Non-equilibrium physics WS 18/19 – Exercise Sheet 1:

Universität Bielefeld
Instructors: Jun.-Prof. Dr. S. Schlichting, D. Schröder

1 Discussion:

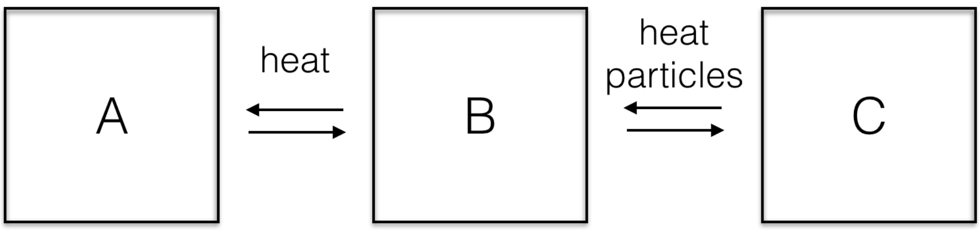
i) Briefly discuss the meaning of the *local equilibrium assumption* for discrete and continuous systems

ii) Briefly discuss the meaning of *affinities and fluxes* for equilibrium and non-equilibrium systems

2 In-class problems:

2.1 Containers

Consider a system composed of three isolated sub-systems A, B, C. Initially each system is in equilibrium, with internal energies U_0^A, U_0^B, U_0^C, containing N_0^A, N_0^B, N_0^C molecules of an ideal gas in volumes V_0^A, V_0^B, V_0^C. Subsequently, the isolation is removed in such a way that sub-systems A and B can only exchange heat with each other, while sub-systems B and C can exchange both particle number and heat.



i) Express the global conservation laws and remaining constraints and deduce the possible variations of the extensive parameters

ii) Based on the possible variations of the extensive parameters, construct the expression for the entropy production rate dS^{tot}/dt

iii) Determine the equilibrium conditions for the system in terms of the intensive quantities $T^{(i)}, p^{(i)}, \mu^{(i)}$ in each sub-system

2.2 Ideal gas

Consider a a classical ideal gas of N identical particles described by the non-interacting Hamiltonian $H_N(\{x\},\{p\}) = \sum_{i=1}^{N} \frac{\vec{p}_i^2}{2m}$.

i) Calculate the canonical partition function

$$Z_C(T,N,V) = \frac{1}{N!}\int \left(\prod_{i=1}^{N} \frac{d^3\vec{x}_i\, d^3\vec{p}_i}{(2\pi\hbar)^3}\right)\, e^{-\frac{H_N(\{x\},\{p\})}{k_B T}}$$

and determine the internal energy $U = k_B T^2 \frac{\partial}{\partial T}\log Z_C(T,N,V)$.

$\left(\text{Cross-check: } U = \frac{3}{2}N k_B T\right)$

ii) Calculate the grand-canonical partition function based on the expansion

$$Z_{GC}(T,\mu,V) = \sum_{N=0}^{\infty} e^{\frac{\mu}{k_B T}N} Z_C(T,N,V)\ ,$$

and determine the average particle number $N = k_B T \frac{\partial}{\partial \mu}\log Z_{GC}(T,\mu,V)$.

$\left(\text{Cross-check: } N = V\left(\frac{m k_B T}{2\pi\hbar^2}\right)^{3/2} e^{\frac{\mu}{k_B T}}\right)$

iii) Based on your results, determine the equations of state $T = T(U,V,N)$ and $\mu = \mu(U,V,N)$ expressing the intensive quantities T,μ in terms of the extensive variables U,V,N

$\left(\text{Cross-check: } k_B T = \frac{2}{3}U/N \text{ and } \frac{\mu}{k_B T} = -\log\left[\frac{V}{N}\left(\frac{mU/N}{3\pi\hbar^2}\right)^{3/2}\right]\right)$

iv) Exploit the relation between the grand-canonical partition function $-k_B T\log Z_{GC} = \phi_G$ and the grand-potential $\phi_G = U - TS - \mu N$ to derive the Sackur-Tetrode equation for the entropy of an ideal gas

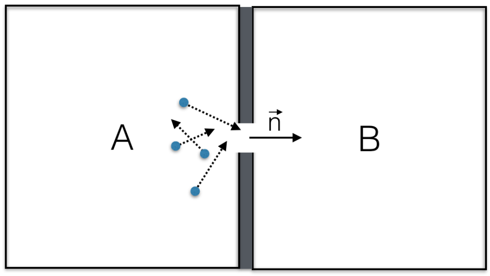
$$S(U,V,N) = N k_B\left\{\frac{5}{2} + \log\left[\frac{V}{N}\left(\frac{4\pi m U}{3N(2\pi\hbar)^2}\right)^{3/2}\right]\right\}$$

v) Based on the entropy function calculate the equation of state $p = p(U,V,N)$ for the pressure of an ideal gas. Convince yourself as a cross check that you re-produce the result $pV = N k_B T$.

3 Homework problems:

3.1 Heat and particle transfer between containers

Consider two containers A and B of identical volumina $V_A = V_B$ each filled with a classical ideal gas. Initially both systems are in equilibrium at temperatures T_A and T_B and chemical potentials μ_A and μ_B. Now a small hole of cross-section S is drilled in the wall separating the containers A and B, allowing for exchange of particle number and heat between the two containers. If we assume that the particle density is uniform in each container, the amount of particles flowing through the hole can be calculated as



$$J_N^{A\to B} = \int \frac{d^3\vec{p}}{(2\pi\hbar)^3} \int_S d^2\vec{x}\ \frac{\vec{n}\cdot\vec{p}}{m}\ f(\vec{p})\ \theta(\vec{n}\cdot\vec{p})\ ,$$

where $\int_S d^2\vec{x}$ denotes the surface integral over the area of the hole, $\vec{n}$ is the direction normal to the surface and $f(\vec{p}) = e^{\frac{\mu}{k_B T}} e^{-\frac{\vec{p}^2}{2mk_B T}}$ is the Maxwell-Boltzmann distribution for the momenta of particles in an ideal gas.

i) Show that the particle flux $J_N^{A\to B}$ through the hole from container A to container B is given by

$$J_N^{A\to B} = \frac{1}{\sqrt{2\pi m k_B T_A}}\ S\ p_A$$

ii) Determine the analogous integral expression for the energy flux $J_E^{A\to B}$ through the hole from container A to container B. Show that $J_E^{A\to B}$ is given by

$$J_E^{A\to B} = \sqrt{\frac{2k_B T_A}{\pi m}}\ S\ p_A$$

iii) Determine the explicit form of the differential equations

$$\frac{d}{dt}N^A = J_N^{B\to A} - J_N^{A\to B}\ , \qquad \frac{d}{dt}U^A = J_E^{B\to A} - J_E^{A\to B}\ ,$$

which govern the relaxation of the particle number and the internal energy, assuming that both sub-systems remain in equilibrium throughout the process.

iv) Expressing the internal energy and particle number in each sub-system in terms of the globally conserved quantity $N^{\text{tot}} = N^A + N^B$ and the difference between $\Delta N = N^A - N^B$ as $N^{A/B} = \frac{1}{2}\left(N^{\text{tot}} \pm \Delta N\right)$ (and similarly for $U^{A/B}$), determine the equations of motion governing the relaxation of ΔN and ΔU. Linearize the equations of motion for $\Delta N \ll N^{\text{tot}}$ and $\Delta U \ll U^{tot}$ and determine the relaxation rates.