EP2210

PRINCIPLES OF QUANTUM MECHANICS

July–November 2014

Lecture schedule and meeting hours

- The course will consist of about 42 lectures, including about 8–10 tutorial sessions. However, note that there will be no separate tutorial sessions, and they will be integrated with the lectures.
- The duration of each lecture will be 50 minutes. We will be meeting in HSB 317.
- The first lecture will be on Thursday, July 31, and the last lecture will be on Friday, November 14.
- We will meet thrice a week. The lectures are scheduled for 1:00–1:50 PM on Tuesdays, 11:00–11:50 AM on Thursdays, and 10:00–10:50 AM on Fridays.
- We may also meet during 4:45–5:35 PM on Tuesdays for either the quizzes or to make up for any lecture that I may have to miss due to, say, travel. Changes in schedule, if any, will be notified sufficiently in advance.
- If you would like to discuss with me about the course outside the lecture hours, you are welcome to meet me at my office (HSB 202A) during 3:00–3:30 PM on Fridays. In case you are unable to find me in my office on more than occasion, please send me an e-mail at `sriram@physics.iitm.ac.in`.

Information about the course

- I will be distributing hard copies containing information such as the schedule of the lectures, the structure and the syllabus of the course, suitable textbooks and additional references, as well as exercise sheets.
- A PDF file containing these information as well as completed quizzes will also made be available at the link on this course at the following URL:
  `http://www.physics.iitm.ac.in/~sriram/professional/teaching/teaching.html`
  I will keep updating the file as we make progress.

Quizzes, end-of-semester exam and grading

- The grading will be based on three scheduled quizzes and an end-of-semester exam.
- I will consider the best two quizzes for grading, and the two will carry 25% weight each.
- The three quizzes will be on August 26, September 23 and October 21. All these three dates are Tuesdays, and the quizzes will be held during 4:45–5:35 PM.
- The end-of-semester exam will be held during 9:00 AM–12:00 NOON on Wednesday, November 19, and the exam will carry 50% weight.

Syllabus and structure

Principles of Quantum Mechanics

1. **Essential classical mechanics** [$\sim$ 3 lectures]

   (a) Generalized coordinates – Lagrangian of a system – The Euler-Lagrange equations of motion
   (b) Symmetries and conserved quantities
   (c) Conjugate variables – The Hamiltonian – The Hamilton's equations of motion
   (d) Poisson brackets
   (e) The state of the system

Exercise sheet 1

2. **Origins of quantum theory and the wave aspects of matter** [$\sim$ 4 lectures]

   (a) Black body radiation – Planck's law
   (b) Photoelectric effect
   (c) Bohr atom model – Frank and Hertz experiment
   (d) de Broglie hypothesis – The Davisson-Germer experiment
   (e) Concept of the wavefunction – The statistical interpretation
   (f) Two-slit experiment – The Heisenberg uncertainty principle

Exercise sheet 2

3. **The postulates of quantum mechanics and the Schrodinger equation** [$\sim$ 5 lectures]

   (a) Observables and operators
   (b) Expectation values and fluctuations
   (c) Measurement and the collapse of the wavefunction
   (d) The time-dependent Schrodinger equation

Exercise sheet 3

Quiz I

4. **The time-independent Schrodinger equation in one dimension** [$\sim$ 8 lectures]

   (a) The time-independent Schrodinger equation – Stationary states
   (b) The infinite square well
   (c) Reflection and transmission in potential barriers
   (d) The delta function potential
   (e) The free particle
   (f) Linear harmonic oscillator
   (g) Kronig-Penney model – Energy bands

Exercise sheets 4 and 5

Additional exercises I

5. **Essential mathematical formalism** [$\sim$ 8 lectures]
   (a) Hilbert space
   (b) Observables – Hermitian operators – Eigen functions and eigen values of hermitian operators
   (c) Orthonormal basis – Expansion in terms of a complete set of states
   (d) Position and momentum representations
   (e) Generalized statistical interpretation – The generalized uncertainty principle
   (f) Studying the simple harmonic oscillator using the operator method
   (g) Unitary evolution

Exercise sheets 6 and 7

Quiz II

6. **Particle in a central potential** [$\sim$ 4 lectures]
   (a) Motion in a central potential – Orbital angular momentum
   (b) Hydrogen atom – Energy levels
   (c) Degeneracy

Exercise sheet 8

Additional exercises II

7. **Angular momentum and spin** [$\sim$ 4 lectures]
   (a) Angular momentum – Eigen values and eigen functions
   (b) Electron spin – Pauli matrices
   (c) Application to magnetic resonance

Exercise sheet 9

Quiz III

8. **Time-independent perturbation theory** [$\sim$ 4 lectures]
   (a) The non-degenerate case
   (b) Fine structure of hydrogen – Hyperfine structure

Exercise sheet 10

9. **Charged particle in a uniform and constant magnetic field** [$\sim$ 2 lectures]
   (a) Landau levels – Wavefunctions
   (b) Elements of the quantum Hall effect

Exercise sheet 11

End-of-semester exam

Basic textbooks

1. P. A. M. Dirac, *The Principles of Quantum Mechanics*, Fourth Edition (Oxford University Press, Oxford, 1958).
2. S. Gasiorowicz, *Quantum Physics*, Third Edition (John Wiley and Sons, New York, 2003).
3. R. L. Liboff, *Introductory Quantum Mechanics*, Fourth Edition (Pearson Education, Delhi, 2003).
4. W. Greiner, *Quantum Mechanics*, Fourth Edition (Springer, Delhi, 2004).
5. D. J. Griffiths, *Introduction to Quantum Mechanics*, Second Edition (Pearson Education, Delhi, 2005).
6. R. Shankar, *Principles of Quantum Mechanics*, Second Edition (Springer, Delhi, 2008).

Advanced textbooks

1. L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Course of Theoretical Physics, Volume 3), Third Edition (Pergamon Press, New York, 1977).
2. J. J. Sakurai, *Modern Quantum Mechanics* (Addison-Wesley, Singapore, 1994).

Other references

1. D. Danin, *Probabilities of the Quantum World* (Mir Publishers, Moscow, 1983).
2. G. Gamow, *Thirty Years that Shook Physics: The Story of Quantum Theory* (Dover Publications, New York, 1985).
3. R. P. Crease and C. C. Mann, *The Second Creation: Makers of the Revolution in Twentieth-Century Physics* (Rutgers University Press, New Jersey, 1996), Chapters 1–4.
4. M. S. Longair, *Theoretical Concepts in Physics*, Second Edition (Cambridge University Press, Cambridge, England, 2003), Chapters 11–15.

Exercise sheet 1

Essential classical mechanics

1. *Geodesics on a cylinder:* A geodesic is a curve that represents the shortest path between two points in any space. Determine the geodesic on a right circular cylinder of a fixed radius, say, R.

2. *Non-relativistic particle in an electromagnetic field:* A non-relativistic particle that is moving in an electromagnetic field described by the scalar potential ϕ and the vector potential $\mathbf{A}$ is governed by the Lagrangian
$$L = \frac{m\,\mathbf{v}^2}{2} + q\,\left(\frac{\mathbf{v}}{c}\cdot\mathbf{A}\right) - q\,\phi,$$
where m and q are the mass and the charge of the particle, while c denotes the velocity of light. Show that the equation of motion of the particle is given by
$$m\,\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = q\,\left(\mathbf{E} + \frac{\mathbf{v}}{c}\times\mathbf{B}\right),$$
where $\mathbf{E}$ and the $\mathbf{B}$ are the electric and the magnetic fields given by
$$\mathbf{E} = -\nabla\phi - \frac{1}{c}\,\frac{\partial\mathbf{A}}{\partial t} \qquad \text{and} \qquad \mathbf{B} = \nabla\times\mathbf{A}.$$
Note: The scalar and the vector potentials, viz. ϕ and $\mathbf{A}$, are dependent on time *as well as* space. Further, given two vectors, say, $\mathbf{C}$ and $\mathbf{D}$, one can write,
$$\nabla\left(\mathbf{C}\cdot\mathbf{D}\right) = \left(\mathbf{D}\cdot\nabla\right)\,\mathbf{C} + \left(\mathbf{C}\cdot\nabla\right)\,\mathbf{D} + \mathbf{D}\times\left(\nabla\times\mathbf{C}\right) + \mathbf{C}\times\left(\nabla\times\mathbf{D}\right).$$
Also, since $\mathbf{A}$ depends on time as well as space, we have,
$$\frac{\mathrm{d}\mathbf{A}}{\mathrm{d}t} = \frac{\partial\mathbf{A}}{\partial t} + \left(\mathbf{v}\cdot\nabla\right)\,\mathbf{A}.$$

3. *Period associated with bounded, one-dimensional motion:* Determine the period of oscillation as a function of the energy, say, E, when a particle of mass m moves in a field governed by the potential $V(x) = V_0\,|x|^n$, where V_0 is a constant and n is a positive integer.

4. *Bead on a helical wire:* A bead is moving on a helical wire under the influence of a uniform gravitational field. Let the helical wire be described by the relations $z = \alpha\,\theta$ and $\rho = constant$. Construct the Hamiltonian of the system and obtain the Hamilton's equations of motion.

5. *Poisson brackets:* Establish the following relations: $\{q_i, q_j\} = 0$, $\{p_i, p_j\} = 0$, $\{q_i, p_j\} = \delta_{ij}$, $\dot{q}_i = \{q_i, H\}$ and $\dot{p}_i = \{p_i, H\}$, where q_i, p_i and H represent the generalized coordinates, the corresponding conjugate momenta and the Hamiltonian, respectively, while the curly brackets denote the Poisson brackets.

   Note: The quantity δ_{ij} is called the Kronecker symbol and it takes on the following values:
$$\delta_{ij} = \begin{cases} 1 & \text{when } i = j, \\ 0 & \text{when } i \neq j. \end{cases}$$

Exercise sheet 2

Origins of quantum theory and the wave aspects of matter

1. *Black body radiation and Planck's law:* Consider a black body maintained at the temperature T. According to Planck's radiation law, the energy per unit volume within the frequency range ν and $\nu + \mathrm{d}\nu$ associated with the electromagnetic radiation emitted by the black body is given by

$$u_\nu \, \mathrm{d}\nu = \frac{8\,\pi\,h}{c^3}\, \frac{\nu^3\,\mathrm{d}\nu}{\exp\left(h\,\nu/k_{\mathrm{B}}\,T\right) - 1},$$

where h and k_{B} denote the Planck and the Boltzmann constants, respectively, while c represents the speed of light.

   (a) Arrive at the Wien's law, viz. that $\lambda_{\mathrm{max}}\,T = b =$ constant, from the above Planck's radiation law. Note that λ_{max} denotes the wavelength at which the energy density of radiation from the black body is the maximum.

   (b) The total energy emitted by the black body is described by the integral

$$u = \int_0^\infty d\nu\; u_\nu.$$

   Using the above expression for u_ν, evaluate the integral and show that

$$u = \frac{4\,\sigma}{c}\,T^4,$$

   where σ denotes the Stefan constant given by

$$\sigma = \frac{\pi^2\,k_{\mathrm{B}}^4}{60\,\hbar^3\,c^2},$$

   with $\hbar = h/(2\,\pi)$.

