Advanced statistical mechanics
(WS 12/13, FU Berlin)

Problem sheet 10 (last sheet!)

Due date: January 23, 2012

Problem 29: Barometric formula (1+3+1+2+1+1)

We want to derive the barometric formula of an ideal gas with particle mass m at temperature T in a homogenous gravitational field $\mathbf{g} = -g\,\mathbf{e}_z$, where $\mathbf{e}_z$ is the unit vector in z-direction. We consider a cubic volume V containing N particles with length, width, and height Δh, whose base is located at height z above the origin.

a) What is the Hamiltonian function of the N particles?

b) Show that the partition function of the canonical ensemble is

$$Z = \frac{(\Delta h)^{2N}}{N!\,h^{3N}} \left(\frac{\mathrm{e}^{-\beta\,m\,g\,z}(\mathrm{e}^{-\beta\,m\,g\,\Delta h} - 1)}{-m\,g\,\beta} \right)^N (2\pi\,m/\beta)^{3N/2}\,. \tag{1}$$

When calculating classically, the factor of $N!$ must be included "by hand". Comment on that!
Hints:

(i) Review the derivation of the partition function of an ideal gas without a gravitational field.
(ii) When using SI units then the volume element of phase space is $\mathrm{d}\gamma = \mathrm{d}^{3N}\mathbf{p}\;\mathrm{d}^{3N}\mathbf{x}/h^{3N}$, where h is Planck's constant.

c) Show that if $\beta\,m\,g\,\Delta h \ll 1$ this can be approximated by

$$Z \approx \frac{V^N}{N!\,h^{3N}}\mathrm{e}^{-\beta\,N\,m\,g\,z}\,(2\pi\,m/\beta)^{3N/2}\,. \tag{2}$$

Now we take V to be so small that the particle density inside of V is approximately constant and so large that the relative particle fluctuations $\Delta N/N$ vanish. In that case the thermodynamic potentials of the canonical and grand canonical ensemble are the same. Consequently, the grand canonical Helmholtz free energy coincides with the canonical free energy

$$F = -\beta^{-1}\ln(Z). \tag{3}$$

d) Using $p\,V = N\,k\,T$, calculate the chemical potential μ as a function only of p, T and z from the Helmholtz free energy. During the calculation, you will have to take derivatives with respect to N. To do this use Stirling's approximation $\ln N! \approx N\ln N - N$.
Hint: It turns out that μ is of the form $\mu(p,T,z) = c_1 z + c_2 \ln p + c_3(T)$, where c_j are constants that might depend on T.

Now we assume that different volumes of the gas are at equilibrium. This implies that μ is constant in z. For simplicity we will further assume that T is also independent of z, but of course, p will depend on z.

e) Find a differential equation for $p(z)$.

f) Solve the differential equation and thereby find a solution for $p(z)$ in terms of $p(0)$.

Problem 30: Equation of state for quantum gases (2+1*+1+3+1)

For the classical ideal gas we know that

$$p\,V = N\,k\,T, \tag{4}$$

here we want to derive the equivalent equation for gases of indistinguishable particles.

The one particle energies of a ideal quantum gas of Bosons or Fermions of mass m and spin S in a d-dimensional cubic Volume V are given by

$$E_{\mathbf{k}} = \frac{\hbar^2 |\mathbf{k}|^2}{2m} \tag{5}$$

where $\mathbf{k} \in \mathbb{R}^d$ is the quantized wave vector whose components are integer multiples of

$$\Delta k = \frac{2\pi}{V^{1/d}}. \tag{6}$$

a) Calculate the density of states

$$D(E) := \frac{2S+1}{\Delta k^d} \Theta(E) \frac{\partial}{\partial E} \varphi(E) \tag{7}$$

where

$$\Theta(E) = \begin{cases} 0 & E < 0 \\ 1 & E \geq 1 \end{cases} \tag{8}$$

$$\varphi(E) = \int_{\mathbf{k}: E_{\mathbf{k}} \leq E} \mathrm{d}^d k \tag{9}$$

Hint: Use that $E_{\mathbf{k}}$ is rotation invariant and that $|\mathbf{k}|$ can be written as a function of E, which allows to calculate the integral in spherical coordinates.

b) *Bonus question:* Explain why (7) is the correct formula for the density of states.

We know from the lecture that

$$p\,V = \beta^{-1} \ln Z \tag{10}$$

where Z is the so called *grand canonical potential* or *grand canonical partition sum* which we had calculated in Problem 28 h) on the last sheet.

c) Write out (10) for Fermions and Bosons.

If the volume V is sufficiently large and the chemical potential sufficiently small, the sums in the expressions from question c) can be approximated by integrals, i.e., you are allowed to make the following replacements

$$\sum_k f(E_k) \quad \longleftrightarrow \quad \int_{-\infty}^{\infty} f(E) D(E) dE. \tag{11}$$

d) Use the above approximation and partial integration to show that for both Fermions and Bosons

$$p\,V = \frac{2}{d} U \tag{12}$$

where

$$U := \sum_k E_k \langle N_k \rangle \tag{13}$$

is the inner energy and $\langle N_k \rangle$ is the Fermi-Dirac or Bose-Einstein distribution we derived in Problem 28 i). *Hint:* You will have to use the approximation in twice. If you were unable to solve a) you can use that the density of states is of the form $D(E) = C E^{d/2-1} \Theta(E)$, with $C = C(S, m, d)$ independent of E.

e) Is the result in Eq. (12) the same as for a classical ideal gas? Justify your answer!