Assignments to Condensed Matter Theory I
Sheet 2

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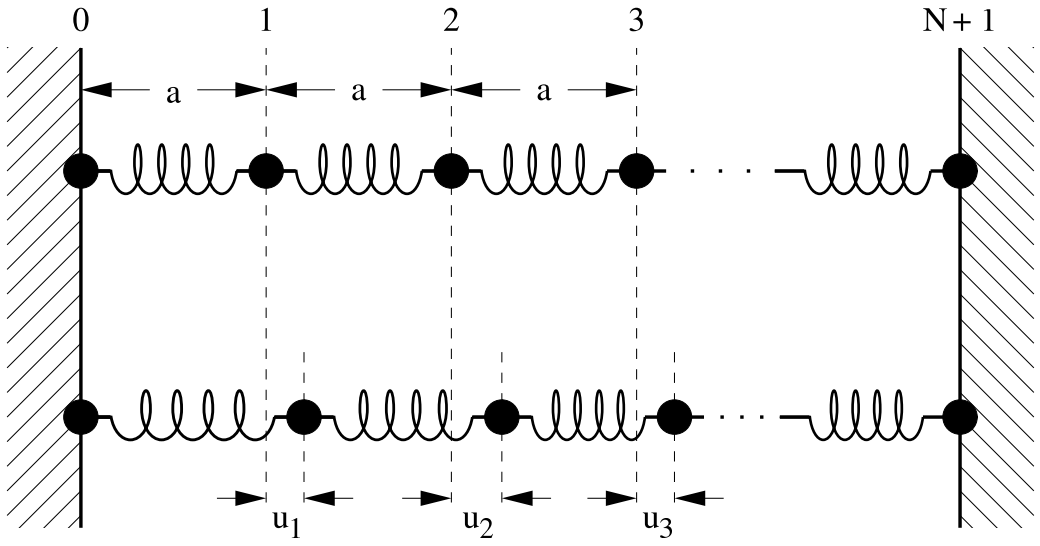
sheet online: http://www-MCG.uni-R.de/teaching/

Problem set: Normal modes of harmonic networks

2.1. Lattice dynamics of a monoatomic linear chain with fixed boundary conditions

Consider a linear chain containing $N+2$ "atoms" (please read "classical particles"!) of mass M. The chain atoms are interacting via nearest neighbor harmonic forces (spring constant k and equilibrium distance a). However *the first and the last atom are constrained to two rigid walls*.



Note that we have $N+1$ springs, but N degrees of freedom. The equilibrium distance of the jth atom is thus $\mathbf{R}_j^0 = ja$. The instantaneous atomic positions are given by specifying the atomic displacements $\boldsymbol{u}_j(t)$ such that $\mathbf{R}_j(t) = \mathbf{R}_j^0 + \boldsymbol{u}_j(t)$. Since we are constrained to strictly 1d we can drop off the vector notation. The coordinates $u_0 = u_{N+1} = 0$ (the displacements of the rigid walls!), so they are *not* dynamical variables. The system Hamiltonian is thus

$$H = \frac{1}{2M}\sum_{j=1}^{N} P_j^2 + \frac{k}{2}\sum_{j=0}^{N}\left(u_{j+1} - u_j\right)^2 .$$

The equations of motion read:

$$M\ddot{u}_j = k\left(u_{j+1} + u_{j-1} - 2u_j\right), \quad j = 1, \ldots, N.$$

(a) Verify that the mth normal mode can be written as

$$u_j^{(m)}(t) \propto \sin\left(\frac{\pi m j}{N+1}\right) \exp\left(-\mathrm{i}\omega_m t\right), 1 \leq m \leq N,$$

and find the correspondent normal (eigen)frequencies ω_m.
Hint: Recall that $\sin(\alpha+\beta)+\sin(\alpha-\beta) = 2\sin\alpha\cos\beta$, and $1-\cos\gamma = 2\sin^2\gamma/2$.

(b) Are the normal modes degenerate or not? What is the value of the maximum frequency? What is the value of the minimum frequency? Does the zero-frequency mode exist in this system or not? Why?

