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

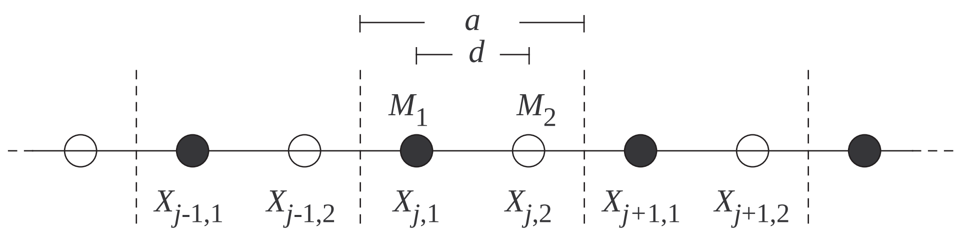
Consider a linear chain with two atoms of masses M_1 and M_2 per unit cell. The atoms are at the positions $X_{j,\nu} = R_j + \tau_\nu + u_{j,\nu}$. The lattice "vector" $R_j = j \cdot a$ and the basis "vector" τ_ν ($\tau_1 = 0$, $\tau_2 = d$) describe the equilibrium positions and $u_{j,\nu}$ gives the elongation of an atom. Two neighboring atoms interact via a potential

$$V(x) = V_0 \left\{ -\mathrm{e}^{-2\alpha(x-d)} + 2\,\mathrm{e}^{-\alpha(x-d)} \right\}$$

with $V_0 < 0$, $\alpha > 0$. Thus, the potential energy of the chain is given by

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

with the equilibrium distance d between the atoms and lattice constand $a = 2d$.



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 $q = \pm\pi/a$. Calculate the sound velocity of the acoustic branch.

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

Problem 5: Linear chain with a point defect **(4 points)**

Consider a linear chain (lattice constant = a) with force constant F between neighbouring atoms (i.e. the simplest textbook case). All atoms have the same mass M, except for one atom (with index $j = 0$) which has the mass M_0.

a) Show that for $M_0 < M$, a localized phonon mode $u_j(t) = (-1)^j\,\mathrm{e}^{-\kappa|j|}\,\bar{u}_0\,\mathrm{e}^{i\bar{\omega}t}$ with $\kappa > 0$ is possible. Calculate its frequency $\bar{\omega}$.

b) Discuss $\bar{\omega}$ as a function of $\dfrac{M_0}{M}$. What do you obtain for $M_0 \to 0$ and for $M_0 \to M$? Compare with the results for a periodic chain ($\to$ see lecture). Plot the mode for $M_0 \ll M$ and for $M_0 \simeq M$.

c) Show that a mode as given in a) is not possible for $M_0 > M$. Is there a simple explanation?