SoSe 2021

# Classical Theoretical Physics II

Lecture: Prof. Dr. K. Melnikov – Exercises: Dr. A. Behring

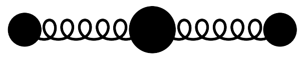
## Exercise Sheet 10

Issue: 25.06. – Submission: 02.07. @ 10:00 Uhr – Discussion: 05./06.07.

### Exercise 1: Tri-atomic molecule

**10 points**

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 $CO_2$. 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 distances between the atoms are $\ell$. We will only consider movement along the axis of the molecule, making it a one-dimensional problem. We denote the position of the central atom as $q_2$ and of the side atoms $q_1$ and $q_3$.



(a) The potential of a spring is given by $U = \frac{k}{2}\xi^2$, where $\xi$ is the displacement from equilibrium. What is the Lagrangian of the system as a function of the coordinates $\vec{q} = (q_1, q_2, q_3)$?

(b) We now perform a change of variables to a new set of coordinates $\vec{\xi} = \vec{q} - \vec{q}_0$ relative to the equilibrium, where $\vec{q}_0 = (-\ell, 0, \ell)$. Show that the Lagrangian has the form

$$L = \sum_{i,j} \left( \frac{1}{2} m_{ij} \dot{\xi}_i \dot{\xi}_j - \frac{1}{2} k_{ij} \xi_i \xi_j \right) \tag{1.1}$$

and determine the $3 \times 3$ matrices $\hat{m}$ and $\hat{k}$. Convince yourself that $\hat{m}$ and $\hat{k}$ are indeed symmetric.

(c) Solve the equations of motion that belong to Eq. (1.1) using a cosine ansatz, $\vec{\xi}_s = \vec{a}_s \cos(\omega_s t + \varphi)$. Show that the amplitudes $\vec{a}$ fulfil the equation

$$\big( -\omega_s^2 \hat{m} + \hat{k} \big) \vec{a}_s = 0 \,. \tag{1.2}$$

(d) Such a system of equations only has non-zero solutions $\vec{a}_s$ if $\det(-\omega_s^2 \hat{m} + \hat{k}) = 0$. What is the reason for this?

(e) Calculate $\det(-\omega_s^2 \hat{m} + \hat{k})$. Use the condition from (d) to show that the eigenfrequencies are

$$\omega_1^2 = 0 \,, \qquad \omega_2^2 = \frac{k}{m} \,, \qquad \omega_3^2 = \frac{k}{m} \left( 1 + \frac{2m}{M} \right) . \tag{1.3}$$

(f) Determine the eigenamplitudes $\vec{a}^{(s)}$ with $s = 1, 2, 3$ associated to the respective $\omega_s^2$ from above. Orthonormalise the eigenvectors using

$$a_i^{(s')}\, m_{ij}\, a_j^{(s)} = \delta^{s's}\,. \tag{1.4}$$

(g) What is the geometric interpretation of each mode of oscillation corresponding to the respective eigenvectors $\vec{a}^{(s)}$?

(h) The eigenvectors $\vec{a}^{(s)}$ also fulfil the condition $a_i^{(s')}\, k_{ij}\, a_j^{(s)} = \omega_s^2 \delta^{s's}$. As we saw in the lectures, the displacements from equilibrium can be written as

$$\vec{\xi}(t) = \sum_{s=1}^{3} r_s(t)\vec{a}^{(s)}\,, \tag{1.5}$$

where $r_s$ are the normal coordinates. The Lagrangian can be written as a sum of three Lagrangians,

$$L = \frac{1}{2}\sum_{s=1}^{3}[\dot{r}_s^2 - \omega_s^2 r_s^2]\,, \tag{1.6}$$

such that the normal coordinates are independent of each other. The equations of motion for the individual $r_s$ have the usual form,

$$\ddot{r}_s + \omega_s^2 r_s = 0 \qquad \Rightarrow r_s(t) = C_s \cos(\omega_s t + \varphi_s)\,, \tag{1.7}$$

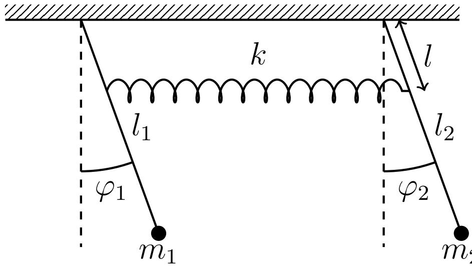
or $r_s(t) = C_s + D_s t$ if $\omega_s = 0$. Assume the following initial conditions at time $t = 0$ for the three atoms:

$$\vec{q}(t=0) = \begin{pmatrix} -\frac{8}{10}\ell \\ -\frac{2m\ell}{10M} \\ \ell \end{pmatrix}, \qquad \dot{\vec{q}}(t=0) = \vec{0}\,. \tag{1.8}$$

Determine the constants $C_s$ and $\varphi_s$ (or $C_s$ and $D_s$) which characterise the motion of the molecule.

