Classical Mechanics

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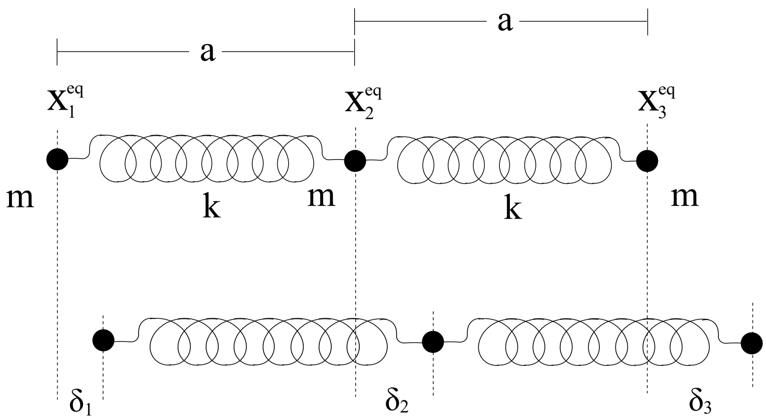
Exercise sheet 6 Due: Thursday December 10 at 24:00

1 Linear molecule with equal masses

In the lecture we considered the vibrations of N particles with periodic boundary conditions. In this exercise we consider a model of a linear molecule consisting of three atoms, each of mass m that interact according to the potential

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

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



Recall from the lecture that 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.

This molecule is in mechanical equilibrium when the positions of the atoms are such that $x_1 = x_1^{eq}$, $x_2 = x_2^{eq}$, and $x_3 = x_3^{eq}$, where $x_2^{eq} - x_1^{eq} = a$ and $x_3^{eq} - x_2^{eq} = a$. It is very convenient to introduce new coordinates $\delta_1 = x_1 - x_1^{eq}$, $\delta_2 = x_2 - x_2^{eq}$, and $\delta_3 = x_3 - x_3^{eq}$ that measure the *deviation* from equilibrium. With respect to these new coordinates, we can write the potential as

$$U(\delta_1, \delta_2, \delta_3) = \frac{k}{2}(\delta_2 - \delta_1)^2 + \frac{k}{2}(\delta_3 - \delta_2)^2.$$

a) In the lecture you have seen that one can write the equations of motion as

$$\frac{d^2}{dt^2}\vec{\delta} = \boldsymbol{M}\vec{\delta}, \quad \vec{\delta} = \begin{bmatrix}\delta_1\\ \delta_2\\ \delta_3\end{bmatrix}, \tag{1}$$

for some matrix $\boldsymbol{M}$. *Determine the matrix* $\boldsymbol{M}$. **(2 points)**

b) In order to find the normal modes one can make the ansatz $\vec{\delta}(t) = e^{i\omega t}\vec{v}$, where $\vec{v}$ is a time-independent vector, and ω a real number. *Show that this leads to an eigenvalue problem of the form*

$$\lambda \vec{v} = \boldsymbol{M}\vec{v}, \tag{2}$$

where the eigenvalue λ is a function of ω. Determine this function. **(1 point)**

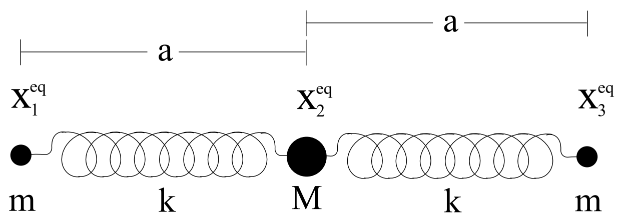
c) *Determine the eigenvalues λ and eigenvectors $\vec{v}$ of (2). For each eigenvalue λ, what are the possible values of ω?* **(3 points)**

d) *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)**

e) *By using the results in c), write down the corresponding solutions to (1). How can you combine these solutions in order to guarantee that the resulting function is real-valued (and thus describes an actual physical motion)?* **(2 points)**

2 Linear molecule with different masses

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, and we still restrict the motion to be one-dimensional).



a) *Show that the equations of motion can be written as*

$$\frac{d^2}{dt^2}\vec{\delta} = \boldsymbol{W}\vec{\delta},$$

and determine the matrix $\boldsymbol{W}$. *Is* $\boldsymbol{W}$ *symmetric? Is* $\boldsymbol{M}$ *in problem 1 symmetric?* **(2 points)**

b) *Determine eigenvalues and corresponding eigenvectors of* $\boldsymbol{W}$.

(4 points)

c) *Are the eigenvectors in b) orthogonal to each other? Are the eigenvectors in 1c) orthogonal to each other?*

(2 points)

d) The spectrum of CO_2 might determine the fate of humanity. The calculation in this exercise can already lead to some predictions about its properties. We cannot deduce the spring constant k, as this requires a quantum mechanical model. However, note that the ratio of the frequencies is independent of k. Thus our simple theory suggests a value for the ratio of some of the frequencies absorbed by atmospheric CO_2. *Compute the ratio, and compare it to experimental results.*

Hint: A suitable source could be “NIST's Tables of Molecular Vibrational Frequencies": https://nvlpubs.nist.gov/nistpubs/Legacy/NSRDS/nbsnsrds39.pdf

Look for the frequencies of the "stretching" modes – there is also a "bending" mode, which we have not considered here. One of the two stretching modes is much more efficient at absorbing light. Can you guess why? **(2 points)**