PX2132: Introductory Quantum Mechanics

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Module information

- Autumn semester: 10 credits.
- Module Organiser: Dr F Flicker.
- Deputy Module Organiser: Prof S Ladak.
- Teaching and feedback methods:
  - pre-recorded videos totalling ~ 10 hours
  - weekly problem sets to be completed before the lecture
  - weekly multiple choice quizzes to be completed before the lecture
  - live 'lectures' (online collaborative discussion classes), 11×1hr
  - two problems classes with the option of in-person attendance
- Assessment: 10 weekly online quizzes 1% each; 2 marked problem sets 5% each; examination 80% [Examination duration: 2 hours].
- Re-assessment : 100% examination.
- Pre-cursors: PX1120*, PX1221 and PX1230* (*excepting joint Maths/Physics students).
- Co-requisites: PX2131.
- Pre-requisites: None.

Aims of the module

- To provide foundations of the description of matter by wave mechanics, in particular through the Schrödinger equation and the interpretation and use of the wave function.
- To introduce more formal aspects of wave mechanics.
- To use worked examples and model systems to develop understanding of the meaning of wave functions, eigenvalues, eigenfunctions and operators.
- To apply quantum mechanics to describing the hydrogen atom.

Learning outcomes

The student will be able to:

- Recall and use basic quantum-mechanical concepts, including Schrödinger's time-independent and time-dependent wave equations, expectation values, operators, and the uncertainty principle.

- Find normalised energy eigenfunctions and eigenvalues in some simple 1D potentials.
- Describe scattering from step potentials.
- Describe quantum-mechanical tunnelling.
- Be able to describe mathematically the time development of quantum states.
- Appreciate how angular momentum appears in quantum mechanics. Solve problems relating to this and quantum states of the hydrogen atom.

Books

All the information relevant to this course appears in a condensed form in the accompanying notes. The online videos provide further detail. There is no course textbook, but the notes provide references to the following books when helpful (all are freely available online):

- J. Binney and D. Skinner, *The Physics of Quantum Mechanics* [https://www-thphys.physics.ox.ac.uk/people/JamesBinney/QBhome.htm]
- P. A. M. Dirac, *The Principles of Quantum Mechanics* [archive.org/details/in.ernet.dli.2015.177580]
- R. P. Feynman, R. B. Leighton, and M. Sands, *The Feynman Lectures on Physics* [feynmanlectures.caltech.edu]

While later editions of the first two books are available for a price, references should be assumed to be made to these free editions. The following books are available as eBooks for free through Cardiff University library and will also be referred to:

- D. J. Griffiths, *Introduction to Quantum Mechanics* (Cambridge University Press, 2nd edition)
- S. Weinberg, *Lectures on Quantum Mechanics* (Cambridge University Press, 2nd edition, 2015).

Other books which you may wish to consult, but which will not be referred to directly in the course:

- A. I. M. Rae and J. Napolitano, Quantum Physics (Routledge, 6th edition, 2015) ISBN 9781482299182
- J. J. Sakurai and J. Napolitano, Modern Quantum Mechanics (Cambridge University Press, 2nd edition, 2017) ISBN 978-1-108-42241-3
- L. D. Landau and E. M. Lifshitz, Course of Theoretical Physics Volume 3 - Quantum Mechanics: Non-Relativistic Theory (Pergamon Press, Third edition, 1977) ISBN 0080291406
- S. Gasiorowicz, Quantum Physics (Wiley, 3rd edition, 2003) ISBN 978-0471057000
- A. P. French and E. Taylor, An Introduction to Quantum Physics (W. W. Norton & Company, 1978) ISBN 0393091066
- R. Eisberg and R. Resnick, Quantum Physics of Atoms, Molecules, Solids, Nuclei, and Particles (Wiley and Sons, 2nd edition, 1985) ISBN 978-0471873730.

How the course will work

- There will be ten online course lectures, Mondays 10am-10.45am from the 5th October to 7th December.
- There will be a revision lecture on Monday 14th December at 10am-10.45am.
- There will be an online office hour from 11am-11.45am following each lecture.
- **Before** each lecture:

- watch the week's videos and take notes. A good plan might be to watch through once without taking notes, then to watch a second time pausing to take notes.
- Read the relevant section of the provided notes. These are intended to aid you in writing your own notes from the videos, not to replace your own notes.
- Complete the corresponding problem set. For example, complete PS1 before lecture 1 on the 5th October. You will mark your own answers during the lecture.
- Complete the online multiple choice quiz. Each quiz will count for 1% of your total grade. The quiz will close 9.45am on the day of the lecture.
- Lecture 1 will include a recap of relevant first-year material covered in problem set PS0. You should complete both PS0 and PS1 in preparation for this lecture.

