Numerische Methoden der Physik

WiSe 2023-2024 – Prof. Marc Wagner

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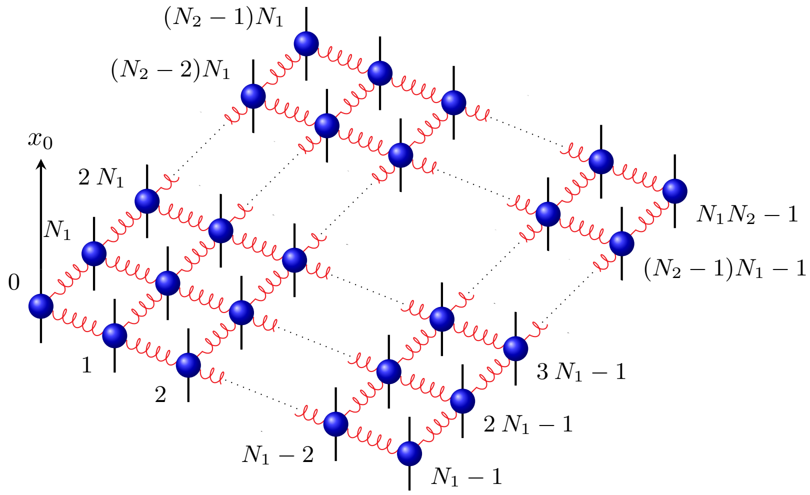
Exercise sheet 10

To be handed in on 20.12.2023 and discussed on 22.12.2023 and 08.01.2024

Exercise 1 [*A simple model for a crystal*] (7+3+5+5=20 pts.)

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 $x_0(t), \dots, x_{M-1}(t)$ from the rest positions are constrained to one dimension.



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.

$$\begin{cases} x_j(t=0) = \delta_{j,0}\, L \\ \dot{x}_j(t=0) = 0 \end{cases} \quad \text{with} \quad \begin{array}{l} j \equiv N_1\, j_2 + j_1 \\ j_1 = 0, 1, \dots, N_1 - 1, \quad j_2 = 0, 1, \dots, N_2 - 1 \end{array} . \tag{1}$$

where L can be used to define dimensionless displacements $\hat{x}_j$.

(i) Consider 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) Rewrite the equations of motions as an eigenvalue problem by using the ansatz

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

The indices $n_1 = 0, 1, ..., N_1 - 1$ and $n_2 = 0, 1, ..., N_2 - 1$ represent the $N_1 \cdot N_2$ modes in the system.

(c) Use the ansatz

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

to derive the eigen frequencies $\hat{\omega}_{n_1,n_2}$.

(d) Write down all the $\hat{\omega}_{n_1,n_2}$ for $N_1 = N_2 = 4$. Determine the coefficients A_{n_1,n_2} of the general solution

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

such that the initial conditions 1 are fulfilled.

(ii) Prepare the problem to be addressed numerically. Start again from the equations of motions from task (i-a). Use an exponential ansatz as in task (i-b) and show that the equations of motion can be reduced to an eigenvector problem,

$$K \cdot \mathbf{v}^n = \hat{\omega}_n^2\, \mathbf{v}^n \qquad \text{with} \qquad \mathbf{v}^n = \begin{pmatrix} v_{0,0}^n \\ v_{1,0}^n \\ \vdots \\ v_{N_1,N_2}^n \end{pmatrix} \; .$$

Determine the stiffness matrix K.

(iii) Write a program to solve the equations of motions of the problem considered in task (i) by reusing your code for the Jacobi method from Sheet 9 Exercise 2 to solve the eigenvalue problem. The stiffness matrix K should satisfy periodic boundary conditions and the initial conditions from Eq. (1) should be used. Verify your numerical solution by comparing to the analytical solution for $N_1 = N_2 = 4$. Compare both v_{j_1,j_2}^n and $\hat{\omega}_n$ and plot the time evolution of $\hat{x}_j(\hat{t})$ for $j = 0, 3, 7, 15$ and $0 \leq \hat{t} \leq 30$ for both the analytical and the numerical solution.

(iv) 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 (*free boundary conditions*). Solve again the problem numerically for $N_1 = N_2 = 4$ and plot the time evolution of $\hat{x}_j(\hat{t})$ for $j = 0, 3, 7, 15$ for $0 \leq \hat{t} \leq 30$. Can you explain the differences in the result compared to the System with periodic boundary conditions, by for example comparing $x_{15}(\hat{t}) = x_{3,3}(\hat{t})$ in both situations?

(v) Optional: $N_1 = N_2 = 4$ models a tiny crystal. Play around with larger N, e.g. repeat task (iv) with $N_1 = N_2 = 10$ or $N_1 = N_2 = 20$.