Submission guidelines for the 10-credit PY4TP2 Research Project, 2019-20

On successful completion of this module, students should be able to carry out a research project through all of its stages, including literature study, data generation and data analysis. Its assessment will be based on the quality of a concise research report prepared by the student, an oral presentation by the student summarising their progress on their project, and short a oral interview.

The STRICT deadline both for submission of soft-bound research reports to the School of Physics office is: Friday 20th March 2020.

Important: Report submission is always the student’s personal responsibility. If a student fails to submit a report or to give their oral presentation then they can obtain no marks for it.
If an ad misericordiam reason, such as illness, appears likely to prevent you from handing in your project report on time you must contact David.O.Regan@tcd.ie as soon as the problem arises. An ad misericordiam reason will not be considered if it is offered after the submission deadline.

Research Report
Each student needs to submit 3 printed copies of her/his own individual report to the School of Physics Office, SNIAM first floor (these copies will then be distributed to the Supervisor, Second Reader, and the External Examiner). You are required to write the report yourself, and evidence will be recognized, in the marking process and interview, of independent thought in the analysis and write-up.

Length of report: approximately 20 printed pages at 12 point, 1.5 spacing, with normal margins. This includes figures, tables, abstract, table of contents, and a list of references (bibliography). Please add page numbers, and consider printing double-sided (if suitably bound). The hard page limit is 25 pages at this font size and spacing, however 20 pages seems adequate for what should be a concise research report. It is accepted that students will inevitably use diverse word processors or LaTeX styles, and different fonts, so that line spacing may vary slightly. This is acceptable, but presentation should be neat and not cramped: do not use smaller font sizes, margins, or figures to fit within the 25 pages.

Appendices may be added on top of these page counts showing additional figures or tables, if needed. This is particularly relevant if the work generates a large volume of data that is worth presenting. It may be reasonable to include original computer code as an appendix, if it forms an important part of your research work. Appendices should not be used to circumvent the above page limit.

Figures should be prepared and exported in a vector format (.pdf or .eps) or at least at high resolution, wherever possible, as low-quality ‘bitmapped’ images will diminish an otherwise well-prepared report.

Layout: You are free to use the report layout that you feel best enables you to present your scientific research. Most students prefer to follow a canonical report structure with the following parts: Title page, Abstract, Acknowledgements, Contents, Introduction, Theory or Background, Theoretical or Computational Method, Results and discussion, Conclusions, Bibliography or References, Appendices.

In the Introduction you should concisely describe the area of physics in which you are working, perhaps beginning at a non-specialist level and ending at a senior undergraduate level. You should clearly outline the problem that you have been set and its motivation, and introduce the theoretical or computational methods (where appropriate) and methods of analysis that you are going to use in later sections. You may wish to include a description of physical theories relevant to your work and these could be included in the Introduction or in a separate Theory or Background section, as appropriate.
In a section that could be titled **Theoretical Method** or **Computational Method**, you should give an adequate, but not overly detailed, description of the methods that you actually used to generate and analyse your results. Include figures here if they can help to illustrate a method or algorithm.

In a section entitled **Results and Discussion**, your results should be presented in a suitable form using tables and graphs. If there are many results then the less important ones may be relegated to an appendix or even omitted. In discussing your results, you should address whether you achieved the goals set for the project, the significance of particular results, how you might have improved the methodology, suggestions for further work, etc. These latter elements can help you to demonstrate that you have properly understood and appreciated the context and future trajectory of your research area. You may find it helpful to look over your lab manuals from previous years for reminders of best practice in reporting. Consider whether error analysis is relevant to your work. Use your figures and tables of data to **illustrate** your discussion if relevant. To this end, always number and caption these (use figure legends if necessary), and always refer to any figures or tables in the text.

Any formal article has a section at the end for a **Bibliography** (list of related works, usually books) and references to books and journal articles *explicitly cited in the text* (e.g. *with a number*). Use a standard format when citing books and articles. Recommended formats are, for a book,


and, for an article,


References in the text to a book or article are cited using either

• a consecutive numbering system (e.g. [1], [2], …) with the references in the bibliography arranged in numerical order, or

• the surname of the first author of the article enclosed in parentheses (e.g. [Bloggs]). In this case the references in the bibliography are arranged in alphabetical order.

