PH 203: Quantum Mechanics I

1. Spreading of a wave packet: For a normalised wave function $\psi(x,t)$ centered at the point x_0, we define the width $\Delta x(t)$ by the formula

$$(\Delta x(t))^2 \; = \; \int_{-\infty}^{\infty} dx \; (x - x_0)^2 \; |\psi(x,t)|^2 \; .$$

(i) Suppose that at $t = 0$, we have a Gaussian wave function of the form

$$\psi(x,0) \; = \; \frac{e^{-(x-x_0)^2/4\sigma^2}}{(2\pi)^{1/4}\sigma^{1/2}} \; .$$

Use the free particle Schrödinger equation to see how this evolves in time, and find an expression for the width $\Delta x(t)$.

Hint: Do a Fourier transform to momentum space and use the result that $\int_{-\infty}^{\infty} dx e^{-a(x-b)^2} = \sqrt{\pi/a}$, where a can be a complex number whose real part is not negative and b can be any complex number.

(ii) Estimate the time required for the wave packet of an electron of mass 9×10^{-31}Kg to double its width starting from $\Delta x(0) = 1$ Å.

2. Consider a normalised wave function at time $t = 0$ given by

$$\psi(x,0) \; = \; \frac{e^{-(x-a)^2/4\sigma^2 + ibx/\hbar}}{(2\pi)^{1/4}\sigma^{1/2}} \; ,$$

where a and b are real constants. Use the free particle Schrödinger equation to see how this evolves in time, and find expressions for the expectation values $< x >$, $< p >$, the uncertainties Δx, Δp, and the product $\Delta x \Delta p$ as functions of t.

3. Quantum mechanics on a lattice: Assume that a particle can only live on the sites of a one-dimensional lattice where the site positions are given by $x_n = na$, a being the lattice spacing. Suppose that the Schrödinger equation for the particle is

$$i\hbar \frac{\partial \psi(x_n,t)}{\partial t} \; = \; - \; \frac{\hbar^2}{2m} \left[\; \frac{\psi(x_{n+1},t) + \psi(x_{n-1},t) - 2\psi(x_n,t)}{a^2} \right] \; .$$

(i) Find all the energy levels and wave functions. (You don't have to normalise the wave functions).

Hint: Assume wave functions of the form $\psi(x_n,t) = e^{(i/\hbar)(px_n - E_p t)}$, and find the energy E_p as a function of the momentum p. (We restrict p to lie in the range $[-\pi\hbar/a, \pi\hbar/a]$).

(ii) Show that you recover the usual continuum result for E_p as a function of p if $|p| << \hbar/a$.

4. For a particle moving on a circle of circumference L, suppose that the Hamiltonian is $H = (\hat{p} - a)^2/2m$, where $\hat{p} = -i\hbar\partial/\partial x$ and a is real.

   (i) Find the energy levels and wave functions.

   (ii) Sketch the ground state energy as a function of a as a goes from $-\infty$ to ∞.

5. Consider an electron with charge q moving on a circle (of circumference L) which encloses a magnetic flux Φ. The Hamiltonian is given by $H = (\hat{p} - a)^2/2m$, where $a = q\Phi/(cL)$ and c is the speed of light.

   (i) Find all the energy levels and the corresponding wave functions.

   (ii) Sketch the energy of the ground state (namely, the minimum energy eigenvalue of H) as a function of a as a goes from $-\infty$ to ∞.

   (iii) In the ground state, sketch the expectation value of the current $< q\hat{v} >$ as a function of a, where we define the velocity operator of the electron as

   $$\hat{v} \; = \; \frac{1}{m} \, (\hat{p} - a).$$

   (Note: This expectation value is time-independent, and is therefore called a persistent current if it is non-zero).

6. A particle is in a one-dimensional box extending from $x = 0$ to $x = L$. ($V(x)$ is zero inside the box and infinity outside the box). We are given a wave function at time $t = 0$ of the form

   $$\psi(x, 0) = \delta(x - \frac{L}{2}) \; .$$

   Find an expression for $\psi(x, t)$ at later times, given that ψ evolves according to the Schrödinger equation. ($\psi(x, 0)$ is not normalisable, but don't worry about that). Show that $|\psi(x, t)|^2$ repeats periodically in time with a time period given by $T = mL^2/(2\pi\hbar)$.

7. A particle is in a box of length L with a δ-function potential in the middle, namely,

   $$\begin{aligned} V(x) \; &= \; c \, \delta(x) \quad \text{if} \quad -L/2 \; < \; x \; < \; L/2, \\ &= \; \infty \qquad\;\; \text{if} \quad x \; < \; -L/2 \quad \text{or} \quad x \; > \; L/2. \end{aligned}$$

   We will assume that $c > 0$.

   (i) What does the ground state wave function look like?

   (ii) Derive an equation which relates the ground state energy E_0 to the parameters c and L. (E_0 cannot be found analytically from this equation, but it can be found numerically if required).

   (iii) What is the value of E_0 in the limit $c \to \infty$? Can you explain this result by a simple physical argument?

8. For a particle moving in the potential $V(x) = c\,\delta(x-a)$, find the scattering matrix

$$S \;=\; \begin{pmatrix} r_p & t_p' \\ t_p & r_p' \end{pmatrix} .$$

The four amplitudes appearing above are defined as in class: for a wave incident from $x=-\infty$, $\psi(x) = e^{ipx/\hbar} \;+\; r_p e^{-ipx/\hbar}$ for $x < a$ and $t_p e^{ipx/\hbar}$ for $x > a$, while for a wave incident from $x = +\infty$, $\psi(x) = e^{-ipx/\hbar} + r_p' e^{ipx/\hbar}$ for $x > a$ and $t_p' e^{-ipx/\hbar}$ for $x < a$. Verify that $S^\dagger S = I$.

