod. Give the rate of entropy production over the whole rod. What do you recognize?

*6. Causal diffusion

Consider a modification of the diffusion equation, where instead of using Fick's law as in the lectures, one supplements the continuity equation

$$\frac{\partial n}{\partial t} + \vec{\nabla} \cdot \vec{\mathcal{J}}_N = 0 \tag{1}$$

by an additional relaxation-type equation

$$\frac{\partial \vec{\mathcal{J}}_N}{\partial t} + \frac{1}{\tau}\big(\vec{\mathcal{J}}_N + D\vec{\nabla} n\big) = 0 \tag{2}$$

for the particle flux density $\vec{\mathcal{J}}_N$, where $\tau > 0$.[1]

i. Decouple the evolution equations for $\vec{\mathcal{J}}_N$ and n to derive the equation for the evolution of the particle-number density $n(t, \vec{r})$, assuming a constant relaxation time τ and diffusion coefficient D.

ii. Introducing the Fourier representation

$$n(t, \vec{r}) \equiv \int \tilde{n}(\omega, \vec{k})\, \mathrm{e}^{-\mathrm{i}(\omega t - \vec{k}\cdot\vec{r})}\, \frac{\mathrm{d}\omega}{2\pi}\, \frac{\mathrm{d}^d\vec{k}}{(2\pi)^d} \tag{3}$$

of the solution of the d-dimensional equation ($\triangle$ denotes the d-dimension Laplacian)

$$\left[\tau\frac{\partial^2}{\partial t^2} + \frac{\partial}{\partial t} - D\triangle\right] n(t, \vec{r}) = 0, \tag{4}$$

determine the dispersion relation $\omega(\vec{k})$.

iii. Show that the retarded Green's function

$$G_R(t, \vec{k}) \equiv \frac{\mathrm{i}}{\tau}\, \frac{\mathrm{e}^{-\mathrm{i}\omega_+(\vec{k})t} - \mathrm{e}^{-\mathrm{i}\omega_-(\vec{k})t}}{\omega_+(\vec{k}) - \omega_-(\vec{k})}\, \Theta(t) \tag{5}$$

with $\omega_\pm(\vec{k}) \equiv \dfrac{1}{2\mathrm{i}\tau} \pm \dfrac{1}{2\tau}\sqrt{4D\vec{k}^2\tau - 1}$ and Θ the Heaviside function is solution to the equation

$$\left[\tau\frac{\partial^2}{\partial t^2} + \frac{\partial}{\partial t} + D\vec{k}^2\right] G_R(t, \vec{k}) = \delta(t), \tag{6}$$

which describes the evolution at $t > 0$ of a density perturbation localized at $\vec{r} = \vec{0}$ at the initial time $t = 0$.

iv. We will now focus on the case of one-dimensional diffusion ($d = 1$). Determine the retarded propagator $G_R(t, x)$ in coordinate space, using the identity

$$\int_{-\infty}^{\infty} \frac{\mathrm{e}^{-\mathrm{i}\omega_+(k)t} - \mathrm{e}^{-\mathrm{i}\omega_-(k)t}}{\omega_+(k) - \omega_-(k)}\, \mathrm{e}^{\mathrm{i}kx}\, \mathrm{d}k = \frac{-\mathrm{i}\pi}{\sqrt{D/\tau}}\, \mathrm{e}^{-t/2\tau} I_0(\xi)\Theta\big(\sqrt{D/\tau}\, t - |x|\big),$$

with I_0 the modified Bessel function[2] and $\xi \equiv \frac{1}{2}\sqrt{t^2/\tau^2 - x^2/D\tau}$. Use you favorite tool to visualize the propagation of the wave packet. Which properties do the coefficients D and τ have to satisfy for the evolution to be *causal*, i.e. respect special relativity?

[1] Such a modification was introduced in 1958 by C. Cattaneo, in the case of heat diffusion: in that context, the analog of Eq. (2) is known as *Maxwell–Cattaneo equation*.

[2] Check chapter 10 of the NIST Digital Library of Mathematical Functions: `https://dlmf.nist.gov`