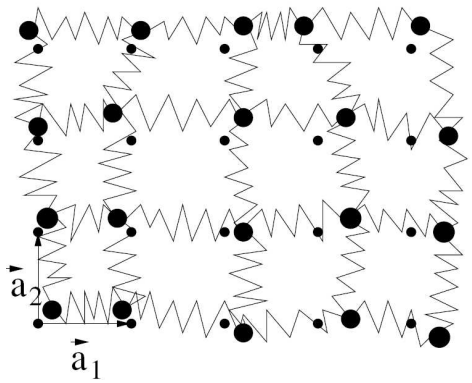
(c) Calculate the mode density in frequencies, in the limit $N \gg 1$. Compare this result with the usual density of modes

$$\mathcal{D}(\omega) = \frac{2N}{\pi} \frac{1}{\sqrt{\omega_{\max}^2 - \omega^2}}$$

calculated (in class[1]) for N masses and N springs with periodic boundary condition.
Note: In the case of the fixed boundary conditions it is *wrong* to speak about group velocity because all modes are stationary.

2.2. Square lattice [Kür]

Consider a monoatomic, two-dimensional square lattice of N^2 atoms of mass M, as shown in the figure.



The basis vectors are $\mathbf{a}_1 = a\hat{x}$ and $\mathbf{a}_2 = a\hat{y}$. Consider periodic boundary conditions with $N \to \infty$.
Consider a potential energy with the form

$$V = \frac{k}{2} \sum_{\langle i,j \rangle} \|\mathbf{u}_i - \mathbf{u}_j\|^2,$$

where $\langle i, j \rangle$ denotes nearest neighbour lattice sites.

[1] C. Kittel, *Quantum Theory of Solids*, *Series in Modern Condensed Matter Physics*, 2nd revised ed. (John Wiley & Sons, Inc., 1987).

(a) Show that the force constant matrices $\mathbf{\Phi}(\mathbf{R}_i^0)$ are diagonal and nonzero up to $\mathbf{R}_i^0 = \mathbf{0}$ or $\mathbf{R}_i^0 = \pm\mathbf{a}_j$ with $(j = 1, 2)$.
Hint: Remember the definition of the force constant matrices and their sum rule:

$$\begin{aligned} \Phi_{\alpha\beta}(\mathbf{R}_i^0, \mathbf{R}_j^0) &= \left. \frac{\partial^2 V}{\partial u_i^{(\alpha)} \partial u_j^{(\beta)}} \right|_{\mathbf{u}_k \equiv 0,\, \forall k}, \\ \sum_{i=1}^{N} \Phi_{\alpha\beta}(\mathbf{R}_i^0) &= 0. \end{aligned}$$

where α, β indicate the x or y component. With a harmless abuse of notation we define, for a periodic lattice, $\Phi_{\alpha\beta}(\mathbf{R}_j^0, \mathbf{R}_k^0) = \Phi_{\alpha\beta}(\mathbf{R}_j^0 - \mathbf{R}_k^0)$ where $\mathbf{R}_i^0 = \mathbf{R}_j^0 - \mathbf{R}_k^0$.

(b) Write the equations of motion in terms of the force constant matrices by making use of the standard exponential Ansatz seen in class. The problem is transformed into the calculus of the 2×2 dynamical matrix

$$D_{\alpha\beta}(\mathbf{q}) = \frac{1}{M} \sum_j \Phi_{\alpha\beta}(\mathbf{R}_j^0) \exp\left(\mathrm{i}\mathbf{q} \cdot \mathbf{R}_j^0\right).$$

(c) The eigenvalues of $\mathbf{D}(\mathbf{q})$ are the squares of the two phonon frequencies $\omega(\mathbf{q})$ (in this case they are degenerate).
Plot the dispersion relation ω vs. $\mathbf{q}$ for the special directions of $\mathbf{q}$: $\Gamma \to \mathsf{X} \to \mathsf{M} \to \Gamma$.
Hint: The high symmetry points Γ, X, M in the reciprocal space lattice are

$$\begin{aligned} \Gamma &= (0, 0), \\ \mathsf{X} &= \left(\frac{\pi}{a}, 0\right), \\ \mathsf{M} &= \left(\frac{\pi}{a}, \frac{\pi}{a}\right). \end{aligned}$$

(d) Alternatively, consider the following bond-stretching potential:

$$V = \frac{k}{2} \sum_{\langle i,j \rangle} \left[\frac{\mathbf{R}_i - \mathbf{R}_j}{\|\mathbf{R}_i - \mathbf{R}_j\|} \cdot (\mathbf{u}_i - \mathbf{u}_j) \right]^2.$$

Is the 2d square lattice stable with this potential? And by extending the sum to second nearest neighbours (diagonals)?
Follow again steps (a)-(c) for this potential in the case of 1st nearest neighbour coupling and then for 1st + 2nd nearest neighbour coupling. Compare the three different results obtained.