Sometimes it is unavoidable to cite an electronic source, e.g. a website, though even here you should emphasise scholarly sources such as University or national research body webpages. For electronic bibliography sources, include the webpage name, its URL, the date that you accessed it, the author’s name, their institution, anything else that may help to identify the source in the long-term.

**Acknowledgements** are necessary to clarify your role in the project and any help received. An example might be: ‘I was shown how to use the analysis software by research student AB. It was necessary to modify the Python script for my jobs, which I did with the advice of PostDoc CD. I analysed the results and interpreted them myself. My Supervisor commented on a draft of my project report. I am grateful for the advice and encouragement given by all members of the research group.’ It is advisable to seek your project Supervisor’s advice **well in advance** of the project submission date on any aspects of the report or oral interview that you remain unsure about. You may offer to show them a draft or outline.

Your Supervisor and a Second Reader will both grade your report. You will be individually invited to a short **oral interview** (following Report submission, organized by your supervisor) to briefly summarise your project and to reply to queries of both the supervisor and second reader. The aim of the interview is to assess your understanding of the project and assist the Supervisor and Second reader in forming their marks for the report. The mark will be finalized at the examiners meeting.
**Coversheet Declaration:** Each Research Report must include a statement signed by the student that the thesis is their own work except where due citations are given. (This is a requirement of the College policy on plagiarism.) Refer to http://tcd-ie.libguides.com/plagiarism/declaration for the exact wording.

**PY4PT2 Research Seminars**

In Michaelmas term each students will individually give a short oral presentation on the context, background, progress to date, and plan for completion of their project. Any .pdf (not Powerpoint and certainly not Open/NeoOffice) slides for a presentation must be emailed to David.O.Regan@tcd.ie by the day before it is given. The quality of each presentation and also the participation of each student throughout the Seminar series (e.g. asking questions and engaging in discussions) will be assessed.

**Marking Scheme**

There are three elements contributing to the final mark for the Module:
1) The Supervisor’s Report mark, informed by the oral interview (45%).
2) The Second Reader’s Report mark, informed by the oral interview (45%).
3) Oral presentation mark from Seminars: PY4TP2 course coordinator (10%).

Guidelines for the **Supervisor’s Mark** (Total 100):
- a) Report quality 30
- b) Results obtained 30
- c) Effort and Performance 20
- d) Initiative and Understanding 20

Guidelines for the **Second Reader’s Mark** for the Report (Total 100):
- a) Introduction / Background 20
- b) Scientific content 50
- c) Presentation 20
- d) Conclusions 10

Guidelines for the **Research Seminar Mark**, provided by PY4TP2 course coordinator (Total 100):
- a) Oral presentation and response to questions 40
- b) Visual presentation, e.g. electronic slides 40
- c) Participation in discussions and questions in the seminar series 20

Please do not hesitate to contact me for any enquiries or clarifications.

David O’Regan, 24th June 2019. 

Email: David.O.Regan@tcd.ie

Theoretical Physics Degree Coordinator for School of Physics
__Project 1: Dr Steve Campbell Steve.Campbell@tcd.ie__

**Equilibration and the thermodynamics of non-Markovian Environments**

1 student

Put a smaller system in contact with a larger environment and, thanks to thermodynamics, the two will equilibrate. If we introduce a second bath at a different temperature, we enter the rich world of non-equilibrium systems. When all of the players in this game are classical systems, the various energy exchanges are fairly well understood. However, for quantum systems and quantum baths things are trickier. In this project we will explore how properties of the baths affect the equilibration of a quantum system to its non-equilibrium steady state. In particular, by exploiting a so called collision-model framework to model the quantum environments, we will examine how Markovian (memoryless) vs. non-Markovian baths affect the rate of equilibration and the ensuing non-equilibrium steady state properties. This is a theoretical project that will involve both analytical and numerical calculations performed with the aid of Mathematica.

