EP2210

PRINCIPLES OF QUANTUM MECHANICS

January–May 2024

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 210.
- The first lecture will be on Wednesday, January 17, and the last lecture will be on Friday, May 3.
- We will meet thrice a week. The lectures are scheduled for 9:00–9:50 AM on Mondays, 8:00–8:50 AM on Tuesdays, and 1:00–1:50 PM on Wednesdays.
- We may also meet during 11:00–11:50 AM on Fridays 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 5:00–6:00 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://coursesnew.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 February 24, March 23 and April 20. The three dates are Saturdays, and the quizzes will be held during 4:00–5:30 PM on these days.
- The end-of-semester exam will be held during 9:00 AM–12:00 NOON on Tuesday, May 7, and the exam will carry 50% weight.

Syllabus and structure

Principles of Quantum Mechanics

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

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

Exercise sheet 1

Additional exercises I

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

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

Exercise sheet 2

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

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

Exercise sheet 3

Quiz I

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

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

Exercise sheets 4 and 5

Additional exercises II

Quiz II

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

Exercise sheets 6, 7 and 8

6. **The Schrodinger equation in three dimensions and particle in a central potential** [$\sim$ 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** [$\sim$ 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** [$\sim$ 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** [$\sim$ 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).

Advanced textbooks

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

Other references

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

Exercise sheet 1

Essential classical mechanics

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

2. *Non-relativistic particle in an electromagnetic field:* A non-relativistic particle that is moving in an electromagnetic field described by the scalar potential ϕ and the vector potential $\boldsymbol{A}$ is governed by the Lagrangian

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

where m and q are the mass and the charge of the particle, while c denotes the velocity of light. Show that the equation of motion of the particle is given by

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

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

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

Note: The scalar and the vector potentials, viz. ϕ and $\boldsymbol{A}$, are dependent on time *as well as* space. Further, given two vectors, say, $\boldsymbol{C}$ and $\boldsymbol{D}$, one can write,

$$\boldsymbol{\nabla}\left(\boldsymbol{C}\cdot\boldsymbol{D}\right) = \left(\boldsymbol{D}\cdot\boldsymbol{\nabla}\right)\boldsymbol{C} + \left(\boldsymbol{C}\cdot\boldsymbol{\nabla}\right)\boldsymbol{D} + \boldsymbol{D}\times\left(\boldsymbol{\nabla}\times\boldsymbol{C}\right) + \boldsymbol{C}\times\left(\boldsymbol{\nabla}\times\boldsymbol{D}\right).$$

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

$$\frac{\mathrm{d}\boldsymbol{A}}{\mathrm{d}t} = \frac{\partial\boldsymbol{A}}{\partial t} + \left(\boldsymbol{v}\cdot\boldsymbol{\nabla}\right)\boldsymbol{A}.$$

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

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

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

   Note: The quantity δ_{ij} is called the Kronecker symbol and it takes on the following values:

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

Additional exercises I

Essential classical mechanics

1. *Snell's law of refraction:* Two homogeneous media of refractive indices n_1 and n_2 are placed adjacent to each other. A ray of light propagates from a point in the first medium to a point in the second medium. According to the Fermat's principle, the light ray will follow a path that minimizes the transit time between the two points. Use Fermat's principle to derive the Snell's law of refraction, viz. that
$$n_1 \sin\theta_1 = n_2 \sin\theta_2,$$
where θ_1 and θ_2 are the angles of incidence and refraction at the interface.

   Note: As the complete path is not differentiable at the interface, actually, the problem is not an Euler equation problem.

2. *Variation involving higher derivatives:* Show that the Euler equation corresponding to the integral
$$J[y(x)] = \int_{x_1}^{x_2} \mathrm{d}x\, f(y, y_x, y_{xx}, , x),$$
where $y_{xx} \equiv \left(\mathrm{d}^2y/\mathrm{d}x^2\right)$, is given by
$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\left(\frac{\partial f}{\partial y_{xx}}\right) - \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial y_x}\right) + \left(\frac{\partial f}{\partial y}\right) = 0.$$

   Note: In order to obtain this equation, the variation as well its first derivative need to be set to zero at the end points.

3. *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.

4. *Action for a free particle:* Given that a free particle that is moving in three dimensions was located at the position $\boldsymbol{r}_1$ at time t_1 and at the position $\boldsymbol{r}_2$ at time t_2, determine the action for the free particle in terms of $\boldsymbol{r}_1$, $\boldsymbol{r}_2$, 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.

