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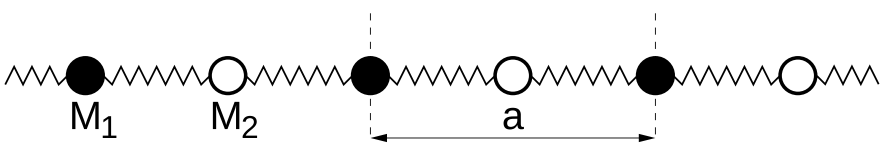
Exercise Set 4

(Due date: Tuesday, November. 17, 2009)

Exercise 9 (Vibrations in a linear chain) (20 points)

Consider a linear chain with two different masses M_1, M_2 per unit cell (lattice constant a) connected by springs (spring constant K).



a) Give the possible different force constants of the model and verify the symmetry properties of the matrix of force constants.

b) Show that the dynamical matrix is given by

$$\underline{\underline{D}} = \begin{pmatrix} \frac{2K}{M_1} & -\frac{2K}{\sqrt{M_1 M_2}} \cos\frac{qa}{2} \\ -\frac{2K}{\sqrt{M_1 M_2}} \cos\frac{qa}{2} & \frac{2K}{M_2} \end{pmatrix}$$

and solve the eigenvalue problem.

c) Discuss the dispersion $\omega_s(\vec{q})$ close to the center and the boundary of the Brillouin zone and visualize the corresponding motion of the masses. What happens for $M_1 = M_2 = M$?

Exercise 10 (Two-dimensinonal lattice dynamics) (15 points)

An ideal two-dimensional crystal consists of only one kind of atom (of mass M), and each atom has an equilibrium location at a point of a square lattice $\vec{R}^{(0)}_{rs} = a\begin{pmatrix} r \\ s \end{pmatrix}$, where $r, s = 1, 2, ..., N$. The displacements from equilibrium are denoted by

$$\vec{u}_{rs} = \begin{pmatrix} u^x_{rs} \\ u^y_{rs} \end{pmatrix}, \quad \textit{i.e.} \quad \vec{R}_{rs} = \vec{R}^{(0)}_{rs} + \vec{u}_{rs} = \begin{pmatrix} ra + u^x_{rs} \\ sa + u^y_{rs} \end{pmatrix}.$$

In the harmonic approximation the potential is given by

$$V(u^x_{rs}, u^y_{rs}) = \sum_{r,s} \left\{ K_1\left[\left(u^x_{(r+1)s} - u^x_{rs}\right)^2 + \left(u^y_{r(s+1)} - u^y_{rs}\right)^2\right] + K_2\left[\left(u^x_{r(s+1)} - u^x_{rs}\right)^2 + \left(u^y_{(r+1)s} - u^y_{rs}\right)^2\right] \right\}.$$

For the case $K_2 = 0.1K_1$:

a) Determine the general phonon dispersion relation $\omega_s(\vec{q})$ throughout the Brillouin zone.

b) Sketch $\omega_s(\vec{q})$ as a function of $\vec{q}$ for

$$\vec{q} = \begin{pmatrix} \xi \\ 0 \end{pmatrix}, \quad 0 \leqslant \xi \leqslant \frac{\pi}{a}.$$