

## **Classical Theoretical Physics II**

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## Exercise Sheet 9

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## Exercise 1: Tri-atomic molecule

In this exercise we will model a linear tri-atomic molecule, with a central atom with mass M, and two identical atoms with mass m at the ends. A real-world example of such a molecule is CO<sub>2</sub>. The

same example was discussed in the lectures in a slightly different way.

We will model the atomic forces between the central atom and the side atoms, as springs with spring constant k that are at equilibrium when the distance between the atoms are b. We will only consider movement along the axis of the molecule, making it a one-dimensional problem. Denoting the position of the central atom  $x_2$ , and of the side atoms  $x_1$  and  $x_3$ , the potential energy is therefore

$$U = \frac{k}{2} \left( (x_2 - x_1 - b)^2 + (x_3 - x_2 - b)^2 \right)$$

- (a) What is the Lagrangian of the system?
- (b) We now do a variable change to a new set of coordinates  $\eta$  that are relative to the equilibrium position. If  $x_{20}$  is the position of the central atom at some specific time (so  $\dot{x}_{20} = 0$ ), these coordinates are  $x_2 = x_{20} + \eta_2$ ,  $x_1 = x_{20} + \eta_1 - b$ ,  $x_3 = x_{20} + \eta_3 + b$ . What is the Lagrangian in the new coordinates?
- (c) The equation of motion for  $\eta_1$  is  $m\ddot{\eta}_1 + k(\eta_1 \eta_2) = 0$ . What are the EOMs for  $\eta_2$  and  $\eta_3$ ?
- (d) Let us assume a sinusoidal form for the solutions, such that  $\ddot{\eta}_i = -\omega^2 \eta_i$ , with  $\omega$  being an oscillation frequency. Show that such an ansatz allows the EOM system to be expressed on matrix form, as  $A\vec{\eta} = 0$ , where  $\vec{\eta} = (\eta_1, \eta_2, \eta_3)$  and

$$A = \begin{bmatrix} k - \omega^2 m & -k & 0 \\ -k & 2k - \omega^2 M & -k \\ 0 & -k & k - \omega^2 m \end{bmatrix}$$

- (e) Such an equation system only allows for non-zero solutions if det(A) = 0. Why is that?
- (f) Show that only three different (non-negative) values of  $\omega$  allow for non-zero solutions:  $\omega = 0$ ,  $\omega = \sqrt{\frac{k}{m}}$ , and  $\omega = \sqrt{\frac{k}{m}(1 + \frac{2m}{M})}$ .

10 points





(g) In the lectures we solved the same problem by finding the eigenvectors and eigenvalues of the matrix

$$B = \begin{bmatrix} k/m & -k/m & 0\\ -k/M & 2k/M & -k/M\\ 0 & -k/m & k/m \end{bmatrix}$$

The eigenvectors were (1, 1, 1), (1, 0, -1), and (1, -2m/M, 1), and the eigenvalues were the squares of three values of  $\omega$  found above. Why are these two approaches to solving the system equivalent?

(h) What is the physical interpretation of the three oscillation modes?

## Exercise 2: Four beads on a ring

Four beads of mass m numbered from one to four, are mounted on a ring with radius r along which they are allowed to slide. The particles are joined with springs, which have the property that the potential energy of a spring connecting two beads at angles  $\theta_i$  and  $\theta_j$ , is  $\frac{1}{2}kr^2(\theta_j - \theta_i)^2$ .

(a) An equilibrium position for the system is  $\theta_1 = 0$ ,  $\theta_2 = \pi/2$ ,  $\theta_3 = \pi$ ,  $\theta_4 = 3\pi/2$ . Changing to coordinates relative to these equilibrium positions:  $\theta_1 = \phi_1$ ,  $\theta_2 = \phi_2 + \pi/2$ ,  $\theta_3 = \phi_3 + \pi$ ,  $\theta_4 = \phi_4 + 3\pi/2$ , write down the Lagrangian and the equations of motion for the beads.



Figure 2

(b) We will now consider small oscillations around that equilibrium position. Argue that an ansatz consisting of oscillations with (angular) frequency  $\omega$ , allows for the system of EOMs to be written as

$$A\vec{\phi} = \vec{0}$$
 with  $A = -\omega^2 I + B$  and  $\vec{\phi} = (\phi_1, \phi_2, \phi_3, \phi_4)$  (1)

where I is the  $4 \times 4$  unit matrix.

- (c) Find the matrix B as a function of m and k.
- (d) Guess an orthogonal set of four eigenvectors of the matrix B and insert them in eq. (1) to extract the corresponding eigenfrequencies  $\omega$ .

Hint 1: When guessing the eigenvectors consider the symmetries of the problem. If one bead moves in a certain way, how should the other beads move for the movement to be stable?

Hint 2: The (positive) eigenfrequencies  $\omega$  should be 0,  $\sqrt{2k/m}$ ,  $\sqrt{2k/m}$ , and  $2\sqrt{k/m}$ .

(e) What is the physical interpretation of these four oscillation modes?

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10 points

- (f) Let U be the 4 × 4 matrix that has as its four rows, an orthonormal (i.e. orthogonal and with length 1) set of eigenvectors of B. Introduce coordinates  $\psi$ , defined by  $\vec{\psi} = U\vec{\phi}$ , and write the Lagrangian and the equations of motion for these new coordinates.
- (g) What makes the  $\psi$  coordinates good? How comes it turns out like that?