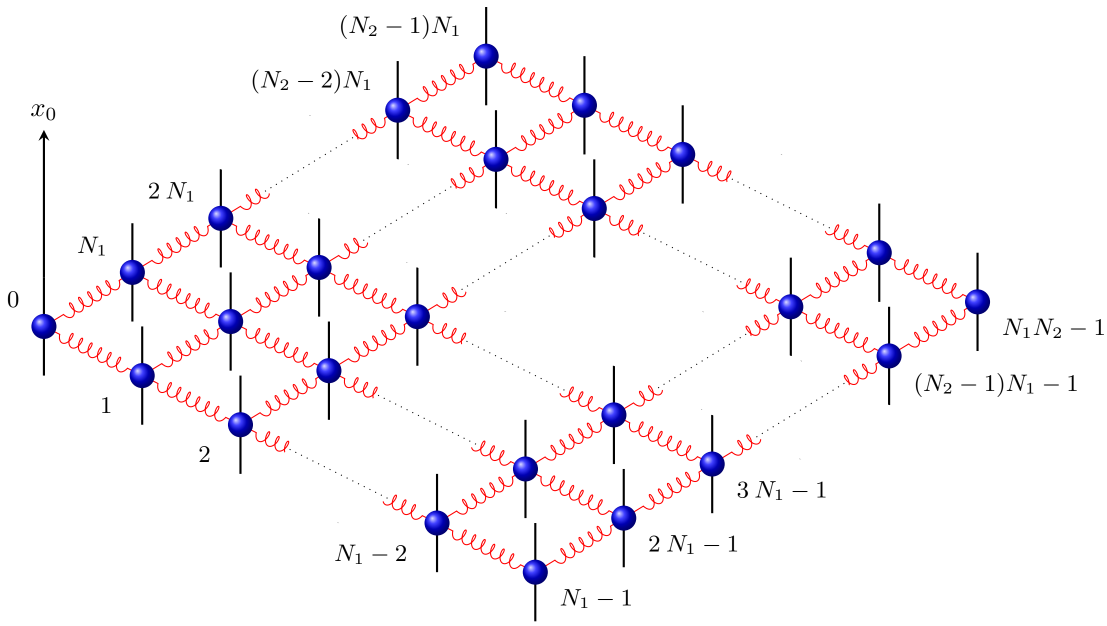
Exercise sheet 7

To be discussed on 22, 25 June and 29, 02 July

Exercise 1 [*A simple model for a crystal*]

Consider a system of $M = N_1 \times N_2$ identical point-like particles located on a 2-dimensional regular lattice. Each particle has mass m and is connected to its nearest neighbours by identical springs of stiffness k as shown in the following figure. The displacements $x_0(t), \ldots, x_{M-1}(t)$ from the rest positions are constrained to one dimension.



FIRST PART

In this problem, focus exclusively on the situation in which the mass on a corner of the lattice is brought out of equilibrium at $t = 0$, i.e.

$$\begin{cases} x_j(t=0) = \delta_{j,0}\,L \\ \dot{x}_j(t=0) = 0 \end{cases} \quad \text{where} \quad \begin{array}{l} j \equiv N_1\,j_2 + j_1 \in [0, M-1] \subset \mathbb{N} \\ (j_1, j_2) \in I \equiv [0, N_1-1] \times [0, N_2-1] \subset \mathbb{N}^2 \end{array} \,,$$

where L can be used as typical length scale of the problem.

(i) Imagine the above sketched lattice to be placed onto a torus in a way such that the points on the boundaries of the system are connected with additional springs and they have as well four nearest neighbours. In this case the problem can be solved analytically.

(a) Write down the Lagrangian of the system and derive the equations of motion in terms of dimensionless quantities.

