Session 6 —Guided problem solving session. Lattice dynamics in periodic systems: phonons.

1. **Classical 1D phonons:** Consider a chain of N particles of mass m in a 1 dimensional space, with periodic boundary conditions. The atoms are at equilibrium in equally spaced positions $\bar{x}_i = ia$, where a is the lattice spacing, and are free to move around those position by a small displacement u_i: $x_i = ia + u_i$, subject to a force from their nearest neighbours with intensity K, linear in $u_i - u_{i\pm1}$.
   a) Write the classical Hamiltonian and relative equations of motion for this system.
   b) Look for a wave-like solution to these equations of motion of the form $u_j = A_k e^{i(kja-\omega_k t)}$: what are the possible values of ω_k as a function of k?
   c) What is the infinite chain $N \to \infty$ limit (phononic dispersion)?

2. **Quantum 1D phonons:** Consider the same system, but this time we want to treat the atoms in a quantum mechanical way. To do this let us consider the quantum displacement operators χ_i corresponding to the classical u_i.
   a) Write the quantum Hamiltonian for this system.
   b) Write the Fourier transform of the displacement operators $\chi_i \to \chi_k$ and the corresponding one for the momenta (hint: take the opposite sign). Verify that these operators still satisfy the commutation relations and rewrite the Hamiltonian in this new basis.
   c) Solve the Hamiltonian as a sum of quantum harmonic oscillators.
   d) Compare your result to the classical one, and the infinite chain limit. What happens at 0 temperature?
   e) How can we count the phonon modes up to a given energy considering the behaviour you found for low temperatures? What would this mean for the heat capacity?

3. **Chain phonons in 3D** Consider the same 1D chain, but embedded in a 3D space, so that each atom is allowed to have a small displacement in any 3 directions.
   a) In the limit of small atomic displacements, write the Hamiltonian for this system.
   b) Solve the equations of motion looking once more for wave-like solutions. Compare the results to the exactly 1D chain.

4. **1D phonons with a basis:** Consider now another 1D chain (in a 1D space), but this time made up of $2N$ particles of alternating types A and B, with masses m and M, respectively.
   a) Write the Hamiltonian and equations of motion for this system.
   b) Find the solutions for each k and compare them to the $M = m$ limit and to the simple A-B dimer case.
   c) How can we count the phonon modes at a given energy for the new modes by just considering an average value $\hbar\bar{\omega}$ for each mode? How would the heat capacity behave?

5. **3D phonons:** How would the problem change for, say, a simple cubic 3D model system?