Exercise 03

Name:	Matriculation number:
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The exercise is due on Wednesday, May 09, 8 am.

3.1 Text book

Read section 2.1 in G.H. Findenegg, T. Hellweg „Statistische Thermodynamik".

3.2 Lagrange multipliers

The area of a rectangular triangle with hypotenuse c is defined as

$$A(x,y) = \frac{1}{2}xy. \tag{1}$$

x and y denote the catheti of the triangle. For a rectangular triangle the sentence of Pythagoras can be applied:

$$g(x,y) = x^2 + y^2 - c^2 = 0 \tag{2}$$

Search for the triangle with the largest area following the methods as described below.

(a) Calculate $A(x,y)$ by reformulation of $g(x,y)$ to a function $y(x,c)$ and inserting in $A(x,y)$

(b) Calculate $A(x,y)$ using the method of Lagrange multipliers.

3.3 Temperature-dependent two-level system

An energy diagram consists of two energy levels with a distance of k_bT. Calculate the ratio of population for $T = 0\text{K}, 298\text{K}, 1000\text{K}$.

3.4 Partition function

The partition function q is an important quantity which links the quantum energy levels of microscopic particles to the thermodynamic state functions. For a single particle the partition function is given as

$$q = \sum_{i=1}^{n} \exp\left(-\beta\epsilon_i\right) \tag{3}$$

The factor

$$\beta = \frac{1}{k_BT} \tag{4}$$

is called thermodynamic temperature, where the k_B is the Boltzmann constant and T is the absolute temperature. ϵ_i are the n accessible quantum energy levels which can be obtained by solving the stationary Schrödinger equation for the particle. Note that q is a sum over these energy levels and the contribution of each energy level to the total value of q is given by the exponential function $\exp(-\beta\epsilon_i)$. Let us consider a particle in a one-dimensional box of length L It's first n energy levels are given as

$$\epsilon_i = \frac{\hbar^2\pi^2}{2mL^2}i^2 \qquad i = 1, 2, ...n \tag{5}$$

(a) Calculate the partition function for an electron ($m = 9.109 \cdot 10^{-31}$ kg) in a one-dimensional box of length $L = 500$ pm at $T = 300$ K. Assume that 10 energy levels are accessible.

Next you will examine the sensitivity of the individual term $\exp(-\beta\epsilon_i)$ on various parameters. Use $m = 9.109 \cdot 10^{-31}$ kg, $L = 500$ pm and ϵ_{10} at $T = 300$ K as a starting point and vary one parameter at a time. Plot $\exp(-\beta\epsilon_i)$ as a function of

(b) i from $i = 1$ to $i = 100$

(c) T from $T = 1$ K to $T = 500$ K

(d) β from $T = 1$ K to $T = 500$ K

(e) L from 1 pm to 1 nm (logarithmic scale)

(f) m from 10^{-31} kg to 10^{-26} kg (logarithmic scale)

(g) Comment on the results.