5. *Motion in one dimension:* Obtain the solutions describing the time evolution of a particle moving in the one-dimensional potential
$$U(x) = \alpha\left(e^{-2\,\beta\,x} - 2\,e^{-\beta\,x}\right), \quad \text{where} \quad \alpha, \beta > 0,$$
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 $E < 0$.

6. *Application of the virial theorem:* Using virial theorem, show that the total mass M of a spherical cluster of stars (or galaxies) of uniform density and radius R is given by
$$M = \frac{5\,R\,\langle v^2\rangle}{3\,G},$$
where $\langle v^2\rangle$ is the mean-squared velocity of the individual stars and G is, of course, the gravitational constant.

Note: The above relation allows us to obtain an estimate of the mass of a cluster if we can measure the mean-squared velocity, say, from the Doppler spread of the spectral lines and the radius of the cluster, say, from its known distance and angular size.

7. *The Laplace-Runge-Lenz vector:* Recall that, for a particle with s degrees of freedom, we require $2\,s-1$ 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 $\boldsymbol{L}$, both of which were conserved. However, these quantities, viz. the energy E and the three components of the angular momentum vector $\boldsymbol{L}$, 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:

   $$\boldsymbol{A} = m\,\boldsymbol{v}\times\boldsymbol{L} - \frac{m\,\alpha\,\boldsymbol{r}}{r}.$$

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

   (b) Show that the vector $\boldsymbol{A}$ lies in the plane of the orbit.

   (c) Indicate the amplitude and the direction of $\boldsymbol{A}$ associated with a planet as it moves in an elliptical orbit around the Sun.

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

   (d) If E, $\boldsymbol{M}$ and $\boldsymbol{A}$ 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 $\boldsymbol{A}$ and $\boldsymbol{L}$ and/or E.

8. *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 $n > 2$.

9. *Hamiltonian of a free particle:* Show that the Hamiltonian of a free particle can be written as

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

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

10. *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 $\nu + \mathrm{d}\nu$ associated with the electromagnetic radiation emitted by the black body is given by

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

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

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

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

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

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

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

   where σ denotes the Stefan constant given by

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

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

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

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

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

2. *Photoelectrons from a zinc plate:* Consider the emission of electrons due to photoelectric effect from a zinc plate. The work function of zinc is known to be $3.6\,\mathrm{eV}$. What is the maximum energy of the electrons ejected when ultra-violet light of wavelength $3000\,\text{Å}$ 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 $2536\,\text{Å}$. The spectrum of mercury has a strong second line at the wavelength of $1849\,\text{Å}$. What will be the voltage corresponding to this line at which we can expect the current in the Frank and Hertz experiment to drop?

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

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

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

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

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

Given the wavefunction

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

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

Exercise sheet 3

The postulates of quantum mechanics and the Schrodinger equation

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

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

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

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

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

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

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

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

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

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

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

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

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

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

4. *Ehrenfest's theorem:* Show that

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

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

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

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

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

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

Quiz I

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

1. _Bounded motion in one dimension:_ Consider a particle moving in the following one-dimensional potential:
$$U(x) = \frac{a}{x^2} + b\,x^2, \quad \text{where} \quad a,\ b > 0.$$
   (a) Obtain the solution describing the time evolution of the particle. 7 marks
   (b) Also, evaluate the time period of the particle as a function of its energy. 3 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 $\boldsymbol{L}$ of a system, 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

3. _Interference pattern on a screen:_ In a double slit experiment, a detector traces across a screen whose coordinate label is y. If one slit is closed, the probability amplitude on the screen is given by
$$\Psi_1(y, t) = \frac{1}{\sqrt{2}}\, \mathrm{e}^{-y^2/2}\, \mathrm{e}^{i\,(\omega\,t - a\,y)},$$
where ω and a are positive and real constants. If the other slit is closed, the probability amplitude is given by
$$\Psi_2(y, t) = \frac{1}{\sqrt{2}}\, \mathrm{e}^{-y^2/2}\, \mathrm{e}^{i\,(\omega\,t - a\,y - b\,y)},$$
where b too is a positive and real constant.
   (a) What is the intensity pattern on the screen if both the slits are open? 4 marks
   (b) Plot the intensity pattern as a function of y. 6 marks

4. _Particle on a circle:_ A particle of mass μ, 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 time-independent Schrodinger equation and obtain the energy eigen functions. 3 marks
   (c) What are the energy eigen values? Are they continuous or discrete? Obtain the normalized the energy eigen functions. 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.

