

EP2210
PRINCIPLES OF QUANTUM MECHANICS
July–November 2018

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 Monday, July 30, and the last lecture will be on Tuesday, November 13.
- We will meet thrice a week. The lectures are scheduled for 11:00–11:50 AM on Mondays, 10:00–10:50 AM on Tuesdays, and 9:00–9:50 AM on Wednesdays.
- We may also meet during 1:00–1:50 PM on Thursdays for either the quizzes or to make up for lectures 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 (in HSB 202) during 5:00–5:30 PM on Mondays. 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 at the start of the course. They will also be available on the course's page on Moodle at the following URL:
<https://courses.iitm.ac.in/>
- The exercise sheets and other additional material will be made available on Moodle.
- 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 this file and the course's page on Moodle 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 held on August 30, September 27 and October 25. The three dates are Thursdays, and the quizzes will be held during 4:30–6:00 PM on these days.
 - The end-of-semester exam will be held during 9:00 AM–12:00 NOON on Monday, November 19, and the exam will carry 50% weight.
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Syllabus and structure

Principles of Quantum Mechanics

1. Essential classical mechanics [~ 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

Additional exercises I

2. Origins of quantum theory and the wave aspects of matter [~ 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 [~ 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 [~ 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 II

Quiz II

5. Essential mathematical formalism [~ 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, 7 and 8

6. The Schrodinger equation in three dimensions and particle in a central potential [~ 4 lectures]

- (a) The Schrodinger equation in three dimensions
- (b) Particle in a three-dimensional box – The harmonic oscillator in three-dimensions
- (c) Motion in a central potential – Orbital angular momentum
- (d) Hydrogen atom – Energy levels
- (e) Degeneracy

Exercise sheet 9

Additional exercises III

Quiz III

7. Angular momentum and spin [~ 4 lectures]

- (a) Angular momentum – Eigen values and eigen functions
- (b) Electron spin – Pauli matrices
- (c) Application to magnetic resonance

Exercise sheet 10

8. Time-independent perturbation theory [~ 4 lectures]

- (a) The non-degenerate case
- (b) Fine structure of hydrogen – Hyperfine structure

Exercise sheet 11

9. Charged particle in a uniform and constant magnetic field [~ 2 lectures]

- (a) Landau levels – Wavefunctions
- (b) Elements of the quantum Hall effect

Exercise sheet 12

End-of-semester exam

Advanced problems

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. W. Robinett, *Quantum Mechanics*, Second Edition (Oxford University Press, Oxford, 2006).
 7. R. Shankar, *Principles of Quantum Mechanics*, Second Edition (Springer, Delhi, 2008).
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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).
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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.
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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

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

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

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

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,

$$\nabla(\mathbf{C} \cdot \mathbf{D}) = (\mathbf{D} \cdot \nabla) \mathbf{C} + (\mathbf{C} \cdot \nabla) \mathbf{D} + \mathbf{D} \times (\nabla \times \mathbf{C}) + \mathbf{C} \times (\nabla \times \mathbf{D}).$$

Also, since \mathbf{A} depends on time as well as space, we have,

$$\frac{d\mathbf{A}}{dt} = \frac{\partial \mathbf{A}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{A}.$$

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 $\rho = \text{constant}$. 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:

$$\delta_{ij} = \begin{cases} 1 & \text{when } i = j, \\ 0 & \text{when } i \neq j. \end{cases}$$

Additional exercises I

Essential classical mechanics

1. Geodesics on a cone: Consider a cone with a semi-vertical angle α .
 - (a) Determine the line element on the cone.
 - (b) Obtain the equations governing the geodesics on the cone.
 - (c) Solve the equations to arrive at the geodesics.
2. Action for a free particle: Given that a free particle that is moving in three dimensions was located at the position \mathbf{r}_1 at time t_1 and at the position \mathbf{r}_2 at time t_2 , determine the action for the free particle in terms of \mathbf{r}_1 , \mathbf{r}_2 , t_1 and t_2 .

Note: Make use of the solution known in the case of the free particle in the integral describing the action.

3. Motion in one dimension: Obtain the solutions describing the time evolution of a particle moving in the one-dimensional potential

$$U(x) = \alpha \left(e^{-2\beta x} - 2e^{-\beta x} \right), \quad \text{where } \alpha, \beta > 0,$$

for the cases $E < 0$, $E = 0$ and $E > 0$, where E is the energy of the particle. Also, evaluate the period of oscillation of the particle when $E < 0$.

4. The Laplace-Runge-Lenz vector: Recall that, for a particle with s degrees of freedom, we require $2s - 1$ constants of motion in order to arrive at a unique trajectory for the particle. According to this argument, for the Kepler problem, we would then need five integrals of motion to obtain the solution. We had expressed the solution in terms of the energy E of the system and the amplitude of the angular momentum vector \mathbf{M} , both of which were conserved. However, these quantities, viz. the energy E and the three components of the angular momentum vector \mathbf{M} , only add up to four constants of motion! Evidently, it will be interesting to examine if we can identify the fifth integral of motion associated with the system.

- (a) Show that, for a particle moving in the Keplerian central potential, i.e. $U(r) = -\alpha/r$ with $\alpha > 0$, the following vector is an integral of motion:

$$\mathbf{A} = m \mathbf{v} \times \mathbf{M} - \frac{m \alpha \mathbf{r}}{r}.$$

Note: The conserved vector \mathbf{A} is known as the Laplace-Runge-Lenz vector.

- (b) Show that the vector \mathbf{A} lies in the plane of the orbit.
- (c) Indicate the amplitude and the direction of \mathbf{A} associated with a planet as it moves in an elliptical orbit around the Sun.

Hint: Determine the amplitude and the direction of \mathbf{A} at, say, the perihelion and the aphelion.

- (d) If E , \mathbf{M} and \mathbf{A} are all constants, then, we seem to have seven integrals of motion instead of the required five to arrive at a unique solution! How does seven reduce to five?

Hint: Examine if there exist any relations between \mathbf{A} and \mathbf{M} and/or E .

5. Phase portraits: Draw the phase portraits of a particle moving in the following one dimensional potentials: (a) $U(x) = \alpha |x|^n$, (b) $U(x) = \alpha x^2 - \beta x^3$, (c) $U(x) = \alpha (x^2 - \beta^2)^2$, and (d) $U(\theta) = -\alpha \cos \theta$, where $(\alpha, \beta) > 0$ and $n > 2$.
6. Hamiltonian of a free particle: Show that the Hamiltonian of a free particle can be written as

$$H = \frac{p_r^2}{2m} + \frac{L^2}{2m r^2},$$

where p_r is the momentum conjugate to the radial coordinate r and $\mathbf{L} = \mathbf{r} \times \mathbf{p}$.

