Problem 1: Tetragonal lattice (15 points)

A hypothetical monoatomic substance crystallizes in a centered tetragonal structure. The conventional unit cell can be described by primitive vectors \((a, 0, 0), (0, a, 0), (0, 0, c)\) with \(c = 3a/2\) and a basis consisting of two atoms at positions \((0, 0, 0)\) and \((a/2, a/2, c/2)\). The lattice constant is \(a = 4.2\ \text{Å}\).

a) Calculate the maximum space filling for this lattice.
b) Find the primitive vectors of the reciprocal lattice.
c) A powder specimen of the substance is analyzed by X-ray diffraction using the Debye-Scherrer method. The wavelength of the X-rays is 1.5 Å. Calculate the angles of the first four diffraction rings.

Problem 2: Phonon dispersion in a chain with long-range interactions (Ashcroft-Mermin 22.1, 15 points)

Consider a one-dimensional chain of identical atoms of mass \(M\). The springs are not only between nearest neighbors but between all pairs of atoms. Thus, the elastic energy reads

\[ E_{el} = \frac{1}{2} \sum_n \sum_{m>0} K_m (u_n - u_{n+m})^2 \]

where \(u_n\) is the displacement of atom \(n\).

a) Find the dispersion relation, i.e., the vibrational frequency \(\omega\) as a function of wave number \(q\).
b) Assume \(K_m = K_0/m^p\) with \(p > 1\) a parameter controlling how rapidly the interaction drops off with distance. Study the long-wavelength limit of the dispersion relation for \(p > 3\). Determine the sound velocity.
c) Investigate the long-wavelength limit of the dispersion relation for \(1 < p < 3\). Show that one gets anomalous sound, i.e., the frequency is not proportional to the wavenumber. (Hint: You may want to approximate the \(m\)-sum by an integral.)

Problem 3: Ionic crystals (10 points)

Consider a material consisting of two types of ions with charges \(+e\) and \(-e\), respectively. In addition to the Coulomb interaction, they have a short-range repulsive potential of the type \(A/r^{12}\).

a) Assume the substance crystalizes in the NaCl structure. Find the lattice constant by minimizing the cohesive energy. The Madelung constant for the NaCl structure is \(\alpha = 1.7476\). (You can restrict the repulsive interaction to the nearest neighbor sites on the lattice.)
b) Do the same for the CsCl structure with a Madelung constant of \(\alpha = 1.7627\).
c) Which structure will the material choose?