# Exercise 06

| Name: | Matriculation number: |
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**The exercise is due on Wednesday, May 30, 8 am.**

## 6.1 Text book

Read sections 3.1 and 4.1 in G.H. Findenegg, T. Hellweg „Statistische Thermodynamik" and https://en.wikipedia.org/wiki/Dulong-Petit_law

## 6.2 Exponential functions

In statistical thermodynamics functions of the form $\exp(\frac{-\epsilon}{kT})$ are of big importance. To get a little insight into these function:

(a) Draw the function $y = \exp(\frac{-\epsilon}{kT})$ as a function of $T$ in the range $0 < T < \infty$.

(b) Expand $y$ for high temperatures $\left(\frac{-\epsilon}{kT} << 1\right)$ using a Taylor expansion

(c) Calculate the derivations $\frac{\mathrm{d}y}{\mathrm{d}T}$, $\frac{\mathrm{d}y}{\mathrm{d}1/T}$ and $\frac{\mathrm{d}(1-y)^{-1}}{\mathrm{d}T}$.

## 6.3 Thermodynamic state functions of the vibrational partition function

Using the vibrational partition function:

$$z_{vib} = \frac{\exp(-h\nu_E/2kT)}{1 - \exp(-h\nu_E/kT)} \tag{1}$$

where $\nu_E$ denotes the frequency of the particles as well as the systems partition function of an ideal crystal

$$Z(N, V, T) = (z_{vib})^{3N} \tag{2}$$

calculate $U, S, A, H, G, \mu$ for an ideal crystal.

## 6.4 Entropy of an Einstein-crystal

Find an expression for the entropy of an Einstein-crystal as a function of the temperature $T$.

## 6.5 Eigen frequencies of the Einstein-function

Fit the eigen frequencies of the Einstein-function $\nu_E$ with respect to the observed molecular heat of KCl (*Hint: Use a data analysis program with a non-linear fitting algorithm like Origin or Python*).

| $T$/K | 10 | 20 | 30 | 40 | 60 | 80 | 100 | 140 | 180 | 220 |
|---|---|---|---|---|---|---|---|---|---|---|
| $c_v$/JK$^{-1}$mol$^{-1}$ | 0.032 | 2.84 | 7.96 | 14.24 | 25.24 | 32.64 | 37.24 | 42.08 | 44.4 | 45.6 |