7. Angular momentum of a free particle: Show that the angular momentum of a free particle can be written as

$$L^2 = L_x^2 + L_y^2 + L_z^2 = p_\theta^2 + \frac{p_\phi^2}{\sin^2\theta}.$$

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 $\nu + d\nu$ associated with the electromagnetic radiation emitted by the black body is given by

$$u_\nu d\nu = \frac{8\pi h}{c^3} \frac{\nu^3 d\nu}{\exp(h\nu/k_B T) - 1},$$

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 $\lambda_{\max} T = b = \text{constant}$, 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

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

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

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

Given that the value of the speed of light is $c = 2.998 \times 10^8 \text{ m s}^{-1}$, 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 $109677.58 \text{ cm}^{-1}$. 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

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

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

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

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

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

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

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

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

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

4. Ehrenfest's theorem: Show that

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

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

$$\langle \Psi_2 | \Psi_1 \rangle \equiv \int dx \Psi_2^*(x, t) \Psi_1(x, t),$$

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

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

Quiz I

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

1. Phase portrait of a system: Consider a particle moving in the one-dimensional potential

$$U(x) = \alpha \left(e^{-2\beta x} - 2e^{-\beta x} \right),$$

where $(\alpha, \beta) > 0$.

- (a) Sketch the potential indicating, in particular, the locations of the extrema and the corresponding values of the potential. 3 marks
- (b) Draw the phase portrait of the system, specifically indicating with arrows the direction of motion of the particle in phase space. 7 marks

2. Poisson brackets for angular momentum: Recall that the Poisson bracket $\{A, B\}$ between two observables $A(q_i, p_i)$ and $B(q_i, p_i)$ is defined as

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

where q_i and p_i denote the generalized coordinates and the corresponding conjugate momenta, respectively, while N denotes the number of degrees of freedom of the system. Let (L_x, L_y, L_z) be the Cartesian components of the angular momentum vector \mathbf{L} , and let $L^2 = L_x^2 + L_y^2 + L_z^2$. Evaluate the following Poisson brackets:

- (a) $\{L_x, L_y\}$, $\{L_y, L_z\}$ and $\{L_z, L_x\}$, 5 marks
- (b) $\{L_x, L^2\}$, $\{L_y, L^2\}$ and $\{L_z, L^2\}$. 5 marks

Hint: For the second set of Poisson brackets, it may be useful to establish and use the result $\{A, BC\} = \{A, B\}C + B\{A, C\}$.

3. Particle in a box I: At time $t = 0$, a particle of mass m that is confined to a box with its walls at $x = 0$ and $x = a$ is equally likely to be found over the domain $0 < x < a/2$.

- (a) What is the initial wave function of the system, i.e. $\Psi(x, 0)$? 3 marks
Hint: Assume that the wave function is real, and make sure you normalize the wave function.
- (b) What is the probability that a measurement of the energy of the particle would yield the value $E_1 = \pi^2 \hbar^2 / (2m a^2)$? 7 marks

4. Particle in a box II: At time $t = 0$, the wave function of a particle that is confined to a box with its walls at $x = 0$ and $x = a$ is given by

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

where ψ_1 and ψ_2 are the ground state and the first excited state of the system.

- (a) Determine the constant A assuming that $\Psi(x, 0)$ is normalized. 1 marks
- (b) What is $\Psi(x, t)$ for $t > 0$? 2 marks
- (c) Determine the expectation values $\langle \hat{x} \rangle$ and $\langle \hat{p}_x \rangle$ in the state $\Psi(x, t)$. Express the results in terms of the angular frequency $\omega = \pi^2 \hbar / (2m a^2)$. 4 marks
- (d) What are probabilities of the system to be found in the ground and the first excited states? What is the expectation value of the Hamiltonian, i.e. $\langle \hat{H} \rangle$, in the state $\Psi(x, t)$? 3 marks

5. *Particle on a circle:* A particle which is otherwise free, is confined to move on a circle of radius R .

(a) Construct the Hamiltonian describing the system. 3 marks

(b) Write down the Schrodinger equation and obtain the energy eigen functions and energy eigen values. 4 marks

Note: The wave function should always have a unique value at any point on the circle. This condition will help you determine the energy eigen values.

(c) Are the energy levels continuous or discrete? Obtain the normalized the wave functions. 3 marks

Exercise sheet 4

The time-independent Schrodinger equation in one dimension

1. Probability of finding an energy eigen value: A particle in a box with its walls at $x = 0$ and $x = a$ is described by the following wave function:

$$\psi(x) = \begin{cases} A (x/a) & \text{for } 0 < x < a/2, \\ A [1 - (x/a)] & \text{for } a/2 < x < a, \end{cases}$$

where A is a real constant. If the energy of the system is measured, what is the probability for finding the energy eigen value to be $E_n = n^2 \pi^2 \hbar^2 / (2 m a^2)$?

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

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

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

- Normalize $\Psi(x, 0)$.
 - Find $\Psi(x, t)$.
 - Plot $\Psi(x, t)$ at $t = 0$ and for large t . Determine qualitatively what happens as time goes on?
 - Find $\langle \hat{x} \rangle$, $\langle \hat{x}^2 \rangle$, $\langle \hat{p} \rangle$, $\langle \hat{p}^2 \rangle$, Δx and Δp .
 - 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 $a > 0$.

- Determine the bound state energy eigen functions.
 - Plot the energy eigen functions.
 - 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 smoothed step that is described by the potential

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

and determine the reflection and the transmission probabilities.

The potential step

Consider the potential

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

where $V_0 > 0$.

For $E < V_0$, over the domain $-\infty < x < 0$, the wavefunction is given by

$$\psi(x) = e^{ikx} + R e^{-ikx},$$

where $k = \sqrt{2mE}/\hbar$, while over $0 < x < \infty$, we have

$$\psi(x) = T e^{-qx},$$

where $q = \sqrt{2m(V_0 - E)}/\hbar$. Matching the wavefunction and its derivative at $x = 0$, we obtain that

$$1 + R = T, \quad ik(1 - R) = -qT,$$

which can be solved to arrive at

$$T = \frac{2k}{k + iq}, \quad R = \frac{k - iq}{k + iq}.$$

Note that $|R|^2 = 1$.

When $E > V_0$, over the domain $-\infty < x < 0$, the wavefunction is again given by

$$\psi(x) = e^{ikx} + R e^{-ikx},$$

with $k = \sqrt{2mE}/\hbar$, whereas over $0 < x < \infty$, we have

$$\psi(x) = T e^{iqx},$$

with $q = \sqrt{2m(E - V_0)}/\hbar$. On matching the wavefunction and its derivative at $x = 0$, we obtain that

$$1 + R = T, \quad ik(1 - R) = iqT.$$

These relations can be easily solved to obtain that

$$T = \frac{2k}{k + q}, \quad R = \frac{k - q}{k + q}.$$

Moreover, it is straightforward to establish that

$$|R|^2 + \frac{q}{k} |T|^2 = 1.$$

The potential barrier

Consider the potential

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

where $V_0 > 0$.

