PHYSICS WITH THEORETICAL PHYSICS

Computing Project (Phys20872)

Academic Year 2024/25

Prof. Michael Seymour, 13/01/2025

Background

All second-year students in Physics with Theoretical Physics do a computing project in the second semester of year two. This project is instead of the laboratory work done by other students in this semester. The project carries a weight equivalent to a lecture course and the pass mark is 40%. No resits are available. Success in the project requires initiative, steady work and independent learning throughout the semester.

Meeting

All second-year students in Physics with Theoretical Physics should meet with Prof. Seymour at 2 pm on Friday 24th January using a zoom link that he will send to your university email address at least 24 hours in advance. At this meeting we shall explain the structure of the first three weeks, the projects, discuss how supervisors will be assigned and answer any questions you have.

Preparation

An online form will be open from Friday 24th January 2pm until Tuesday 28th January 5pm for you to nominate a list of 4 preferred projects (in order of preference) and a choice of partner. If you have not submitted your form by the deadline, you will be assigned a project. If you do not nominate a partner, you will be assigned one.

The choice of computer language

The choice of language to program in is completely up to you. We recommend using an interpreted language: We particularly recommend Python and/or Mathematica. Other good choices could be Matlab, C++ or Java, as well as lots of other languages. We expect each team of two students to collaborate on their codes, so they **must** use the same language. Additional support material for Python and Mathematica is available on Blackboard.

The first 3 weeks of the course

In the first three weeks of the course you will work through a set of materials available on the Blackboard site of the course, individually or in your own choice of small groups; we require satisfactory completion of a set of tasks before you will be allowed to start the project stage of the course. You can complete these tasks on your own computer, or by logging in to our jupyter server. You can do this in your own time, at your own pace, but on **Tuesdays and Fridays from 2–5**, Prof. Seymour and at least one Graduate Teaching Assistant will be available to assist you in the Schuster library "glass box" rooms. Each week, you submit your work on Blackboard, and will meet your project supervisor to discuss it, normally on the following **Tuesday afternoon**, unless your supervisor arranges a different time with you. You must submit your work and attend this meeting to receive the corresponding (pass/fail) mark.

Project arrangements

Students will normally work together as a team of two. It is not normally recommended to work without a partner. You can nominate a choice of partner, and students with no preference will be assigned one.

The Project Supervisor will outline the topic in Week 4 of the semester. This project will involve some reading on background physics and associated computational work. The physics and computing will become more sophisticated as the project develops.

The projects should be completed in the following six weeks of the Semester.

Students will normally use their own computers. If this will be a problem, you should contact Prof. Seymour as soon as possible.

Generic support for computing will be provided through Blackboard and a GTA; specific support normally by the supervisor.

Students should meet with their project supervisor once a week to discuss progress and to decide on the next step(s). In exceptional circumstances a meeting can be skipped for one week. Lack of engagement may lead to students being removed from the course. Supervisors will also make themselves available for a one-hour drop-in session once a week. These meetings and drop-in sessions normally take place on Tuesdays and Fridays between 2pm and 5pm, or by arrangement with the supervisor.

Reports

One of the most important aspects of carrying out a research or development project lies in presenting and analysing your results clearly. To this end we ask you to produce a joint report of about 10 pages, in the style of a scientific paper, aimed at an audience of your fellow students, that

1. introduces the problem and its related physics;
2. gives a succinct description of the computational context of your work (we do not want to see your code!);
3. analyses and illustrates the results in a physical context, concisely and in an appropriate form (normally using suitable high-quality graphical representations);
4. summarizes your conclusions about the quality and limitations of the techniques you applied;
5. makes some recommendations about the direction of future work.

Structure of report:

We do not provide a template, since we expect a variety of software packages to be used for typesetting the highly mathematical content. Microsoft Word is probably not the most appropriate choice; LaTeX, maybe using overleaf may be a much better choice. We require you to start with a title, abstract and introduction, and end with conclusions and references—the middle part should contain theory and results, following the generic structure of a scientific paper. The department's lab report "house style" is also helpful, sensibly adapted for a theory report. Students should submit a pdf version of the report of about 10 pages in length, but no more than 12, using a font no smaller than 10 points, before **2 p.m. on Friday, April 4th 2025**, using Blackboard.

Interviews

Interviews will take place on Tuesday 6th and Wednesday 7th May (the last week of the semester); these will be assigned a given time, and cannot *normally* be rearranged or moved (i.e., except in exceptional circumstances, which should be communicated well in advance).

Each interview will last 25 minutes, and will start with a 5-minute presentation.

Assessment

- 25% of the marks will be allocated by the supervisor, based on effort and progress.
- 25% of the marks are available for the interview and presentation.
- 50% will be allocated to the report, with quality of writing, presentation, physics and use of computing all carrying equal weight.

In the first instance, marks will be assigned equally to each student in a team. If there is a clear indication of a disparity of effort and/or contribution, the marks will be modified accordingly.

Note that, in accordance with University policy, Automatic Extensions do not apply to group work.