   (c) The experimentally determined values of the Stefan's constant σ and the Wien's constant b are found to be

$$\sigma = 5.67 \times 10^{-8}\,\mathrm{J\,m^{-2}\,s^{-1}\,K^{-4}} \quad \text{and} \quad b = 2.9 \times 10^{-3}\,\mathrm{m\,K}.$$

   Given that the value of the speed of light is $c = 2.998 \times 10^8\,\mathrm{m\,s^{-1}}$, determine the values of the Planck's constant h and the Boltzmann's constant k_{B} from these values.

2. *Photoelectrons from a zinc plate:* Consider the emission of electrons due to photoelectric effect from a zinc plate. The work function of zinc is known to be 3.6 eV. What is the maximum energy of the electrons ejected when ultra-violet light of wavelength 3000 Å is incident on the zinc plate?

3. *Radiation emitted in the Frank and Hertz experiment:* Recall that, in the Frank and Hertz experiment, the emission line from the mercury vapor was at the wavelength of 2536 Å. The spectrum of mercury has a strong second line at the wavelength of 1849 Å. What will be the voltage corresponding to this line at which we can expect the current in the Frank and Hertz experiment to drop?

4. *Value of the Rydberg's constant:* Evaluate the numerical value of the Rydberg's constant R_{H} and compare with its experimental value of $109677.58\,\mathrm{cm}^{-1}$. How does the numerical value change if the finite mass of the nucleus is taken into account?

5. *Mean values and fluctuations:* The expectation values $\langle \hat{A} \rangle$ and $\langle \hat{A}^2 \rangle$ associated with the operator $\hat{A}$ and the wavefunction Ψ are defined as

$$\langle \hat{A} \rangle = \int \mathrm{d}x\ \Psi^* \hat{A}\, \Psi \quad \text{and} \quad \langle \hat{A}^2 \rangle = \int \mathrm{d}x\ \Psi^* \hat{A}^2\, \Psi,$$

where the integrals are to be carried out over the domain of interest. Note that the momentum operator is given by

$$\hat{p}_x = -i\,\hbar\,\frac{\partial}{\partial x}.$$

Given the wavefunction

$$\Psi(x) = \left(\frac{\pi}{\alpha}\right)^{-1/4}\ \mathrm{e}^{-\alpha\, x^2/2},$$

calculate the following quantities: (i) $\langle \hat{x} \rangle$, (ii) $\langle \hat{x}^2 \rangle$, (iii) $\Delta x = \left[\langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2\right]^{1/2}$, (iv) $\langle \hat{p}_x \rangle$, (v) $\langle \hat{p}_x^2 \rangle$, (vi) $\Delta p_x = \left[\langle \hat{p}_x^2 \rangle - \langle \hat{p}_x \rangle^2\right]^{1/2}$, and (vii) $\Delta x\, \Delta p_x$.

Exercise sheet 3

The postulates of quantum mechanics and the Schrodinger equation

1. *Hermitian operators:* Recall that the expectation value of an operator $\hat{A}$ is defined as

$$\langle \hat{A} \rangle = \int \mathrm{d}x \; \Psi^* \hat{A} \, \Psi.$$

An operator $\hat{A}$ is said to be hermitian if

$$\langle \hat{A} \rangle = \langle \hat{A} \rangle^*.$$

Show that the position, the momentum and the Hamiltonian operators are hermitian.

2. *Motivating the momentum operator:* Using the time-dependent Schrodinger equation, show that

$$\frac{\mathrm{d}\langle x \rangle}{\mathrm{d}t} = -\frac{i\,\hbar}{m} \int \mathrm{d}x \; \Psi^* \frac{\partial \Psi}{\partial x} = \langle \hat{p}_x \rangle,$$

a relation which can be said to motivate the expression for the momentum operator, viz. that $\hat{p}_x = -i\,\hbar\,\partial/\partial x$.

3. *The conserved current:* Consider a quantum mechanical particle propagating in a given potential and described by the wave function $\Psi(x,t)$. The probability $P(x,t)$ of finding the particle at the position x and the time t is given by

$$P(x,t) = |\Psi(x,t)|^2.$$

Using the one-dimensional Schrodinger equation, show that the probability $P(x,t)$ satisfies the conservation law

$$\frac{\partial P(x,t)}{\partial t} + \frac{\partial j(x,t)}{\partial x} = 0,$$

where the quantity $j(x,t)$ represents the conserved current given by

$$j(x,t) = \frac{\hbar}{2\,i\,m} \left[\Psi^*(x,t) \left(\frac{\partial \Psi(x,t)}{\partial x}\right) - \Psi(x,t) \left(\frac{\partial \Psi^*(x,t)}{\partial x}\right)\right].$$

4. *Ehrenfest's theorem:* Show that

$$\frac{\mathrm{d}\langle \hat{p}_x \rangle}{\mathrm{d}t} = -\left\langle \frac{\partial V}{\partial x} \right\rangle,$$

a relation that is often referred to as the Ehrenfest's theorem.

5. *Conservation of the scalar product:* The scalar product between two normalizable wavefunctions, say, Ψ_1 and Ψ_2, which describe a one-dimensional system is defined as

$$\langle \Psi_2 | \Psi_1 \rangle \equiv \int \mathrm{d}x \; \Psi_2^*(x,t)\, \Psi_1(x,t),$$

where the integral is to be carried out over the domain of interest. Show that

$$\frac{\mathrm{d}\langle \Psi_2 | \Psi_1 \rangle}{\mathrm{d}t} = 0.$$

Quiz I

From the origins of quantum theory and wave aspects of matter to the postulates of quantum mechanics and the Schrodinger equation

1. *Bohr's quantization rule:* Consider a particle that is moving in the central potential $V(r) = V_0\,(r/a)^k$, where V_0, a and k are constants.

   (a) Using Bohr's quantization procedure, determine the energy levels of the system. 5 marks
   Note: Assume, for simplicity, that the orbits are circular.

   (b) Show that, for large n, the frequency of a photon emitted in a transition from the level n to the level $(n-1)$ is the same as the rotational frequency. 5 marks
   Note: This is a version of the quantum-classical correspondence.

2. *Probabilities, normalization and expectation values:* Consider a one-dimensional quantum system that is described by the wavefunction

$$\Psi(x,t) = A\,\mathrm{e}^{-i\,\omega\,t}\,\mathrm{e}^{-|x|/\alpha},$$

   where A, ω and α are real constants.

   (a) Determine the value of A from the condition that the total probability (over the complete domain, viz. $-\infty < x < \infty$) associated with the above wavefunction is unity. 3 marks
   Note: A wavefunction $\Psi(x,t)$ is said to be normalized if the integral of the corresponding probability density over the allowed domain is unity.

   (b) Determine the expectation values of the operators $\hat{x}$ and $\hat{x}^2$ in the given state. 4 marks

   (c) What is the probability of finding the particle in the domain $-\alpha < x < \alpha$? 3 marks

3. *Eigen functions and eigen values:* The Hamiltonian operator corresponding to that of a free particle which is moving in one-dimension is given by

$$\hat{H} = \frac{\hat{p}_x^2}{2\,m} = -\frac{\hbar^2}{2\,m}\,\frac{\mathrm{d}^2}{\mathrm{d}x^2}.$$

   (a) Let $\psi_E(x)$ denote the eigen functions with the eigen values E associated with the above Hamiltonian operator so that $\hat{H}\,\psi_E(x) = E\,\psi_E(x)$. Determine the function $\psi_E(x)$ and the allowed values of E. 5 marks

   (b) What are the eigen functions of the Hamiltonian operator if we additionally demand that they should vanish at $x=0$? What are the corresponding eigen values? 5 marks

4. *Poisson brackets and commutation relations:* Consider first a classical particle in three dimensions. Let the spatial coordinates of the particle be denoted as $\boldsymbol{x} \equiv x_i = (x,y,z)$ and let $\boldsymbol{p} \equiv p_i = (p_x,p_y,p_z)$ represent the corresponding conjugate momenta. Also, let $L = \boldsymbol{x}\times\boldsymbol{p}$ be the angular momentum associated with the particle. Recall that the Poisson bracket between two classical quantities, say, A and B, that are functions of the coordinates $\boldsymbol{x}$ and the conjugate momenta $\boldsymbol{p}$ is defined as

$$\{A,B\} = \sum_{i=1}^{3}\left(\frac{\partial A}{\partial x_i}\,\frac{\partial B}{\partial p_i} - \frac{\partial B}{\partial x_i}\,\frac{\partial A}{\partial p_i}\right).$$

   Now, consider the quantum version of the system wherein the particle is described by the wavefunction $\Psi(\boldsymbol{x},t)$. The so-called commutation relation between the two operators $\hat{A}$ and $\hat{B}$ is defined as

$$\left[\hat{A},\hat{B}\right]\,\Psi(\boldsymbol{x},t) = (\hat{A}\,\hat{B} - \hat{B}\,\hat{A})\,\Psi(\boldsymbol{x},t).$$

(a) Evaluate $\{x, y\}$, $\{x, p_x\}$, $\{x, L_x\}$, and $\{L_x, L_y\}$. 4 marks

(b) Determine $[\hat{x}, \hat{y}]$, $[\hat{x}, \hat{p}_x]$, $\left[\hat{x}, \hat{L}_x\right]$, and $\left[\hat{L}_x, \hat{L}_y\right]$. 4 marks

Note: Recall that, in quantum mechanics, $\hat{\boldsymbol{p}} \equiv -i\,\hbar\,\boldsymbol{\nabla}$.

(c) Identify the 'correspondence' between the commutation relations $\left[\hat{A}, \hat{B}\right]$ and the Poisson brackets $\{A, B\}$ that you have evaluated. 2 marks

Note: This is another version of the quantum-classical correspondence.

5. *Translations:* Given $\hat{p}_x \equiv -i\,\hbar\,\partial/\partial x$, show that 4+6 marks

$$\exp\,(i\,\hat{p}_x\,a/\hbar)\;\psi(x) = \psi(x+a)$$

and

$$\exp\,(i\,\hat{p}_x\,a/\hbar)\;\hat{x}\,\exp\,(-i\,\hat{p}_x\,a/\hbar)\;\psi(x) = (x+a)\,\psi(x).$$

Exercise sheet 4

The time-independent Schrodinger equation in one dimension

1. *Superposition of energy eigen states:* Consider a particle in the infinite square well. Let the initial wave function of the particle be given by

$$\Psi(x,0) = A\,[\psi_1(x) + \psi_2(x)]\,,$$

where $\psi_1(x)$ and $\psi_2(x)$ denote the ground and the first excited states of the particle.

(a) Normalize the wave function $\Psi(x,0)$.

(b) Obtain the wave function at a later time t, viz. $\Psi(x,t)$, and show that the probability $|\Psi(x,t)|^2$ is an oscillating function of time.

(c) Evaluate the expectation value of the position in the state $\Psi(x,t)$ and show that it oscillates. What are the angular frequency and the amplitude of the oscillation?

(d) What will be the values that you will obtain if you measure the energy of the particle? What are the probabilities for obtaining these values?

(e) Evaluate the expectation value of the Hamiltonian operator corresponding to the particle in the state $\Psi(x,t)$. How does it compare with the energy eigen values of the ground and the first excited states?