5. *Wave function describing a free particle:* Consider the following wave function describing a system in one dimension:

$$\Psi(x,t) = \frac{\mathrm{e}^{-i\,\theta(t)/2}}{\left[\pi\,\alpha^2\,\hbar^2\,\mathcal{F}_1(t)\right]^{1/4}}\,\mathrm{e}^{i\,\left[p_0\,(x-x_0)-(p_0^2\,t/2\,m)\right]/\hbar}\;\mathrm{e}^{-[x-x_0-(p_0\,t/m)]^2/\left[2\,\alpha^2\,\hbar^2\,\mathcal{F}(t)\right]},$$

where α is a real constant, while $\mathcal{F}(t)$ and $\mathcal{F}_1(t)$ are given by

$$\mathcal{F}(t) = 1 + \frac{i\,t}{m\,\hbar\,\alpha^2}, \qquad \frac{1}{\mathcal{F}_1(t)} = \frac{1}{\mathcal{F}(t)} + \frac{1}{\mathcal{F}^*(t)}, \qquad \theta(t) = \tan^{-1}\left(\frac{t}{m\,\hbar\,\alpha^2}\right).$$

(a) Show that the wave function is normalized. $\boxed{\text{1 marks}}$

(b) Prove that the wave function describes a free particle. $\boxed{\text{5 marks}}$

(c) Evaluate $\langle\hat{x}\rangle$ and $\langle\hat{p}_x\rangle$ in the given state. $\boxed{\text{2+2 marks}}$

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

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

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

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

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

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

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

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

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

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

where $a > 0$.

(a) Determine the bound state energy eigen functions.

(b) Plot the energy eigen functions.

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

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

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

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

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

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

and determine the reflection and the transmission probabilities.

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

$$\psi(x) = \mathrm{e}^{i\,k\,x} + R\,\mathrm{e}^{-i\,k\,x},$$

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

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

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

$$1 + R = T, \quad i\,k\,(1 - R) = -q\,T,$$

which can be solved to arrive at

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

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

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

$$\psi(x) = \mathrm{e}^{i\,k\,x} + R\,\mathrm{e}^{-i\,k\,x},$$

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

$$\psi(x) = T\,\mathrm{e}^{i\,q\,x},$$

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

$$1 + R = T, \quad i\,k\,(1 - R) = i\,q\,T.$$

These relations can be easily solved to obtain that

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

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

$$\psi(x) = \mathrm{e}^{i\,k\,x} + R\,\mathrm{e}^{-i\,k\,x},$$

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

$$\psi(x) = T\,\mathrm{e}^{i\,k\,x},$$

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

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

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

$$\begin{aligned} \mathrm{e}^{-i\,k\,a} + R\,\mathrm{e}^{i\,k\,a} &= A\,\mathrm{e}^{-q\,a} + B\,\mathrm{e}^{q\,a}, \\ i\,k\left(\mathrm{e}^{-i\,k\,a} - R\,\mathrm{e}^{i\,k\,a}\right) &= q\left(A\,\mathrm{e}^{-q\,a} - B\,\mathrm{e}^{q\,a}\right). \end{aligned}$$

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

$$B = \frac{-2\,i\,k}{q - i\,k}\,\mathrm{e}^{(q+i\,k)\,a} + A\,\frac{q + i\,k}{q - i\,k}\,\mathrm{e}^{-2\,q\,a}.$$

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

$$\begin{aligned} A\,\mathrm{e}^{q\,a} + B\,\mathrm{e}^{-q\,a} &= T\,\mathrm{e}^{i\,k\,a}, \\ q\left(A\,\mathrm{e}^{q\,a} - B\,\mathrm{e}^{q\,a}\right) &= i\,k\,T\,\mathrm{e}^{i\,k\,a}. \end{aligned}$$

On eliminating T from these two relations, we obtain that

$$A = B\,\frac{q + i\,k}{q - i\,k}\,\mathrm{e}^{-2\,q\,a}.$$

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

$$B = -\frac{-2\,i\,k\,(q - i\,k)\,\mathrm{e}^{-(q+i\,k)\,a}}{(q - i\,k)^2 - (q + i\,k)^2\,\mathrm{e}^{-4\,q\,a}}.$$

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

$$T = \frac{2\,k\,q\,\mathrm{e}^{-2\,i\,k\,a}}{2\,q\,k\cosh(2\,q\,a) - i\,(k^2 - q^2)\sinh(2\,q\,a)}$$

leading to

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

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

$$|T|^2 \simeq \frac{(4\,k\,q)^2}{(k^2 + q^2)^2}\,\mathrm{e}^{-4\,q\,a}.$$

Exercise sheet 5

The harmonic oscillator

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

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

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

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

   (b) Utilize the following recursion relation:

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

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

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

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

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

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

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

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

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

   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

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

   In terms of the dimensionless variable

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

   the above time-independent Schrodinger equation reduces to

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

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

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

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

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

Additional exercises 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 $E = L^2/(2\, I)$, where L is the angular momentum and I is the moment of inertia.
   (a) Using Bohr's rule, determine the quantized energy levels of the rigid rotator.
   (b) Molecules are known to behave sometimes as rigid rotators. If the rotational spectra of molecules are characterized by radiation of wavelength of the order of 10^6 nm, estimate the interatomic distances in a molecule such as H_2.