9. Consider the periodic δ-function potential

$$V(x) \;=\; \sum_{n=-\infty}^{\infty} c\,\delta(x-na) \;.$$

(i) Sketch the ground state wave function for $c > 0$ and for $c < 0$.

(ii) Derive equations which relate the ground state energy E_0 to c for $c > 0$ and for $c < 0$. (E_0 cannot be found analytically from these equations).

(iii) Find the ground state energy in the limit $c \to +\infty$.

(iv) Evaluate E_0 numerically (in eV) if $c = -1$ eV-Å, $a = 2$ Å, and $m = 9 \times 10^{-31}$Kg.

(Remember: $\hbar = 6.58 \times 10^{-16}$ eV-sec).

10. For the case of two attractive δ-function potentials, namely,

$$V(x) \;=\; c\,\delta(x+\frac{a}{2}) \;+\; c\,\delta(x-\frac{a}{2})$$

with $c < 0$, find the energy splitting ΔE between the two bound states for a large separation a. You should express ΔE in terms of a and the bound state E_0 of a single δ-function potential.

11. A particle moving in a one-dimensional potential $V(x)$ has a bound state wave function of the form

$$\psi(x) \;=\; \frac{c}{\cosh\,(x/a)} \;,$$

where a is some distance scale, and c is a constant.

(i) Find the potential $V(x)$ (assuming that $V(x) \to 0$ as $x \to \pm\infty$), and the bound state energy E.

(ii) Find the value of c for which ψ is normalised to unity.

12. A particle is moving in one dimension in the presence of the potential $V(x) = -\hbar^2/(ma^2\cosh^2(x/a))$, where $a > 0$.

(i) Show that the wave function

$$\psi = (1 \;+\; \frac{i}{ka}\;\tanh\frac{x}{a}\;)\;e^{ikx} \;,$$

satisfies the time-independent Schrödinger equation with energy $E_k = \hbar^2 k^2/(2m)$.

(ii) Show that this wave function can be multiplied by a suitable constant so that it takes the form e^{ikx} as $x \to -\infty$ and $t_k e^{ikx}$ as $x \to \infty$. Hence find the expression for the transmission amplitude t_k. (Since there is no term like $r_k e^{-ikx}$ as $x \to -\infty$, this potential is *reflectionless* for any energy E_k).

(iii) Show that t_k diverges when k is equal to a particular positive imaginary number, and use this to find the bound state energy and wave function for this potential.

13. Consider a particle moving in the presence of a potential $V(x)$ which is localised in some region. For a wave incident from the left (i.e., from $x = -\infty$) with momentum p, let $t_p = |t_p| e^{i\phi_p}$ be the transmission amplitude; ϕ_p is called the transmission phase shift. Now consider a wave packet incident from the left which is a superposition of many plane waves centered around $p = p_0$.

    (i) Show that the transmitted wave packet is centered around the point

    $$x \ = \ v_0 \left[t \ - \ \frac{\hbar}{v_0} \left(\frac{d\phi_p}{dp} \right)_{p=p_0} \right] ,$$

    where $v_0 = p_0/m$. The quantity $(\hbar/v_0)(d\phi_p/dp)_{p=p_0}$ is called the time delay.

    (ii) Calculate the time delay when the potential is given by $V(x) = c\ \delta(x)$ and the momentum $p_0 >> m|c|/\hbar$. (You may use the expression for t_p that was derived in class for a δ-function potential).

    (iii) Can you give a physical argument to explain the sign of the time delay? (Hint: classically, do you expect the particle to slow down or speed up at $x = 0$ if $c > 0$?)

14. Coherent states:

    (i) For the simple harmonic oscillator with the time-independent wave functions $\psi_n(x)$ satisfying

    $$H\psi_n(x) \ = \ \hbar\omega \ (n + \frac{1}{2}) \ \psi_n(x) \ ,$$

    consider the superposition

    $$\psi(x, 0) \ = \ \sum_{n=0}^{\infty} \ c_n \ \psi_n(x)$$

    at time $t = 0$. How should the coefficients c_n be chosen so that $\psi(x, 0)$ is an eigenstate of the lowering operator a, namely, $a\psi(x, 0) = \alpha\psi(x, 0)$, where the eigenvalue α is some given complex number?

    Eigenstates of a are called coherent states.

    (ii) Using the expression for a, find the explicit form of the wave function $\psi(x, 0)$. Make sure that $\psi(x, 0)$ is correctly normalised.

(iii) Now let ψ evolve in time according to the Schrödinger equation $i\hbar\partial\psi(x,t)/\partial t = H\psi(x,t)$. Show that $\psi(x,t)$ remains a coherent state at all times, except that the eigenvalue of a changes with time; how does it change?

(iv) The mean position $< x >$ and uncertainty Δx of the wave function $\psi(x,t)$ are defined as

$$\begin{aligned} < x > &= \int_{-\infty}^{\infty} dx \; x \; |\psi|^2 \; , \\ (\Delta x)^2 &= \int_{-\infty}^{\infty} dx \; (x \; - \; < x >)^2 \; |\psi|^2 \; , \end{aligned}$$

assuming that $\psi(x,t)$ is normalised. Show that $< x >$ varies with time according to the classical equation of motion, while Δx does not change at all.

(v) Calculate the mean momentum $< p >$ and uncertainty Δp, and show that they have similar properties as $< x >$ and Δx in part (iv). How much is $\Delta x \Delta p$ equal to?

All these are important properties of coherent states.

15. Squeezed states:

Recall that for the simple harmonic oscillator, the uncertainties Δx and Δp of the ground state wave function (and all coherent states) are equal to the 'natural' values $\sqrt{\hbar/2m\omega}$ and $\sqrt{\hbar m\omega/2}$ respectively.