The University policy on Late Submissions applies to the report submission. It must be submitted through Blackboard by 2p.m. on the submission day. Multiple submissions can be made up to that point. Only one student from each pair may submit the report (otherwise the plagiarism system will report a 100% match!).

Plagiarism and AI use

Of course, the report is subject to the University's policies on Plagiarism and AI use. It is important to realise that **both** members of a pair are responsible for the content of their report and for ensuring that it complies with these policies. It is an important part of collaborating together to keep an open record of your sources, so that you can both take responsibility for them.

AI tools such as ChatGPT can be extremely helpful in software development and their use is not forbidden. However, you should treat them in the same way you would treat input from friends, staff members or the internet – it is helpful input to your research process, but you must take full responsibility for all code produced, understand how it works and how to adapt it if needed, and you must devise strategies to validate that it is working correctly and producing the expected results. These are all important skills needed in "real world" applications of AI to software development. All text and figures written in your report must, however, be generated by yourselves, except where properly acknowledged, and must not be AI-generated.

You will be asked to fill in an online form about two weeks before report submission, confirming that you understand these policies, and are encouraged to discuss them with your supervisor or the course leader if in any doubt.

SCHEDULE

A summary of the schedule of the course:

- Meeting at 2 pm on Friday 24th January
- Tuesday 28th January: Support available for introductory work 2-5p.m., Schuster library "glass boxes".
- Fridays 31st January and 7th and 14th February: Support available for introductory work 2-5p.m., Schuster library "glass boxes".
- Tuesdays 4th and 11th February: Support available for introductory work 2-5p.m., Schuster library "glass boxes", plus meeting with project supervisor to discuss introductory work, or as arranged by supervisor.
- February 17th – March 28th: perform computational work, weekly meeting with supervisor.
- March 24th – 28th: complete computational work, final meeting with supervisor.
- March 31st – April 4th: write report (start well before this!), optional meeting with supervisor.
- April 4th, 2p.m.: joint report handed in on Blackboard.
- April 7th – 25th: Easter break.
- May 6th and 7th: interviews. Pre-assigned time, 25 minutes per pair (including 5 minutes presentation).

List of projects

Please note that we will assign multiple teams to each project; supervisors will be determined later.

Details appear on the next pages.

Project Supervisors and contact details

- Dr Oznur Apsimon (Oznur.Apsimon@manchester.ac.uk)
- Dr Michael Keith (Michael.Keith@manchester.ac.uk)
- Dr Andrea Mattioni (Andrea.Mattioni@manchester.ac.uk)
- Dr James McHugh (James.McHugh@manchester.ac.uk)
- Dr Harry Miller (Harry.Miller@manchester.ac.uk)
- Dr Ahsan Nazir (Ahsan.Nazir@manchester.ac.uk)
- Dr Draga Pihler-Puzovic (Draga.Pihler-Puzovic@manchester.ac.uk)
- Prof Michael Seymour (Michael.Seymour@manchester.ac.uk)
- Prof Robert-Jan Slager (Robert-Jan.Slager@manchester.ac.uk)

Lab Demonstrators (Tuesday and Friday 2-5pm of weeks 1–3)

- Prof Michael Seymour (Michael.Seymour@manchester.ac.uk)
- Tom Harvey (Thomas.Harvey-3@manchester.ac.uk)

List of projects

1: The classical H_2^+ ion

This project provides a simple introduction to the "many body problem". The aim is to simulate (using purely classical physics), a positive ion of molecular hydrogen. The motion of the electron will be calculated from the equation of motion, which requires integration of the set of ordinary differential equations, with the force arising from the two protons (initially taken to be fixed). Then, the covalent binding force due to the electron will be considered, and the effects of also allowing the protons to move will be explored.

Physics Background
Classical Mechanics

References:
M L De Jong "Introduction to computational Physics" (Addison-Wesley, 1991)

2: Monte Carlo simulation of phase transitions

Monte Carlo algorithms are a key tool in computational physics, and are used in statistical physics, in quantum field theory and in particle physics. In this project you will implement a Monte Carlo simulation and study the Ising model, a very simple model of magnets, and you will study its thermal properties, including most importantly the study of phase transitions. If time permits we shall look at cluster algorithms.

Physics Background
Statistical Physics and Thermodynamics

References
1. F. Mandl, Statistical Physics, 2nd ed (Wiley, 1988)
2. C. J. Adkins, Equilibrium Thermodynamics, 3d ed (Cambridge UP, 1983)
3. S. E. Koonin, Computational physics (Benjamin/Cummings Pub. Co., 1986).

3. Simulation of road traffic

The main objective is to develop computer modelling skills of random events in the context of real life problems. Students will be asked to consider some of the following problems using a simplified cellular automaton model:

- The clumping of buses. How does it arise? What is the effect of the frequency of buses, and of the arrival and departure rates of passengers?
- The optimum design of traffic lights at an intersection. For a given traffic flow, what are the optimum time intervals between red and green lights?
- Traffic flow at roundabouts. Can they replace traffic lights?

