Exercise 2

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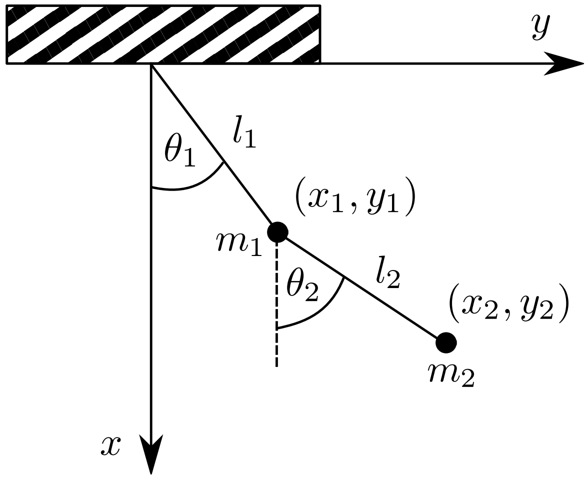
Problem 1: Classical Mechanics – The Double Pendulum

The goal of this exercise is to illustrate the application of *analytical mechanics* (Lagrangian and Hamiltonian formulations) in the context of a practical example. To this purpose, we consider the *double pendulum*, illustrated in the figure below.



The masses m_1 and m_2 as well as the lengths l_1 and l_2 are fixed (these are *parameters* of the problem). For simplicity, it is assumed here that $m_1 = m_2 = m$ and $l_1 = l_2 = l$. The two masses are subject to the gravitational acceleration g. Their initial velocities have no component along the orthogonal z-direction, so that the pendulum only swings within the displayed xy-plane.

Due to the constraints introduced by the fix rod lengths, the dynamics of this system can be formulated in terms of two degrees of freedom (defining the four *variables* of the problem). As the most obvious choice, this formulation can rely on the *generalized coordinates* $\mathbf{q} = \{\theta_1, \theta_2\}$, along with either the *generalized velocities* $\dot{\mathbf{q}} = \{\dot{\theta}_1, \dot{\theta}_2\}$ (*Lagrangian* formulation) or the *conjugate momenta* $\mathbf{p} = \{p_1, p_2\}$ (*Hamiltonian* formulation), where p_1 and p_2 are the momenta conjugate to θ_1 and θ_2, respectively. The two variants will be considered in turn, as you perform in sequence the following tasks.

a) Express the Cartesian coordinates $\{x_1, y_1\}$ and $\{x_2, y_2\}$ of the two masses as functions of $\mathbf{q}$ (four equations).

b) Express the Cartesian velocities $\{\dot{x}_1, \dot{y}_1\}$ and $\{\dot{x}_2, \dot{y}_2\}$ of the two masses as functions of $\mathbf{q}$ and $\dot{\mathbf{q}}$ (four equations).

c) Write the expression for the potential energy $\mathcal{V}(\mathbf{q})$ as a function of $\mathbf{q}$, with its zero set to the situation where the pendulum is at rest ($\theta_1 = \theta_2 = 0$).

d) Write the expression for the kinetic energy $\mathcal{K}(\mathbf{q}, \dot{\mathbf{q}})$ as a function of $\mathbf{q}$ and $\dot{\mathbf{q}}$, and simplify your final equation using the addition theorem for cosines ($\sin a \sin b + \cos a \cos b = \cos a - b$).

e) Write the expression fot the Lagrangian $\mathcal{L}(\mathbf{q}, \dot{\mathbf{q}})$ of the system.

f) To apply the Lagrangian formalism, write down the Lagrange equations of motion, which provide a relationship between $\ddot{\mathbf{q}}$, $\dot{\mathbf{q}}$ and $\mathbf{q}$ for the system (two equations).

g) To move on to the Hamiltonian formalism, start by using the definition of the conjugate momenta (derivatives of the Lagrangian with respect to $\dot{\mathbf{q}}$) to write the expressions for the conjugate momenta $\mathbf{p}$ as functions of $\mathbf{q}$ and $\dot{\mathbf{q}}$ (two equations).

h) Derive the expressions providing $\dot{\mathbf{q}}$ as functions of $\mathbf{p}$ and $\mathbf{q}$ (two equations), using the symbol c in place of $\cos(\theta_1 - \theta_2)$ to simplify the notation (tip: consider the linear combinations $p_1 - cp_2$ and $2p_2 - cp_1$).

i) Insert the above expressions into the equation for $\mathcal{K}(\mathbf{q}, \dot{\mathbf{q}})$, so as to derive an expression for the kinetic energy $\mathcal{K}(\mathbf{q}, \mathbf{p})$ as a function of $\mathbf{q}$ and $\mathbf{p}$.

