

## Sheet 9

Hand in via OLAT until 26.01.2020 18:00.

### 25) Rotating Boltzmann gas ( $8=5+3$ Points)

Consider a Boltzmann gas, that is inside a cylindrical container of radius  $R$  and height  $h$ . The gas is rotating inside the container, with a angular momentum  $\mathbf{\Omega} = \Omega \mathbf{e}_z$ . It is possible to describe the effect of rotation on the gas molecules by considering an additional potential (that is connected to the centrifugal force)

$$V_{rot}(\mathbf{r}) = -\frac{1}{2}m(\mathbf{\Omega} \times \mathbf{r})^2.$$

- (i) Show that the free energy of the rotating gas can be written as

$$F = F_0 - NT \ln \left( \frac{1}{V} \int e^{-V_{rot}(\mathbf{r})/T} dV \right),$$

with  $F_0$  the free energy of the Boltzmann gas, familiar from the lecture. Afterwards, calculate the volume integral in the rotating coordinate system.

- (ii) Calculate the inner energy  $E$  of the rotating gas.

*Hint: You can consider the inner energy  $E_0$  of the non-rotating gas as known and you do not have to calculate it.*

## 27) Gas of diatomic molecules (12=2+4+4+2 Points)

Consider an ideal gas of molecules, build from two different kinds of atoms. In the lecture the free energy of an ideal Boltzmann-gas has been derived

$$F = -NT \ln \left[ \frac{eV}{N} \left( \frac{mT}{2\pi\hbar^2} \right)^{3/2} \sum_k e^{-\frac{\epsilon'_k}{T}} \right],$$

with  $\epsilon'_k$  denoting the energy of the quantum states of each molecule, with quantum numbers  $k$ . In the following we assume, that the electrons of the diatomic gas molecules are in the lowest quantum states, writing their energy as a constant  $\epsilon_0$ . The quantum energy levels of a diatomic molecule are then given as

$$\epsilon_{n,K} = \epsilon_0 + \hbar\omega \left( n + \frac{1}{2} \right) + \frac{\hbar^2}{2I} K(K+1),$$

with a contribution to the energy from oscillations, with oscillation quantum number  $n$  and a contribution from rotations, with rotation quantum number  $K$  and moment of inertia  $I$  of the molecule.

- (i) Show that the free energy is given as a superposition of the different energy contributions

$$F = -NT \ln \left[ \frac{eV}{N} \left( \frac{mT}{2\pi\hbar^2} \right)^{3/2} \right] + F_{osc} + F_{rot} + N\epsilon_0.$$

*Hint: When summing all rotation quantum states  $K$ , a degeneracy factor  $g_K = 2K + 1$  has to be included in the partition function of rotations  $Z_{rot}$ , counting the degeneracy of rotation modes along the direction of angular momentum.*

- (ii) Let us determine the contribution of rotations to the free energy  $F_{rot}$  first. Consider the limit of large temperatures  $T \gg \frac{\hbar^2}{2I}$  and calculate the free energy  $F_{rot}$ . Continue by calculating the contribution of rotations to the heat capacity  $c_V$  in the limit of large temperatures.

*Hint: Argue, that in the limit of large temperatures the summation of rotation quantum numbers  $K$  can be expressed as an integral and that large quantum numbers  $K$  are dominating, making it possible to approximate  $K + 1 \approx K$ .*

- (iii) Next calculate the contribution to the free energy coming from oscillations  $F_{osc}$ . Use your result to determine the contribution to the heat capacity and comment on the temperature dependence. Afterwards consider the limit of high temperatures  $T \gg \hbar\omega$  and expand the heat capacity up to order  $\mathcal{O}\left(\frac{\hbar\omega}{T}\right)$ .

*Hint: When summing the quantum numbers, make use of the geometric sum.*

- (iv) Give the heat capacity  $c_V$  of the diatomic molecule gas and compare your result to the result obtained from the equipartition theorem that was derived in the lecture

$$c_V = \frac{l}{2},$$

for a suitable choice of  $l$  in case of a diatomic molecule gas.