Let us focus on the case wherein $E < V_0$. For $-\infty < x < -a$, the wavefunction is given by

$$\psi(x) = e^{ikx} + R e^{-ikx},$$

where $k = \sqrt{2mE}/\hbar$. Similarly, over $a < x < \infty$, we can write

$$\psi(x) = T e^{ikx},$$

Over the domain $-a < x < a$, we can write

$$\psi(x) = A e^{qx} + B e^{-qx},$$

where $q = \sqrt{2m(V_0 - E)}/\hbar$. Matching the wavefunction and its derivative at $x = -a$, we obtain that

$$\begin{aligned} e^{-ika} + R e^{ika} &= A e^{-qa} + B e^{qa}, \\ ik (e^{-ika} - R e^{ika}) &= q (A e^{-qa} - B e^{qa}). \end{aligned}$$

We can use these two equations to eliminate R and arrive at the following relation between A and B

$$B = \frac{-2ik}{q-ik} e^{(q+ik)a} + A \frac{q+ik}{q-ik} e^{-2qa}.$$

Similarly, at $x = a$, the matching conditions lead to the relations

$$\begin{aligned} A e^{qa} + B e^{-qa} &= T e^{ika}, \\ q (A e^{qa} - B e^{-qa}) &= ik T e^{ika}. \end{aligned}$$

On eliminating T from these two relations, we obtain that

$$A = B \frac{q+ik}{q-ik} e^{-2qa}.$$

The two equations relations between A and B can be used to determine B to be

$$B = -\frac{-2ik(q-ik)e^{-(q+ik)a}}{(q-ik)^2 - (q+ik)^2 e^{-4qa}}.$$

From the second set of relations, we can then obtain T to be

$$T = \frac{2kq e^{-2ika}}{2kq \cosh(2qa) - i(k^2 - q^2) \sinh(2qa)}$$

leading to

$$|T|^2 = \frac{(2kq)^2}{(2kq)^2 + (k^2 + q^2)^2 \sinh^2(2qa)},$$

which, for $(qa) \gg 1$, can be approximated to be

$$|T|^2 \simeq \frac{(4kq)^2}{(k^2 + q^2)^2} e^{-4qa}.$$

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

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

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

(b) Utilize the following recursion relation:

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

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:

$$\frac{dH_n}{dx} = 2n H_{n-1}(x).$$

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

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

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 n th 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 $x \leq 0$.

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

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_E}{dx^2} + \frac{1}{2} m \omega^2 x^2 \psi_E = E \psi_E.$$

In terms of the dimensionless variable

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

the above time-independent Schrodinger equation reduces to

$$\frac{d^2\psi_E}{d\xi^2} + (\mathcal{E} - \xi^2) \psi_E = 0,$$

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

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

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 II

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

1. Semi-classical quantization procedure: Consider a particle moving in one spatial 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. Why does the semi-classical result exactly match the result from the complete quantum theory?

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 $E = L^2/(2I)$, 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

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

- (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. Quantum revival: Consider an arbitrary wavefunction describing a particle in the infinite square well.
- (a) Show that the wave function will return to its original form after a time $T_Q = 4 m a^2 / (\pi \hbar)$.
 Note: The time T_Q is known as the *quantum revival time*.
 (b) Determine the classical revival time T_C for a particle of energy E bouncing back and forth between the walls.
 (c) What is the energy for which $T_Q = T_C$?

5. Absence of degenerate bound states in one spatial dimension: Two or more quantum states are said to be degenerate if they are described by distinct solutions to the time-independent Schrodinger equation corresponding to the *same* energy. For example, the free particle states are doubly degenerate—one solution describes motion to the right and the other motion to the left. It is

not an accident that we have not encountered normalizable degenerate solutions in one spatial dimension. By following the steps listed below, prove that there are no degenerate bound states in one spatial dimension.

- (a) Suppose that there are two solutions, say, ψ_1 and ψ_2 , with the same energy E . Multiply the Schrodinger equation for ψ_1 by ψ_2 and the equation for ψ_2 by ψ_1 , and show that the quantity

$$\mathcal{W} = \psi_1 \frac{d\psi_2}{dx} - \psi_2 \frac{d\psi_1}{dx}$$

is a constant.

- (b) Use further the fact that, since the wavefunctions ψ_1 and ψ_2 are normalizable, the quantity \mathcal{W} defined above must vanish.
- (c) If $\mathcal{W} = 0$, integrate the above equation to show that ψ_2 is a multiple of ψ_1 and hence the solutions are not distinct.

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

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

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

- (d) Argue that the odd eigen states are ‘less bound’ than 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

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

which leads to

$$(e^{iqx_0})^N = 1$$

or, equivalently, $q = 2\pi n/(Nx_0)$, where $n = 0, 1, 2, \dots, N$. For large N , q ranges almost continuously between 0 and 2π .

- (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

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

where $\kappa = \sqrt{-2mE}/\hbar$ and $z = \cos(qx_0)$.

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

$$z = \cos(kx_0) - \frac{ma}{\hbar^2 k} \sin(kx_0),$$

where $k = \sqrt{2mE}/\hbar$.

- (c) Argue that, for $2ma x_0/\hbar^2 \gg 1$, 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

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

- (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:

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

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

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

- (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

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

where

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

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. Tunneling probability: An electron with energy 1.0 eV is incident on a rectangular potential barrier of height 1.5 eV and thickness 5 Å. Estimate the probability for the electron to tunnel through the barrier. 10 marks

Note: The mass of an electron is 9.11×10^{-31} kg, the value of the Planck's constant is $h = 6.626 \times 10^{-34}$ J s, and $1 \text{ eV} = 1.602 \times 10^{-19}$ J.

2. Time derivative of an expectation value: Show that, in one dimension, 10 marks

$$m \frac{d\langle \hat{x}^2 \rangle}{dt} = \langle \hat{x} \hat{p}_x \rangle + \langle \hat{p}_x \hat{x} \rangle,$$

where, as usual, the angular brackets denote expectation values.

3. Energy from the wavefunction: Consider a particle moving in the potential

$$V(x) = \frac{\hbar^2}{2m} \left(\frac{4}{225} \sinh^2 x - \frac{2}{5} \cosh x \right).$$

- (a) Sketch the potential $V(x)$, roughly indicating the locations of the two minima. 3 marks

- (b) Does the wavefunction

$$\psi(x) = (1 + 4 \cosh x) \exp -[(2/15) \cosh x],$$

correspond to an energy eigen state of the system? If it does, determine the corresponding energy eigen value, and indicate it in the plot of $V(x)$. 3 marks

- (c) Plot the wavefunction above the potential $V(x)$, specifically illustrating the behavior of the wavefunction in the classically forbidden regions. 4 marks

4. Constructing the energy eigen states of the harmonic oscillator: If $\psi_n(x)$ denotes the n -th energy eigen state of the harmonic oscillator and \hat{a} represents the lowering operator, then, recall that

$$\hat{a} \psi_n(x) = \sqrt{n} \psi_{n-1}(x).$$

- (a) Using the fact that $\hat{a} \psi_0(x) = 0$, construct the ground state wave function $\psi_0(x)$, ensuring that it is normalized. 5 marks

- (b) Also, recall that

$$\hat{a}^\dagger \psi_n(x) = \sqrt{n+1} \psi_{n+1}(x),$$

where \hat{a}^\dagger is the raising operator. Operate the raising operator on $\psi_0(x)$ successively to construct the wavefunctions describing the first and the second excited states, i.e. $\psi_1(x)$ and $\psi_2(x)$. 5 marks

5. Oscillating charge in an electric field: Let a particle of mass m and charge q be oscillating in the simple harmonic potential $V(x) = m\omega^2 x^2/2$. A constant electric field of strength \mathcal{E} is turned on along the positive x -direction.