- Assessment: in addition to the weekly quizzes [10% total] and the exam [80%], there will be two marked pieces of work.
  - M1 should be submitted by Tuesday 17th November at 2pm. It will cover the material in the first four lectures, and will count for 5% of your total course mark.
  - M2 should be submitted by Tuesday 8th December at 2pm. It will cover the material in the final six lectures, and will count for 5% of your total course mark.
- There will be two classes, C1 and C2, which you will have the option of attending in person. The PhD students who mark your submitted work M1 and M2 will go through the answers to M1 and M2 in these classes, and will be available to answer any further questions.

Lecture outline

Week 1: Introduction to quantum mechanics

Lecture: Monday 5/10/20 10am-10.45am
Office hours: Monday 5/10/20 11am-11.45am
Complete quiz Q1 before 9.45am 5/10/20
Bring answers to PS0 and PS1
Videos:

- V1.0: Introduction to course
- V1.1: Historical motivation for quantum mechanics
- V1.2: The Schrödinger equation
- V1.3: Plane waves
- V1.4: Amplitudes and probabilities
- V1.5: Two slit demo

Topics:

- recap of vectors, matrices, and differential equations
- the experimental necessity of quantum mechanics: Compton scattering, de Broglie relation $p = h/\lambda = \hbar k$; single particle interference; photoelectric effect and $E = hf = \hbar\omega$
- the time-dependent Schrodinger equation (TDSE)
- the time-independent Schrodinger equation (TISE)
- the wavefunction
- probability density

- probability current density
- general boundary conditions.

For the exam you should be able to:

- understand and apply $p = \hbar k$, $E = \hbar\omega$
- write down the TDSE and TISE
- derive the TISE from the TDSE using separation of variables
- deduce the time dependence of a solution to the TISE
- state the Born rule
- state the meaning of the probability density and to calculate it for a given wavefunction
- derive the continuity equation for the local conservation of probability
- derive the probability current density and calculate it for a given wavefunction
- state the two boundary conditions which always apply to the wavefunction.

Week 2: Scattering and tunnelling

Lecture: Monday 12/10/20 10am-10.45am
Office hours: Monday 12/10/20 11am-11.45am
Complete quiz Q2 before 9.45am 12/10/20
Bring answers to PS2
Videos:

- V2.1a–d: Scattering from a potential step
- V2.2: Quantum tunnelling
- V2.3: Evanescent waves demo

Topics:

- plane waves
- recovering $p = \hbar k$ and $E = \hbar\omega$ from the Schrödinger equation
- scattering from a potential step
- tunnelling and barrier penetration
- scanning tunnelling microscopes.

For the exam you should be able to:

- write down the form of a plane wave
- use this form to show the Schrödinger equation is compatible with $p = \hbar k$ and $E = \hbar\omega$
- state the forms of the TISE in regions of constant potential
- find the transmission and reflection amplitudes for scattering from a potential step
- find the probability current densities for scattering from a potential step
- find the probabilities of transmission and reflection from a potential step
- explain the steps necessary to solve scattering from a potential barrier of finite width
- explain the physical significance of quantum tunnelling

- explain the relevance to scanning tunnelling spectroscopy and microscopy

For the exam you will not be required to:

- rote learn any solutions
- solve explicitly for the amplitudes associated with the finite-width barrier

Week 3: Bound states (I)

Lecture: Monday 19/10/20 10am-10.45am
Office hours: Monday 19/10/20 11am-11.45am
Complete quiz Q3 before 9.45am 19/10/20
Bring answers to PS3
Videos:

- V3.1: Infinite potential well
- V3.2: Normalisation
- V3.3 Stationary states
- V3.4 Orthonormality of eigenstates
- V3.5 Fourier decomposition

Topics:

- The infinite potential well (particle in a box)
- energy eigenvalues and eigenfunctions
- normalisation of wavefunctions
- orthogonality of eigenstates
- energy eigenstates as stationary states
- complete orthonormal bases.

