Session 7 -Individual problem solving session.

- **1D phonons with a basis:** Consider a 1D chain (in a 1D space) made up of $2N$ particles of alternating types A and B, with masses m and M, respectively, uniformly spaced at distance a, with periodic boundary conditions.

  1. Write the Hamiltonian and the equations of motion for the system.
  2. Assume periodic Bloch-type solutions and determine the allowed values of the corresponding wavevector k. How many modes per k are defined ?
  3. Find the solutions for each k and compare them to the $M = m$ limit and to the simple A-B dimer case.
  4. Assume the extra phonon modes can be approximated as having an average, k-independent, energy $\hbar\bar{\omega}$. How would the heat capacity of the system behave?

- **Parallel monoatomic chains**
  Consider two monoatomic chains of N atoms with periodic boundary conditions, each lying along x, parallel to one another such that the position of the i^{th} atom in the first chain is $(x_i, -Y)$ while the position of the i^{th} atom in the second chain is (x_i, Y). The interatomic distance in each chain is a, the masses of the atoms in the chains are m_A and m_B respectively for the first and the second chain.

  1. $Y \to \infty$ limit: Let us assume that the two chains do not interact. Let us also assume that the Born-Oppenheimer approximation is valid. Within the harmonic approximation, assuming the radial force constant is the same, c_X, for each bond between two adjacent atoms, and is non-zero only for the nearest neighbors, describe the phonons of the system and draw the dispersion relation between the eigenfrequency ω and the wavevector of the vibration, k. Assume that the motion of the atoms is confined to the x axis alone.
  2. Finite Y: Now, as the chains approach one another, assume that a bond is formed between the i^{th} atom of each chain and the chains are at the equilibrium distance of this new bond. The radial force constant associated to this bond is c_Y and $c_Y < c_X$. Within the harmonic approximation, again, how do the phonons of the system change w.r.t. the previous exercise? Draw the new dispersion relation between ω and k, assuming again that the motion of the atoms is confined to the x axis alone.
  3. Y = r_m - Lennard Jones interaction: Now assume that the interatomic interaction between the chains is of the Lennard Jones type: $V(r) = \epsilon\left[-2r_m^6/r^6 + r_m^{12}/r^{12}\right]$, where ϵ is the depth of the potential at its minimum, and r_m is the interchain separation at this minimum. Starting from two chains that are not in their equilibrium separation, Y=r_m, solve the coupled equations for the atoms in each chain and determine the phonon dispersion. How does it differ from the previous problem? As earlier, assume that the motion of the atoms is confined to the x axis alone.
  4. Y = $2r_m$: Consider now an alternating array of 2N chains along the y-direction and the chain separation to be at its equilibrium value. Allowing the atoms to move both in x and y directions, determine the eigenfrequency of the system that corresponds to a wavevector $\boldsymbol{k} = (0, \frac{\pi}{2r_m})$.

- **Test of the Adiabatic Approximation:**

  Consider two 1D harmonic oscillators with normal frequencies $\omega_1 = \omega$ and $\omega_2 = \mu\omega$ (assume $\mu \gg 1$) coupled by a bi-linear potential $V_{12} = \frac{1}{2}m\lambda^2\omega^2 q_1 q_2$, where q_1 and q_2 measure the displacement from equilibrium of the two oscillators.

  1. Write down the Hamiltonian of the system.

2. By considering a suitable unitary linear variable transformation

$$Q_1 = f_1(q_1, q_2) = U_{11} q_1 + U_{12} q_2,$$

$$Q_2 = f_2(q_1, q_2) = U_{21} q_1 + U_{22} q_2,$$

   show that the system is equivalent to a system of two decoupled harmonic oscillators.
3. Find the exact eigenvalues of the system
4. Find the conditions to be satisfied by the λ and μ parameters so that the V_{12} coupling does not make the system unstable.
5. Assume those conditions are satisfied, and write the equations of the two original oscillators described in the beginning within the adiabatic approximation.
6. Find the eigenvalues of the system in the adiabatic approximation and compare them with the exact ones computed previously.

The End.