- (a) What is the complete potential influencing the charge in the presence of the electric field? 1 marks

- (b) Draw the classical trajectory of the charge in phase space when the electric field has been turned on. How does it compare with the original trajectory? 2 marks

- (c) What are the energy eigen values of the system when it is quantized? 3 marks

- (d) Plot the ground state wave function of the system with and without the electric field. 4 marks

Quiz II again

The time-independent Schrodinger equation in one dimension

1. Wavefunctions in a finite square well: Consider a particle in the following finite square well potential:

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

where $V_0 > 0$. Illustrate the behavior of the wavefunctions corresponding to the ground and the first two excited states of the particle. 2+4+4 marks

2. The twin Dirac delta function potential: Consider the following *attractive* potential involving two Dirac delta functions:

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

where $\alpha = \hbar^2/(ma) > 0$.

- (a) For a bound state with $E < 0$, write down the wavefunctions in the three domains, i.e. over $-\infty < x < -a$, $-a < x < a$ and $a < x < \infty$. 2 marks
- (b) Match the wavefunctions and their derivatives suitably to arrive at the relations between the coefficients in the three domains. 3 marks
- (c) Construct the two possible bound state wavefunctions. Highlight their behavior as $x \rightarrow -x$ in the domain $-a < x < a$. 5 marks
3. 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

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

where the expectation values are evaluated in a *stationary* 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

$$\int_{-\infty}^{\infty} dx \psi x \frac{dV}{dx} \psi = -\langle \hat{V} \rangle - 2 \int_{-\infty}^{\infty} dx \frac{d\psi}{dx} x V \psi$$

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

$$-2 \int_{-\infty}^{\infty} dx \frac{d\psi}{dx} x V \psi = E + \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} dx \left(\frac{d\psi}{dx} \right)^2.$$

4. More about oscillators: Let $|0\rangle$ represent the ground state of a one dimensional quantum oscillator. Show that 10 marks

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

where \hat{x} is the position operator.

5. A time-dependent solution to the simple harmonic oscillator: Consider the following wave function:

$$\psi(x, t) = \left(\frac{m\omega}{\pi\hbar} \right)^{1/2} \exp - (m\omega/2\hbar) \left[x^2 + (a^2/2) (1 + e^{-2i\omega t}) + (i\hbar t/m) - 2ax e^{-i\omega t} \right],$$

where a is a real constant with dimensions of length.

- (a) Examine if this wave function satisfies the *time-dependent* Schrodinger equation for the simple harmonic oscillator with mass m and frequency ω . 3 marks
- (b) Evaluate $|\psi(x, t)|^2$, and describe the evolution of the wave packet. 3 marks
- (c) Compute $\langle \hat{x} \rangle$ and $\langle \hat{p}_x \rangle$ in the above state, and examine if the Ehrenfest's theorem, viz.

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

is satisfied.

4 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

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

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 $p_0 = ma/\hbar$?
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:

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

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

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

(c) Defining

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

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:

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

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

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

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 α ?

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

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

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

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

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

Essential mathematical formalism III

1. Expectation values in momentum space: Given a wave function, say, $\Psi(x, t)$, in the position space, the corresponding wave function in momentum space is given by

$$\Phi(p, t) = \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi\hbar}} \Psi(x, t) e^{-ipx/\hbar}.$$

- (a) Show that, if the wavefunction $\Psi(x, t)$ is normalized in position space, it is normalized in momentum space as well, i.e.

$$\int_{-\infty}^{\infty} dx |\Psi(x, t)|^2 = \int_{-\infty}^{\infty} dp |\Phi(p, t)|^2 = 1.$$

- (b) Recall that, in the position representation, the expectation value of the momentum operator can be expressed as follows:

$$\langle \hat{p} \rangle = -i\hbar \int_{-\infty}^{\infty} dx \Psi^*(x, t) \frac{\partial \Psi(x, t)}{\partial x}.$$

Show that, in momentum space, it can be expressed as

$$\langle \hat{p} \rangle = \int_{-\infty}^{\infty} dp p |\Phi(p, t)|^2.$$

- (c) Similarly, show that the following expectation value of the position operator in position space

$$\langle \hat{x} \rangle = \int_{-\infty}^{\infty} dx x |\Psi(x, t)|^2,$$

can be written as

$$\langle \hat{x} \rangle = i\hbar \int_{-\infty}^{\infty} dp \Phi^*(p, t) \frac{\partial \Phi(p, t)}{\partial p}.$$

2. The Schrodinger equation in momentum space: Assuming that the potential $V(x)$ can be expanded in a Taylor series, show that the time-dependent Schrodinger equation in momentum space can be written as

$$\frac{p^2}{2m} \Phi(p, t) + V \left(i\hbar \frac{\partial}{\partial p} \right) \Phi(p, t) = i\hbar \frac{\partial \Phi(p, t)}{\partial t}.$$

3. Uniformly accelerating particle: A simple system wherein it turns out to be easier to solve the Schrodinger equation in momentum space is the case of a particle that is exerted by a constant force, say, F , so that $V(x) = -Fx$. Classically, this corresponds to a uniformly accelerating particle.

- (a) Show that, in such a case, the momentum space wavefunction can be written as

$$\Phi(p, t) = \Phi_0(p - Ft) e^{-ip^3/(6mF\hbar)}.$$

where $\Phi_0(p - Ft)$ is an arbitrary function.

- (b) Since $\Phi_0(p - Ft)$ is arbitrary, argue that we can write the above wave function as

$$\Phi(p, t) = \phi_0(p - Ft) e^{-i[(p-Ft)^3 - p^3]/(6mF\hbar)},$$

where $\phi_0(p)$ is the momentum space amplitude at $t = 0$, i.e. $\phi_0(p, t = 0) = \phi_0(p)$.

- (c) Note that the expectation value of the operator \hat{p} at $t = 0$, say, $\langle \hat{p} \rangle_0$, is determined by the initial momentum space amplitude $\phi_0(p)$. Show that, for $t > 0$, the expectation value $\langle \hat{p} \rangle$ is given by

$$\langle \hat{p} \rangle = \langle \hat{p} \rangle_0 + F t,$$

which is the same as the corresponding classical result.

4. Commutator in momentum space: Working in the momentum space representation, establish that $[\hat{x}, \hat{p}] = i \hbar$.
5. Feynman-Kac formula: Given that a quantum mechanical particle is at the location x at time t , show that the probability amplitude for finding the particle at the location x' at a *later* time t' can be expressed as

$$K(x', t' | x, t) = \langle x', t' | x, t \rangle = \sum_{\text{all } n} \psi_n(x') \psi_n^*(x) e^{-i E_n (t' - t) / \hbar},$$

where $\psi_n(x)$ denote the energy eigen states corresponding to the energy eigen values E_n and the sum over n represents either the sum or a suitable integral in the case of a continuum of states over all the energy eigen values. Evaluate the quantity $\langle x', t' | x, t \rangle$ for the case of a free particle.

Note: The above expression for the probability amplitude is known as the Feynman-Kac formula. The probability amplitude $\langle x', t' | x, t \rangle$ can be given a so-called path integral interpretation, i.e. it can be expressed as a sum over all paths with the probability amplitude for each path given the same weightage, being proportional to $\exp \{i S[x(t)] / \hbar\}$, with $S[x(t)]$ denoting the corresponding classical action.

