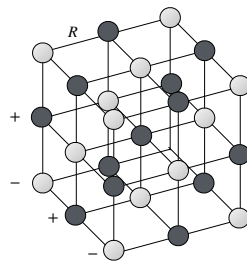


Sheet 01: Introduction

Discussion: Thursday, 11.05.23

Exercise 1 Ionic Crystals: Why is Interaction Short-Ranged?

Consider a face-centered cubic NaCl crystal, consisting of Na^+ (dark grey dots) and Cl^- ions (light grey dots in the sketch of the unit cell).



(1.a) Show that the Coulomb interaction of an ion with all others leads to the energy

$$E_{\text{Coul}} = -\frac{e^2}{4\pi\epsilon_0} \frac{a_M}{R} \quad (1)$$

R is the distance between two ions and a_M the Madelung constant. Find a formal expression for a_M and show that a_M depends only on the lattice structure.

Calculating the Madelung constant a_M is usually not trivial.

(1.b) In the Evcjen method one considers the atoms on the surface of a cube (with arbitrary sidelength nR , $n = 2, 3, \dots$) with a correcting factor $1/2$, the atoms on the edges with $1/4$ and the atoms on the corners with $1/8$. Calculate a_M for a cubic crystal of side length $4R$. For computer lovers: Find computer-based solutions for larger side lengths. (Hint: for an infinitely large cube $a_M = 1.748$.)

Exercise 2 Interaction energy: bulk versus surface

Consider a homogeneous system in a volume $V = L^3$, in which interactions are (effectively) screened on a length scale $\xi \ll L$. Argue that the interaction energy in the bulk scales as $L^3\xi^3$, while the interaction energy on the surface scales as $L^2\xi^4$.

Exercise 3 Isotherms in the Van der Waals gas

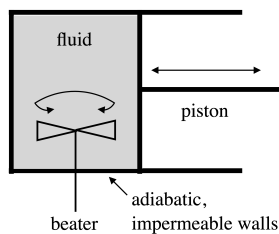
Plot the isotherms (curves of equal temperature Θ) of nitrogen (N_2) in a Π - V diagram for $\Theta = 20K, 40K, \dots 300K$. Consider N_2 as

- a Van der Waals gas with coefficients $a = 1.370 \text{ bar dm}^6 \text{ mol}^{-2}$ and $b = 0.0387 \text{ dm}^3 \text{ mol}^{-1}$ (these values are also found in Chapter 3 of the notes) and
- an ideal gas.

Some of the Van der Waals isotherms should show something special. Do these curves look physically meaningful?

Exercise 4 Adiabatic state changes

We go back to Section 5.4 in the notes. We considered the following process in a container with a beater and a piston and adiabatic impermeable walls.



- beater is active $(\Pi_1, V_1) \rightarrow (\Pi'_1, V_1)$.
- piston is pulled out $(\Pi'_1, V_1) \rightarrow (\Pi'_2, V_2)$.
- beater is active $(\Pi'_2, V_2) \rightarrow (\Pi_2, V_2)$.

This process should leave environment \mathcal{E} unchanged except for the lowering of a mass. Pulling out the piston (ii) obviously involves a change of volume of \mathcal{E} .

- Under which circumstances can we neglect this?

Moreover we discussed that process (i)-(iii) cannot be done adiabatically reversibly. Yet, apart from the adiabatic process (ii) we only considered partial processes at constant volume V .

- Explain that (Π_2, V_2) is reachable from (Π_1, V_1) also with partial processes at constant pressure Π apart from (ii).
- Is the complete process you have thought up adiabatically reversible?