(i) Now consider an eigenstate of the operator $Q = \mu a + \nu a^\dagger$ with eigenvalue α, where μ, ν and α are three complex numbers satisfying $|\mu|^2 - |\nu|^2 = 1$. For this state, calculate the uncertainties Δx and Δp as functions of μ, ν and α. Is $\Delta x \Delta p \geq \hbar/2$?

This is called a squeezed state if either Δx or Δp is less than its 'natural' value given above.

(ii) Now let this state evolve in time according to the Schrödinger equation. Show that it continues to be an eigenstate of the operator $Q(t) = \mu(t)a + \nu(t)a^\dagger$ with the *same* eigenvalue α, where $\mu(t)$ and $\nu(t)$ are some functions of time that you have to determine.

(iii) From this, find Δx and Δp as functions of time, and show that they periodically get squeezed and 'unsqueezed'. What is the time period of maximum squeezing of Δx? Sketch Δx, Δp and $\Delta x \Delta p$ as functions of time.

16. Consider the eigenstates $\psi_n(x)$ of the one-dimensional simple harmonic oscillator Hamiltonian. (We assume these are normalised so that $\int_{-\infty}^{\infty} dx \; \psi_n^\star(x)\psi_n(x) = 1$). Use the raising and lowering operators to find the expectation values

$$\begin{aligned} < x^3 >_n &= \int_{-\infty}^{\infty} dx \; \psi_n^\star(x) \; x^3 \; \psi_n(x) \\ \text{and} \qquad < x^4 >_n &= \int_{-\infty}^{\infty} dx \; \psi_n^\star(x) \; x^4 \; \psi_n(x) \end{aligned}$$

as functions of n.

17. A particle is moving in two dimensions with the Hamiltonian

$$H = \frac{p_x^2 + p_y^2}{2m} + \frac{1}{2} m\omega^2 \left(x^2 + y^2 + 2\lambda xy\right) .$$

(i) Find all the energy levels and the corresponding wave functions for $-1 < \lambda < 1$.

(ii) What are the energy levels and corresponding wave functions if $\lambda = \pm 1$?

18. A triatomic molecule is moving in one dimension with the Hamiltonian

$$H = \frac{p_1^2 + p_2^2 + p_3^2}{2m} + \frac{1}{2} m\omega^2 \left[(x_2 - x_1)^2 + (x_2 - x_3)^2\right] ,$$

where x_n denotes the displacement of the n^{th} particle from its equilibrium position. Find all the energy levels and write down the corresponding wave functions.

19. An electron with charge q is placed in a three-dimensional isotropic harmonic oscillator potential so that

$$H = \frac{\vec{p}^2}{2m} + \frac{1}{2} m\omega^2 \vec{r}^2 .$$

Now we apply a uniform electric field with magnitude A along the $\hat{z}$-direction.

(i) Find all the energy levels and their degeneracies. Does the answer depend on the direction of the electric field? Give a reason for your answer.

(ii) If E_0 is the ground state energy in the presence of the electric field, the electric dipole moment (in the $\hat{z}$-direction) is defined as $-dE_0/dA$ and the electric polarisability is defined as $-d^2E_0/dA^2$. Calculate these quantities in this problem.

20. A particle with mass m and charge q is placed in a one-dimensional simple harmonic potential with frequency ω and a uniform electric field $\mathcal{E}$ which is applied along the $+\,\hat{x}$ direction. Find the exact ground state energy and wave function. Hence find the induced dipole moment and explain its value using the form of the wave function.

21. Consider N particles arranged around a circle (of circumference L) with the Hamiltonian

$$H = \sum_{n=1}^{N} \left[\frac{p_n^2}{2m} + \frac{1}{2} m\omega^2 \left(x_{n+1} - x_n\right)^2 \right] ,$$

where $x_{N+1} = x_1$. (Here x_n denotes the displacement of the n^{th} particle from its equilibrium position). Find all the energy levels.

22. A particle is in a potential

$$\begin{aligned} V(x) &= \frac{1}{2} m\omega^2 x^2 \quad \text{if} \quad x > 0, \\ &= \infty \qquad\qquad \text{if} \quad x < 0. \end{aligned}$$

(i) Use a simple argument to find all the energy levels.

(ii) Show that for any initial state $\psi(x,0)$ which is given by an arbitrary superposition of the eigenstates of the Hamiltonian, the probability density $|\psi(x,t)|^2$ will repeat in time with a period π/ω.

23. Suppose that a particle moves in a one-dimensional potential of the form

$$\begin{aligned} V(x) &= \frac{1}{2} m\omega^2 x^2 \quad \text{for} \quad x > 0 \ , \\ &= \infty \quad \text{for} \quad x < 0 \ . \end{aligned}$$

Find all the energy levels and corresponding wave functions.

24. Virial theorem in quantum mechanics: For a one-dimensional problem described by

$$\hat{H} = \frac{\hat{p}^2}{2m} + a|\hat{x}|^n \ ,$$

(where $a, n > 0$), the virial theorem states that in any *eigenstate* of $\hat{H}$, the expectation values satisfy the relations

$$< \frac{\hat{p}^2}{2m} > = \frac{n}{n+2} < \hat{H} > \quad \text{and} \quad < a|\hat{x}|^n > = \frac{2}{n+2} < \hat{H} > .$$

To prove this theorem, consider the Hermitian operator

$$\hat{D} = \frac{\hat{x}\hat{p} + \hat{p}\hat{x}}{2\hbar}.$$

(i) Calculate the commutator $[\hat{D}, \hat{H}]$. (We have written the potential as $a|\hat{x}|^n$ instead of $a\hat{x}^n$ to avoid any difficulties if n is not an integer. But when you are calculating $[\hat{D}, \hat{H}]$, you may take $a|\hat{x}|^n$ to be equivalent to $a\hat{x}^n$).