For the exam you should be able to:

- solve for the energy eigenstates and eigenvalues of the infinite potential well (particle in a box)
- explain the physical relevance of normalisation
- normalise a given wavefunction
- explain the relevance of the orthogonality of eigenstates
- demonstrate the orthogonality of given wavefunctions
- explain what is meant by energy eigenstates being stationary states and to prove this mathematically
- explain the significance of sets of eigenstates forming complete orthonormal bases
- explain the significance of expectation values of observable quantities (observables)
- find the expectation values of powers of position and momentum for a given wavefunction

Week 4: Bound states (II)

Lecture: Monday 26/10/20 10am-10.45am
Office hours: Monday 26/10/20 11am-11.45am
Complete quiz Q4 before 9.45am 26/10/20
Bring answers to PS4
Videos:

- V4.1: Quantum superposition
- V4.2: The finite potential well

Topics:

- Quantum superposition
- the finite potential well.

For the exam you should be able to:

- explain the principle of quantum superposition
- calculate properties of superposed states
- decompose a given wavefunction into a superposition of energy eigenstates
- find the time dependence of a given spatial wavefunction
- justify the forms of the wavefunctions solving the TISE for the finite potential well
- explain the steps involved in solving the TISE in the finite potential well
- prove that there is at least one bound state in any finite potential well

For the exam you will not be required to:

- provide a full solution for the finite potential well

Week 5: Finite-dimensional Hilbert spaces

Lecture: Monday 2/11/20 10am-10.45am
Office hours: Monday 2/11/20 11am-11.45am
Complete quiz Q5 before 9.45am 2/11/20
Bring answers to PS5
Videos:

- V5.1: Complex vectors
- V5.2: Hermitian matrices
- V5.3a–c: Spin-1/2
- V5.4: Polarisation demo

Topics:

- Complex vectors and matrices
- Dirac notation
- Hermitian matrices: eigenvalues and eigenvectors, properties
- complete orthonormal bases, resolution of the identity
- Spin-1/2: Stern-Gerlach experiment, Pauli matrices, commutation relations

For the exam you should be able to:

- work with complex vectors and matrices
- employ Dirac notation for complex vectors
- state and derive the properties of Hermitian matrices of use in quantum mechanics
- describe spin-1/2 particles using a 2-dimensional Hilbert space.

Week 6: Operators and observables

Lecture: Monday 9/11/20 10am-10.45am
Office hours: Monday 9/11/20 11am-11.45am
Complete quiz Q6 before 9.45am 9/11/20
Bring answers to PS6
Videos:

- V6.1: Operators and observables
- V6.2: The Heisenberg uncertainty principle
- V6.3: The Heisenberg picture
- V6.4 Conserved quantities

Topics:

- $\hat{p}$ and $\hat{x}$ operators
- canonical commutation relations
- complete sets of states
- quantum numbers
- the Heisenberg uncertainty principle
- the Heisenberg and Schrödinger pictures
- the Heisenberg equations of motion
- Ehrenfest's theorem.

For the exam you should be able to:

- state the canonical commutation relations
- find the commutators of given operators
- explain the significance of operators commuting
- state the Heisenberg uncertainty principle
- show that given wavefunctions obey the uncertainty principle
- explain what is meant by the Heisenberg and Schrodinger pictures
- deduce the Heisenberg equation of motion
- state Ehrenfest's theorem and explain its physical significance
- discuss the correspondence principle
- deduce Ehrenfest's theorem from the Heisenberg equation of motion
- state the meaning of a conserved quantity

- show that the observable quantity associated to a given operator is conserved
- explain the meaning of quantum numbers.

For the exam you will not be required to:

- derive the Heisenberg uncertainty principle.

Week 7: Quantum mechanics

Lecture: Monday 16/11/20 10am-10.45am
Office hours: Monday 16/11/20 11am-11.45am
Complete quiz Q7 before 9.45am 16/11/20
Bring answers to PS7
Marked problems M1 due 2pm Tuesday 17th November
Videos:

- V7.1: Infinite dimensional Hilbert spaces
- V7.2: Fourier transforms
- V7.3: Differential operators
- V7.4: The postulates of quantum mechanics
- V7.5: Schrödinger's cat demo

Topics:

- Functions as infinite-dimensional vectors: examples of operators
- Equivalence of Schrödinger, Heisenberg, and Dirac notations: $\psi(x) = \langle x|\psi\rangle$
- expectation values
- wavefunction overlap
- The postulates of quantum mechanics
- interpretations of quantum mechanics

For the exam you should be able to:

- work with functions as elements of a vector space, including taking inner products
- state the forms of the operators $\hat{H}$, $\hat{V}$, $\hat{\boldsymbol{p}}$, and $\hat{\boldsymbol{x}}$ in the position basis
- confirm the Hermiticity of given differential operators in the position basis

For the exam you will not be required to:

- recount details of different interpretations of quantum mechanics
- understand the dead cat.