Exercise sheet 9

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

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

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

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

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

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

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 10

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.

$$r_c = \frac{e^2}{4\pi\epsilon_0 m_e c^2}$$

where e and m_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

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

- (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 $\hat{\mathbf{S}} = \hat{S}_x \hat{i} + \hat{S}_y \hat{j} + \hat{S}_z \hat{k}$ 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 $\omega = \gamma B$.

Additional exercises III

From essential mathematical formalism to angular momentum and spin

1. Sequential measurements: An operator \hat{A} , representing the observable A , has two normalized eigenstates 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:

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

- (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

$$\begin{aligned} \hat{S}_x &= \frac{\hbar}{2} (|+\rangle\langle-| + |-\rangle\langle+|), \\ \hat{S}_y &= \frac{i\hbar}{2} (-|+\rangle\langle-| + |-\rangle\langle+|), \\ \hat{S}_z &= \frac{\hbar}{2} (|+\rangle\langle+| - |-\rangle\langle-|). \end{aligned}$$

- (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 n th 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

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

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) $[f(\hat{x}), \hat{p}_x] = i\hbar (df(\hat{x})/d\hat{x})$,

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

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

- (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

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

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

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

- (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 $I_1 \neq I_2$?

Quiz III

Essential mathematical formalism

1. Time derivatives of expectation values:

5+5 marks

(a) If \hat{A} and \hat{B} are arbitrary, time-dependent operators, show that

$$\frac{d\langle\hat{A}\hat{B}\rangle}{dt} = \left\langle \frac{\partial\hat{A}}{\partial t} \hat{B} \right\rangle + \left\langle \hat{A} \frac{\partial\hat{B}}{\partial t} \right\rangle + \frac{i}{\hbar} \langle [\hat{H}, \hat{A}] \hat{B} \rangle + \frac{i}{\hbar} \langle \hat{A} [\hat{H}, \hat{B}] \rangle.$$

(b) Show that, in the case of an operator, say, \hat{A} , that is *not* explicitly dependent on time,

$$\frac{d^2\langle\hat{A}\rangle}{dt^2} = -\frac{1}{\hbar^2} \langle [\hat{H}, [\hat{H}, \hat{A}]] \rangle.$$

2. Wave function describing the coherent state: Earlier, that we had arrived at the wave function $\psi_0(x) = \langle x|0\rangle$ describing the ground state of the oscillator using the following definition of the ground state $|0\rangle$:

$$\hat{a}|0\rangle = 0$$

and the position representation of the lowering operator \hat{a} . Recall that the coherent state $|\alpha\rangle$ is defined through the relation

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

where α is a complex quantity.(a) How is the state $|\alpha(t)\rangle$ at a later time described?

2 marks

(b) Evaluate $\langle\hat{x}(t)\rangle$ and $\langle\hat{p}_x(t)\rangle$ in the state $|\alpha(t)\rangle$.

2 marks

(c) Using the above definition of $|\alpha\rangle$, obtain the wave function $\Psi_\alpha(x, t) = \langle x|\alpha(t)\rangle$. Express the wavefunction $\Psi_\alpha(x, t)$ in terms of $\langle\hat{x}(t)\rangle$ and $\langle\hat{p}_x(t)\rangle$.

6 marks

3. The number-phase uncertainty relation: The lowering and raising operators \hat{a} and \hat{a}^\dagger can be represented in the following polar form:

$$\hat{a} = \sqrt{\hat{N} + 1} e^{i\hat{\phi}}, \quad \hat{a}^\dagger = e^{-i\hat{\phi}} \sqrt{\hat{N} + 1},$$

where the operators \hat{N} and $\hat{\phi}$ are hermitian.(a) Using the commutation relation between the operators \hat{a} and \hat{a}^\dagger , evaluate the following commutators:

8 marks

- i. $[e^{i\hat{\phi}}, \hat{N}]$,
- ii. $[e^{-i\hat{\phi}}, \hat{N}]$,
- iii. $[\cos \hat{\phi}, \hat{N}]$,
- iv. $[\sin \hat{\phi}, \hat{N}]$.

(b) What is $(\Delta N)^2 (\Delta \sin \phi)^2$ in a general state?

2 marks

4. 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

$$\begin{aligned} \hat{S}_x &= \frac{\hbar}{2} (|+\rangle\langle-| + |-\rangle\langle+|), \\ \hat{S}_y &= \frac{i\hbar}{2} (-|+\rangle\langle-| + |-\rangle\langle+|), \\ \hat{S}_z &= \frac{\hbar}{2} (|+\rangle\langle+| - |-\rangle\langle-|). \end{aligned}$$

- (a) Construct the matrices corresponding to the three operators \hat{S}_x , \hat{S}_y and \hat{S}_z in the basis $|+\rangle$ and $|-\rangle$. 2 marks
- (b) Evaluate the commutators $[\hat{S}_x, \hat{S}_y]$, $[\hat{S}_y, \hat{S}_z]$ and $[\hat{S}_z, \hat{S}_x]$ and express the results in terms of the operators \hat{S}_x , \hat{S}_y or \hat{S}_z ? 4 marks
- (c) Let $\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$. Evaluate the commutators $[\hat{S}_z, \hat{S}_\pm]$ and express them in terms of the original operators \hat{S}_x , \hat{S}_y and \hat{S}_z . 4 marks

5. Orthogonality and completeness of coherent states:

- (a) Let $|\alpha\rangle$ and $|\beta\rangle$ describe two normalized coherent states. If $\alpha \neq \beta$, are $|\alpha\rangle$ and $|\beta\rangle$ orthogonal? 3 marks
- (b) Do the coherent states $|\alpha\rangle$ form a complete basis? 7 marks

Hints: To begin with, note that α is a complex quantity. Therefore, if we write $\alpha = \alpha_R + i\alpha_I$, then the completeness relation can be expressed as

$$\frac{1}{\pi} \int_{-\infty}^{\infty} d\alpha_R \int_{-\infty}^{\infty} d\alpha_I |\alpha\rangle\langle\alpha| = \hat{\mathcal{I}},$$

where $\hat{\mathcal{I}}$ is the identity operator. The integral can be carried out easily if you convert the integral over the α_R - α_I plane into a radial and angular integral. Also, note that

$$\int_0^{\infty} dx e^{-x} x^n = n!.$$

Exercise sheet 11

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 $a_0 = 4\pi\epsilon_0 \hbar^2 / (m_e e^2)$ is the Bohr radius, with m_e denoting the mass of the electron, e the electronic charge, and ϵ_0 the permittivity of free space.

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

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

Given that $\hat{\mathbf{S}}_p$ and $\hat{\mathbf{S}}_e$ denote the spin of the proton and the electron, use the above result to demonstrate that

$$\left\langle \frac{3 (\hat{\mathbf{S}}_p \cdot \hat{r}) (\hat{\mathbf{S}}_e \cdot \hat{r}) - \hat{\mathbf{S}}_p \cdot \hat{\mathbf{S}}_e}{r^3} \right\rangle = 0,$$

in states wherein $l = 0$.