(ii) Now calculate the expectation value of $[\hat{D}, \hat{H}]$ in an eigenstate of $\hat{H}$ and use the result to prove the virial theorem.

(iii) How does the unitary operator $U = e^{i\theta\hat{D}}$ transform $\hat{x}$ and $\hat{p}$, namely, what are $U\hat{x}U^{-1}$ and $U\hat{p}U^{-1}$ equal to? Show that for $\theta = i\pi$, the operator U does the parity transformation, $x \to -x$ and $p \to -p$.

[$\hat{D}$ is sometimes called the scaling operator].

25. For a Hermitian operator $\mathcal{O}$, show that the expectation values $< \mathcal{O} >$ and $< \mathcal{O}^2 >$ in any normalised state $|\psi>$ satisfy $< \mathcal{O}^2 > \ \geq \ < \mathcal{O} >^2$. Prove that equality holds if and only if $|\psi>$ is an eigenstate of $\mathcal{O}$.

26. For the one-dimensional Hamiltonian

$$H = \frac{p^2}{2m} + \lambda x^4 \ ,$$

where λ is positive, use the position-momentum uncertainty relation to show that the ground state energy satisfies

$$E_0 \ \geq \ \frac{3}{4} \left(\frac{\lambda \hbar^4}{4m^2}\right)^{1/3} .$$

[Use the inequality, which follows from the previous problem, that $< x^4 > \ \geq \ < x^2 >^2$ in any state].

27. Let A, B and C be three Hermitian operators such that $[A, B] = iC$. If $|\psi>$ is a normalised eigenstate of C with eigenvalue λ, show that the uncertainties ΔA and ΔB in the state $|\psi>$ must satisfy $\Delta A \Delta B \geq |\lambda|/2$.

    [We define ΔA as the square root of the expectation value of $(A - <A>)^2$ in the state $|\psi>$, where $<A>$ is the expectation value of A in $|\psi>$. ΔB is defined in a similar way].

28. Find all the 2×2 Hermitian matrices A whose square is equal to the identity matrix I. For all such matrices, calculate $e^{i\theta A}$, where θ is a real number, and show that the answer can be written in terms of the matrices I and A.

29. Suppose that there are four operators L_z, A_x, A_y and A_z satisfying $[L_z, A_x] = i\hbar A_y$, $[L_z, A_y] = -i\hbar A_x$, and $[L_z, A_z] = 0$. Show that the operator $U = e^{i\theta L_z/\hbar}$ satisfies

$$\begin{aligned} U A_x U^{-1} &= A_x \cos\theta \ - \ A_y \sin\theta \ , \\ U A_y U^{-1} &= A_y \cos\theta \ + \ A_x \sin\theta \ , \\ U A_z U^{-1} &= A_z \ . \end{aligned}$$

30. Let L_i denote the three angular momentum operators; i may denote x, y or z. We say that an operator $\mathcal{O}$ transforms like a scalar under rotations if $[L_i, \mathcal{O}] = 0$ for all i. Similarly, three operators $A_i = (A_x, A_y, A_z)$ are said to transform like a vector under rotations if

$$[L_i, A_j] \ = \ i\hbar \sum_{k=x,y,z} \epsilon_{ijk} \ A_k \ .$$

    (i) If $\mathcal{O}$ and $\vec{A}$ transform like a scalar and vector respectively, show that $\mathcal{O}\vec{A}$ transforms like a vector. If $\vec{A}$ and $\vec{B}$ transform like vectors, show that $\vec{A} \cdot \vec{B}$ transforms like a scalar, and $\vec{A} \times \vec{B}$ transforms like a vector. (All this is true whether or not $\mathcal{O}$, $\vec{A}$ and $\vec{B}$ commute with each other).

    (ii) Verify that $\vec{r}$ and $\vec{p}$ transform like vectors.

31. Consider the matrices

$$T_z \ = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad T_x \ = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad T_y \ = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix},$$

and

$$T'_z \;=\; \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad T'_x \;=\; \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad T'_y \;=\; \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix},$$

Construct a unitary matrix U such that $UT_iU^{-1} = T'_i$ for $i = x, y$ and z.

Hint: If x_n are the three normalised eigenvectors of T_z with the eigenvalues λ_n, and x'_n are the corresponding eigenvectors of T'_z with the same eigenvalues, then $U = \sum_n x'_n x^\dagger_n$ satisfies $UT_zU^{-1} = T'_z$. Note that the vectors x_n and x'_n have some phase ambiguities; these ambiguities can be fixed by explicitly checking that the same matrix U also satisfies $UT_xU^{-1} = T'_x$ and $UT_yU^{-1} = T'_y$.

32. The Hamiltonian governing the rotational motion of a system with angular momentum $l = 1$ is given by

$$H \;=\; aL_x^2 \;+\; bL_y^2 \;+\; cL_z^2 \;.$$

Find all the energy levels.

33. Consider an eigenstate of $\vec{L}^2$ and L_z denoted by $|l, m>$. Let $A = \hat{n} \cdot \vec{L}$ denote an operator, where $\hat{n}$ is a unit vector; we can parametrise it in terms of two angles as $(n_x, n_y, n_z) = (\sin\alpha\cos\beta, \sin\alpha\sin\beta, \cos\alpha)$. In terms of (α, β), calculate the expectation value $< A >$ and the uncertainty ΔA in the state $|l, m>$.

(Note: The angles α and β are fixed numbers, and the operators L_x, L_y, L_z do not act on them).

34. Consider a particle with angular momentum $\vec{J}$ with $\vec{J}^2 = j(j+1)\hbar^2$. Let $\hat{n} = (\sin\alpha\cos\beta, \sin\alpha\sin\beta, \cos$ be a unit vector. Verify that the state $|\psi>$ given by

$$|\psi> \;=\; \sum_{m=-j}^{j} e^{i(j-m)\beta} \left(\frac{(2j)!}{(j-m)!(j+m)!}\right)^{1/2} \left(\cos\frac{\alpha}{2}\right)^{j+m} \left(\sin\frac{\alpha}{2}\right)^{j-m} |j_z = m>$$

satisfies $\hat{n} \cdot \vec{J}|\psi >= j\hbar|\psi >$.