Physics Background
Non-linear dynamics

References
K. Nagel, M. Schreckenberg: "A cellular automaton model for freeway traffic", J. Phys. I France 2 (1992) 2221–2229, https://jp1.journaldephysique.org/articles/jp1/pdf/1992/12/jp1v2p2221.pdf

4: Neutron stars

Neutron stars are very dense objects created in supernova explosions. They are prevented from collapsing by the pressure of dense nuclear matter. We will study the differential equations describing such stars using Newtonian and general relativity. Runge-Kutta or similar methods will be used to solve non-linear differential equations for the density as a function of radius. Dependence of the radii of such objects on the equation of state will also be investigated.

Physics Background
Statistical Physics and Thermodynamics; Nuclear Physics

References
1. A. C. Phillips, The physics of stars (Wiley, 1994)

2. S. E. Koonin, Computational physics (Benjamin/Cummings Pub. Co., 1986).

5: Random sampling and Monte-Carlo simulation

The Monte-Carlo method is very widely used to simulate physical processes, and is also used do numerical integration, particularly in the field of finance.

In this project you will develop an understanding of Monte-Carlo radiation transport, and apply it to the movement of neutrons in a nuclear reactor. The example of a dilute thermal homogenous nuclear reactor will be modelled, and you will obtain by Monte Carlo simulation the parameters of such a reactor such that it becomes critical.

Physics Background
Random Processes

References
"Elements of Nuclear Power" (3rd edition), D J Bennet (Longman, 1989)

6: Scars in the wave function of the stadium billiard

Infinite square wells are the simplest problems to solve in quantum mechanics; indeed most QM textbooks (e.g., [1]) discuss such problems in detail. In two dimensions the situation is quite different: in certain cases the problem can be solved in closed form, but those that correspond to classically chaotic systems, such as the stadium billiard[2], a system that has now been realized experimentally [3], are quite interesting.

In this project we shall study the eigenstates of the stadium billiard. This requires solution of the simple problem $\Delta\psi = E\psi$ with the requirement that ψ vanishes on an interesting boundary.

This can be turned into a simple diagonalisation problem by applying finite differences, where the boundary condition is turned into an enumeration (labelling) problem. Using standard routines [4], we will then find the eigenfunctions of this problem, and show how they are influenced by (unstable) periodic orbits of the classical problem [5].

Physics Background
Quantum Mechanics; Partial Differential Equations

References
1. F. Mandl, Quantum mechanics (Wiley, 1992)

2. http://serendip.brynmawr.edu/chaos/doc.html

3. http://arXiv.org/abs/chao-dyn/9906032,

4. W. H. Press et al, Numerical recipes : the art of scientific computing either C or C++ version; Alternatively, look at http://www.netlib.org

5. L. E. Reichl, The transition to chaos: conservative classical systems and quantum manifestations (Springer, 2004)

7: Solitons in wave equations

There are many nonlinear wave equations that allow for exact non-dispersive solutions. We shall study one of these equations, the non-linear Schrödinger equation, and numerically determine the solitons of this equation. We shall then study their scattering, and look how the solutions change if we modify the equations.

Physics Background
Mathematical Methods; Partial Differential Equations

References
1. R. Rajaraman, Solitons and Instantons (North-Holland, 1982)

2. W. H. Press et al, Numerical recipes : the art of scientific computing either C or C++ version; Alternatively, look at http://www.netlib.org

8: Numerical solution of the Schrödinger equation

We shall study the behaviour of the Schrödinger equation for simple one dimensional problems, solving the initial value problem for an incoming wave packet on various barriers. We will also compare different numerical techniques for this problem, with an emphasis on the probability density.

Physics Background
Mathematical Methods; Partial Differential Equations

References
1. S. E. Koonin, Computational physics (Benjamin/Cummings Pub. Co., 1986).

2. W. H. Press et al, Numerical recipes : the art of scientific computing either C or C++ version; Alternatively, look at http://www.netlib.org

3. Joshua Izaac, Jingbo Wang, Computational Quantum Mechanics (Springer 2018)
https://www.librarysearch.manchester.ac.uk/permalink/44MAN_INST/bofker/alma992979784517501631

9: The chaotic pendulum

The motion of a forced, damped pendulum can be solved analytically when the amplitude of oscillations is small. This is not true in general, however, and the solution can even be chaotic (i.e. the long-term behaviour of the system is unpredictable). The aim of this project will be to investigate the general behaviour of the pendulum. Students will write a code to numerically solve the approximation to the equation of motion for small oscillations and compare with the analytic solution for various situations. They will then solve the exact equation and investigate how different choices for the model parameters (e.g. strength of damping, forcing frequency) lead to regular or chaotic behaviour.

Physics Background
Vibrations and Waves

References
1. W. H. Press et al., Numerical recipes: the art of scientific computing (CUP 2007, see www.n-r.com)

2. G. King, Vibrations and Waves (Wiley, 2009)