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

$$E_{\text{hf}}^1 = \frac{\mu_0 g_p e^2}{8\pi m_p m_e} \left\langle \frac{3 (\hat{\mathbf{S}}_p \cdot \hat{r}) (\hat{\mathbf{S}}_e \cdot \hat{r}) - (\hat{\mathbf{S}}_p \cdot \hat{\mathbf{S}}_e)}{r^3} \right\rangle + \frac{\mu_0 g_p e^2}{3 m_p m_e} \langle \hat{\mathbf{S}}_p \cdot \hat{\mathbf{S}}_e \rangle |\psi(0)|^2,$$

where m_p denotes the mass of the proton, $g_p = 5.58$ 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:

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

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

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

- (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 12

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

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

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

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

- (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: $\mathbf{B} = B \hat{z}$. 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 $V(\mathbf{x})$. Show that, if $V(\mathbf{x}) \rightarrow V(\mathbf{x}) + V_0(t)$, the wavefunction describing the particle transforms as

$$\Psi(\mathbf{x}, t) \rightarrow \Psi(\mathbf{x}, t) \exp -\frac{i}{\hbar} \int^t dt' V_0(t').$$

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

$$\Psi(\mathbf{x}, t) \rightarrow \Psi(\mathbf{x}, t) \exp - [i q \chi(\mathbf{x}, t)/\hbar],$$

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. Angular momentum and Hamiltonian of a free particle: Consider a free particle in three dimensions.

- (a) Express the Lagrangian of the free particle in terms of the spherical polar coordinates (r, θ, ϕ) . 2 marks
- (b) What are the conjugate momenta p_r , p_θ and p_ϕ ? Express the corresponding Hamiltonian H in terms of the conjugate momenta. 3 marks
- (c) If $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ is the angular momentum of the particle, show that 3 marks

$$L^2 = p_\theta^2 + \frac{p_\phi^2}{\sin^2 \theta}.$$

Hint: Recall that the Hamiltonian of the free particle is given by $H = p^2/(2m) = \mathbf{p} \cdot \mathbf{p}/(2m)$. Use this relation to construct p^2 in terms of p_r , p_θ and p_ϕ . Then, utilize the fact that $L^2 = (\mathbf{r} \times \mathbf{p})^2 = r^2 p^2 - (\mathbf{r} \cdot \mathbf{p})^2 = r^2 (p^2 - p_r^2)$.

- (d) Show that the Hamiltonian of the free particle can then be expressed as 2 marks

$$H = \frac{p_r^2}{2m} + \frac{L^2}{2m r^2}.$$

2. Particle in a box: Consider a particle in a one-dimensional box of width 1 mm.

- (a) Roughly, what value of n corresponds to a state with energy $E = 10^{-2}$ eV? 6 marks
- (b) The density of states $g(E)$ of a system is defined as $g(E) = dn/dE$. Show that, for the system, $g(E) = n/(2E)$. What is the number of states within an interval of 10^{-4} eV about the energy 10^{-2} eV? 4 marks

3. Repulsive Dirac delta function potential: Consider a particle moving in the following repulsive Dirac function potential:

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

where $a > 0$. Calculate the reflection and transmission coefficients for the system. 10 marks

4. Operator describing a two level system: Let the states $|\psi_1\rangle$ and $|\psi_2\rangle$ form an orthonormal basis of a two level system. Let us define new basis vectors $|\phi_1\rangle$ and $|\phi_2\rangle$ which are related to the original basis vectors as follows:

$$|\phi_1\rangle = \frac{1}{\sqrt{2}} (|\psi_1\rangle + |\psi_2\rangle), \quad |\phi_2\rangle = \frac{1}{\sqrt{2}} (|\psi_1\rangle - |\psi_2\rangle).$$

An operator \hat{A} in the original basis is given by the matrix

$$\hat{A} = \begin{pmatrix} a & c \\ c & b \end{pmatrix}.$$

Determine the matrix describing the operator in the new basis. 10 marks

5. Testing the energy-time uncertainty principle: Consider a particle in an infinite square well with its walls located at $x = 0$ and $x = a$. At an initial time, say, $t = 0$, the system is described by the wavefunction

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

where the $\psi_1(x)$ and $\psi_2(x)$ are the energy eigen functions corresponding to the ground and the first excited states of the system.

- (a) Evaluate the expectation values $\langle \hat{x} \rangle$ and $\langle \hat{H} \rangle$ at time $t > 0$. 3 marks
- (b) What are ΔE and Δx at time $t > 0$? 3 marks
- (c) Estimate Δt , where $\Delta t = \Delta x / (|d\langle x \rangle / dt|)$. 2 marks
- (d) What is $\Delta E \Delta t$? Is the energy-time uncertainty principle satisfied? 2 marks

Hint: It is useful to note that

$$\int_0^a dx x^2 \sin^2 \left(\frac{n \pi x}{a} \right) = a^3 \left(\frac{1}{6} - \frac{1}{(2n\pi)^2} \right)$$

and, when $n \neq m$,

$$\int_0^a dx x^2 \sin \left(\frac{n \pi x}{a} \right) \sin \left(\frac{m \pi x}{a} \right) = a^3 \left(\frac{\cos [(n-m)\pi]}{[(n-m)\pi]^2} - \frac{\cos [(n+m)\pi]}{[(n+m)\pi]^2} \right).$$

6. The ground state of hydrogen: Recall that, in three dimensions, given a wavefunction $\psi(\mathbf{r})$ in real space, the wavefunction in momentum space is described by the integral

$$\phi(\mathbf{p}) = \int \frac{d^3 \mathbf{r}}{(2\pi\hbar)^{3/2}} \psi(\mathbf{r}) e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar}.$$

The ground state wavefunction of hydrogen is given by

$$\psi_{100}(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0},$$

where a_0 denotes the Bohr radius.

- (a) Using $\psi(\mathbf{r})$, evaluate the expectation value of the potential energy $\langle \hat{V} \rangle$ of the system. 3 marks
- (b) Obtain the momentum space wavefunction $\phi(\mathbf{p})$ describing the ground state of hydrogen. Check if $\phi(\mathbf{p})$ is normalized. 3 marks
- (c) Using $\phi(\mathbf{p})$, evaluate the expectation value of the kinetic energy $\langle \hat{T} \rangle$ of the system. How do $\langle \hat{T} \rangle$ and $\langle \hat{V} \rangle$ compare? 4 marks

Hint: It is useful to note that

$$\int_0^\infty \frac{x^2}{(1+x^2)^4} = \int_0^\infty \frac{x^4}{(1+x^2)^4} = \frac{\pi}{32}.$$

7. Ehrenfest's theorem for angular momentum: Consider a particle moving in a potential $V(\mathbf{r})$.

- (a) If $\hat{\mathbf{L}}$ and $\hat{\mathbf{N}}$ are the operators representing angular momentum and torque, show that 7 marks

$$\frac{d\langle \hat{\mathbf{L}} \rangle}{dt} = \langle \hat{\mathbf{N}} \rangle,$$

where $\mathbf{N} = \mathbf{r} \times (-\nabla V)$.

- (b) Show that $d\langle \hat{\mathbf{L}} \rangle / dt = 0$ for any spherically symmetric potential, i.e. when $V(\mathbf{r}) = V(r)$. 3 marks

8. Energy eigen functions and eigen values of the rigid rotator: Two particles of mass m are attached to the ends of a massless rigid rod of length a . The system is free to rotate in three dimensions about its center, but with the center point itself being fixed.