2. *Spreading of wave packets:* A free particle has the initial wave function

$$\Psi(x,0) = A\,\mathrm{e}^{-a\,x^2},$$

where A and a are constants, with a being real and positive.

(a) Normalize $\Psi(x,0)$.

(b) Find $\Psi(x,t)$.

(c) Plot $\Psi(x,t)$ at $t=0$ and for large t. Determine qualitatively what happens as time goes on?

(d) Find $\langle\hat{x}\rangle$, $\langle\hat{x}^2\rangle$, $\langle\hat{p}\rangle$, $\langle\hat{p}^2\rangle$, Δx and Δp.

(e) Does the uncertainty principle hold? At what time does the system have the minimum uncertainty?

3. *Particle in an attractive delta function potential:* Consider a particle moving in one-dimension in the following attractive delta function potential:

$$V(x) = -a\,\delta^{(1)}(x),$$

where $a > 0$.

(a) Determine the bound state energy eigen functions.

(b) Plot the energy eigen functions.

(c) How many bound states exist? What are the corresponding energy eigen values?

4. *From the wavefunction to the potential:* Consider the one dimensional wave function

$$\psi(x) = A\,(x/x_0)^n\,\exp-(x/x_0),$$

where A, n and x_0 are constants. Determine the time-independent potential $V(x)$ and the energy eigen value E for which this wave function is an energy eigen function.

5. *Encountering special functions:* Solve the Schrodinger equation in a smoothened step that is described by the potential

$$V(x) = \frac{V_0}{2}\,\left[1+\tanh\left(\frac{x}{2\,a}\right)\right],$$

and determine the reflection and the transmission probabilities.

Exercise sheet 5

The harmonic oscillator

1. *Properties of Hermite polynomials:* In this problem, we shall explore a few useful relations involving the Hermite polynomials.

   (a) According to the so-called Rodrigues's formula

   $$H_n(x) = (-1)^n \, \mathrm{e}^{x^2} \left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^n \left(\mathrm{e}^{-x^2}\right).$$

   Use this relation to obtain $H_3(x)$ and $H_4(x)$.

   (b) Utilize the following recursion relation:

   $$H_{n+1}(x) = 2\,x\; H_n(x) - 2\,n\; H_{n-1}(x),$$

   and the results of the above problem to arrive at $H_5(x)$ and $H_6(x)$.

   (c) Using the expressions for $H_5(x)$ and $H_6(x)$ that you have obtained, check that the following relation is satisfied:

   $$\frac{\mathrm{d}H_n}{\mathrm{d}x} = 2\,n\,H_{n-1}(x).$$

   (d) Obtain $H_0(x)$, $H_1(x)$ and $H_2(x)$ from the following generating function for the Hermite polynomials:

   $$e^{-\left(z^2 - 2\,z\,x\right)} = \sum_{n=0}^{\infty} \frac{z^n}{n!}\, H_n(x).$$

2. *Orthonormality conditions:* Explicitly carry out the integrals to show that the energy eigen functions of the ground, the first and the second excited states of the harmonic oscillator are normalized and orthogonal.

3. *Expectation values in the excited states of the harmonic oscillator:* Determine the following expectation values in the nth excited state of the harmonic oscillator: $\langle\hat{x}\rangle$, $\langle\hat{p}_x\rangle$, $\langle\hat{x}^2\rangle$, $\langle\hat{p}_x^2\rangle$, $\langle\hat{T}\rangle$, $\langle\hat{V}\rangle$ and $\langle\hat{H}\rangle$, where T and V denote the kinetic and the potential energies of the system.

4. *Half-an-oscillator:* Determine the energy levels and the corresponding eigen functions of an oscillator which is subjected to the additional condition that the potential is infinite for $x \le 0$.

   Note: You do not have to separately solve the Schrodinger equation. You can easily identify the allowed eigen functions and eigen values from the solutions of the original, complete, oscillator!

5. *Wagging the dog:* Recall that the time-independent Schrodinger equation satisfied by a simple harmonic oscillator of mass m and frequency ω is given by

   $$-\frac{\hbar^2}{2\,m}\,\frac{\mathrm{d}^2\psi_{_E}}{\mathrm{d}x^2} + \frac{1}{2}\,m\,\omega^2\,x^2\,\psi_{_E} = E\,\psi_{_E}.$$

   In terms of the dimensionless variable

   $$\xi = \sqrt{\frac{m\,\omega}{\hbar}}\;x,$$

   the above time-independent Schrodinger equation reduces to

   $$\frac{\mathrm{d}^2\psi_{_E}}{\mathrm{d}\xi^2} + \left(\mathcal{E} - \xi^2\right)\,\psi_{_E} = 0,$$

where $\mathcal{E}$ is the energy expressed in units of $(\hbar\,\omega/2)$, and is given by

$$\mathcal{E} = \frac{2\,E}{\hbar\,\omega}.$$

According to the 'wag-the-dog' method, one solves the above differential equation numerically, say, using Mathematica, varying $\mathcal{E}$ until a wave function that goes to zero at large ξ is obtained.

Find the ground state energy and the energies of the first two excited states of the harmonic oscillator to five significant digits by the 'wag-the-dog' method.

Additional exercises I

From essential classical mechanics to the time-independent Schrodinger equation in one dimension

1. *Semi-classical quantization precedure:* Consider a particle moving in one-dimension. Let the particle be described by the generalized coordinate q, and let the corresponding conjugate momentum be p. According to Bohr's semi-classical quantization rule, the so-called action I satisfies the following relation:
$$I \equiv \int dq\, p = n\, h,$$
where n is an integer, while h is the Planck constant. Using such a quantization procedure, determine the energy levels of a particle in an infinite square well and the simple harmonic oscillator.

2. *Molecules as rigid rotators:* A rigid rotator is a particle which rotates about an axis and is located at a fixed length from the axis. Also, the particle moves *only* along the azimuthal direction. The classical energy of such a plane rotator is given by $E = L^2/(2\, I)$, where L is the angular momentum and I is the moment of inertia.
   (a) Using Bohr's rule, determine the quantized energy levels of the rigid rotator.
   (b) Molecules are known to behave sometimes as rigid rotators. If the rotational spectra of molecules are characterized by radiation of wavelength of the order of 10^6 nm, estimate the interatomic distances in a molecule such as H_2.

3. *The Klein-Gordon equation:* Consider the following Klein-Gordon equation governing a wavefunction $\Psi(x, t)$:
$$\frac{1}{c^2}\,\frac{\partial^2\Psi(x,t)}{\partial t^2} - \frac{\partial^2\Psi(x,t)}{\partial x^2} + \left(\frac{\mu\, c}{\hbar}\right)^2\, \Psi(x,t) = 0,$$
where c and μ are constants. Show that there exists a corresponding 'probability' conservation law of the form
$$\frac{\partial P(x,t)}{\partial t} + \frac{\partial j(x,t)}{\partial x} = 0,$$
where the quantity $j(x, t)$ represents the conserved current given by
$$j(x,t) = \frac{\hbar}{2\, i\, \mu}\, \left[\Psi^*(x,t)\, \left(\frac{\partial\Psi(x,t)}{\partial x}\right) - \Psi(x,t)\, \left(\frac{\partial\Psi^*(x,t)}{\partial x}\right)\right].$$
   (a) Express the 'probability' $P(x, t)$ in terms of the wavefunction $\Psi(x, t)$.
   (b) Can you identify any issue with interpreting $P(x, t)$ as the probability?

4. *A simple superposition of energy eigen states:* A particle in the infinite square well is described by the following wavefunction at time $t = 0$:
$$\Psi(x, 0) = A \sin^3(\pi\, x/L),$$
where L is the width of the well. Evaluate the expectation value $\langle x\rangle$ at a time $t > 0$.

5. *An infinite superposition of states:* Consider a particle in an infinite square well, whose walls are located at $x = 0$ and $x = L$. Let the wavefunction of the particle be given by
$$\psi(x) = \begin{cases} A\,(x/L) & \text{for } \ 0 < x < L/2, \\ A\,[1-(x/L)] & \text{for } \ L/2 < x < L. \end{cases}$$
What is the probability that, upon measuring its energy, the particle is found to be in the n-th energy level?

6. *'Wagging the dog' in the case of the infinite square well:* Find the first three allowed energies numerically to, say, five significant digits, of a particle in the infinite square well, by the 'wagging the dog' method.

7. *The twin delta function potential:* Consider a particle moving in the following twin delta function potential:

$$V(x) = -a\,\left[\delta^{(1)}(x+x_0) + \delta^{(1)}(x-x_0)\right],$$

where $a > 0$.

   (a) Obtain the bound energy eigen states.

   (b) Do the states have definite parity? Or, in other words, do the energy eigen functions $\psi_E(x)$ satisfy the conditions $\psi_E(\pm x) = \pm\psi_E(x)$?

   (c) Show that the energy eigen values corresponding to the states with even and odd parity are determined by the conditions

$$\begin{aligned}\kappa\, x_0\,\left[1+\tanh\left(\kappa\, x_0\right)\right] &= 2\, m\, a\, x_0/\hbar^2,\\ \kappa\, x_0\,\left[1+\coth\left(\kappa\, x_0\right)\right] &= 2\, m\, a\, x_0/\hbar^2,\end{aligned}$$

   respectively, where $\kappa = \sqrt{-2\, m\, E}/\hbar$.

   (d) Argue that the odd eigen states are 'less bound' that the corresponding even ones.

8. *The Dirac 'comb':* Consider a particle propagating in an infinite series of evenly spaced, attractive, Dirac delta function potentials of the following form:

$$V(x) = -a\sum_{n=-\infty}^{\infty}\delta^{(1)}(x-n\, x_0),$$

where $a > 0$. Such a situation can describe, for instance, the potential encountered by an electron as it traverses along a given direction in a solid. Due to the periodic nature of the potential, one can expect that the energy eigen states satisfy the condition $\psi_E(x+x_0) = e^{i\,q\,x_0}\,\psi_E(x)$ so that $|\psi_E(x+x_0)|^2 = |\psi_E(x)|^2$. Further, to avoid boundary effects, one often imposes the periodic boundary condition

$$\psi(x+N\, x_0) = \psi(x),$$

where $N \gg 1$. In such a case, we obtain that

$$\psi(x+N\, x_0) = \left(\mathrm{e}^{i\,q\,x_0}\right)^N\,\psi(x) = \psi(x),$$

which leads to

$$\left(\mathrm{e}^{i\,q\,x_0}\right)^N = 1$$

or, equivalently, $q = 2\,\pi\, n/(N\, x_0)$, where $n = 0, 1, 2, \ldots, N$. For large N, q ranges almost continuously between 0 and $2\,\pi$.

   (a) By matching the wavefunction and its derivative suitably across one of the delta functions, show that, for bound states wherein $E < 0$, the energy eigen values satisfy the equation

$$\frac{2\,\kappa\, x_0\,\left[\cosh\left(\kappa\, x_0\right) - z\right]}{\sinh\left(\kappa\, x_0\right)} = \frac{2\, m\, a\, x_0}{\hbar^2},$$

   where $\kappa = \sqrt{-2\, m\, E}/\hbar$ and $z = \cos\left(q\, x_0\right)$.

