



3. Fourier transformation and Hamiltonian (20 points)

To be discussed on Wednesday, 18th October, 2023 in the tutorial.

Please indicate your preferences until Friday, 13/10/2023, 21:00:00 on the website.

Exercise 3.1: Solving the differential equation

We have defined a linear 1D chain by the Lagrangian

$$L = \sum_{n=1}^N \left[\frac{m}{2} \dot{q}_n^2 - \frac{\kappa}{2} (q_{n+1} - q_n)^2 \right].$$

a) (3 points) Prove that the equation of motion for said Lagrangian is

$$m\ddot{q}_n = \kappa(q_{n+1} + q_{n-1} - 2q_n) \tag{1}$$

In solving the equation of motion, the normal coordinates

$$u_n^k = \frac{1}{\sqrt{N}} e^{ikan}$$

will prove useful.

b) (4 points) Prove that u_n^k are orthonormal

$$\sum_n \bar{u}_n^k u_n^{k'} = \delta^{kk'}$$

and complete

$$\sum_k \bar{u}_n^k u_{n'}^k = \delta_{nn'}.$$

Hint: Use

$$\sum_{n=1}^N x^n = x \frac{1-x^N}{1-x}, \quad \frac{1}{N} \sum_{l=1}^N e^{2\pi i(n-n')\frac{l}{N}} = \delta_{nn'}$$

and periodic boundary conditions, that is $u_{N+n}^k = u_n^k$.

c) (5 points) Using the discrete Fourier transform we have written the real solution of (1) in the following form:

$$q_n(t) = \frac{1}{\sqrt{N}} \sum_k [b_k e^{-i(\omega_k t - kan)} + \bar{b}_k e^{i(\omega_k t - kan)}], \quad \omega_k = 2\sqrt{\frac{\kappa}{m}} \left| \sin \frac{ka}{2} \right|. \tag{2}$$

Derive above solution.

Hint: Make the substitution

$$q_n(t) = \sum_k a_k(t) u_n^k$$

in (1); use also

$$e^{ix} + e^{-ix} - 2 = -4 \sin^2 \frac{x}{2}$$

and that q_n are real.

Exercise 3.2: The Hamiltonian

We will now derive the Hamiltonian of the linear chain

$$H = T + V = \frac{1}{2m} \sum_{n=1}^N p_n^2 + \frac{\kappa}{2} \sum_{n=1}^N (q_{n+1} - q_n)^2, \quad p_n = \frac{\partial L}{\partial \dot{q}_n}$$

in terms of the normal coordinates b_k and \bar{b}_k .

- a) (3 points) Compute the kinetic energy T .

Hint: Expressing p_n in terms of u_n^k and making use of orthonormality and completeness will facilitate your computations.

- b) (3 points) Compute the potential energy V .

Hint: Again, expressing q_n in terms of u_n^k and making use of orthonormality and completeness will help with your calculations.

- c) (2 points) Prove that the Hamiltonian of the linear chain reduces to

$$H = 2m \sum_k \omega_k^2 \bar{b}_k b_k$$