Classical Mechanics

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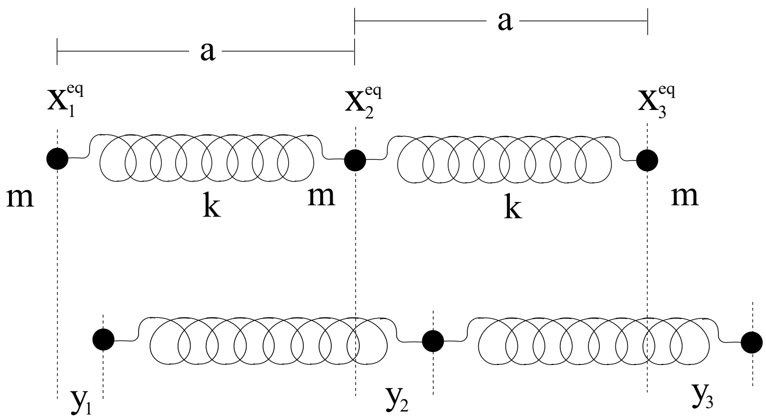
Exercise sheet 5 **Due: November, 15 at 12:00**

1 Normal modes



The motion of particles that interact harmonically can be decomposed into especially simple components, the *normal modes*. For each such normal mode, the particles perform a collective periodic motion with respect to one single frequency.

As an example we consider a model of a linear molecule consisting of three atoms, each of mass m that interact according to the potential

$$V(x_1, x_2, x_3) = \frac{k}{2}(x_2 - x_1 - a)^2 + \frac{k}{2}(x_3 - x_2 - a)^2,$$

where $k > 0$ and $a > 0$. For the sake of simplicity we here only consider the motion of the atoms along the axis of the molecule.

This molecule is in mechanical equilibrium when the positions of the atoms are such that $x_1 = x_1^{\text{eq}}$, $x_2 = x_2^{\text{eq}}$, and $x_3 = x_3^{\text{eq}}$, where $x_2^{\text{eq}} - x_1^{\text{eq}} = a$ and $x_3^{\text{eq}} - x_2^{\text{eq}} = a$. It is very convenient to introduce new coordinates $y_1 = x_1 - x_1^{\text{eq}}$, $y_2 = x_2 - x_2^{\text{eq}}$, and $y_3 = x_3 - x_3^{\text{eq}}$ that measure the *deviation* from equilibrium. With respect to these new coordinates, we can write the potential as

$$V(y_1, y_2, y_3) = \frac{k}{2}(y_2 - y_1)^2 + \frac{k}{2}(y_3 - y_2)^2 = \frac{1}{2}\vec{y}^t \boldsymbol{V} \vec{y}, \quad \vec{y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}, \tag{1}$$

where $\boldsymbol{V}$ is a 3×3 matrix, and t denotes the transpose, i.e., $\vec{y}^t = [y_1, y_2, y_3]$. One can also realize that $\ddot{y}_1 = \ddot{x}_1$, $\ddot{y}_2 = \ddot{x}_2$, and $\ddot{y}_2 = \ddot{x}_3$.

a) Before we start to investigate the molecule, let us first look at some more general questions concerning how to find normal modes. Suppose that

$$U(y_1, y_2, \ldots, y_N) = \frac{1}{2}\vec{y}^t \boldsymbol{U} \vec{y}, \quad \vec{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}, \tag{2}$$

for some matrix $\boldsymbol{U}$. *Show that one always can find a symmetric matrix $\boldsymbol{U}'$ such that $U(y_1, y_2, \ldots, y_N) = \frac{1}{2}\vec{y}^t \boldsymbol{U}' \vec{y}$.*

Hint: Recall that a matrix $\boldsymbol{U}'$ is symmetric if $\boldsymbol{U}'_{kl} = \boldsymbol{U}'_{lk}$. **(1 points)**

b) Suppose that the function U defined in (2) is the potential of a collection of particles of mass m, and that we choose $\boldsymbol{U}$ to be symmetric. *Show that the equation of motion can be written*

$$m\frac{d^2}{dt^2}\vec{y} = -\boldsymbol{U}\vec{y}. \tag{3}$$

(1 points)

c) In order to find the normal modes one can make the ansatz $\vec{y}(t) = e^{i\omega t}\vec{q}$, where $\vec{q}$ is a time-independent vector, and ω a real number. *Show that this leads to an eigenvalue problem. For a given eigenvalue, what are the allowed values of the frequency ω? Write down the corresponding solutions to (3). How can you combine these solutions in order to guarantee that the resulting function is real-valued (and thus describe an actual physical motion)?*

Hint: You can use the fact that if $\boldsymbol{U}$ comes from a harmonic potential, then the eigenvalues of $\boldsymbol{U}$ always have to be real and non-negative. (This follows from $\boldsymbol{U}$ being positive semi-definite.)

(3 points)

d) Unfortunately the type of ansatz in c) does not give all solutions in the case that $\vec{q}$ is an eigenvector corresponding to eigenvalue 0. In this case we can instead try an ansatz on the form $\vec{y} = f(t)\vec{q}$ in (3). *Show that this leads to a differential equation that f has to satisfy. What is the general solution to this differential equation? Write down the corresponding solutions to (3).* **(2 points)**

e) After these general considerations, let us now turn to the linear molecule defined by the potential V. *Determine the symmetric matrix $\mathbf{V}$ in (1).* **(2 points)**

f) *Find the eigenvalues and corresponding eigenvectors of the matrix $\mathbf{V}$ that you found in e).* **(3 points)**

g) *Sketch the motion of the normal modes of the linear molecule. What kind of motion does the zero eigenvalue correspond to? What conservation law is it related to?* **(2 points)**

h) *Write down the general solution of the equations of motion of the linear molecule in terms of its normal modes. Make sure that the functions that you write down are real-valued.* **(2 points)**

i) Let us now change the problem such that the middle particle (the one with equilibrium position x_2^{eq}) could have a mass M different from m (but we let the interaction potential be the same as before). *Show that the equations of motion can be written as*

$$\frac{d^2}{dt^2}\vec{y} = -\mathbf{W}\vec{y}, \tag{4}$$

and determine the matrix $\mathbf{W}$.

Hint: Note that there is no mass at the left hand side of (4) (as opposed to what we did in (3)). Hence, the masses m and M have to be incorporated into $\mathbf{W}$. **(1 points)**

j) *Determine eigenvalues and corresponding eigenvectors of $\mathbf{W}$, and compare with what you found in f).*

(3 points)

Comment: The purpose of this exercise is to get used to concepts like harmonic motion and normal modes, and how this relates to eigenvalues and eigenvectors.