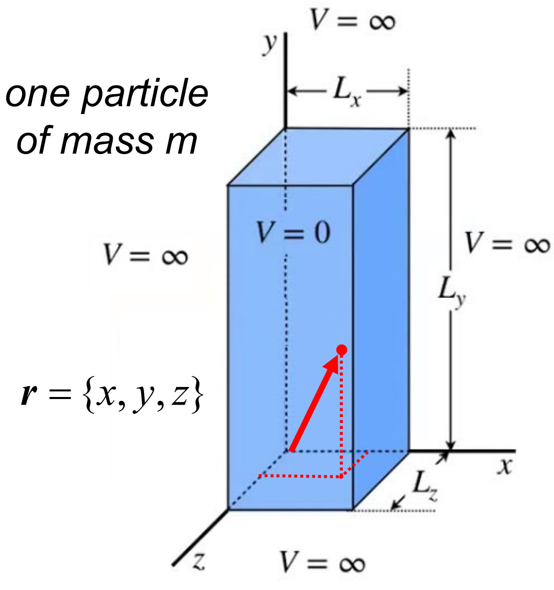
j) Write the expression for the Hamiltonian $\mathcal{H}(\mathbf{q}, \mathbf{p})$ of the system.

k) Formulate the first Hamiltonian equation of motion (the one giving $\dot{\mathbf{q}}$) and verify that the resulting expression indeed returns $\dot{\mathbf{q}} = \{\dot{\theta}_1, \dot{\theta}_2\}$.

l) Formulate the second Hamiltonian equation of motion (the one giving $-\dot{\mathbf{p}}$), not forgetting to consider the derivative of c, the symbol we introduced above in place of $\cos(\theta_1 - \theta_2)$.

Problem 2: Quantum Mechanics – The Particle in a Box

The goal of this exercise is to illustrate the solution of the *time-independent Schrödinger equation* (TISE) in the context of a relatively simple (yet extremely important!) example, namely the *particle in a box* problem *in three dimensions*, as illustrated in the figure below.



The edges L_x, L_y and L_z of the box as well as the mass m of the particle are fixed (these are *parameters* of the problem). Positions in the box are described by the Cartesian coordinate vector $\mathbf{r} = \{x, y, z\}$ (note that quantum mechanically, it would be misleading to refer to $\mathbf{r}$ as the "position of the particle").

It is assumed that the system is isolated (no coupling to the surroundings, no time-dependent interactions), so that the *Hamiltonian operator* is given by

$$\hat{\mathcal{H}} \;=\; -\frac{\hbar^2}{2m}\nabla^2 + \mathcal{V}(\mathbf{r}) = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right) + \mathcal{V}(x,y,z)\,,$$

where $\mathcal{V}$ is the potential energy. The latter only involves the hard (impenetrable) walls at the box surface, *i.e.*

$$V(\mathbf{r}) = \begin{cases} 0 & \text{for } x\in[0,L_x],\ y\in[0,L_y] \text{ and } z\in[0,L_z]\ , \\ \infty & \text{otherwise} \end{cases} \quad .$$

The TISE for this problem is an *eigenvalue equation* that can be written

$$\hat{\mathcal{H}}\,\Psi(\mathbf{r}) \;=\; E\,\Psi(\mathbf{r})\,.$$

Here, $\Psi(\mathbf{r})$ is the stationary (*i.e.* time-independent) wavefunction of the system (*eigenfunction*), *i.e.* a complex-valued function of the position vector $\mathbf{r}$, and E is the total energy (*eigenvalue*). Because the system is confined, we expect that the TISE solutions will span a discrete (but infinite) spectrum of energy values (*energy levels*), and that every allowed energy value will be associated with a discrete set of (degenerate) solutions for the wavefunction (*system states*).