   (b) Also, show that, for scattering states wherein $E > 0$, the corresponding condition is given by

$$z = \cos\left(k\, x_0\right) - \frac{m\, a}{\hbar^2\, k}\,\sin\left(k\, x_0\right),$$

   where $k = \sqrt{2\, m\, E}/\hbar$.

(c) Argue that, for $2\,m\,a\,x_0/\hbar^2 \gg 1$, these conditions lead to a series of energy bands, i.e. an almost continuous range of allowed energy levels, separated by disallowed energy gaps.

9. *A smooth potential barrier:* Consider a particle moving in the following smooth potential barrier:

$$V(x) = \frac{V_0}{\cosh^2(\alpha\, x)},$$

where $V_0 > 0$. Evaluate the reflection and the tunneling probabilities for a particle that is being scattered by the potential.

10. *Quasi-probabilities in phase space:* Given a normalized wave function $\Psi(x,t)$, the Wigner function $W(x,p,t)$ is defined as

$$W(x,p,t) = \frac{1}{\pi\,\hbar} \int_{-\infty}^{\infty} dy\;\; \Psi^*[(x+y),t]\;\; \Psi[(x-y),t]\;\; \mathrm{e}^{2\,i\,p\,y/\hbar}.$$

(a) Show that the Wigner function $W(x,p,t)$ can also be expressed in terms of the momentum space wave function $\Phi(p,t)$ as follows:

$$W(x,p,t) = \frac{1}{\pi\,\hbar} \int_{-\infty}^{\infty} dq\;\; \Phi^*[(p+q),t]\;\; \Phi[(p-q),t]\;\; \mathrm{e}^{-2\,i\,q\,x/\hbar}.$$

Note: Recall that, given the wave function $\Psi(x,t)$, the momentum space wavefunction $\Phi(p,t)$ is described by the integral

$$\Phi(p,t) = \frac{1}{\sqrt{2\,\pi\,\hbar}} \int_{-\infty}^{\infty} dx\; \Psi(x,t)\; \mathrm{e}^{-i\,p\,x/\hbar}.$$

(b) Show that the Wigner function is a real quantity.

(c) Show that

$$\int_{-\infty}^{\infty} dp\;\; W(x,p,t) = |\Psi(x,t)|^2 \quad \text{and} \quad \int_{-\infty}^{\infty} dx\;\; W(x,p,t) = |\Phi(p,t)|^2.$$

(d) Consider the following normalized Gaussian wave packet

$$\Psi(x,t) = \left(\sqrt{\pi}\,\alpha\,\mathcal{F}\,\hbar\right)^{-1/2}\;\; \mathrm{e}^{i\,\left[p_0\,(x-x_0)-(p_0^2\,t/2\,m)\right]/\hbar}\;\; \mathrm{e}^{-[x-x_0-(p_0\,t/m)]^2/\left(2\,\alpha^2\,\hbar^2\,\mathcal{F}\right)},$$

where

$$\mathcal{F} = 1 + i\,(t/\tau) \quad \text{and} \quad \tau = m\,\hbar\,\alpha^2.$$

The peak of wave function is located at $x = x_0 + (p_0\,t/m)$, and the peak follows the trajectory of a classical free particle of mass m, whose position and momentum at the initial time $t = 0$ were x_0 and p_0, respectively.

i. Evaluate the Wigner function corresponding to this wave function.

ii. Plot the Wigner function, say, using Mathematica, at different times.

Quiz II

The time-independent Schrodinger equation in one dimension

1. *Wave function in momentum space and Parseval's theorem:* A one-dimensional quantum mechanical system is described by the following position space wavefunction:

$$\psi(x) = A\, \mathrm{e}^{-|x|/a},$$

where A and a are real constants, over the domain $-\infty < x < \infty$.

   (a) Obtain the corresponding momentum space wavefunction $\phi(p)$. 5 marks

   Note: The momentum space wave function $\phi(p)$ corresponding to the spatial wave function $\psi(x)$ is described by the integral

$$\phi(p) = \int\limits_{-\infty}^{\infty} \frac{\mathrm{d}x}{\sqrt{2\,\pi\,\hbar}}\, \psi(x)\, \mathrm{e}^{-i\,p\,x/\hbar}.$$

   (b) For the above $\psi(x)$ and $\phi(p)$, establish that 5 marks

$$\int\limits_{-\infty}^{\infty} \mathrm{d}x\, |\psi(x)|^2 = \int\limits_{-\infty}^{\infty} \mathrm{d}p\, |\phi(p)|^2.$$

   Note: This relation, in general, is known as Parseval's theorem.

   Hint: It is helpful to note that

$$\frac{2}{(1+z^2)^2} = \frac{1}{(1+z^2)} + \frac{1-z^2}{(1+z^2)^2}$$

   and

$$\frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{z}{1+z^2}\right) = \frac{1-z^2}{(1+z^2)^2}.$$

2. *Virial theorem:* Let x and p_x denote the position and momentum of a particle moving in a given time-independent potential $V(x)$. Show that the system satisfies the equation 10 marks

$$\frac{\langle \hat{p}_x^2 \rangle}{2\,m} = \frac{1}{2}\left\langle \hat{x}\, \widehat{\frac{\partial V}{\partial x}} \right\rangle,$$

where the expectation values are evaluated in a state described by a *real* wavefunction.

Note: The above relation is often referred to as the virial theorem.

Hint: Establish the virial theorem in the following two steps. To begin with, show that

$$\int\limits_{-\infty}^{\infty} \mathrm{d}x\, \psi\, x\, \frac{\mathrm{d}V}{\mathrm{d}x}\, \psi = -\langle \hat{V} \rangle - 2 \int\limits_{-\infty}^{\infty} \mathrm{d}x\, \frac{\mathrm{d}\psi}{\mathrm{d}x}\, x\, V\, \psi$$

and then, using the time-independent Schrodinger equation, illustrate that

$$-2 \int\limits_{-\infty}^{\infty} \mathrm{d}x\, \frac{\mathrm{d}\psi}{\mathrm{d}x}\, x\, V\, \psi = E + \frac{\hbar^2}{2\,m} \int\limits_{-\infty}^{\infty} \mathrm{d}x\, \left(\frac{\mathrm{d}\psi}{\mathrm{d}x}\right)^2.$$

3. *Scattering at a 'cliff':* The wavefunction corresponding to positive energy E and propagating from $x \to -\infty$ is scattered by the cliff-like potential

$$V(x) = \begin{cases} 0 & \text{for } x \leq 0, \\ -V_0 & \text{for } x > 0. \end{cases}$$

Determine the probability for the particle to be reflected back if $E = V_0/3$. **10 marks**

4. *Shifting the sides of a box:* A particle is in the ground state of a box whose sides are located at $x = 0$ and $x = a$. The side of the box located at $x = a$ is *suddenly* moved to $x = b$, where $b > a$.

   (a) Obtain the probability for the particle to be found in the ground state of the new potential. **4 marks**

   (b) What is the probability for the particle to be found in the first excited state? **3 marks**

   (c) Determine the behavior of these two probabilities as $b \to a$. **3 marks**

5. *Uninterrupted propagation across a potential well:* Consider a particle that is being scattered by the following smooth potential well:

$$V(x) = -\frac{\hbar^2 a^2}{m} \operatorname{sech}^2(a\,x),$$

where a is a positive constant.

   (a) Show that the potential admits the bound state

$$\psi(x) = A \operatorname{sech}(a\,x),$$

   and determine the energy associated with the state. **5 marks**

   (b) Show that the function

$$\psi(x) = A \left(\frac{i\,k - a \tanh(a\,x)}{i\,k + a}\right) \mathrm{e}^{i\,k\,x},$$

   where, as usual, $k = \sqrt{2\,m\,E}/\hbar$, satisfies the Schrodinger equation for any positive energy E. Obtain the behavior of the wavefunction as $x \to \pm\infty$ and determine the reflection and the transmission probabilities. **5 marks**

Exercise sheet 6

Essential mathematical formalism I

1. *Eigen values and eigen functions of the momentum operator:* Determine the eigen values and the eigen functions of the momentum operator. Establish the completeness of the momentum eigen functions.

2. *The angular momentum operator:* Consider the operator

$$L_\phi = -i\,\hbar\,\frac{\mathrm{d}}{\mathrm{d}\,\phi},$$

where ϕ is an angular variable. Is the operator hermitian? Determine its eigenfunctions and eigenvalues.

Note: The operator L_ϕ, for instance, could describe the conjugate momentum of a bead that is constrained to move on a circle of a fixed radius.

3. *Probabilities in momentum space:* A particle of mass m is bound in the delta function well $V(x) = -a\,\delta(x)$, where $a > 0$. What is the probability that a measurement of the particle's momentum would yield a value greater than $p_0 = m\,a/\hbar$?

4. *The energy-time uncertainty principle:* Consider a system that is described by the Hamiltonian operator $\hat{H}$.

   (a) Given an operator, say, $\hat{Q}$, establish the following relation:

$$\frac{\mathrm{d}\langle\hat{Q}\rangle}{\mathrm{d}t} = \frac{i}{\hbar}\,\langle[\hat{H},\hat{Q}]\rangle + \left\langle\frac{\partial\hat{Q}}{\partial t}\right\rangle,$$

   where the expectation values are evaluated in a specific state.

   (b) When $\hat{Q}$ does not explicitly depend on time, using the generalized uncertainty principle, show that

$$\Delta H\,\Delta Q \geq \frac{\hbar}{2}\,\left|\frac{\mathrm{d}\langle\hat{Q}\rangle}{\mathrm{d}t}\right|.$$

   (c) Defining

$$\Delta t \equiv \frac{\Delta Q}{|\mathrm{d}\langle\hat{Q}\rangle/\mathrm{d}t|},$$

   establish that

$$\Delta E\,\Delta t \geq \frac{\hbar}{2},$$

   and interpret this result.

5. *Two-dimensional Hilbert space:* Imagine a system in which there are only two linearly independent states, viz.

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

The most general state would then be a normalized linear combination, i.e.

$$|\psi\rangle = \alpha\,|1\rangle + \beta\,|2\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix},$$

with $|\alpha|^2+|\beta|^2 = 1$. The Hamiltonian of the system can, evidently, be expressed as a 2×2 hermitian matrix. Suppose it has the following form:

$$\mathsf{H} = \begin{pmatrix} a & b \\ b & a \end{pmatrix},$$

where a and b are *real* constants. If the system starts in the state $|1\rangle$ at an initial time, say, $t = 0$, determine the state of the system at a later time t.

Exercise sheet 7

Essential mathematical formalism II

1. *A three-dimensional vector space:* Consider a three-dimensional vector space spanned by the orthonormal basis $|1\rangle$, $|2\rangle$ and $|3\rangle$. Let two kets, say, $|\alpha\rangle$ and $|\beta\rangle$ be given by

$$|\alpha\rangle = i\,|1\rangle - 2\,|2\rangle - i\,|3\rangle \quad \text{and} \quad |\beta\rangle = i\,|1\rangle + 2\,|3\rangle.$$

   (a) Construct $\langle\alpha|$ and $\langle\beta|$ in terms of the dual basis, i.e. $\langle 1|$, $\langle 2|$ and $\langle 3|$.

