Problem 16: Vibrations of a linear chain **(4 points)**

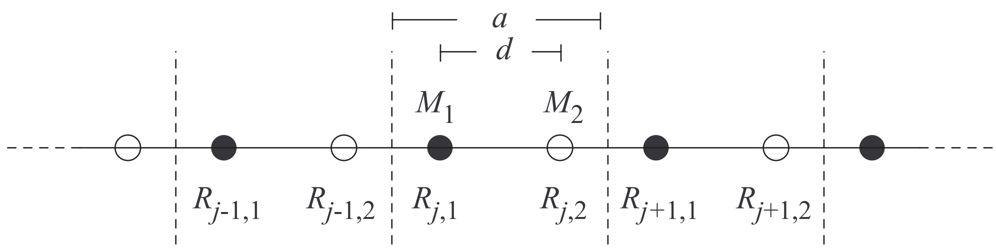
Consider a linear chain with two atoms of masses M_1 and M_2 per unit cell. The atoms are at the positions $X_{j,\nu} = R_j + \tau_\nu + u_{j,\nu}$. The lattice vector $R_j = j \cdot a$ and the basis vector τ_ν describe the equilibrium position and $u_{j,\nu}$ gives the elongation of an atom. Two neighboring atoms interact via a potential

$$V(x) = D\left\{\mathrm{e}^{-2\alpha x} - 2\,\mathrm{e}^{-\alpha x}\right\} .$$

Thus, the potential energy of the chain is given by

$$E^{\mathrm{el}} = \sum_i \left\{V\left((X_{i,1} - X_{i-1,2}) - d\right) + V\left((X_{i,2} - X_{i,1}) - d\right)\right\}$$

with the equilibrium distance d between the atoms.



a) Plot the pair potential $V(x)$.

b) Calculate the force constants $\Phi(j\,\nu,\, j'\,\nu')$.

c) Set up the dynamic matrix $D_{\nu,\nu'}(q)$ and calculate the vibrational frequencies $\omega(q)$ of the chain. Give the values of $\omega(q)$ for $q = 0$ and $q = \pm\pi/a$.

d) Consider the case $M_1 = M_2 = M$. Give the frequencies $\omega(q)$.

Problem 17: Phonons of a hexagonal lattice (8 points)

A two-dimensional lattice is described by the vectors

$$\vec{a}_1 = (1,\, 0)\, a \qquad \text{and} \qquad \vec{a}_2 = \left(-1,\, \sqrt{3}\right) \frac{a}{2} \,.$$

The atoms of the lattice interact via central forces with spring constant K between nearest neighbors. The potential energy of this system has the form

$$E^{\text{el}} = \frac{1}{2} \sum_j \sum_{j'} \frac{K}{2} \left[|\vec{R}_j + \vec{u}_j - \vec{R}_{j'} - \vec{u}_{j'}| - |\vec{R}_j - \vec{R}_{j'}| \right]^2 \,.$$

The sum over j' includes only nearest neighbors of $\vec{R}_j$. Derivatives with respect to the elongations $\vec{u}_j$ and $\vec{u}_{j'}$ give the force constants. They have for $j \neq j'$ the form

$$\Phi_{\alpha,\alpha'}(\vec{R}_j, \vec{R}_{j'}) = \begin{cases} -K \dfrac{(\vec{R}_j - \vec{R}_{j'})_\alpha (\vec{R}_j - \vec{R}_{j'})_\alpha}{|\vec{R}_j - \vec{R}_{j'}|^2} & \text{for} \quad |\vec{R}_j - \vec{R}_{j'}| = 1\,\text{n. N. distance} \\ 0 & \text{else} \end{cases} \,.$$

The force constants for $j = j'$ can be calculated from the *acoustic sum rule*.

a) Calculate the force constants $\Phi_{\alpha\alpha'}(\vec{R}_j, 0)$ for the six $\vec{R}_j$ of the nearest neighbors of an atom at $\vec{R}_{j'} = \vec{0}$ and *then* for $\vec{R}_j = \vec{0}$.

b) Set up the dynamical matrix.

c) Calculate the vibrational frequencies $\omega(\vec{q})$ at the high-symmetry points

$$\vec{q} = (0,0)\,\frac{2\pi}{a} \quad (\Gamma\,\text{point}) \qquad\qquad \vec{q} = \left(0,\, \frac{1}{\sqrt{3}}\right) \frac{2\pi}{a} \quad (M\,\text{point})$$

$$\vec{q} = \left(\frac{1}{3},\, \frac{1}{\sqrt{3}}\right) \frac{2\pi}{a} \quad (K\,\text{point}) \qquad\qquad \vec{q} = \left(\frac{2}{3},\, 0\right) \frac{2\pi}{a} \quad (K'\,\text{point})$$

and along the high-symmetry lines Γ-M, M-K, K-Γ of the Brillouin zone. Plot $\omega(\vec{q})$ along these lines.

Problem 18: Phonons of a linear chain (4 points)

The Hamilton operator of a linear chain (lattice constant a) with atoms of mass M is given by

$$\hat{H} = \frac{1}{2} \sum_j \frac{\hat{P}_j^2}{M} + \frac{1}{2} K \sum_j (u_j - u_{j-1})^2 \,.$$

Show that $\hat{H}$ can be transformed into a sum of Hamilton operators of decoupled harmonic oscillators by employing (see lecture)

$$u_j = \sqrt{\frac{\hbar}{N M}} \sum_q \frac{1}{\sqrt{2\,\omega(q)}} \left(\hat{a}(q) + \hat{a}^+(-q)\right) \mathrm{e}^{i\,q\,R_j} \,,$$

$$\hat{P}_j = \sqrt{\frac{\hbar M}{N}} \sum_q \sqrt{\frac{\omega(q)}{2}} \frac{1}{i} \left(\hat{a}(q) - \hat{a}^+(-q)\right) \mathrm{e}^{-i\,q\,R_j}$$

with $R_j = j \cdot a$.

Hint: use the explicit form of the dispersion relation $\omega(q)$ of the linear chain.