__Project 2: Prof. Mauro Ferreira ferreirm@tcd.ie__

**Quantum Full-Waveform Inversion**

1 student

Full-Waveform Inversion (FWI) is a technique used in seismology that generates high-resolution images that can map the subsurface of the Earth, with applications in oil and gas prospection as well as earthquake risk-assessment. While this is a technique fully based on classical Physics, it can also be extended to the quantum realm. The goal of this project is to implement FWI methods to the propagation of quantum particles with the objective of reverse-engineering the potential-energy landscape of a quantum system. The project involves a good balance between analytical and numerical work.

__Project 3: Prof. John Goold gooldj@tcd.ie__

**Propagation of typical states with Krylov subspace techniques in non-integrable Heisenberg chains**

1 student

In this project we will use typical states (uniformly drawn from the Haar measure) as initial conditions for massively parallel time evolution of non integrable quantum spin chains. The idea is to first generate the states and then develop a state of the art code to do time evolution for the XXZ spin chain with integrability breaking perturbations. Special emphasis will be placed on the connection with the Kubo theory for high temperature transport and we will explore the ramifications for the temporal evolution of entanglement.
Project 4: Prof. John Goold gooldj@tcd.ie

Quantum dynamics of confinement

1 student

Some fundamental constituents of matter, the quarks, cannot be observed free in nature because they are confined into baryons and mesons. This is a consequence of the fact that the strong interaction between them increases with their separation. This phenomenon also occurs in condensed matter and statistical field theory. The goal of this project is to study the dynamics of confinement after a quench in a spin chain namely the Ising model in the transverse field with an integrability perturbation. In particular we will focus on the dynamics of quantum entanglement and mutual information following the quench.

Reference: http://www.nature.com/articles/nphys3934

Project 5: Prof. Stefan Hutzler shutzler@tcd.ie

Using the foam drainage equation to model the perfect pint

1 student

The drainage of liquid out of a foam is described by the nonlinear partial differential Foam Drainage Equation [1]. With the appropriate boundary conditions the equation describes the drying out of a foam under gravity, the propagation of a solitary wave of liquid through a foam, or the rise of a foam column due to continuous bubbling.

This project solves the Foam Drainage Equation numerically, by further developing some existing Python code. The aim is to model a rising column of foam to gain insight into foam stability. Such an understanding is of importance for many processes, for example in the food and drinks industry or for mineral extraction.

With the addition of good graphics this project should also result in a computer animation of the pouring and decay of a pint of beer.

Correcting DFT calculations for spurious electron self-interaction - the riddle of Prussian blue

1 student

The computer simulation of molecules and materials using density-functional theory (DFT) is beset by a number of well understood, but difficult to correct, systematic errors. The most notorious of these is electron self-interaction error — it is hard to inform a theory based only on the total electron density that electrons are discrete particles. Hence, the electrons are allowed to partially self-interact in DFT, often with severe adverse consequences for the prediction of energy gaps, magnetism, bond lengths and energies, etc. An established route to addressing this involves a parameter known as the Hubbard U. Adding a free parameter to DFT is undesirable, and a number of recipes have been developed for calculating an optimal value for U for a given system, whereby the theory again becomes parameter-free. We have been developing a new such recipe with attractive properties and promising results, including a second parameter targeting spin, Hund’s J, for small molecules [1] and oxides.

Having confirmed its capabilities, we have decided to step into the unknown with this method together with Prof. García-Melchor’s group at the School of Chemistry, investigating the complex electronic structure of Prussian blue. This substance has long been used as a pigment and as a medicine, but it has recently started to attract increasing attention due to its diverse range of functionality driven by its unusually ‘hollow’ crystal structure and multiple-valence effects on the correlated iron sites (the atoms can switch from 2+ to 3+, and may form quantum superpositions of these): controllable ferromagnetism, ferroelectricity, adsorption of molecules (potential for heterogeneous catalysis), ionic conductivity, etc. While it is understood that, in principle, the Fe 2+ and 3+ atoms should require different U parameters and particularly so in Prussian blue, there has been no systematic study to date directly exploring this effect and its ramifications for any material. This project will run a series of pioneering tests for a strongly charge-dependent-U in Prussian blue, calculating U & J values for different sites and dopants that can be used by Prof. García-Melchor’s group in close collaboration.