(Note: The angles α and β are fixed numbers, and the operators J_x, J_y, J_z do not act on them).

35. Consider the angular momentum matrices

$$L_z \;= \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad \text{and} \quad L_x \;= \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

for a particle with orbital angular momentum $l = 1$. Find the normalised eigenvectors of L_x corresponding to the eigenvalues $\hbar$, 0 and $-\hbar$. (The phases of the three eigenvectors are unimportant; hence you can choose the phases in any way you like).

Show that the state with eigenvalue $L_x = \hbar$ can be transformed to the state with eigenvalue $L_x = -\hbar$ by rotating around the $\hat{z}$ axis by an appropriate angle; find this angle. Show that it is impossible to transform the state with eigenvalue $L_x = \hbar$ to the state with eigenvalue $L_x = 0$ by rotating around the $\hat{z}$ axis by any angle.

36. Find the energy levels and corresponding wave functions of the isotropic simple harmonic oscillator in three dimensions using polar coordinates (r, θ, ϕ). (You don't have to normalise the wave functions).

    If the energy levels are written as $E_N = (N + 3/2)\hbar\omega$, where $N = 0, 1, 2, \cdots$, what are the allowed values of the orbital angular momentum l for a given value of N? Using this information, show that the degeneracy of the energy level E_N is given by $(N+1)(N+2)/2$.

37. Hidden symmetry:

    (i) Find the energy levels and degeneracies of the two-dimensional isotropic simple harmonic oscillator.

    (ii) Use the two sets of raising and lowering operators (given in terms of the coordinates x, y) to construct three operators which commute with the Hamiltonian and also satisfy the commutations relations of 'angular momentum' amongst each other. Show that these operators can be used to explain the degeneracies in this problem. Which representation of 'angular momentum' describes states with a given energy E?

    (iii) Can you write the angular momentum operator L_z in terms of the above operators?

38. (i) A two-dimensional representation of the angular momentum algebra is given by the three matrices

$$J_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad J_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \text{and} \quad J_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

    Given a unit vector $\hat{n} = (n_x, n_y, n_z)$, use various properties of the Pauli matrices to find the rotation matrix $R = \exp(i\alpha\hat{n} \cdot \vec{J}/\hbar)$. (This operator rotates by an angle α about the direction $\hat{n}$).

    What is the value of R for $\alpha = 2\pi$?

    (ii) A three-dimensional representation of angular momentum is given by

$$J_x = \hbar\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad J_y = \hbar\begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, \quad J_z = \hbar\begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

    (These matrices can be written in short as $(J_i)_{jk} = -i\hbar\epsilon_{ijk}$). Calculate the rotation matrix $R = \exp(i\alpha\hat{n} \cdot \vec{J}/\hbar)$.

    Hint: By symmetry, the matrix elements R_{ij} can only be a linear combination of the three matrices δ_{ij}, $n_i n_j$ and $\sum_k \epsilon_{ijk} n_k$, with coefficients which can only be functions of α. Find the three coefficients by considering the special case $\hat{n} = (0, 0, 1)$.

39. Find all the Clebsch-Gordan coefficients when two angular momenta $\vec{J}_1$ and $\vec{J}_2$ are combined to give $\vec{J} = \vec{J}_1 + \vec{J}_2$, if $j_1 = 3/2$ and $j_2 = 1/2$, namely, find the inner products $< j, j_z | j_1 = 3/2, j_{1z}; j_2 = 1/2, j_{2z} >$ for all the possible values of j, j_z, j_{1z} and j_{2z}. What are the eigenvalues of the operator $\vec{J}_1 \cdot \vec{J}_2$ in the various possible states $|j, j_z >$?

40. Consider an electron whose spin is initially pointing along the direction $\hat{n}$, where $\hat{n} = (\sin\theta, 0, \cos\theta)$ is a unit vector. It is then acted on by a magnetic field of the form $\vec{B} = B\ \hat{z}$. Find the spin wave function of the electron as a function of time, and use that to calculate the three expectation values $< S_x >$, $< S_y >$, and $< S_z >$.

41. Consider an electron whose spin is pointing in the $+\hat{z}$ direction at time $t = 0$. The Hamiltonian is given by $H = \mu_B \vec{\sigma} \cdot \vec{B}$ when a magnetic field $\vec{B}$ is applied. Suppose that $\vec{B} = B(t)\ \hat{x}$ where

$$\begin{aligned} B(t) &= B_0 \quad \text{for} \quad 0 \le t \le T, \\ &= 0 \quad \text{for} \quad t > T. \end{aligned}$$

(i) In which direction will the spin point at time $t > T$?

(ii) Find the minimum value of B_0 such that the spin will point in the $-\hat{z}$ direction at time $t > T$.

42. Consider three $s = 1/2$ spins coupled to each other by the Hamiltonian

$$H = -A\,[\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3 + \vec{S}_3 \cdot \vec{S}_1] - BS_z,$$

where A and B are some constants, and $S_z = S_{1z} + S_{2z} + S_{3z}$.

(i) Find all the energy levels and label all the eigenstates using the total spin $\vec{S}^2 = (\vec{S}_1 + \vec{S}_2 + \vec{S}_3)^2$ and S_z. (You don't have to find the eigenstates of H).

(ii) Let us set $B = 0$. What is the energy, total spin and degeneracy of the ground state if (i) $A > 0$ (called a ferromagnetic system), and (ii) $A < 0$ (called antiferromagnetic)?

