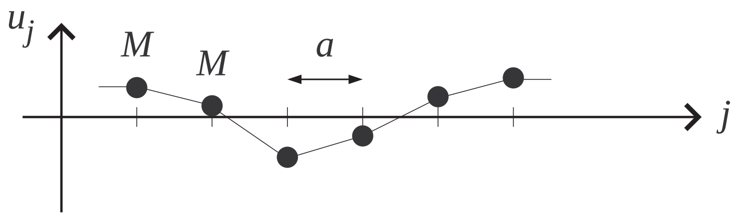
Problem 6: Phonons in stiff layers [2 points]

Consider a two-dimensional sheet of material or (simpler but analogous) a one-dimensional wire. The system is stiff, i.e. bending costs elastic energy.

A simple linear-chain model might look as follows (for small vertical displacements u_j):



$$V = \sum_{j=-\infty}^{\infty} \alpha \cdot (u_{j+1} + u_{j-1} - 2u_j)^2 \ .$$

Notice that different from a vibrating string, drum etc. the elastic energy does <u>not</u> result from elongation of the bonds, but from resistance of the material against bending.

a) Calculate the elastic energy per atom if the system is bent into a ring or coil of Radius $R \gg a$.

b) Calculate and plot the phonon dispersion $\omega(k)$ and show that $\omega(k) \approx \beta \cdot k^2$ for small k. Calculate β.

Remark: as a consequence of this effect, all two-dimensional systems with stiffness (i.e. resistance against bending) show low-frequency sound waves /phonon modes / ... with quadratic dispersion.

Problem 7: Phonons of a hexagonal lattice [7 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 8: Phonons of a linear chain [3 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

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

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

with $R_j = j\cdot a$ and N denotes the number of unit cells in a Born-von Karman supercell.

[Here, $\hat{a}(q) = \frac{1}{\sqrt{2\,M\,\hbar\,\omega(q)}}\left(M\,\omega(q)\,x(q) + i\,p(q)\right)$ and the corresponding $\hat{a}^+(q)$ are the ladder operators for mode q, while $x(q) = \sum_{j=1}^{N}\mathrm{e}^{-i\,q\,R_j}\,u_j$ and $p(q) = \sum_{j=1}^{N}\mathrm{e}^{-i\,q\,R_j}\,p_j$ denote the transformation of the displacements to the normal modes.]

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