- (a) Express the classical energy of the system in terms of its total angular momentum. 2 marks
- (b) What are the allowed energies of the quantum rigid rotator? 3 marks

- (c) What are the energy eigen functions of the system? 3 marks
- (d) What is the degeneracy of a given energy level? 2 marks

9. Spin- $\frac{3}{2}$ particle: Consider a particle with spin $\frac{3}{2}$.

- (a) What are the eigen values and eigen states of the \hat{S}_z operator for the system? 2 marks
- (b) Determine the effects of the operators \hat{S}_+ and \hat{S}_- on these eigen states. 3 marks
- (c) Construct the matrices describing the operators \hat{S}_+ and \hat{S}_- . 3 marks
- (d) Obtain the matrix describing the operator \hat{S}_x . 2 marks

10. Relations involving angular momentum operators: Establish the following operator relations:

- (a) $[\hat{\phi}, \hat{L}_z] = i\hbar$, 1 marks
- (b) $\exp(i\hat{L}_z\alpha/\hbar)\psi(\phi) = \psi(\phi + \alpha)$, 2 marks
- (c) $[L^2, [L^2, \mathbf{r}]] = 2\hbar^2(\mathbf{r}L^2 + L^2\mathbf{r})$. 7 marks
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Advanced problems

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

1. Particle in a uniform gravitational field: The potential describing a particle in a uniform gravitational field is given by $V(x) = -m g x$, where g denotes acceleration due to gravity and we have assumed that g is directed towards the negative x -direction. Earlier, we had solved the Schrodinger equation in momentum space to arrive at the corresponding wave function.
 - (a) Solve the Schrodinger equation in position space for vanishing energy eigen value in the domains of large positive and negative x .
 - (b) Show that the solution to the Schrodinger equation in position space can be expressed in terms of the Airy functions.
 - (c) Plot the energy eigen functions for a few different eigen values.
2. Simple harmonic oscillator in momentum space: Earlier, we had arrived at the Schrodinger equation governing the wave function of a system in momentum space. Solve the time-independent Schrodinger equation governing the harmonic oscillator *in momentum space* to arrive at the corresponding energy eigen functions. Can you recognize the form of the eigen functions?
3. Classical and quantum probability distributions for the harmonic oscillator: Consider a particle moving in the time independent potential $V(x)$ with energy E . The classical probability of finding the particle in the region between x and $x + dx$ is simply the ratio of the time spent in the domain, say, dt , to the total time taken for one traversal, i.e.

$$P_C(x) dx = \frac{dt}{T/2} = \frac{2}{T} \frac{dx}{v(x)},$$

where, evidently, $v(x)$ is the velocity at the location x , while T is the time period of the system. We can rewrite the above expression for $P_C(x)$ as

$$P_C(x) = \frac{2}{T} \frac{\sqrt{m/2}}{\sqrt{E - V(x)}}.$$

- (a) Plot the classical probability for the case of a harmonic oscillator for a given energy E and specific sets of values for the parameters m and ω .
 - (b) We had earlier discussed the energy eigen functions $\psi_n(x)$ for the case of the harmonic oscillator, with n denoting the different states. Plot the probability density $|\psi_n(x)|^2$ for an integer n which corresponds to an energy eigen value that is closest to the energy E chosen in the classical case.
 - (c) How do the two plots compare as you keep increasing the energy E ?
4. Baker-Campbell-Hausdorff formulae: Consider two operators \hat{A} and \hat{B} .

- (a) Show that, when $[\hat{A}, \hat{B}] = c$, where c is, in general, a complex number,

$$e^{\hat{A}} e^{\hat{B}} = e^{\hat{A} + \hat{B} + \frac{1}{2}[\hat{A}, \hat{B}]}$$

- (b) Establish that, in general,

$$e^{\hat{A}} e^{\hat{B}} = e^{\hat{A} + \hat{B} + \frac{1}{2}[\hat{A}, \hat{B}] + \frac{1}{12}([\hat{A}, [\hat{A}, \hat{B}]] + [\hat{B}, [\hat{B}, \hat{A}]] + \dots)}$$

- (c) Further, show that, for a complex number α ,

$$e^{-\alpha \hat{A}} \hat{B} e^{\alpha \hat{A}} = \hat{B} - \alpha [\hat{A}, \hat{B}] + \frac{\alpha^2}{2} [\hat{A}, [\hat{A}, \hat{B}]] + \frac{\alpha^3}{3!} [\hat{A}, [\hat{A}, [\hat{A}, \hat{B}]]] + \dots$$

Note: Such relations are known as Baker-Campbell-Hausdorff formulae.

5. Non-trivial commutation relations: If \hat{a} and \hat{a}^\dagger denote the raising and lowering operators, show that

$$(a) [\hat{a}, e^{-\alpha \hat{a}^\dagger \hat{a}}] = (e^{-\alpha} - 1) e^{-\alpha \hat{a}^\dagger \hat{a}} \hat{a},$$

$$(b) [\hat{a}^\dagger, e^{-\alpha \hat{a}^\dagger \hat{a}}] = (e^\alpha - 1) e^{-\alpha \hat{a}^\dagger \hat{a}} \hat{a}^\dagger.$$

6. Interpreting Wigner function as a probability distribution: Consider two distinct states $\Psi(x, t)$ and $\chi(x, t)$ describing a system. Let the Wigner functions corresponding to the two states be represented as $W_\Psi(x, p, t)$ and $W_\chi(x, p, t)$.

(a) Show that

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dp W_\Psi(x, p, t) W_\chi(x, p, t) = \frac{2}{\pi \hbar} \left| \int_{-\infty}^{\infty} dx \Psi^*(x, t) \chi(x, t) \right|^2.$$

(b) Using this result, argue that, if $\Psi(x, t)$ and $\chi(x, t)$ are orthogonal states, then the Wigner functions cannot be positive definite.

(c) As an explicit example, evaluate the Wigner function for the excited energy eigen states of the harmonic oscillator and show that it is indeed not positive definite.

Note: It is for this reason that the Wigner function is often referred to as a *quasi*-probability distribution.

7. Wigner function for a coherent state: Earlier, we had determined the wave function describing a coherent state in the position representation.

(a) Assuming the wave function to be the wave function at time, say, $t = 0$, determine the wavefunction at later times.

(b) Evaluate the Wigner function corresponding to the wave function.

(c) Choose a large amplitude for the parameter α describing the coherent state and plot the behavior of the corresponding Wigner function as a function of time. Compare the evolution of the peak of the Wigner function with the classical trajectory in phase space.

8. Quantum mechanical kernels: Recall that, the probability amplitude for finding the particle at the location x_2 at a *later* time t_2 , given that it was located at x_1 at time t_1 , can be expressed as

$$K(x_2, t_2 | x_1, t_1) = \langle x_2, t_2 | x_1, t_1 \rangle = \sum_{\text{all } n} \psi_n^*(x_2) \psi_n(x_1) e^{-i E_n (t_2 - t_1) / \hbar},$$

where $\psi_n(x)$ denote the energy eigen states corresponding to the energy eigen values E_n and the sum over n represents either the sum or a suitable integral (in the case of a continuum of states) over all the energy eigen values.