43. Consider three spins each of which has $s = 1/2$. Find all the eigenvalues and the explicit forms of the corresponding eigenstates of both the total spin squared $\vec{S}^2$ (where $\vec{S} = \vec{S}_1 + \vec{S}_2 + \vec{S}_3$) and the total $S_z = S_{1z} + S_{2z} + S_{3z}$. You have to write the eigenstates as superpositions of the eight states $|\uparrow\uparrow\uparrow\rangle$, $|\uparrow\uparrow\downarrow\rangle$, $\cdots$, $|\downarrow\downarrow\downarrow\rangle$. Make sure that the eigenstates are orthonormal.

44. Consider four spin-1/2 objects coupled to each other by the following Hamiltonian

$$H = -A\,[\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_1 \cdot \vec{S}_3 + \vec{S}_1 \cdot \vec{S}_4 + \vec{S}_2 \cdot \vec{S}_3 + \vec{S}_2 \cdot \vec{S}_4 + \vec{S}_3 \cdot \vec{S}_4].$$

Show that the total spin component $S_z = S_{1z} + S_{2z} + S_{3z} + S_{4z}$ commutes with H. In the same way, we can show that total S_x and S_y commute with H, but you don't have to show this. Now show that the total spin squared, $\vec{S}^2 = (\vec{S}_1 + \vec{S}_2 + \vec{S}_3 + \vec{S}_4)^2$, also commutes with H.

For $A > 0$, it turns out that one of the ground states is given by the state in which all the four spins have $S_{iz} = \hbar/2$. What is the energy and total spin of this state? Hence find the degeneracy of the ground state.

45. For the $j = 3/2$ representation of the angular momentum algebra, find the 4×4 matrices for J_x, J_y and J_z using the relations

$$\begin{aligned} J_z \; |j, m> \quad &= \quad m\hbar \; |j, m> \;\; , \\ J_+ \; |j, m> \quad &= \quad \hbar \; \sqrt{j(j+1) - m(m+1)} \; |j, m+1> \;\; , \\ J_- \; |j, m> \quad &= \quad \hbar \; \sqrt{j(j+1) - m(m-1)} \; |j, m-1> \;\; . \end{aligned}$$

Verify explicitly that $\vec{J}^2 = j(j+1)\hbar^2 \; I$.

46. Holstein-Primakoff transformation: There is a striking similarity between the equal spacing of the eigenvalues of J_z (in any particular representation of angular momentum labelled by an integer or half-integer value of j) and the raising and lowering operators J_+ and J_- on the one hand, and the equal spacing of the energy levels of a simple harmonic oscillator and the raising and lowering operators $a^\dagger$ and a on the other hand.

(i) Show that if we define

$$\begin{aligned} J_z \quad &= \quad \hbar \; (j - a^\dagger a) \;\; , \\ J_+ \quad &= \quad \hbar \; (2j - a^\dagger a)^{1/2} \; a \;\; , \\ J_- \quad &= \quad \hbar \; a^\dagger (2j - a^\dagger a)^{1/2} \;\; , \end{aligned}$$

then they satisfy the angular momentum commutation relations and the relation $\vec{J}^2 = j(j+1)\hbar^2$ if $[a, a^\dagger] = 1$. (Do these calculations using only J_z, J_+ and J_-. You don't have to introduce J_x and J_y).

[The square root of an operator is defined as a Taylor expansion, namely,

$$(2j - a^\dagger a)^{1/2} \;\; = \;\; (2j)^{1/2} \; [\; 1 \; - \; \frac{1}{2}\Big(\frac{a^\dagger a}{2j}\Big) \; - \; \frac{1}{8}\Big(\frac{a^\dagger a}{2j}\Big)^2 \; - \; \ldots \;] \; .$$

However, you do not need to make this expansion in this problem].

(ii) What are the maximum and minimum possibles values of $a^\dagger a$ in this representation?

47. Landau levels: Consider a particle with charge q and mass m moving in a uniform magnetic field $\vec{B} = B\hat{z}$. Let the vector potential be given by $A_x = 0$, $A_y = Bx$, $A_z = 0$. Find all the energy levels and the corresponding wave functions in terms of the cyclotron frequency $\omega_c = |qB|/mc$. Show that each energy level has an infinite degeneracy if the plane perpendicular to $\vec{B}$ has an infinite area (ignore any degeneracy arising from motion in the $\hat{z}$ direction).

48. Landau levels: Consider an electron with charge $-e$ and mass m moving in two dimensions in the presence of a magnetic field $\vec{B} = B\hat{z}$ with a vector potential given by $A_x = 0$ and $A_y = Bx$. [Ignore the z coordinate in this problem. Also, assume that $eB > 0$ and define $\omega_c = eB/(mc)$]. Let us define the four operators

$$\begin{aligned}
a &= \sqrt{\frac{c}{2\hbar eB}}\, [p_x - i\,(p_y + \frac{eBx}{c})], \\
a^\dagger &= \sqrt{\frac{c}{2\hbar eB}}\, [p_x + i\,(p_y + \frac{eBx}{c})], \\
b &= \sqrt{\frac{c}{2\hbar eB}}\, [(p_x + \frac{eBy}{c}) + ip_y], \\
b^\dagger &= \sqrt{\frac{c}{2\hbar eB}}\, [(p_x + \frac{eBy}{c}) - ip_y].
\end{aligned}$$

(i) Calculate the commutators between all possible pairs of these operators.

(ii) Write the Hamiltonian

$$H = \frac{1}{2m}\,(\vec{p} - \frac{q}{c}\vec{A})^2 + \frac{e}{mc}\,\vec{S}\cdot\vec{B}$$

in terms of a, $a^\dagger$, b, $b^\dagger$ and σ^z.