   (b) Find $\langle\alpha|\beta\rangle$ and $\langle\beta|\alpha\rangle$ and show that $\langle\beta|\alpha\rangle = \langle\alpha|\beta\rangle^*$.

   (c) Determine all the matrix elements of the operator $\hat{A} = |\alpha\rangle\langle\beta|$ in this basis and construct the corresponding matrix. Is the matrix hermitian?

2. *A two level system:* The Hamiltonian operator of a certain two level system is given by

$$\hat{H} = E\left(|1\rangle\langle 1| - |2\rangle\langle 2| + |1\rangle\langle 2| + |2\rangle\langle 1|\right),$$

   where $|1\rangle$ and $|2\rangle$ form an orthonormal basis, while E is a number with the dimensions of energy.

   (a) Find the eigen values and the normalized eigen vectors, i.e. as a linear combination of the basis vectors $|1\rangle$ and $|2\rangle$, of the above Hamiltonian operator.

   (b) What is the matrix that represents the operator $\hat{H}$ in this basis?

3. *Matrix elements for the harmonic oscillator:* Let $|n\rangle$ denote the orthonormal basis of energy eigen states of the harmonic oscillator. Determine the matrix elements $\langle n|\hat{x}|m\rangle$ and $\langle n|\hat{p}_x|m\rangle$ in this basis.

4. *Coherent states of the harmonic oscillator:* Consider states, say, $|\alpha\rangle$, which are eigen states of the annihilation (or, more precisely, the lowering) operator, i.e.

$$\hat{a}|\alpha\rangle = \alpha\,|\alpha\rangle,$$

   where α is a complex number.

   Note: The state $|\alpha\rangle$ is called the coherent state.

   (a) Calculate the quantities $\langle\hat{x}\rangle$, $\langle\hat{x}^2\rangle$, $\langle\hat{p}_x\rangle$ and $\langle\hat{p}_x^2\rangle$ in the coherent state.

   (b) Also, evaluate the quantities Δx and Δp_x in the state, and show that $\Delta x\,\Delta p_x = \hbar/2$.

   (c) Like any other general state, the coherent state can be expanded in terms of the energy eigen states $|n\rangle$ of the harmonic oscillator as follows:

$$|\alpha\rangle = \sum_{n=0}^{\infty} c_n\,|n\rangle.$$

   Show that the quantities c_n are given by

$$c_n = \frac{\alpha^n}{\sqrt{n!}}\,c_0.$$

   (d) Determine c_0 by normalizing $|\alpha\rangle$.

   (e) Upon including the time dependence, show that the coherent state continues to be an eigen state of the lowering operator $\hat{a}$ with the eigen value evolving in time as

$$\alpha(t) = e^{-i\,\omega\,t}\,\alpha.$$

   Note: Therefore, a coherent state *remains* coherent, and continues to minimize the uncertainty.

(f) Is the ground state $|0\rangle$ itself a coherent state? If so, what is the eigen value?

5. *A three level system:* The Hamiltonian for a three level system is represented by the matrix

$$\mathsf{H} = \hbar\omega \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

Two other observables, say, A and B, are represented by the matrices

$$\mathsf{A} = \lambda \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 2 \end{pmatrix} \qquad \text{and} \qquad \mathsf{B} = \mu \begin{pmatrix} 2 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

where ω, λ and μ are positive real numbers.

(a) Find the eigen values and normalized eigen vectors of H, A, and B.

(b) Suppose the system starts in the generic state

$$|\psi(t=0)\rangle = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix},$$

with $|c_1|^2 + |c_2|^2 + |c_3|^2 = 1$. Find the expectation values of H, A and B in the state at $t = 0$.

(c) What is $|\psi(t)\rangle$ for $t > 0$? If you measure the energy of the state at a time t, what are the values of energies that you will get and what would be the probability for obtaining each of the values?

(d) Also, arrive at the corresponding answers for the quantities A and B.

Exercise sheet 8

The Schrodinger equation in three dimensions and particle in a central potential

1. *Commutation relations:* Establish the following commutation relations between the components of the position and the momentum operators in three dimensions:

$$[\hat{x}_i, \hat{x}_j] = 0, \quad [\hat{p}_i, \hat{p}_j] = 0 \quad \text{and} \quad [\hat{x}_i, \hat{p}_j] = i\,\hbar\,\delta_{ij},$$

   where $(i, j) = (1, 2, 3)$.

2. *Particle in a three dimensional box:* Consider a particle that is confined to a three dimensional box of side, say, a. In other words, the particle is free inside the box, but the potential energy is infinite on the walls of the box, thereby confining the particle to the box.

   (a) Determine the energy eigen functions and the corresponding energy eigen values.

   (b) Does there exist degenerate energy eigen states? Identify a few of them.

3. *Particle in a spherical well:* Consider a particle that is confined to the following spherical well:

$$V(r) = \begin{cases} 0 & \text{for } r < a, \\ \infty & \text{for } r \geq a. \end{cases}$$

   Find the energy eigen functions and the corresponding energy eigen values of the particle.

4. *Orthogonality of Legendre polynomials:* Recall that, according to the Rodrigues formula, the Legendre polynomials $P_l(x)$ are given by

$$P_l(x) = \frac{1}{2^l\,l!}\,\frac{\mathrm{d}^l}{\mathrm{d}x^l}\,\left[\left(x^2 - 1\right)^l\right].$$

   Using this representation, arrive at the following orthonormality condition for the Legendre polynomials:

$$\int_{-1}^{1} \mathrm{d}\,x\,P_l(x)\,P_{l'}(x) = \frac{2}{2\,l + 1}\,\delta_{ll'}.$$

   Hint: The differentials appearing in the representation suggests integration by parts.

5. *Expectation values in the energy eigen states of the hydrogen atom:* Recall that, the normalized wavefunctions that describe the energy eigen states of the electron in the hydrogen atom are given by

$$\psi_{nlm}(r, \theta, \phi) = \left[\left(\frac{2}{n\,a_0}\right)^3 \frac{(n - l - 1)!}{2\,n\,[(n + l)!]^3}\right]^{1/2} e^{-r/(n\,a_0)}\,\left(\frac{2\,r}{n\,a_0}\right)^l\,L_{n-l-1}^{2\,l+1}(2\,r/n\,a_0)\;Y_l^m(\theta, \phi),$$

   where $L_p^q(x)$ and Y_l^m represent the associated Laguerre polynomials and the spherical harmonics, respectively, while a_0 denotes the Bohr radius.

   (a) Evaluate $\langle\hat{r}\rangle$ and $\langle\hat{r}^2\rangle$ for the electron in the ground state of the hydrogen atom, and express it in terms of the Bohr radius.

   (b) Find $\langle\hat{x}\rangle$ and $\langle\hat{x}^2\rangle$ for the electron in the ground state of hydrogen.
   Hint: Express r^2 as $x^2 + y^2 + z^2$ and exploit the symmetry of the ground state.

   (c) Calculate $\langle\hat{x}^2\rangle$ in the state $n = 2$, $l = 1$ and $m = 1$.
   Note: This state is not symmetrical in x, y and z. Use $x = r\sin\theta\cos\phi$.

Exercise sheet 9

Angular momentum and spin

1. *The raising and lowering angular momentum operators:* As we have discussed, the raising and lowering angular momentum operators L_+ and L_- change the value of the z-component of angular momentum, viz. the eigen value m (corresponding to the operator L_z) by one unit, i.e.

$$L_\pm\, f_l^m = A_l^m\, f_l^{m\pm 1},$$

where A_l^m are constants, while f_l^m are simultaneous eigen functions of the operators L^2 and L_z. What are A_l^m, if f_l^m are normalized eigen functions?

2. *Velocity on the surface of a spinning electron:* Consider the electron to be a classical solid sphere. Assume that the radius of the electron is given by the classical electron radius, viz.

$$r_{\rm c} = \frac{e^2}{4\,\pi\,\epsilon_0\, m_{\rm e}\, c^2}$$

where e and $m_{\rm e}$ denote the charge and the mass of the electron, while c represents the speed of light. Also, assume that the angular momentum of the electron is $\hbar/2$. Evaluate the speed on the surface of the electron under these conditions.

3. *Probabilities for a spin state:* Suppose a spin 1/2 particle is in the state

$$\chi = \frac{1}{\sqrt{6}} \begin{pmatrix} 1+i \\ 2 \end{pmatrix}.$$

What are the probabilities of getting $\hbar/2$ and $-\hbar/2$, if you measure S_z and S_x?

4. *Mean values and uncertainties associated with spin operators:* An electron is in the spin state

$$\chi = A \begin{pmatrix} 3\,i \\ 4 \end{pmatrix}.$$

   (a) Determine the normalization constant A.
   (b) Find the expectation values of the operators $\hat{S}_x$, $\hat{S}_y$ and $\hat{S}_z$ in the above state.
   (c) Evaluate the corresponding uncertainties, i.e. ΔS_x, ΔS_y and ΔS_z.
   (d) Examine if the products of any two of these quantities are consistent with the corresponding uncertainty principles.

5. *Larmor precession:* Consider a charged, spin 1/2 particle that is at rest in an external and uniform magnetic field, say, $\mathbf{B}$, that is oriented along the z-direction, i.e. $\mathbf{B} = B\,\hat{k}$, where B is a constant. The Hamiltonian of the particle is then given by

$$\hat{H} = -\gamma\, B\, \hat{S}_z,$$

where γ is known as the gyromagnetic ratio of the particle.

   (a) Determine the most general, time dependent, solution that describes the state of the particle.
   (b) Evaluate the expectation values of the operators $\hat{S}_x$, $\hat{S}_y$ and $\hat{S}_z$ in the state.
   (c) Show that the expectation value of the operator $\hat{\mathbf{S}} = \hat{S}_x\,\hat{\imath} + \hat{S}_y\,\hat{\jmath} + \hat{S}_z\,\hat{k}$ is tilted at a constant angle with respect to the direction of the magnetic field and precesses about the field at the so-called Larmor frequency $\omega = \gamma\, B$.