## Exercise 2: Coupled pendulums **10 points**

Two pendulums of lengths $l_1$ and $l_2$ are connected via a spring with spring constant $k$. The distance between the two pendulums should be much larger than the distance $l$ between the point where the spring is connected to the pendulum and the point from where the pendulum is suspended. Then the spring is always approximately horizontal. At the end of each pendulum there is a mass $m_1$ and $m_2$, respectively.



(a) Find the Lagrangian of the system and derive the equations of motion for the displacement angles $\varphi_1$ and $\varphi_2$ of the pendulums.

(b) Approximate the Lagrangian and the equations of motion for the case of small displacements. In what follows, we will always work in this approximation.

(c) Solve the equations of motion for the special case $m_1 = m_2$ and $l_1 = l_2$ with the initial conditions

$$\varphi_1(0) = \varphi_0\,, \qquad \varphi_2(0) = 0\,, \tag{2.1}$$

$$\dot{\varphi}_1(0) = 0\,, \qquad \dot{\varphi}_2(0) = 0\,. \tag{2.2}$$

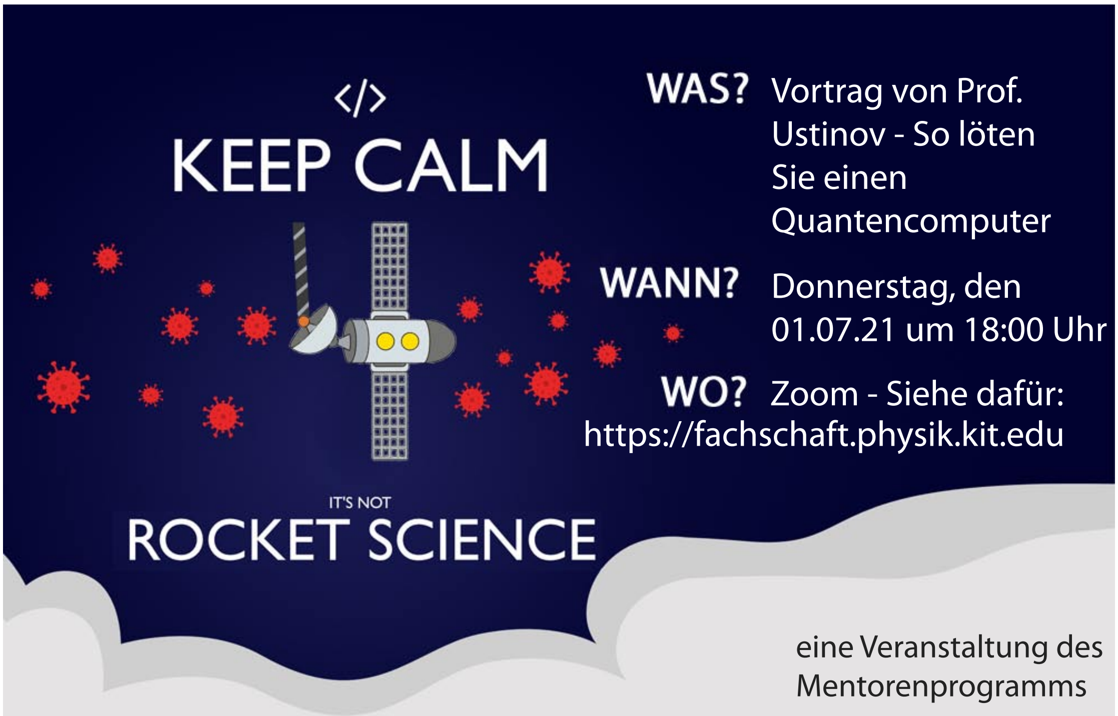
Show that the solutions can be brought into the form

$$\varphi_1(t) = A\cos(\Omega t)\cos(\omega t)\,, \qquad \varphi_2(t) = A\sin(\Omega t)\sin(\omega t)\,. \tag{2.3}$$

(d) Describe qualitatively how the pendulums behave according to these solutions. What are the roles of $\Omega$ and $\omega$? Sketch the behaviour of $\varphi_1(t)$ and $\varphi_2(t)$.

(e) Solve the equations of motion for the case $m_1 \neq m_2$ and $l_1 = l_2$ with the same initial conditions as above.

(f) Plot the behaviour of $\varphi_1(t)$ and $\varphi_2(t)$. You can use a computer algebra system of your choice for that. A free online tool to plot graphs can be found, for example, at `https://www.geogebra.org/`. Describe again qualitatively the behaviour of both pendulums.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KEEP CALM
IT'S NOT
ROCKET SCIENCE
WAS? Vortrag von Prof. Ustinov - So löten Sie einen Quantencomputer
WANN? Donnerstag, den 01.07.21 um 18:00 Uhr
WO? Zoom - Siehe dafür: https://fachschaft.physik.kit.edu
eine Veranstaltung des Mentorenprogramms