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

4. *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 $T_{\mathrm{Q}} = 4\, m\, a^2/(\pi\, \hbar)$. 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 $T_{\mathrm{Q}} = T_{\mathrm{C}}$?

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

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

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

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

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

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

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

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

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

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

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

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

which leads to

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

(c) Show that

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

(d) Consider the following normalized Gaussian wave packet

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

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.

Exercise sheet 6

Essential mathematical formalism I

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

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

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

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

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

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

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

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

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

   where the expectation values are evaluated in a specific state.

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

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

   (c) Defining

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

   establish that

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

   and interpret this result.

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

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

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

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

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

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

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

Quiz II

From time-independent Schrodinger equation in one dimension to essential mathematical formalism

1. *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]

2. *Particle in a box:* The wave function of a particle that is confined to a box with its walls at $x = 0$ and $x = a$ is given by

$$\psi(x) = A \sin^3\left(\frac{\pi\,x}{a}\right).$$

   (a) Determine the constant A assuming that $\psi(x)$ is normalized. [2 marks]

   (b) If $\psi(x)$ above is the complete wavefunction of the system at $t = 0$ [i.e. $\Psi(x, t = 0) = \psi(x)$], then what is the wavefunction $\Psi(x, t)$ for $t > 0$? [4 marks]

   (c) What is the expectation value of the operator $\hat{p}_x^2$ in the state $\Psi(x, t)$ at time $t > 0$? [4 marks]

3. *Coherent states of the harmonic oscillator:* Consider states, say, $|\alpha\rangle$, which are eigen states of the 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 $\psi_\alpha(x) = \langle x|\alpha\rangle$. [4 marks]

   (b) 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:

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

   Determine c_n. Determine c_0 by normalizing $|\alpha\rangle$. [4 marks]

   (c) 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 [2 marks]

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

4. *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 $\alpha = \hbar^2/(m\,a) > 0$.

   (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 $x \to -x$ in the domain $-a < x < a$. 5 marks

5. *Quantum revival:* Consider an *arbitrary* wavefunction describing a particle in the infinite square well.

(a) Determine the so-called quantum revival time, say, T_{Q}, when the wave function will return to its original form. 6 marks

(b) What is the classical revival time T_{C} for a particle of energy E bouncing back and forth between the walls? 2 marks

Note: Essentially, the classical revival time is the time period of the particle.

(c) What is the energy for which $T_{\mathrm{Q}} = T_{\mathrm{C}}$? 2 marks

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. *Wigner function for coherent states of the harmonic oscillator:* Recall that the coherent states of the harmonic oscillator are the eigen states of the lowering operator, i.e.

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

   where α is a complex number.

   (a) Obtain the wave function $\Psi(x,t)$ describing the coherent state.

   (b) Calculate the expectation values $\langle\hat{x}\rangle$ and $\langle\hat{p}_x\rangle$ in the state at any time t.

   (c) Earlier, we had defined the Wigner function associated with a wave function $\Psi(x,t)$ as follows:

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

   Evaluate the Wigner function $W(x,p,t)$ associated with the coherent state.

   (d) 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 quantities $\langle\hat{x}\rangle$ and $\langle\hat{p}_x\rangle$ as well as the classical trajectory in phase space.

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

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

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

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

where ω, λ and μ are positive real numbers.

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

(b) Suppose the system starts in the generic state

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

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

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

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

Exercise sheet 8

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

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

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

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

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

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

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

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

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

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

   can be written as

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

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

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

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 $V(x) = -F\,x$. Classically, this corresponds to a uniformly accelerating particle.

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

$$\Phi(p,t) = \Phi_0(p - F\,t)\,\mathrm{e}^{-i\,p^3/(6\,m\,F\,\hbar)}.$$

   where $\Phi_0(p - F\,t)$ is an arbitrary function.

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

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

   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

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

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

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

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

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

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

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

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

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

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

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

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

Exercise sheet 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.

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

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

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

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

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

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

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

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

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

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

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

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