Quiz III

From essential mathematical formalism to angular momentum and spin

1. *Eigen values and eigen vectors of a hermitian matrix:* Consider the following hermitian matrix:

$$\mathsf{A} = \begin{pmatrix} 1 & 1-i \\ 1+i & 0 \end{pmatrix}.$$

   (a) Determine the eigen values of the matrix. 3 marks

   (b) Obtain the corresponding eigen vectors. 5 marks

   (c) Are the eigen vectors orthonormal? 2 marks

2. *Expectation value in the momentum representation:* Let $\psi(x)$ be the wavefunction describing a one-dimensional quantum system. Let $\phi(p)$ be the associated momentum space wavefunction. Recall that the expectation value of the position operator in the state ψ is given by

$$\langle \hat{x} \rangle = \int \mathrm{d}x\, \psi^*(x)\, x\, \psi(x).$$

   Show that we can also write 10 marks

$$\langle \hat{x} \rangle = \int_{-\infty}^{\infty} \mathrm{d}p\, \phi^*(p) \left(i\,\hbar\, \frac{\partial \phi(p)}{\partial p}\right),$$

3. *A version of the energy-time uncertainty principle:* Consider two orthonormal energy eigen states of a system, say, ψ_1 and ψ_2. Let the system start, say, at $t = 0$, in the initial state $\Psi(x,0) = \psi(x) = [\psi_1(x) + \psi_2(x)]/\sqrt{2}$. In an interesting version of the energy-time uncertainty principle applicable to such situations, it is stated that $\Delta t = \tau/\pi$, where τ is the time it takes for the wavefunction $\Psi(x,t)$ to evolve to a situation wherein it is orthogonal to the initial state $\Psi(x,0)$, while ΔE is the uncertainty of the Hamiltonian operator in the initial state $\Psi(x,0)$. Establish such a version of the energy-time uncertainty principle. 10 marks

4. *The radial wave functions of the hydrogen atom:* The radial wavefunctions associated with the first four energy eigen states of the hydrogen atom are given by

$$\begin{aligned}
R_{10}(r) &= \frac{1}{2\, a_0^{3/2}}\, \exp -(r/a_0), \\
R_{20}(r) &= \frac{1}{\sqrt{2}\, a_0^{3/2}} \left(1 - \frac{r}{2\, a_0}\right) \exp -(r/2\, a_0), \\
R_{21}(r) &= \frac{1}{\sqrt{24}\, a_0^{3/2}}\, \frac{r}{a_0}\, \exp -(r/2\, a_0), \\
R_{30}(r) &= \frac{2}{\sqrt{27}\, a_0^{3/2}} \left(1 - \frac{2\, r}{3\, a_0} + \frac{2\, r^2}{27\, a_0^2}\right) \exp -(r/3\, a_0),
\end{aligned}$$

   where $a_0 = 4\,\pi\,\epsilon_0\,\hbar^2/(m\, e^2)$ is the Bohr radius. Plot these functions. 2+3+2+3 marks

5. *Commutation relations involving angular momentum:* Establish the following commutation relations: 2+2+3+3 marks

   (a) $[\hat{L}_z, \hat{x}] = i\,\hbar\,\hat{y}$,

   (b) $[\hat{L}_z, \hat{p}_x] = i\,\hbar\,\hat{p}_y$,

   (c) $[\hat{L}_z, \hat{x}^2] = 2\,i\,\hbar\,\hat{x}\,\hat{y}$,

   (d) $[\hat{L}_z, \hat{x}\,\hat{p}_x] = i\,\hbar\,(\hat{x}\,\hat{p}_y + \hat{y}\,\hat{p}_x)$.

Additional exercises II

From essential mathematical formalism to angular momentum and spin

1. *Sequential measurements:* An operator $\hat{A}$, representing the observable A, has two normalized eigen states ψ_1 and ψ_2, with eigen values a_1 and a_2. Operator $\hat{B}$, representing another observable B, has two normalized eigen states ϕ_1 and ϕ_2, with eigen values b_1 and b_2. These eigen states are related as follows:
$$\psi_1 = \frac{3}{5}\,\phi_1 + \frac{4}{5}\,\phi_2 \qquad \text{and} \qquad \psi_2 = \frac{4}{5}\,\phi_1 - \frac{3}{5}\,\phi_2.$$
   (a) Observable A is measured and the value a_1 is obtained. What is the state of the system immediately after this measurement?
   (b) If B is now measured, what are the possible results, and what are their probabilities?
   (c) Immediately after the measurement of B, A is measured again. What is the probability of getting a_1?

2. *Operators describing spin:* A two level system is described by two orthonormal states, say, $|+\rangle$ and $|-\rangle$. There exist three operators, $\hat{S}_x$, $\hat{S}_y$ and $\hat{S}_z$, called the spin operators along the three axes, which are defined as
$$\begin{aligned}\hat{S}_x &= \frac{\hbar}{2}\,\left(|+\rangle\langle-| + |-\rangle\langle+|\right),\\ \hat{S}_y &= \frac{i\,\hbar}{2}\,\left(-|+\rangle\langle-| + |-\rangle\langle+|\right),\\ \hat{S}_z &= \frac{\hbar}{2}\,\left(|+\rangle\langle+| - |-\rangle\langle-|\right).\end{aligned}$$
   (a) Construct the matrices corresponding to the three operators $\hat{S}_x$, $\hat{S}_y$ and $\hat{S}_z$ in the basis $|+\rangle$ and $|-\rangle$.
   (b) Evaluate the commutators $[\hat{S}_x, \hat{S}_y]$, $[\hat{S}_y, \hat{S}_z]$ and $[\hat{S}_z, \hat{S}_x]$.
   (c) Can you express the results in terms of the operators $\hat{S}_x$, $\hat{S}_y$ or $\hat{S}_z$?

3. *Momentum space wave functions:* Consider a particle that is confined to an infinite square well with its walls located at $x = 0$ and $x = a$.
   (a) Determine the momentum space wave functions, say, $\phi_n(p,t)$, for the particle in the nth energy eigen state described by the position wave functions $\psi_n(x,t)$.
   (b) Evaluate $|\phi_1(p,t)|^2$ and $|\phi_2(p,t)|^2$.

4. *More about oscillators:* Let $|0\rangle$ represent the ground state of a one dimensional quantum oscillator. Show that
$$\langle 0|e^{i\,k\,\hat{x}}|0\rangle = \exp -\left(k^2\,\langle 0|\hat{x}^2|0\rangle/2\right),$$
where $\hat{x}$ is the position operator.

5. *Commutator identities:* Establish the following identities involving the commutators of operators:
   (a) $[\hat{A}\,\hat{B}, \hat{C}] = \hat{A}\,[\hat{B}, \hat{C}] + [\hat{A},\,\hat{C}]\,\hat{B}$,
   (b) $[\hat{x}^n, \hat{p}_x] = i\,\hbar\,n\,\hat{x}^{n-1}$,
   (c) $[f(\hat{x}), \hat{p}_x] = i\,\hbar\,\left(\mathrm{d}f(\hat{x})/\mathrm{d}\hat{x}\right)$,

   where $f(x)$ is a function that can be expanded in a power series.

6. *Properties of unitary operators:* An operator say, $\hat{U}$, is said to be unitary if its hermitian conjugate is the same as its inverse, i.e. $\hat{U}^\dagger = \hat{U}^{-1}$ so that $\hat{U}^{-1}\,\hat{U} = \hat{U}^\dagger\,\hat{U} = 1$.

(a) Show that unitary transformations preserve inner products in the sense that $\langle \hat{U}\,\beta|\hat{U}\,\alpha\rangle = \langle\beta|\alpha\rangle$, for all $|\alpha\rangle$ and $|\beta\rangle$.

(b) Show that the eigen values of a unitary operator have unit modulus.

(c) Show that the eigen vectors of a unitary operator belonging to distinct eigen values are orthogonal.

7. *Superposition of states of the hydrogen atom:* An electron in the Coulomb field of a proton is in the state described by the wave function

$$\psi(\boldsymbol{r}) = \frac{1}{6}\,\left[4\,\psi_{100}(\boldsymbol{r}) + 3\,\psi_{211}(\boldsymbol{r}) - \psi_{210}(\boldsymbol{r}) + \sqrt{10}\,\psi_{21-1}(\boldsymbol{r})\right].$$

(a) What is the expectation value of the energy of the electron in the state?

(b) What is the expectation value of $\hat{\mathbf{L}}^2$?

(c) What is the expectation value of $\hat{L}_z$?

8. *A model of angular momentum:* Let

$$\hat{L}_{\pm} = \left(\hat{a}_{\pm}^{\dagger}\,\hat{a}_{\mp}\right)\hbar, \qquad \hat{L}_z = \left(\hat{a}_{+}^{\dagger}\,\hat{a}_{+} - \hat{a}_{-}^{\dagger}\,\hat{a}_{-}\right)\hbar/2 \qquad \text{and} \qquad \hat{N} = \hat{a}_{+}^{\dagger}\,\hat{a}_{+} + \hat{a}_{-}^{\dagger}\,\hat{a}_{-},$$

where $\hat{a}_{\pm}$ and $\hat{a}_{\pm}^{\dagger}$ are the annihilation and the creation operators of two *independent* simple harmonic oscillators satisfying the usual commutation relations. Show that

(a) $[\hat{L}_z, \hat{L}_{\pm}] = \pm\,\hbar\,\hat{L}_{\pm}$,

(b) $\hat{\mathbf{L}}^2 = \hat{N}\,\left[\left(\hat{N}/2\right) + 1\right]\,\left(\hbar^2/2\right)$,

(c) $[\hat{\mathbf{L}}^2, \hat{L}_z] = 0$.

Note: This representation of the angular momentum operators in terms of creation and the annihilation operators of oscillators is known as the Schwinger model.

9. *Operators and eigen functions for a spin 1 particle:* Consider a particle with spin 1.

(a) Construct the operators $\hat{S}_x$, $\hat{S}_y$ and $\hat{S}_z$ corresponding to the particle.

(b) Determine the eigen values of the operator $\hat{S}_x$ and express the corresponding eigen functions in terms of the eigen functions of the $\hat{S}_z$ operator.

10. *Hamiltonian involving angular momentum:* The Hamiltonian of a system is described in terms of the angular momentum operators as follows:

$$H = \frac{L_x^2}{2\,I_1} + \frac{L_y^2}{2\,I_2} + \frac{L_z^2}{2\,I_3}.$$

(a) What are the eigen values of the Hamiltonian when $I_1 = I_2$?

(b) What are the eigen values of the Hamiltonian if the angular momentum of the system is unity and $I_1 \neq I_2$?

Exercise sheet 10

Time-independent perturbation theory

1. *The perturbed wavefunction:* Using time-independent perturbation theory, show that the wave function of the n-th eigen state of system at the first order in the perturbation is given by

$$\psi_n^1 = \sum_{m\neq n} \frac{\langle\psi_m^0|\hat{H}'|\psi_n^0\rangle}{E_n^0 - E_m^0}\, \psi_m^0,$$

where $\hat{H}'$ is the Hamiltonian describing the perturbation, while ψ_n^0 and E_n^0 denote the eigen functions and the eigen values of the unperturbed Hamiltonian $\hat{H}_0$.

2. *A delta function perturbation:* Suppose we introduce the following perturbation:

$$\hat{H}' = \alpha\, \delta^{(1)}(x - a/2),$$

where α is a constant, at the centre of an infinite potential well with its walls located at $x = 0$ and $x = a$. Determine the change in the energy eigen values at the first order in the perturbation. Also, explain why the original energy eigen values with even n are not affected by the perturbation.

3. *Expectation values of inverse powers of radii:* Show that, for an electron in the hydrogen atom,

$$\begin{aligned}
\left\langle\frac{1}{r}\right\rangle &= \frac{1}{n^2\, a_0},\\
\left\langle\frac{1}{r^2}\right\rangle &= \frac{1}{[l + (1/2)]\; n^3\, a_0^2},\\
\left\langle\frac{1}{r^3}\right\rangle &= \frac{1}{l\; [l + (1/2)]\; (l+1)\, n^3\, a_0^3},
\end{aligned}$$

where n and l are the principal and the azimuthal quantum numbers, and $a_0 = 4\,\pi\,\epsilon_0\,\hbar^2/\left(m_{\rm e}\, e^2\right)$ is the Bohr radius, with $m_{\rm e}$ denoting the mass of the electron, e the electronic charge, and ϵ_0 the permitivity of free space.