In the following, we will omit $\mathcal{V}$ from the Hamiltonian. This is allowed considering that the energy of the particle is entirely due to its motion (kinetic energy), and if we keep in mind that the expressions derived below for $\Psi(\mathbf{r})$ should be substituted by $\Psi(\mathbf{r})=0$ for any point $\mathbf{r}$ located outside the box. Given this convention, inserting the Hamiltonian expression into the TISE leads to

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\Psi \;=\; E\Psi\,,$$

which is a partial differential equation in the three dimensions x, y and z. To solve it, you have to perform in sequence the following tasks.

a) Show that this equation is separable, using the *ansatz* $\Psi(x,y,z)=\Psi_x(x)\Psi_y(y)\Psi_z(z)$. In practice, you have to insert this expansion for $\Psi(x,y,z)$ into the equation, divide by the product $\Psi_x(x)\Psi_y(y)\Psi_z(z)$ (ignore any potential roots of these functions), and split the result into individual equations (one for each spatial direction).

b) Each of these three equations corresponds to the problem of a particle in a one-dimensional box. The solution to this problem has been given in the lecture without proof, namely (considering the x-direction as an example)

$$\Psi_x(x) = \left(\frac{2}{L_x}\right)^{1/2}\sin\left(\frac{\pi n_x}{L_x}\,x\right) \quad \text{with} \quad E_x = \frac{h^2}{8mL_x^2}\,n_x^2 \quad \text{for} \quad n_x = 1,2,\ldots\,.$$

Remember that this expression should be substituted by $\Psi_x(x)=0$ for $x\notin[0,L_x]$. Before proceeding to the three-dimensional case, we ask you to verify that the function $\Psi_x(x)$ satisfies the following conditions: (*i*) it vanishes at 0 and L_x, so that it is continuous at the edges of the interval (towards the value of zero outside); (*ii*) it is normalized over the interval $[0,L_x]$, *i.e.* the integral of its complex square evaluates to one over this interval; (*iii*) it satisfies the one-dimensional TISE, *i.e.* $-\hbar^2/(2m)\,\mathrm{d}^2/\mathrm{d}x^2\,\Psi_x(x) = E\Psi_x(x)$ for all n_x; (*iv*) it has n_x-1 nodes (excluding 0 and L_x) over the interval $[0,L_x]$. By doing these checks, you will actually have proved (if not derived) the results reported in the lecture slides for the one-dimensional case.

c) Use the previous considerations to formulate the solution to the three-dimensional TISE, *i.e.* write the general expression for the wavefunction (using a vector of three integer quantum numbers $\mathbf{n} = \{n_x, n_y, n_z\}$ to label the solutions) along with the equation that gives the associated energy (as a function of $\mathbf{n}$).

d) State the allowed ranges of the quantum numbers n_x, n_y and n_z. Write the expression for the energy of the ground level (*i.e.* the level with the lowest-possible energy), and give its degeneracy (*i.e.* the number of possible states, *i.e.* wavefunctions, compatible with this energy level).

e) Considering the special case $L_x = L_y = L = V^{1/3}$, where V is the box volume, show that the energy E_n of a level depends only on the norm of n. Considering the resulting expression connecting E_n to n, give the scaling with which the degeneracy (number of states, *i.e.* of wavefunctions, associated with a given energy level) grows with the energy E_n of the level in the limit of large n. Calculate the numerical value (in kJ·mol^{-1}) of the constant relating E_n to n^2 for the specific case of a hydrogen atom (mass $m = 1$ g·mol^{-1}) in a nanometric cubic box (volume $V = 1$ nm^3). Compare this value to the average classical kinetic energy $(3/2)k_BT$ of an atom in an ideal gas at room temperature ($T = 300$ K), and briefly discuss your observations.

Problem 3: Quantum and Classical Mechanics – Revision Questions

This last "problem" is not really a problem, but rather a pointer to additional material you may wish to consider, either during or after this exercise session, or later during your exam preparations (*i.e.* you are *not* expected to do this right now!).

On the course web site, you will find a collection of previous examinations, together with detailed written solutions. Below, we use the labels S (spring) and F (fall), along with the year, the exercise number, and the task index.

The following questions refer to classical mechanics (considered: F2020-S2023)

- F2020.2(a): Hamiltonian equations of motion
- S2021.2(b): Newtonian equations of motion
- F2021.2(a): Lagrangian equations of motion

The following questions refer to quantum mechanics (considered: F2020-S2023)

- F2020.3(b): Time (in)dependent Schrödinger equation
- S2021.1(b): Correspondence principle
- S2022.2(a): Time (in)dependent Schrödinger equation