PHY321 Classical Mechanics 1

Final project, due Friday April 30

midnight (1159pm)

Apr 22, 2021

Practicalities about homeworks and projects

1. You can work in groups (optimal groups are often 2-3 people) or by yourself. If you work as a group you can hand in one answer only if you wish. **Remember to write your name(s)!**

2. How do I(we) hand in? Due to the extraordinary situation we are in now, the final projec should be handed in fully via D2L. You can scan your handwritten notes and upload to D2L or you can hand in everyhting (if you are ok with typing mathematical formulae using say Latex) as a jupyter notebook at D2L. The numerical part should always be handed in as a jupyter notebook.

Introduction to the final project, total score: 160 points. The relevant reading background is

1. chapters 2-8 and 14 of Taylor

2. lecture notes throughout the semester and previous homework and midterm projects.

The final project aims at covering most of the topics we have discussed during the semester. You should feel free to use either paper and pencil and/or symbolic software (sympy, Mathematica or similar) for the non-computational exercises.

Exercise 1, Two-body Problems and Conservative Forces. The relevant material from Taylor aree chapters 4 and 8. Homework sets 6-9 and the chapters on forces and two-body problems from the lecture notes may also be of use.

This exercise is a follow-up of hw6. There we studied the so-called Lennard-Jones potential which is widely used in molecular dynamics calculations. This potential is based on parametrizations from expertiments. In molecular dynamics calculations the assumption is that atoms move according to the laws of Newton,

given the correct model for interactions. We can say then that quantum-mechanical degrees of freedom stemming from the interactions between electrons and protons in an atom, are parametrized in terms of an effective potential.

We will limit ourselves to a two-body problem.

The goal of this exercise is to model a gas of argon atoms (here two atoms only interacting), where the atoms interact according to the famous Lennard-Jones potential,

$$V(r) = 4\varepsilon \left((\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^6 \right), \tag{1}$$

where r is the distance between two atoms, $r = |\boldsymbol{r}_i - \boldsymbol{r}_j|$, that is the norm of the relative distance vector $\boldsymbol{r}$. The quantities σ and ε are parameters which determine which chemical compound is modelled. This potential is a good approximation for noble gases like helium, neon, argon and other.

We start first with a basic study of the potential

- **1a (5pt):** Plot the potential as a function of r with $\varepsilon = 1$ and $\sigma = 1$, for example for $r \in [0.9, 3]$.

- **1b (5pt):** The behaviour of $V(r)$ is vastly different for $r < \sigma$ and $r > \sigma$. Which term in the potential, (1), dominates in each case and what is the effect?

- **1c (5pt):** Find and characterise the equilibrium points of the potential.

- **1d (5pt):** Describe qualitatively the motion of two atoms which start at rest separated by a distance of 1.5σ. What if they start with a separation of 0.95σ? (Hint: use the graph of the potential.)

- **1e (5pt):** Describe the shape of the potential close to the stable equilibrium point. Can you think of other force(s) with the same behaviour?

Then we switch our attention to the equations of motion.

- **1f (5pt):** Find the force on atom i at position $\boldsymbol{r}_i$ from atom j at position $\boldsymbol{r}_j$.

- **1g (5pt):** Is this a conservative force? Show that the **curl** is zero.

- **1h (5pt):** Are linear and angular momentum conserved? You need to show this by calculating the relevant quantities.

- **1i (5pt):** Show that the equation of motion for atom i is

$$\frac{d^2 \boldsymbol{r}_i}{dt^2} = \frac{24\varepsilon}{m} \sum_{j \neq i} \left(2(\frac{\sigma}{|\boldsymbol{r}_i - \boldsymbol{r}_j|})^{12} - (\frac{\sigma}{|\boldsymbol{r}_i - \boldsymbol{r}_j|})^6 \right) \frac{\boldsymbol{r}_i - \boldsymbol{r}_j}{|\boldsymbol{r}_i - \boldsymbol{r}_j|^2}.$$

Numerical accuracy is reduced when computing with values which are many orders of magnitude apart. This is often an issue in physics, and molecular

dynamics is no exception. For example, the mass of argon is smaller than $10e - 25$kg, while typical length scales are on the order of nanometers, $10e - 9$m.

The remedy is to change units so that most quantities are close to 1. From (1) it is clear that σ and ε are the typical scales for length and energy.

- **1j (5pt):** Introduce the scaled coordinates $\boldsymbol{r}_i{'} = \boldsymbol{r}_i/\sigma$ and show that the equation of motion can be rewritten in terms of these coordinates as (where $t' = t/\tau$ for a suitable choice of τ.)

$$\frac{d^2 \boldsymbol{r}_i{'}}{dt'^2} = 24 \sum_{j \neq i} \left(2|\boldsymbol{r}_i{'} - \boldsymbol{r}_j{'}|^{-12} - |\boldsymbol{r}_i{'} - \boldsymbol{r}_j|^{-6} \right) \boldsymbol{r}_i{'} - \boldsymbol{r}_j{'}$$

$$\overline{|\boldsymbol{r}_i{'} - \boldsymbol{r}_j{'}|^2}, (2)$$

- **1k (5pt):** What is the characteristic time scale τ, and what is its value for argon, which has $\sigma = 3.405$Å (1Å$= 1e - 10$m), $m = 39.95u$ (with $1u = 1.66e - 27$kg) and $\varepsilon = 1.0318e - 2$eV ($1eV=1.602e - 19$J)?