Week 8: The quantum harmonic oscillator

Lecture: Monday 23/11/20 10am-10.45am
Office hours: Monday 23/11/20 11am-11.45am
Complete quiz Q8 before 9.45am 23/11/20
Bring answers to PS8
Videos:

- V8.1: The quantum harmonic oscillator
- V8.2: Ladder operators
- V8.3: The number operator
- V8.4: Second quantisation

Topics:

- converting the quantum harmonic oscillator (QHO) TISE to Hermite's equation
- solution with Hermite polynomials
- raising and lowering (ladder) operators
- ladder operator commutation relations
- Energy eigenstates and eigenvalues of the QHO
- Second quantization

For the exam you should be able to:

- work with Hermite polynomials, checking properties such as orthogonality
- find the commutators between the raising and lowering (ladder) operators, and with the Hamiltonian
- demonstrate that these commutation relations lead to an infinite ladder of equally-spaced energy eigenvalues
- justify the normalisation of the ladder operators
- deduce the ground state of the QHO from the existence of a bottom rung of the ladder
- explain the concepts of first and second quantization.

For the exam you will not be required to:

- rote learn the form of the Hermite polynomials
- rote learn the form of the ladder operators.

Week 9: The Schrödinger equation in three dimensions

Lecture: Monday 30/11/20 10am-10.45am
Office hours: Monday 30/11/20 11am-11.45am
Complete quiz Q9 before 9.45am 30/11/20
Bring answers to PS9
Videos:

- V9.1: The 3D infinite potential well
- V9.2: The 3D quantum harmonic oscillator
- V9.3: Angular momentum
- V9.4: Angular momentum ladder operators

Topics:

- 3D infinite potential well
- 3D quantum harmonic oscillator
- polar co-ordinates
- angular momentum
- commutation relations for angular momentum operators
- $\hat{L}_z$ and $\hat{L}^2$ as a maximal set of commuting operators
- angular momentum ladder operators

For the exam you should be able to:

- solve the TISE/TDSE for the 3D infinite potential well
- solve the TISE/TDSE for the 3D quantum harmonic oscillator
- state the form of the angular momentum operator
- derive the position-basis form of the angular momentum operator in cartesian co-ordinates
- derive the position-basis form of $\hat{L}_z$ in polar co-ordinates
- find the commutation relations between the x, y, and z-projections of the angular momentum operator
- show that $\hat{L}^2$ commutes with all three of $\hat{L}_i$, $i \in [x, y, z]$
- find the commutation relations between the angular momentum raising and lowering operators $\hat{L}_\pm$
- use the commutation relations between $\hat{L}_\pm$ to deduce the existence of a ladder of states with different $\hat{L}_z$ eigenvalues.

For the exam you will not be required to:

- rote learn the form of ∇^2 in spherical polar co-ordinates.

Week 10: The hydrogen atom

Lecture: Monday 7/12/20 10am-10.45am
Office hours: Monday 7/12/20 11am-11.45am
Complete quiz Q10 before 9.45am 14/12/20
Bring answers to PS10
Marked problems M2 due 2pm Tuesday 8th December
Videos:

- V10.1: Spherically symmetric potentials: angular equation
- V10.2: Spherically symmetric potentials: radial equation
- V10.3: The hydrogen atom

Topics:

- the TISE in spherical polar co-ordinates
- separating into radial and angular equations
- separating the angular equation into the azimuthal and polar equations
- solution of the azimuthal equation using associated Legendre polynomials

- solution of the angular equation using spherical harmonics
- rewriting the radial equation as the 1D TDSE with a centrifugal barrier term
- the TISE for the electron in the hydrogen atom
- solution to the radial equation by reduction to La Guerre's equation
- quantum numbers of the electron in the hydrogen atom

For the exam you should be able to:

- separate the TISE in spherical polar co-ordinates into radial, azimuthal, and polar parts (given the TISE itself)
- rewrite the radial equation of the TISE for a spherically-symmetric potential as a 1D TISE with centrifugal barrier term
- explain the origin of the quantum numbers of the electron in the hydrogen atom
- state the origin of atomic line spectra
- recount the basic idea of the Bohr model of the atom

For the exam you will not be required to:

- rote learn the forms of the spherical harmonics (although you should have a basic familiarity with them)
- learn detailed properties of the associated Legendre equation or La Guerre's equation
- rote learn the solutions to the TISE for the hydrogen atom

Week 11: Revision

Lecture: Monday 14/12/21 10am-10.45am
Office hours: Monday 14/12/21 11am-11.45am