(iii) Use the result in (ii) to find all the energy levels and show that each of these levels has an infinite degeneracy. (We are assuming that the coordinates x and y go from $-\infty$ to $+\infty$, so that the system has an infinite area).

49. Landau levels:

(i) Consider a spinless particle with charge q and mass m moving in a uniform magnetic field, say, $\vec{B} = B\hat{z}$. Use the 'symmetric gauge' $\vec{A} = (1/2)\vec{B}\times\vec{r}$ and cylindrical coordinates (r, ϕ, z). [In these coordinates, the Laplacian is $\vec{\nabla}^2 = \partial^2/\partial r^2 + (1/r)\partial/\partial r + (1/r^2)\partial^2/\partial\phi^2$]. Find the energy levels in terms of the cyclotron frequency $\omega_c = |qB|/mc$. Show that each energy level has an infinite degeneracy if the plane perpendicular to $\vec{B}$ has an infinite area (ignore any degeneracy arising from motion in the $\hat{z}$ direction).

(ii) Let us now concentrate on the ground states. What do the probability densities $|\psi|^2$ look like in the different states? Suppose that the particle is constrained to move inside a large circular disc in the $x-y$ plane; *large* means that the area of the disc $\pi R^2 >>$ the 'Landau area' $2\pi\hbar c/|qB|$. What is the degeneracy of the ground state in terms of these two areas?

(iii) Finally, assume that the particle is a spin-1/2 electron. Find the energy levels and degeneracies in that case.

50. Consider a particle with charge q and mass m moving in a uniform magnetic field $\vec{B} = B\hat{z}$ and a uniform electric field $\vec{E} = F\hat{x}$. Let the vector potential be given by $A_x = 0$, $A_y = Bx$, $A_z = 0$. (Assume that the particle is moving in the $x-y$ plane and ignore its motion in the $\hat{z}$-direction).

(i) Find all the energy levels and show that they depend on the momentum in the $\hat{y}$-direction denoted by p_y.

(ii) Find the group velocity in the $\hat{y}$-direction given by $v_y = \partial E/\partial p_y$.

51. Consider a simple model of a one-dimensional ferromagnet, namely, N spin-1/2 objects placed around a circle with the Hamiltonian

$$H \;=\; -\; J \sum_{n=1}^{N} \vec{S}_n \cdot \vec{S}_{n+1} \;,$$

where we assume the periodic boundary condition $\vec{S}_{N+1} \equiv \vec{S}_1$ and $J > 0$.

(i) Show that the total $S_z = \sum_n S_{nz}$ and the total spin $\vec{S}^2 = (\sum_n \vec{S}_n)^2$ are good quantum numbers, namely, they commute with H.

(ii) A ground state of this system is the state $|\psi_0>$ in which all spins point up, namely, $S_{nz} = \hbar/2$ (denoted by $\uparrow$) for all n. What is the total spin S of $|\psi_0>$, i.e., $\vec{S}^2|\psi_0>= S(S+1)\hbar^2|\psi_0>$? Find the ground state energy E_0 and degeneracy.

(iii) Now consider a state

$$|k> \;\equiv\; \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{ikn} \;|n> \;\;,$$

where $|n>$ denotes the state in which the spin at site n points down and the spins at all the other states point up. (Note that k must be equal to $2\pi p/N$, where $p = 0, 1, 2, \ldots, N-1$). Show that $|k>$ is an eigenstate of H, and find its energy $E(k)$ as a function of k. What is the total spin of $|k>$ as a function of k?

The state $|k>$ is called a spin wave or magnon of wave number k, and the function $E(k) - E_0$ is called its dispersion relation.

52. Fine structure: The normalised wave functions in the $2P$ states of an electron in a hydrogen atom are given by

$$\psi_{n=2,l=1,m,s_z} \;=\; \frac{r}{a_0^{5/2}\sqrt{24}} \; e^{-r/2a_0} \; Y_1^m \; (\theta, \phi)$$

times

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \text{for} \quad s_z \;=\; \pm\,\hbar/2 \;.$$

The wave functions have been normalised such that

$$\begin{aligned} \int \sin\theta d\theta d\phi \; Y_1^{m'\star} \; Y_1^m \;&=\; \delta_{mm'} \\ \text{and} \quad \int d^3\vec{r} \; \psi^\dagger_{2,1,m',s_z'} \; \psi_{2,1,m,s_z} \;&=\; \delta_{mm'} \; \delta_{s_z s_z'} \;. \end{aligned}$$

Use first order perturbation theory to calculate the energy splitting between the $j = 3/2$ and $j = 1/2$ states produced by the spin-orbit interaction

$$\frac{e^2}{2m^2c^2r^3}\,\vec{L}\cdot\vec{S}\ .$$

Express your answer in eV using the values of the fine structure constant $\alpha = e^2/\hbar c \simeq 1/137$, the Bohr radius $a_0 = \hbar^2/me^2 = 0.529$ Å, and $e^2/2a_0 = 13.6$ eV.

53. Hyperfine structure: The hyperfine splitting in the hydrogen atom is produced by the interaction between the proton's magnetic dipole moment $\vec{\mu}_p = (g_p e/2Mc)\vec{S}_p$ and the electron's dipole moment $\vec{\mu}_e = -(e/mc)\vec{S}_e$. Here M and m denote the proton and electron masses, $-e$ is the electron charge, $\vec{S}_p$ and $\vec{S}_e$ are the proton and electron spin operators, and $g_p = 5.59$ is the g-factor of the proton.

