Exercise 1. *Ideal phonons in a harmonic trap.*

In this exercise we consider an ideal gas of phonons as an example of bosonic particles confined in a three-dimensional harmonic potential. Observe the differences to the cases of classical and fermionic particles in the same harmonic potential, which we discussed in Sheet 1, Exercise 3, and for Sheet 3, Exercise 2, respectively.

The energy states of the phonons are given by

$$E_{\boldsymbol{a}} = \hbar\omega(3/2 + a_x + a_y + a_z) \ , \tag{1}$$

including the zero point energy of $E_0 = 3\,\hbar\omega/2$. The occupation number of the oscillator modes of the state $E_{\boldsymbol{a}}$ is given by $\boldsymbol{a} = (a_x, a_y, a_z)$ with $a_i \in \{0, 1, 2, ...\}$.

(a) Consider the high-temperature, low-density limit ($z \ll 1$). Derive the grand canonical partition function for the phonons, $\mathcal{Z}_\mathrm{b}$, and compute the grand potential Ω_b. Take into account also the zero-point energy of the harmonic oscillators. Show that

$$\Omega_\mathrm{b} \propto g_4\left(z\mathrm{e}^{-3\beta\hbar\omega/2}\right) \ , \tag{2}$$

where the function $g_s(z)$ is defined as

$$g_s(z) = \sum_{l=1}^{\infty} \frac{z^l}{l^s} \ . \tag{3}$$

(b) Derive the internal energy U and the average particle number $\langle N\rangle$. Follow the same approach as in Sheet 3, Exercise 2 in order to obtain U in terms of N.

(c) Compute the specific heat C_N for constant particle number.

Compute the thermal expansion coefficient α. Use the average square displacement of the harmonic oscillator $r_\mathrm{eff} = x_0^2(a_x + a_y + a_z)$ in order to define an effective volume $V_\mathrm{eff} = 4\pi/3\,\langle r^2\rangle^{3/2}$. Give an interpretation of V_eff.

(d) Plot your results for U, C, and α for the classical, the fermionic, and the bosonic case and note the differences.

(e) Find the critical temperature T_c at which Bose-Einstein condensation occurs. How can this be reconciled with the high-temperature, low-density limit?

Hint. The chemical potential can not be larger than the lowest energy level of the particles.

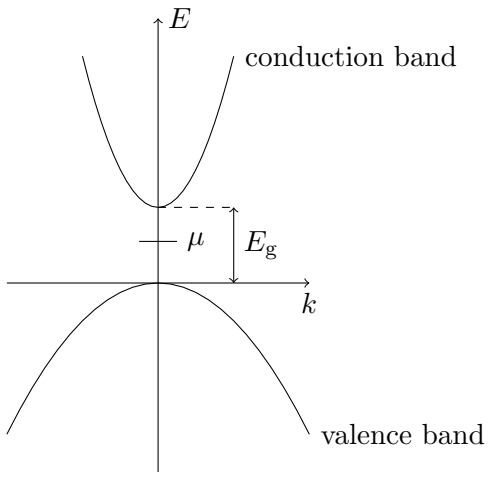
Exercise 2. *Behavior of excitations in a semiconductor.*

In this exercise we analyze the properties and behavior of electron-excitations of a semiconductor at finite temperature. In solid state theory, electronic states $|\boldsymbol{k}, \alpha\rangle$ are usually labeled by a *pseudomomentum* $\boldsymbol{k} = (k_x, k_y, k_z)$ and a band-index $\alpha \in \{1, 2, \dots\}$. For a crystal with lattice constant a, the pseudomomentum takes values in the so-called *Brillouin zone* $\{-\pi/a, \pi/a\}^3$. Assuming a cubic crystal with side-length L there exist $(L/a)^3$ equally distributed $\boldsymbol{k}$-vectors in this Brillouin zone. Each of the states is doubly degenerate due to the spin, such that there are in total $2(L/a)^3$ states for each band.

In order to simplify the treatment, we only take into account two bands whose energies are approximated as parabolic,

$$\epsilon_{\mathrm{v}}(\boldsymbol{k}) = -\frac{\hbar^2 \boldsymbol{k}^2}{2m_{\mathrm{v}}} \qquad \epsilon_{\mathrm{c}}(\boldsymbol{k}) = E_{\mathrm{g}} + \frac{\hbar^2 \boldsymbol{k}^2}{2m_{\mathrm{c}}} \ , \quad (4)$$

as shown in the figure. Here the indices v and c stand for valence and conduction band, respectively. The parameters m_{v} and m_{c} which define the curvature of the two bands are called *effective masses* and can in general be different from one another and from the electron mass. The *bandgap*, E_{g}, is the energy difference between the bottom of the conduction band and the top of the valence band.



Assume for this exercise that the bandgap is much larger than the thermal energy and the chemical potential lies within the gap, $\beta E_{\mathrm{g}} \gg \beta\mu \gg 1$.

(a) Assume at first that the particle number is not fixed and calculate the grand potential Ω of this system.

Hint. For large L, a sum over $\boldsymbol{k}$ can be approximated by an integral:

$$\sum_{\boldsymbol{k}} \approx \int_{-\pi/a}^{\pi/a} \mathrm{d}^3 k \, \frac{L^3}{8\pi^3} \quad (5)$$

(b) In a realistic system, the particle number is fixed, as every atom in the solid contributes a specific number of electrons. We assume here a particle number, such that the lower band is completely filled at zero temperature, i. e. $N = 2(L/a)^3$. Calculate the chemical potential $\mu(T)$ at finite temperature.

(c) Starting from your result for Ω, calculate the internal energy $U(T,N) - U(T=0,N)$ (for $N = 2(L/a)^3$), using a Legendre transform.

Hint. The final result is given by

$$U(T,N) - U(T=0,N) = N \left(\frac{k_{\mathrm{B}}T}{2\pi\hbar^3}\right)^{3/2} \mathrm{e}^{-\beta E_{\mathrm{g}}/2} \, (m_{\mathrm{v}} m_{\mathrm{c}})^{3/4} \, (3k_{\mathrm{B}}T + E_{\mathrm{g}}) \ . \quad (6)$$

(d) A picture that is frequently used in solid state theory is that of electrons and *holes*: When an electron is excited to the conduction band, it leaves an empty state in the valence band. This empty state now behaves like a particle itself and is called a *hole*. Therefore an excitation can be regarded as a creation of two particles, similar to the creation of particle-antiparticle pairs in particle physics.

Use this scheme to interpret the calculated internal energy in terms of the equipartition law for an ideal gas. How many electrons are in the conduction band?