4. *Nature of $l = 0$ states:* Let $\mathbf{a}$ and $\mathbf{b}$ be two constant vectors. Show that

$$\int_0^\pi {\rm d}\theta \int_0^{2\pi} {\rm d}\phi\, \sin\theta\; (\boldsymbol{a}\cdot\hat{r})\; (\boldsymbol{b}\cdot\hat{r}) = \frac{4\,\pi}{3}\; (\boldsymbol{a}\cdot\boldsymbol{b})\,.$$

Given that $\hat{\boldsymbol{S}}_{\rm p}$ and $\hat{\boldsymbol{S}}_{\rm e}$ denote the spin of the proton and the electron, use the above result to demonstrate that

$$\left\langle\frac{3\,(\hat{\boldsymbol{S}}_{\rm p}\cdot\hat{r})\,(\hat{\boldsymbol{S}}_{\rm e}\cdot\hat{r}) - \hat{\boldsymbol{S}}_{\rm p}\cdot\hat{\boldsymbol{S}}_{\rm e}}{r^3}\right\rangle = 0,$$

in states wherein $l = 0$.

5. *The 21-cm transition:* Recall that the hyperfine structure of hydrogen is given by

$$E_{\rm hf}^1 = \frac{\mu_0\, g_{\rm p}\, e^2}{8\,\pi\, m_{\rm p}\, m_{\rm e}} \left\langle\frac{3\;(\hat{\boldsymbol{S}}_{\rm p}\cdot\hat{r})\;(\hat{\boldsymbol{S}}_{\rm e}\cdot\hat{r}) - (\hat{\boldsymbol{S}}_{\rm p}\cdot\hat{\boldsymbol{S}}_{\rm e})}{r^3}\right\rangle + \frac{\mu_0\, g_{\rm p}\, e^2}{3\, m_{\rm p}\, m_{\rm e}}\,\langle\hat{\boldsymbol{S}}_{\rm p}\cdot\hat{\boldsymbol{S}}_{\rm e}\rangle\; |\psi(0)|^2,$$

where $m_{\rm p}$ denotes the mass of the proton, $g_{\rm p} = 5.59$ its gyromagnetic ratio, and μ_0 is the magnetic permeability of free space.

(a) As we discussed, when $l = 0$, the first term always vanishes. Establish that, the ground state of hydrogen splits into a singlet and triplet state with the following energies:

$$E^1_{\rm hf} = \frac{4\, g_{\rm p}\, \hbar^4}{3\, m_{\rm p}\, m_{\rm e}\, c^2\, a_0^4} \begin{cases} +(1/4), \\ -(3/4). \end{cases}$$

(b) Also show that the gap between these two energy levels is

$$\Delta E = \frac{4\, g_{\rm p}\, \hbar^4}{3\, m_{\rm p}\, m_{\rm e}\, c^2\, a_0^4} = 5.88 \times 10^{-6}\, {\rm eV}.$$

(c) Further, establish that this energy gap corresponds to the wavelength of 21 cm and the frequency of 1420 MHz.

Note: Due to the abundance of hydrogen, this 21-cm transition is one of the most ubiquitous forms of radiation in the universe.

Exercise sheet 11

Charged particle in a uniform and constant magnetic field

1. *Hamiltonian and Hamilton's equations for a particle in an electromagnetic field:* Recall that, a non-relativistic particle that is moving in an electromagnetic field described by the scalar potential ϕ and the vector potential $\mathbf{A}$ is governed by the Lagrangian

$$L = \frac{m\,\mathbf{v}^2}{2} + q\,\left(\frac{\mathbf{v}}{c}\cdot\mathbf{A}\right) - q\,\phi,$$

where m and q are the mass and the charge of the particle, while c denotes the velocity of light. From the above Lagrangian, we had obtained the equation of motion satisfied by the particle to be

$$m\,\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = q\,\left(\mathbf{E} + \frac{\mathbf{v}}{c}\times\mathbf{B}\right),$$

where $\mathbf{E}$ and the $\mathbf{B}$ are the electric and the magnetic fields given by

$$\mathbf{E} = -\boldsymbol{\nabla}\phi - \frac{1}{c}\,\frac{\partial\mathbf{A}}{\partial t} \qquad \text{and} \qquad \mathbf{B} = \boldsymbol{\nabla}\times\mathbf{A}.$$

   (a) Construct the Hamiltonian corresponding to the above Lagrangian.

   (b) Obtain the corresponding Hamilton's equations of motion.

   (c) Arrive at the above Lorentz force law satisfied by the particle from the Hamilton's equations.

2. *Gauges and gauge transformations:* Consider a constant and uniform magnetic field of strength B that is directed along the positive z-direction as follows: $\boldsymbol{B} = B\,\hat{z}$. Construct three different gauges that can lead to such a magnetic field and also obtain the gauge transformations that relate these gauges.

3. *Motion in a constant and uniform magnetic field:* Solve the above of motion to arrive at the trajectory of a particle in a uniform and constant magnetic field that is pointed towards, say, the positive z-direction.

4. *Transformation of the wavefunction I:* Consider a particle moving in the three-dimensional potential $V(\boldsymbol{x})$. Show that, if $V(\boldsymbol{x}) \to V(\boldsymbol{x}) + V_0(t)$, the wavefunction describing the particle transforms as

$$\Psi(\boldsymbol{x},t) \to \Psi(\boldsymbol{x},t)\,\exp -\frac{i}{\hbar}\int^t \mathrm{d}t'\,V_0(t').$$

5. *Transformation of the wavefunction II:* Consider a charged particle moving in an electromagnetic background. Show that, under a gauge transformation of the form $\phi \to \phi + (1/c)\,(\partial\chi/\partial t)$ and $\boldsymbol{A} \to \boldsymbol{A} - \boldsymbol{\nabla}\,\chi$, where χ is an arbitrary function of space and time, the wavefunction describing the particle transforms as

$$\Psi(\boldsymbol{x},t) \to \Psi(\boldsymbol{x},t)\,\exp\,-\left[i\,q\,\chi(\boldsymbol{x},t)/\hbar\right],$$

with q being the charge associated with the particle.

End-of-semester exam

From the origins of quantum theory and the wave aspects of matter until charged particles in a uniform magnetic field

1. *Warming up with numbers:* Recall that the fine structure constant is defined as $\alpha = e^2/(4\,\pi\,\epsilon_0\,\hbar\,c)$.

   (a) Calculate the value of α^{-1} to the second decimal place. **[2 marks]**

   (b) Express the Rydberg constant in terms of the fine structure constant α and the mass $m_{\rm e}$ of the electron, and evaluate the quantity in electron volts. **[2 marks]**

   (c) If the energy associated with the fine structure of hydrogen is $\alpha^4\, m_{\rm e}\, c^2$, estimate the wavelength corresponding to these energies. **[3 marks]**

   (d) If the energy associated with the hyperfine structure of hydrogen is $(m_{\rm e}/m_{\rm p})\,\alpha^4\, m_{\rm e}\, c^2$, where $m_{\rm p}$ is the mass of the proton, estimate the wavelength corresponding to these transitions. **[3 marks]**

   Note: The mass and the charge of the electron are $m_{\rm e} = 9.109 \times 10^{-31}\,{\rm kg}$ and $e = 1.602 \times 10^{-19}\,{\rm C}$, respectively, the value of the Planck's constant is $h = 6.626 \times 10^{-34}\,{\rm J\,s}$, the speed of light is $c = 2.998 \times 10^8\,{\rm m/s}$, while $(4\,\pi\,\epsilon_0)^{-1} = 8.987 \times 10^9\,{\rm N\,m^2/C^2}$ and the mass of the proton is $m_{\rm p} = 1.675 \times 10^{-27}\,{\rm kg}$. Also, $1\,{\rm eV} = 1.602 \times 10^{-19}\,{\rm J}$.

2. *Molecules as rigid rotators:* A rigid rotator is a system of two masses connected by a rigid rod, which rotates about an axis that lies midway between the two masses and runs perpendicular to the rod. Assume that, the rod, along with the masses fixed at its ends, rotates *only* along the azimuthal direction. The classical energy of such a plane rotator is given by $E = L^2/(2\,I)$, where L is the angular momentum and I is the moment of inertia of the system.

   (a) Using Bohr's semi-classical quantization rule, viz. that

   $$\oint {\rm d}q\; p = n\,h,$$

   where p is the momentum conjugate to the coordinate q, determine the quantized energy levels of the rigid rotator. **[6 marks]**

   Note: The angular momentum L is conjugate to the azimuthal angle, say, ϕ.

   (b) Molecules are known to behave sometimes as rigid rotators. If the rotational spectra of molecules are characterized by radiation of wavelength of the order of $10^6\,{\rm nm}$, estimate the interatomic distances in a molecule such as H_2. **[4 marks]**

   Note: The values of the Planck's constant h and the mass $m_{\rm p}$ of the proton that you may require are listed in the previous problem.

3. (a) *Incoherent super-position:* Consider a double slit experiment involving electrons in which the wave function of the electrons at, say, the slit 1, acquires an arbitrary random phase, say, ϕ, that is to be eventually averaged over. The total wave function at the screen is given by $\psi(x,t) = e^{i\,\phi}\,\psi_1(x,t) + \psi_2(x,t)$, where $\psi_1(x,t)$ and $\psi_2(x,t)$ are the wave functions describing the electrons at the slits 1 and 2. What will happen to the interference pattern on the screen in such a case? **[5 marks]**

   Note: Such a situation may arise if there are two incoherent electron sources, one at each slit.

   (b) *Sequential measurements:* An operator $\hat{A}$, representing the observable A, has two normalized eigen states ψ_1 and ψ_2, with eigen values a_1 and a_2. Operator $\hat{B}$, representing another observable B, has two normalized eigen states ϕ_1 and ϕ_2, with eigen values b_1 and b_2. These eigen states are related as follows:

   $$\psi_1 = \frac{3}{5}\,\phi_1 + \frac{4}{5}\,\phi_2 \qquad \text{and} \qquad \psi_2 = \frac{4}{5}\,\phi_1 - \frac{3}{5}\,\phi_2.$$

i. Observable A is measured and the value a_1 is obtained. What is the state of the system immediately after this measurement? 1 marks

ii. If B is now measured, what are the possible results, and what are their probabilities? 2 marks

iii. Immediately after the measurement of B, A is measured again. What is the probability of getting a_1? 2 marks

4. *Wavefunctions in a potential well:* Consider a particle that is moving in the following one-dimensional potential well:

$$V(x) = \begin{cases} 0 & \text{for} \quad x < 0, \\ -V_0 & \text{for} \quad 0 < x < a, \\ 0 & \text{for} \quad x > a, \end{cases}$$

where $V_0 > 0$.

(a) Determine the wave functions in the three domains for energies $E < 0$. 3 marks

(b) Obtain the wave functions in the three domains for positive energies. 3 marks

(c) Match the necessary conditions at $x = 0$ and $x = a$ and arrive at the relations between the coefficients in the three domains for $E > 0$. 4 marks

Note: As usual, assume that there are incoming and reflected waves in the domain $x < 0$ and there is a transmitted wave in the domain $x > a$.