    In a state with $l = 0$, the hyperfine interaction is given by

$$V \;=\; -\;\frac{8\pi}{3}\;\vec{\mu}_e\cdot\vec{\mu}_p\;\delta^3(\vec{r})\ .$$

    Use first order perturbation theory to calculate the energy splitting in eV between the $j = 0$ and $j = 1$ states in the $1S$ state of the H atom. Note that the normalised wave functions of these states are given by

$$\psi_{n=1,l=0,m=0} \;=\; \frac{1}{a_0^{3/2}\sqrt{\pi}}\;e^{-r/a_0}$$

    times the appropriate spin wave functions of the electron and proton. What is the wavelength of the photon emitted in a transition between the two states? (Use the values of α and a_0 given in the previous problem, $M/m = 1840$, and $2\pi\hbar c = 12400$ eV-Å).

54. Consider a particle with orbital angular momentum $l = 1$ and spin $s = 1/2$. (Ignore the radial part of the wave function in this problem). Suppose that the Hamiltonian is given by

$$H \;=\; A\,\vec{L}\cdot\vec{S} \;+\; B\,(L_z \;+\; 2S_z),$$

    where A and B are some constants.

    (i) Show that $J_z = L_z + S_z$ commutes with H. This implies that we can work in the basis of eigenstates of J_z.

    (ii) Find all the six energy levels exactly in terms of A and B. What are the values of J_z in these six levels?
    (Hint: Note that in the basis of eigenstates of J_z, the 6×6 matrix for H breaks up into blocks of sizes 1, 2, 2 and 1. So you will not need to find the eigenvalues of any matrix bigger than 2×2).

    (iii) What happens to all these energy levels in the two limits $A = 0$ and $B = 0$ respectively?

55. Three distinguishable particles have the same spin S, namely, $\vec{S}_n^2 = S(S+1)\hbar^2$ for $n = 1, 2, 3$. If the Hamiltonian is $H = A(\vec{S}_1 + \vec{S}_2 + \vec{S}_3)^2$ and $A > 0$, what is the energy, spin and degeneracy of the ground state if (i) S is an integer, and (ii) S is a half-odd-integer?

56. Consider a two-dimensional isotropic harmonic oscillator with

$$H_0 = \frac{1}{2m}(p_x^2 + p_y^2) + \frac{1}{2}m\omega^2(x^2 + y^2).$$

(i) We know that the second excited states with $E_2^{(0)} = 3\hbar\omega$ have a three-fold degeneracy. Use degenerate perturbation theory to calculate the shifts in these three energy levels, to first order in λ, if we add a perturbation $V = \lambda m\omega^2 xy$. What are the eigenstates corresponding to these energy levels?

(ii) Find the same three energy levels exactly for the Hamiltonian

$$H = \frac{1}{2m}(p_x^2 + p_y^2) + \frac{1}{2}m\omega^2(x^2 + y^2) + \lambda m\omega^2 xy.$$

(iii) Show that the perturbative results and exact results agree to first order in λ.

57. Consider a three-dimensional isotropic harmonic oscillator with

$$H_0 = \frac{\vec{p}^2}{2m} + \frac{1}{2}m\omega^2\vec{r}^2 .$$

We know that the first excited states with $E_1^{(0)} = \frac{5}{2}\hbar\omega$ have a three-fold degeneracy.

(i) Use degenerate perturbation theory to calculate the shifts in these three energy levels, to first order in λ, if we add a perturbation $V = \lambda m\omega^2(xy + yz)$.

(ii) Now calculate these three energy levels exactly for the total Hamiltonian $H = H_0 + V$.

(iii) Show that your exact answers agree to first order in λ with those obtained using perturbation theory.

(iv) Use the exact calculation to show that the problem becomes ill-defined if $|\lambda| > 1/\sqrt{2}$.

58. Consider the one-dimensional anharmonic oscillator with

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + \lambda x^4$$

where λ is small compared to the other parameters in the problem.

(i) Use first order perturbation theory to calculate the change in the energy of the n^{th} state.

(ii) Use second order perturbation theory to calculate the change in the ground state energy.

59. Consider a one-dimensional anharmonic oscillator with $H = H_0 + V$, where

$$H_0 \;=\; \frac{p^2}{2m} \;+\; \frac{1}{2} m\omega^2 x^2 \quad \text{and} \quad V \;=\; \lambda_1 x^3 \;+\; \lambda_2 x^4 \;,$$

and λ_1 and λ_2 are small compared to the other parameters in the problem.

Use first and second order perturbation theory to calculate the change in the energy of the ground state up to second order in λ_1 and λ_2, i.e., terms proportional to $\lambda_1,\ \lambda_2,\ \lambda_1^2,\ \lambda_2^2$ and $\lambda_1 \lambda_2$.

60. Consider a one-dimensional oscillator with $H = H_0 + V$, where

$$H_0 \;=\; \frac{p^2}{2m} \;+\; \frac{1}{2} m\omega^2 x^2 \quad \text{and} \quad V \;=\; \lambda x^2,$$

and λ is small compared to the other parameters in the problem.

(i) Calculate all the energy levels of H exactly.

(ii) Use first and second order perturbation theory to calculate the change in the energy of the n-th state of H_0 up to second order in λ. Show that the perturbative result agrees with the exact expression up to order λ^2.

61. Consider a one-dimensional problem with a Hamiltonian given by

$$H \;=\; \frac{p^2}{2m} \;+\; V(x),$$

where x and p are operators. Let us denote the eigenstates and eigenvalues of H by $|n\rangle$ and E_n respectively; we will assume that E_n only takes a discrete set of values.

(i) Calculate the double commutator $[x, [H, x]]$.

(ii) Use this and the fact that the identity operator can be written as the sum $I = \sum_{n'} |n'\rangle\langle n'|$ to derive the equation

$$\sum_{n'} \; (E_{n'} \;-\; E_n) \; |\langle n'|x|n\rangle|^2 \;=\; \frac{\hbar^2}{2m}.$$

This is an example of a 'sum rule'. Note that it holds for every eigenstate $|n\rangle$.

(iii) Show explicitly that the above sum rule is satisfied for every eigenstate of H for the case $V = (1/2) m\omega^2 x^2$.