We switch now to a numerical procedure and study the simulation of two interacting atoms.

- **1l (5pt):** Write a function which solves () for two atoms and finds the positions and velocities of the atoms as a function of time. Implement either the Euler-Cromer or the Velocity-Verlet method to solve the equations od motion.

- **1m (5pt):** Simulate the motion of two atoms which start at rest separated by a distance of 1.5σ. Use $\Delta t' = 0.01$, simulate until $t' = 5$ and integrate with one of the above methods.

- **1n (5pt):** Plot the distance between the atoms as a function of time.

- **1o (5pt):** How does the motion fit with your expectations?

- **1p (5pt):** Repeat the previous tasks, but now with an initial separation of 0.95σ. Explain your results.

- **1q (5pt):** Compute and plot the kinetic, potential and total energy as a function of time for. Should the total energy be conserved? Why, or why not? Does your program fulfil this? If not, what could be the cause?

Exercise 2, Coupled Harmonic Oscillators. The relevant chapters from Taylor are chapters 5-7 and the lectures notes on harmonic oscillations and the Lagrangian Formalism and Calculus of Variations. Your codes from homework sets 5-8 and the first midterm may also be of interest.

Consider a mass m that is connected to a wall by a spring with spring constant k. A second identical mass m is connected to the first mass by an identical spring. Motion is confined to the x direction only.

- **2a (10pt):** Make a drawing of the system, set up forces and define variables x_1 and x_2 for the two masses.

- **2b (10pt):** Write the Lagrangian in terms of the positions of the two masses x_1 and x_2.

- **2c (10pt):** Use the Euler-Lagrange equations to find the equations of motion.

- **2d (10pt):** Find the analytical solutions using a guess of the type

$$x_1 = Ae^{i\omega t}, \quad x_2 = Be^{i\omega t}.$$

Solve for A/B and ω. Express your answers in terms of $\omega_0^2 = k/m$.

- **2e (20pt):** Write now a program which solves these two coupled differential equations for x_1 and x_2. Compute the positions x_1 and x_2 by choosing your initial conditions and compare with the analytical answers from 2d.

Classical Mechanics Extra Credit Assignment: Scientific Writing and attending Talks. The following gives you an opportunity to earn **five extra credit points** on each of the remaining homeworks and **ten extra credit points** on the midterms and finals. This assignment also covers an aspect of the scientific process that is not taught in most undergraduate programs: scientific writing. Writing scientific reports is how scientist communicate their results to the rest of the field. Knowing how to assemble a well written scientific report will greatly benefit you in you upper level classes, in graduate school, and in the work place.

The full information on extra credits is found at `https://github.com/mhjensen/Physics321/blob/master/doc/Homeworks/ExtraCredits/`. There you will also find examples on how to write a scientific article. Below you can also find a description on how to gain extra credits by attending scientific talks.

This assignment allows you to gain extra credit points by practicing your scientific writing. For each of the remaining homeworks you can submit the specified section of a scientific report (written about the numerical aspect of the homework) for five extra credit points on the assignment. For the two midterms and the final, submitting a full scientific report covering the numerical analysis problem will be worth ten extra points. For credit the grader must be able to tell that you put effort into the assignment (i.e. well written, well formatted, etc.). If you are unfamiliar with writing scientific reports, see the information here

The following table explains what aspect of a scientific report is due with which homework. You can submit the assignment in any format you like, in the same document as your homework, or in a different one. Remember to cite any external references you use and include a reference list. There are no length requirements, but make sure what you turn in is complete and through. If you have any questions, please contact Julie Butler at butler@frib.msu.edu.

HW/Project	Due Date	Extra Credit Assignment
HW 3	2-8	Abstract
HW 4	2-15	Introduction
HW 5	2-22	Methods
HW 6	3-1	Results and Discussion
Midterm 1	**3-12**	*Full Written Report*
HW 7	3-22	Abstract
HW 8	3-29	Introduction
HW 9	4-5	Results and Discussion
Midterm 2	**4-16**	*Full Written Report*
HW 10	4-26	Abstract
Final	**4-30**	*Full Written Report*

You can also gain extra credits if you attend scientific talks. This is described here.

Integrating Classwork With Research. This opportunity will allow you to earn up to 5 extra credit points on a Homework per week. These points can push you above 100% or help make up for missed exercises. In order to earn all points you must:

1. Attend an MSU research talk (recommended research oriented Clubs is provided below)

2. Summarize the talk using at least 150 words

3. Turn in the summary along with your Homework.

Approved talks: Talks given by researchers through the following clubs:

- Research and Idea Sharing Enterprise (RAISE): Meets Wednesday Nights Society for Physics Students (SPS): Meets Monday Nights

- Astronomy Club: Meets Monday Nights

- Facility For Rare Isotope Beam (FRIB) Seminars: Occur multiple times a week

If you have any questions please consult Jeremy Rebenstock, rebensto@msu.edu.

All the material on extra credits is at https://github.com/mhjensen/Physics321/blob/master/doc/Homeworks/ExtraCredits/.