5. *Energy eigen functions of the harmonic oscillator:* Consider a one-dimensional simple harmonic oscillator of mass m and angular frequency ω. Recall that the Hamiltonian operator of the oscillator can be written as

$$\hat{H} = \left(\hat{a}^\dagger\, \hat{a} + \frac{1}{2}\right) \hbar\, \omega,$$

where $\hat{a}$ and $\hat{a}^\dagger$ are the lowering and the raising operators, respectively. They are related to the position operator $\hat{x}$ and the momentum operator $\hat{p}_x$ by the following relations:

$$\hat{a} = \sqrt{\frac{m\,\omega}{2\,\hbar}}\,\left(\hat{x} + \frac{i\,\hat{p}_x}{m\,\omega}\right) \qquad \text{and} \qquad \hat{a}^\dagger = \sqrt{\frac{m\,\omega}{2\,\hbar}}\,\left(\hat{x} - \frac{i\,\hat{p}_x}{m\,\omega}\right),$$

In units such that $m = \hbar = \omega = 1$, let the un-normalized energy eigen function of a particular state be given by

$$\psi(x) = \left(2\,x^3 - 3\,x\right)\, \exp -(x^2/2).$$

Find that other two (un-normalized) eigen states that are closest in energy to the eigen state $\psi(x)$ above. 10 marks

6. *Spherical harmonics:* Recall that, $\langle \theta, \phi | l, m\rangle = Y_l^m(\theta, \phi)$. Using the relations $\hat{L}_+|l, l\rangle = 0$ and $\hat{L}_z|l, l\rangle = l\,\hbar |l, l\rangle$, determine the functional form of $Y_l^l(\theta, \phi)$. 10 marks

Hint: Using the representations of $\hat{L}_+$ and $\hat{L}_z$ as differential operators, write the two relations above as differential equations and solve them.

Note: You need not have to normalize the wavefunction.

7. *Commutation relations involving angular momentum and spin:* Establish the following commutation relations involving the angular momentum and the spin operators $\hat{\boldsymbol{L}}$ and $\hat{\boldsymbol{S}}$:

(a) $[\hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}, \hat{\boldsymbol{L}}] = i\,\hbar\, \left(\hat{\boldsymbol{L}} \times \hat{\boldsymbol{S}}\right)$, 4 marks

(b) $[\hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}, \hat{\boldsymbol{S}}] = i\,\hbar\, \left(\hat{\boldsymbol{S}} \times \hat{\boldsymbol{L}}\right)$, 4 marks

(c) $[\hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}, \hat{\boldsymbol{J}}] = 0$, 2 marks where $\hat{\boldsymbol{J}} = \hat{\boldsymbol{L}} + \hat{\boldsymbol{S}}$.

Note: These relations imply that, in the case of the electron in the hydrogen atom, when the contribution to the Hamiltonian due to the spin-orbit coupling is taken into account, it is the total angular momentum $\boldsymbol{J}$ of the electron which is conserved.

8. *The three-dimensional harmonic oscillator:* Consider the following three-dimensional oscillator:

$$V(r) = \frac{m}{2}\,\omega^2\,r^2.$$

   (a) What are the energy eigen functions describing the oscillator? [3 marks]
   Hint: For this problem, despite the spherical symmetry, it proves to be more convenient to work in the Cartesian coordinates.

   (b) What are the corresponding energy eigen values? [3 marks]

   (c) Determine the degeneracy of the eigen states of the oscillator. [4 marks]

9. *Orienting spin along an arbitrary direction:* Let $\hat{\boldsymbol{n}}$ be a three-dimensional unit vector whose polar angle (i.e. the angle with respect to the z-axis) is θ and the azimuthal angle (i.e. the angle with respect to the x-axis, when the unit vector $\hat{\boldsymbol{n}}$ has been projected on to the x-y plane) is ϕ, i.e.

$$\hat{\boldsymbol{n}} = \sin\theta\,\cos\phi\;\hat{i} + \sin\theta\,\sin\phi\;\hat{j} + \cos\theta\;\hat{k}.$$

   (a) Obtain the eigen values of the operator $\hat{\boldsymbol{S}}\cdot\hat{\boldsymbol{n}}$ describing a spin-1/2 particle. [4 marks]

   (b) Construct the corresponding eigen vectors. [4 marks]

   (c) Show that the eigen vectors are orthonormal. [2 marks]

10. (a) *'Tilting' the floor of a box:* Consider a particle confined to a box with its walls located at $x = 0$ and $x = a$. Let the floor of the box be 'tilted' with the introduction of the following additional potential:

$$V_1(x) = V_0\,x/a,$$

   where V_0 is a constant. Calculate the shift in the energy levels of the particle due to this additional potential using first order perturbation theory. [5 marks]

   (b) *Perturbing the harmonic oscillator:* Consider the following perturbation to the standard potential of the harmonic oscillator:

$$V_1(x) = \lambda\,x^4.$$

   Evaluate the shift in the ground state of the oscillator due to such a perturbation using first order perturbation theory. [5 marks]

Supplementary end-of-semester exam

From the origins of quantum theory and the wave aspects of matter until charged particles in a uniform magnetic field

1. *Warming up with numbers:* Recall that the fine structure constant is defined as $\alpha = e^2/(4\,\pi\,\epsilon_0\,\hbar\,c)$.

   (a) Calculate the value of α^{-1} to the second decimal place. [2 marks]

   (b) Express the Rydberg constant in terms of the fine structure constant α and the mass $m_{\rm e}$ of the electron, and evaluate the quantity in electron volts. [2 marks]

   (c) If the energy associated with the fine structure of hydrogen is $\alpha^4\, m_{\rm e}\, c^2$, estimate the wavelength corresponding to these energies. [3 marks]

   (d) If the energy associated with the hyperfine structure of hydrogen is $(m_{\rm e}/m_{\rm p})\,\alpha^4\, m_{\rm e}\, c^2$, where $m_{\rm p}$ is the mass of the proton, estimate the wavelength corresponding to these transitions. [3 marks]

   Note: The mass and the charge of the electron are $m_{\rm e} = 9.109 \times 10^{-31}\,{\rm kg}$ and $e = 1.602 \times 10^{-19}\,{\rm C}$, respectively, the value of the Planck's constant is $h = 6.626 \times 10^{-34}\,{\rm J\,s}$, the speed of light is $c = 2.998 \times 10^8\,{\rm m/s}$, while $(4\,\pi\,\epsilon_0)^{-1} = 8.987 \times 10^9\,{\rm N\,m^2/C^2}$ and the mass of the proton is $m_{\rm p} = 1.675 \times 10^{-27}\,{\rm kg}$. Also, $1\,{\rm eV} = 1.602 \times 10^{-19}\,{\rm J}$.

2. *Bohr's quantization rule:* Consider a particle that is moving in the central potential $V(r) = V_0\,(r/a)^k$, where V_0, a and k are constants.

   (a) Using Bohr's quantization procedure, determine the energy levels of the system. [5 marks]
   Note: Assume, for simplicity, that the orbits are circular.

   (b) Show that, for large n, the frequency of a photon emitted in a transition from the level n to the level $(n-1)$ is the same as the rotational frequency. [5 marks]
   Note: This is a version of the quantum-classical correspondence.

3. *A simple superposition of energy eigen states:* A particle in the infinite square well is described by the following wavefunction at time $t = 0$:

$$\Psi(x, 0) = A \sin^3(\pi\, x/L),$$

   where L is the width of the well. Evaluate the expectation value $\langle x\rangle$ at a time $t > 0$. [10 marks]

4. *Scattering at a 'cliff':* The wavefunction corresponding to positive energy E and propagating from $x \to -\infty$ is scattered by the cliff-like potential

$$V(x) = \begin{cases} 0 & \text{for } x \le 0, \\ -V_0 & \text{for } x > 0. \end{cases}$$

   Determine the probability for the particle to be reflected back if $E = V_0/3$. [10 marks]

5. *More about oscillators:* Let $|0\rangle$ represent the ground state of a one dimensional quantum oscillator. Show that

$$\langle 0|e^{i\,k\,\hat{x}}|0\rangle = \exp -\left(k^2\,\langle 0|\hat{x}^2|0\rangle/2\right),$$

   where $\hat{x}$ is the position operator. [10 marks]

6. *Superposition of states of the hydrogen atom:* An electron in the Coulomb field of a proton is in the state described by the wave function

$$\psi(\boldsymbol{r}) = \frac{1}{6}\,\left[4\,\psi_{100}(\boldsymbol{r}) + 3\,\psi_{211}(\boldsymbol{r}) - \psi_{210}(\boldsymbol{r}) + \sqrt{10}\,\psi_{21-1}(\boldsymbol{r})\right].$$

(a) What is the expectation value of the energy of the electron in the state? 3 marks

(b) What is the expectation value of $\hat{\mathbf{L}}^2$? 4 marks

(c) What is the expectation value of $\hat{L}_z$? 3 marks

7. *Spherical harmonics:* Recall that, $\langle \theta, \phi | l, m \rangle = Y_l^m(\theta, \phi)$. Using the relations $\hat{L}_+ |l, l\rangle = 0$ and $\hat{L}_z |l, l\rangle = l\,\hbar |l, l\rangle$, determine the functional form of $Y_l^l(\theta, \phi)$. 10 marks

   Hint: Using the representations of $\hat{L}_+$ and $\hat{L}_z$ as differential operators, write the two relations above as differential equations and solve them.

   Note: You need not have to normalize the wavefunction.

8. *Mean values and uncertainties associated with spin operators:* An electron is in the spin state

$$\chi = A \begin{pmatrix} 3\,i \\ 4 \end{pmatrix}.$$

(a) Determine the normalization constant A. 2 marks

(b) Find the expectation values of the operators $\hat{S}_x$, $\hat{S}_y$ and $\hat{S}_z$ in the above state. 3 marks

(c) Evaluate the corresponding uncertainties, i.e. ΔS_x, ΔS_y and ΔS_z. 5 marks

9. *Transformation of the wavefunction:* Consider a charged particle moving in an electromagnetic background. Show that, under a gauge transformation of the form $\phi \to \phi + (1/c)\,(\partial\chi/\partial t)$ and $\boldsymbol{A} \to \boldsymbol{A} - \boldsymbol{\nabla}\,\chi$, where χ is an arbitrary function of space and time, the wavefunction describing the particle transforms as

$$\Psi(\boldsymbol{x}, t) \to \Psi(\boldsymbol{x}, t)\ \exp\ -\left[i\,q\,\chi(\boldsymbol{x}, t)/\hbar\right],$$

   with q being the charge associated with the particle. 10 marks

10. (a) *'Tilting' the floor of a box:* Consider a particle confined to a box with its walls located at $x = 0$ and $x = a$. Let the floor of the box be 'tilted' with the introduction of the following additional potential:

$$V_1(x) = V_0\, x/a,$$

   where V_0 is a constant. Calculate the shift in the energy levels of the particle due to this additional potential using first order perturbation theory. 5 marks

   (b) *Perturbing the harmonic oscillator:* Consider the following perturbation to the standard potential of the harmonic oscillator:

$$V_1(x) = \lambda\, x^4.$$

   Evaluate the shift in the ground state of the oscillator due to such a perturbation using first order perturbation theory. 5 marks