(b) A first step valid in general to simplify the equations of motion is to make an ansatz about the form of the time dependence of the solution. As already discussed in the lecture, this can be assumed to be

$$x_{j_1,j_2}(\hat{t}) = v_{j_1,j_2}^{n_1,n_2}\ \exp\big(\imath\,\hat{\omega}_{n_1,n_2}\,\hat{t}\big) \,,$$

where it has been taken into account with the indices $(n_1, n_2) \in I$ that there are $N_1 \cdot N_2$ modes in the system and therefore $N_1 \cdot N_2$ possible values of $\hat{\omega}$. To be precise, the general solution of the problem is a linear combination of all possible modes, but this is a known fact and it can be considered just before imposing the initial conditions. Rewrite the equations of motions in terms of v.

(c) The following step depends on the problem and it consists in making an ansatz on the functions v. Use the assumption

$$v_{j_1,j_2}^{n_1,n_2} = \exp\left[2\pi\imath\left(\frac{j_1\, n_1}{N_1} + \frac{j_2\, n_2}{N_2}\right)\right]$$

to obtain $\hat{\omega}_{n_1,n_2}$.

(d) Write down all the $\hat{\omega}$ in the case $N_1 = N_2 = 4$. Consider the general solution of the problem combining all the 16 modes and impose the previously mentioned initial conditions.

(ii) Prepare the problem to be addressed numerically. Start again from the equations of motions written in terms of v obtained in task (i-b) and combine them using a vector notation into the following form,

$$K \cdot \mathbf{v}^{n_1,n_2} = \hat{\omega}_{n_1,n_2}\, \mathbf{v}^{n_1,n_2} \qquad \text{with} \qquad \mathbf{v} = \begin{pmatrix} v_{0,0} \\ v_{1,0} \\ \vdots \\ v_{N_1,N_2} \end{pmatrix} .$$

Determine the stiffness matrix K analogously to what was done in the lecture in the 1-dimensional case. Which are, in particular, the non-zero entries?

(iii) In a preliminary program implement the Jacobi algorithm to find out the eigenvalues and the eigenvectors of a matrix. Test it properly to be sure it works.

———————— SECOND PART ————————

(iv) Write a program to solve the equations of motions of the problem considered in task (i). Compare your numerical solution with the analytical one for $N_1 = N_2 = 4$.

(v) Change now the boundary conditions of the system, considering exactly the situation sketched in the figure, where the mass points on the boundaries have only three or two nearest neighbours (the so-called *free boundary conditions*). Solve again the problem numerically in the case $N_1 = N_2 = 4$. Can you explain the differences in the result, for example comparing $x_{15}(\hat{t}) = x_{3,3}(\hat{t})$ in both situations?

(vi) In the following, set $N_1 = N_2 = 7$, use free boundary conditions and consider $0 \leqslant \hat{t} \leqslant 30$.

(a) Solve the problem for the given initial conditions and plot $x_j(\hat{t})$ for $j \in \{0, 6, 24, 48\}$.

(b) From your plot you should be able to estimate the time needed to make the initial perturbation propagate through the lattice, e.g. compare $x_0(\hat{t})$ and $x_{48}(\hat{t})$, and you should then be able to estimate the stiffness k of iron. Typical values for the speed of sound, the mass and the lattice spacing of an iron crystal are, respectively, $c_s \approx 5\,\text{km/s}$, $m \approx 10^{-25}\,\text{kg}$ and $a \approx 3 \cdot 10^{-10}\,\text{m}$.

(c) Solve again the problem changing the stiffness of the springs connected to the points in the middle row, $j \in [21, 27] \subset \mathbb{N}$, reducing it to $k' = 0.2\,k$. Have a look again to $x_j(\hat{t})$ for $j \in \{0, 6, 24, 48\}$ and try to understand which kind of physical situation is reproduced.

(d) Repeat again task (vi-a), but connect the crystal to the origin via a different spring of stiffness $k' = 5k$ attached to the central point of the lattice, i.e. the potential in the Lagrangian has an additional term

$$V' = \frac{1}{2}\, k' \left[x_{24}(\hat{t})\right]^2 = \frac{5}{2}\, k \left[x_{3,3}(\hat{t})\right]^2 .$$

Do you notice any characteristic difference in the eigenvalues? Why is there no zero mode any more (i.e. a vanishing eigenvalue)?