(a) We had earlier evaluated the kernel for the case of a free particle. Show that the kernel can be expressed as follows:

$$K(x_2, t_2 | x_1, t_1) = \sqrt{\frac{m}{2\pi i \hbar T}} \exp\left(\frac{i S_{\text{FP}}[x(t)]}{\hbar}\right),$$

where $T = t_2 - t_1$ and $S_{\text{FP}}[x(t)]$ is the classical action governing the free particle, given that the particle is at locations x_1 and x_2 at times t_1 and t_2 .

(b) Evaluate the above sum describing the kernel for the case of a harmonic oscillator and show that it is given by

$$K(x_2, t_2 | x_1, t_1) = \sqrt{\frac{m\omega}{2\pi i \hbar \sin(\omega T)}} \exp\left\{\frac{i m \omega}{2 \hbar \sin(\omega T)} [(x_1^2 + x_2^2) \cos(\omega T) - 2 x_1 x_2]\right\}.$$

- (c) Show that this kernel reduces to the kernel of a free particle in the limit $\omega \rightarrow 0$, as required.
- (d) Show that the kernel for the oscillator can also be expressed as

$$K(x_2, t_2 | x_1, t_1) = \sqrt{\frac{m\omega}{2\pi i \hbar \sin(\omega T)}} \exp\left(\frac{i S_{\text{HO}}[x(t)]}{\hbar}\right),$$

where $S_{\text{HO}}[x(t)]$ is the classical action governing the oscillator.

- (e) Can you evaluate the kernel for a particle in a uniform gravitational field and also express it in terms of the action governing the system?
9. Equation governing the kernel: Recall that the quantum mechanical kernel $K(x_2, t_2 | x_1, t_1)$ is defined through the relation

$$\Psi(x_2, t_2) = \int dx_1 K(x_2, t_2 | x_1, t_1) \Psi(x_1, t_1).$$

Note: As it propagates the wave function, the kernel $K(x_2, t_2 | x_1, t_1)$ is also referred to as the quantum mechanical propagator.

- (a) Using the time-dependent Schrodinger equation, arrive at the equation of motion governing the kernel $K(x_2, t_2 | x_1, t_1)$.
 Note: It is important to appreciate that $t_2 > t_1$. In other words, to ensure causality, the kernel should actually be multiplied by the step function $\Theta(t_2 - t_1)$.
- (b) Solve the equation to arrive at the kernel for the free particle, the harmonic oscillator and a particle in a uniform gravitational field.

10. An important property of the propogator: An important property of the kernel $K(x', t' | x, t)$ is the following:

$$K(x_3, t_3 | x_1, t_1) = \int dx_2 K(x_3, t_3 | x_2, t_2) K(x_2, t_2 | x_1, t_1),$$

where $t_3 > t_2 > t_1$.

Note: It is this property which permits one to provide a path integral interpretation for the quantum mechanical propagator.

- (a) Establish this result for a generic system using the Feynman-Kac formula we had discussed earlier.
- (b) Establish this result explicitly for the cases of the free particle and the simple harmonic oscillator using the kernels we have obtained above.
11. The isotropic oscillator in spherical polar coordinates: We had earlier discussed the case of the isotropic harmonic oscillator in three dimensions that is described by the potential

$$V(x, y, z) = \frac{m\omega^2}{2} (x^2 + y^2 + z^2).$$

In the cartesian coordinates, it had proved to be easy to determine the energy eigen functions and the corresponding energy eigen values. Evidently, the above potential can also be written in the following spherically symmetric fashion:

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

which suggests that the system can also be studied in the spherical polar coordinates.

- (a) Working in the spherical polar coordinates, determine the energy eigen functions of the isotropic oscillator.

(b) What are the energy eigen values? How are they related to the eigen values obtained in the cartesian coordinates?

12. The quantum Runge-Lenz vector: Consider the Kepler problem of a particle moving in the following spherically symmetric potential:

$$V(r) = -\frac{\alpha}{r},$$

where α is a positive quantity. In such a case, it is well known that the energy and angular momentum of the particle are conserved quantities. The energy is conserved due to the fact that the potential is time-independent, while angular momentum is conserved because of the spherical symmetry. Apart from these quantities, it is also found that the following quantity, often referred to as the Runge-Lenz vector, is conserved as well:

$$\mathbf{R} = \frac{\mathbf{r}}{r} - \frac{1}{m\alpha} (\mathbf{p} \times \mathbf{L}),$$

where \mathbf{r} is the position vector, while \mathbf{p} and \mathbf{L} are the momentum and the angular momentum of the particle. Construct the quantum operator corresponding to the above Runge-Lenz vector and show that it commutes with the Hamiltonian describing the system, suggesting that it is conserved quantum mechanically as well.

13. A modified Coulomb potential: Consider the following modified Coulomb potential

$$V(r) = -\frac{Z e^2}{4\pi\epsilon_0 r} \left(1 + b \frac{a_0}{r}\right),$$

where b is a dimensionless quantity and $a_0 = 4\pi\epsilon_0 \hbar^2 / (m_e c^2)$ is the Bohr radius, with m_e being the mass of the electron. Solve the Schrodinger equation for this case and show that the energy eigen values are given by

$$E_{nl} = -\frac{(Z\alpha)^2 \mu c^2}{2} \frac{1}{\left[n + \sqrt{\left(l + \frac{1}{2}\right)^2 - 2b} - \left(l + \frac{1}{2}\right)\right]^2},$$

where μ is the reduced mass of the proton and $\alpha = e^2 / (4\pi\epsilon_0 \hbar c)$ is the fine structure constant.

Note: In contrast to the standard Coulomb case, the energy levels now depend on the quantum numbers n as well as l .

14. The classical limit and the Hamilton-Jacobi equation: Consider the time-dependent Schrodinger equation in three dimensions. Let us write the time-dependent wavefunction $\Psi(\mathbf{x}, t)$ as follows:

$$\Psi(\mathbf{x}, t) = \sqrt{\rho(\mathbf{x}, t)} \exp[iS(\mathbf{x}, t)/\hbar],$$

where $\rho(\mathbf{x}, t)$ and $S(\mathbf{x}, t)$ are real functions of space and time.

- (a) Substituting the above form of $\Psi(\mathbf{x}, t)$ in the time-dependent Schrodinger equation, show that, under certain conditions, the imaginary part of the equation leads to following conservation equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0,$$

where $\mathbf{v} = \nabla S / m$.

- (b) Also, show that, under certain conditions, one can arrive at the following so-called Hamilton-Jacobi equation that governs the action S in classical mechanics:

$$\frac{\partial S}{\partial t} + \frac{1}{2m} |\nabla S|^2 + V(\mathbf{x}) = 0,$$

where $V(\mathbf{x})$ denotes the potential energy of the system.

(c) What are the conditions under which the above two equations are arrived at? Can you physically interpret these conditions?

15. The no-cloning theorem: Consider a quantum photocopying machine which produces an exact replica of the original state, say, $|\psi\rangle$, i.e.

$$|\psi\rangle \rightarrow |\psi\rangle \otimes |\psi\rangle.$$

Argue that, such a machine cannot produce a copy of a superposition of states such as $(\alpha|\psi_1\rangle + \beta|\psi_2\rangle)$.

Note: This statement is known as the no-cloning theorem.