Project 7: Prof. Charles Patterson Charles.Patterson@tcd.ie

Many-body methods applied to excitons in molecules and solids

Up to 2 students

Many-body methods for treating electronic properties of materials are commonly expressed in terms of Feynman diagrams, which describe how electrons and holes scatter from each other in either the ground state or excited states of any system. This project will involve using a code developed in TCD in C and MPI for calculating optical excitations in molecules and crystalline matter. It will afford you the opportunity to learn the Green’s function theory that lies behind the methods, to use the code to compute optical excitations in molecules used for technological applications and, if desired, to gain some experience in developing the code further.

Quantum Theory of Many-Particle Systems, Fetter and Walecka (Dover or McGraw-Hill)
A Guide to Feynman Diagrams in the Many-Body Problem, Mattuck, (Dover)
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**Project 8: Dr Stephen Power stpower@tcd.ie**

Electron scattering from bilayer islands in graphene

1 student

See abstract overleaf

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**Project 9: Dr Stephen Power stpower@tcd.ie**

Electron scattering from spin-orbit enhanced quantum dots in graphene

1 student

See abstract overleaf

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**Project 10: Dr Stephen Power stpower@tcd.ie**

Machine-learning prediction of edge-state magnetism in graphene

Up to 2 students

See abstract overleaf

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**Project 11: Prof. Stefano Sanvito sanvitos@tcd.ie**

Generating molecules with GANs

1 student

See abstract overleaf

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**Project 12: Prof. Stefano Sanvito sanvitos@tcd.ie**

3D representation of molecules with a variable number of atoms

1 student

See abstract overleaf

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Electron scattering from bilayer islands in graphene

Analytic project / Python or Mathematica / Quantum Mechanics
Supervisor: Dr. Stephen Power *(Lloyd building, 232)*
1 student

![Figure 1: Bilayer islands surrounding by single layer graphene during CVD growth (from Luo et al, J. Mat. Chem C, 4, 7464 (2016))](image)

Graphene has an unusual electronic properties that are well-described using the relativistic Dirac equation in place of the more standard Schrodinger equation. The electronic properties of graphene are strongly dependent on the number of atomic layers, with electrons in a system of two layers (*bilayer graphene*) behaving very different to the single layer case.

This project will simulate how electrons in single layer graphene scatter from bilayer regions, which commonly form during some growth processes (see Figure 1). The aim is to determine whether this scattering can be controlled by applying an electric field. The project will also determine if such a setup has potential *valleytronic* applications. The student will:

- Learn the tight-binding and Dirac spinor representations of electrons in single layer and bilayer graphene
- Examine how barrier and spherically-symmetric scattering geometries can be solved using the Dirac approach for simple potential terms
- Solve the full scattering problem for a range of realistic parameters, and calculate the valley-splitting efficiencies of these systems.
Electron scattering from spin-orbit enhanced quantum dots in graphene

Analytic project / Mathematica / Quantum Mechanics

Supervisor: Dr. Stephen Power (Lloyd building, 232)

1 student

Figure 1: Caustics formed by electron scattering from a potential dot in graphene (from Heinisch et al, Phys. Rev. B. 87 155409 (2013))

Graphene has an unusual electronic dispersion relation that bears closer resemblance to that of light than to that of a conventional semiconductor. In fact, many features of graphene are well-described using the relativistic Dirac equation from quantum electrodynamics in place of the more standard Schrodinger equation.

Very recent research proposes using other materials to induce features such as spin-orbit coupling (SOC -- which is naturally weak in graphene) in graphene whilst maintaining the excellent electronic transport that makes it so appealing for applications. This would allow a higher degree of control over the “spin” degree of freedom than is currently possible.

This project will study the analytics of electron scattering from regions of enhanced SOC in graphene in order to determine the characteristics of materials that give the greatest degree of control of spin behaviour. The student will:

- Learn the tight-binding and Dirac spinor representations of electrons in graphene
- Examine how barrier and spherically-symmetric scattering geometries can be solved using the Dirac approach for simple potential terms
- Investigate the different Hamiltonians required to describe proximity-induced spin-orbit coupling in graphene, and how these are written in Dirac notation
- Solve the full scattering problem for a range of realistic parameters, and calculate the spin-filtering and spin-splitting efficiencies of these systems.
Machine-learning prediction of edge-state magnetism in graphene

Computational project / Coding (Python/C/etc.) / Machine Learning
Supervisor: Dr. Stephen Power (Lloyd building, 232)
1-2 students

Figure 1: Section of a graphene ribbon with mixed edges grown using chemical "bottom-up" techniques (from Ruffieux et al, Nature 531, 489 (2016))

Graphene is a two-dimensional hexagonal lattice of carbon atoms whose ground-breaking physical and electronic properties have been investigated in great detail over the last decade. Recent experimental techniques allow graphene to be produced both at very large scales for industrial purposes, and at the nanometre scale required for investigating fundamental physics.

The latter approach allows for a high-degree of control over the edge geometries of finite flakes or narrow ribbons of graphene. This is particularly exciting because, although carbon is generally considered nonmagnetic, local magnetism can arise near edges with particular geometries. Magnetic edge features have received much attention from theorists, and recent experiments show convincing signatures of their presence.

Although the expected magnetic behaviour of small scale or periodic systems can be easily predicted, the computational power required increases rapidly when larger or disorder systems (with a mix of different edge types) are considered. This project aims to solve some of these problems by training a machine-learning algorithm to predict the magnetic properties of arbitrary graphene systems using only their geometry and a knowledge of the properties of similar structures.

The student(s) will

- Learn tight-binding methods required describe non-magnetic graphene samples
- Implement a self-consistent procedure to calculate magnetic profiles
- Generate a training set and develop a suitable descriptor to capture its important features
- Train machine-learning algorithms to predict the magnetic profiles of unseen samples using its knowledge of the training set.
Generating molecules with GANs

Generative Adversarial Networks (GANs) belong to a class of machine learning algorithms, where two neural networks compete against each other [1]. These have widespread applications in several fields, with the most celebrated success being in image processing/recognition. A classical example of how GANs work is that of picture generation. In this case a first neural network (call it “Alice”) generates pictures (for example, human faces), which are included in a database of images of real people. Then a second neural network (call it “Bob”) sort the real images of people from the computer-generated ones. Bob and Alice then play against each other, namely Alice generates increasingly more realistic pictures and Bob refines its discrimination ability. The game ends when Bob is no longer able to distinguish the real images from the computer-generated ones. At this point Alice ability is to generate pictures of people indistinguishable from those of real people. An example of this scheme at work can be found at https://thispersondoesnotexist.com/

Similar methods have been used to generate characters of Anime cartoons [2] or to age people photographs [3]

In this project we will attempt to use GANs for computing temperature-dependent properties of molecules. The idea is to replace standard Monte-Carlo schemes for finite-temperature predictions with GANs, where the generative part of the network is used to create statistical distributions of molecules at a given temperature. In this project the students will:

1. Learn the basics of machine learning
2. Construct a simple GAN model
3. Extract finite-temperature properties of a molecule at finite temperature

References


3D representation of molecules with a variable number of atoms

Machine learning is rapidly becoming an important tool in materials modelling and in the design of new compounds [1]. A fundamental issue in developing these methods is that of providing a compact representation of the atomic distribution. In fact, one typically needs a way to describe a three dimensional structure, which is rotational and translational invariant. Furthermore the representation needs to be invariant against permutations of the atomic order and should be able to describe on the same footing molecules (or solids) with different number of atoms. Although several strategies have been proposed [2] a fully satisfactory solution is still at large.

In this project we will explore different strategies for representing the atomic distribution in molecules. We will use as a test bench artificial molecules in which uneven atoms are arranged in 2D and are kept together by simple van der Waals forces. We will then explore different ways to describe their spacial arrangement and establish, which representation can provide the best description of the structure against the prediction of neural networks. In this project the students will:

1. Learn the basics of machine learning
2. Construct a several molecule representation
3. Extract atomisation energies via neural network

References
