Problem 1: Warming up

1. If A and B are two operators such that $[A, B] = \lambda$, where λ is a complex number, and if μ is a second complex number, prove that

$$\exp\left[\mu(A+B)\right] = \exp(\mu A)\exp(\mu B)\exp(-\mu^2\lambda/2)$$

2. **The Ehrenfest theorem**

   Consider the quantum mechanical description of a particle of mass m falling freely under gravity. The Hamiltonian of the particle is given by

$$\hat{H} = \frac{\hat{p}_z^2}{2m} + mg\hat{z}$$

   (a) Find the equations of motion satisfied by the expectation values of position and momentum operators, i.e., calculate $d\langle\hat{z}\rangle(t)/dt$ and $d\langle\hat{p}_z\rangle(t)/dt$.

   (b) Show that the total energy is conserved.

   (c) Set yp and solve the second order differential equation of motion for $\langle\hat{z}\rangle(0) = h$ and $\langle\hat{p}_z\rangle(0) = 0$. Compare your result with the classical equation of motion.

3. **Particle in 1D square well**

   Consider a quantum mechanical particle of mass m in the ground state of a 1D infinite square well of width a.

   (a) If the energy of the particle is measured, what are the possible outcomes and corresponding probabilities?

   (b) If the position of the particle is measured, what are the possible outcomes and corresponding probability densities?

   (c) If the momentum of the particle is measured, what are the possible outcomes and corresponding probabilities? (Hint: Express the wave function as a superposition of the eigenstates of the momentum operator, p_x)

4. **Radial momentum operator**

   (a) Show that $\hat{r}\cdot\vec{p}$ is not hermitian and find it's hermitian conjugate.

   (b) The hermitian radial momentum pr is then constructed as follows

$$\hat{p}_r = \frac{(\hat{r}\cdot\vec{p}) + (\hat{r}\cdot\vec{p})^\dagger}{2}.$$

Show that p_r is given by the expression

$$\hat{p}_r = -i\hbar \frac{1}{r}\left(\frac{\partial}{\partial r} r\right).$$

(c) calculate the commutator $[\hat{r}, \hat{p}_r]$ between the position operator $\hat{r}$ and the radial momentum operator.

(d) Calculate the expectation value of p_r for the ground state Hydrogen atom.

5. **Hydrogenic atoms**

(a) Calculate $\langle \vec{p} \rangle$ for the ground state of the Hydrogen atom.

(b) Calculate $\langle p \rangle$ for the ground state of the Hydrogen atom, where p is the magnitude of momentum.

(c) Using the generating function for the associated Laguerre polynomials

$$\begin{aligned} U_p(\rho, 2) &= \frac{(-s)^p \exp[-\rho s/(1-s)]}{(1-s)^{p+1}} \\ &= \sum_{q=p}^{\infty} \frac{L_q^p(\rho)}{q!} s^q, \qquad\qquad |s| < 1 \end{aligned}$$

show that the average values

$$\langle r^k \rangle_{nlm} = \int \psi_{nlm}^*(\mathbf{r}) r^k \psi_{nlm}(\mathbf{r}) d\mathbf{r} = \int_0^\infty |R_{nl}(r)|^2 r^{k+2} dr$$

are given respectively for $k = 1, -1, -2,$ and -3 by

$$\langle r \rangle_{nlm} = a_\mu \frac{n^2}{Z}\left\{1 + \frac{1}{2}\left[1 - \frac{l(l+1)}{n^2}\right]\right\}$$

$$\langle r^{-1} \rangle_{nlm} = \frac{Z}{a_\mu n^2}$$

$$\langle r^{-2} \rangle_{nlm} = \frac{Z^2}{a_\mu^2 n^3 \left(l + \frac{1}{2}\right)}$$

$$\langle r^{-3} \rangle_{nlm} = \frac{Z^3}{a_{mu}^3 n^3 l \left(l + \frac{1}{2}\right)(L+1)}.$$

Problem 2: Angular Momenta

1. **Angular Momenta and Uncertainty**

   (a) Using the basic commutator relations, $[\hat{x}_a, \hat{p}_b] = i\hbar\delta_{ab}$, show that

   $$[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z, \quad [\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x, \quad [\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y.$$

   (b) The commutator relations you derived above imply an important set of uncertainty relations amongst the angular momenta,

   $$\Delta L_x \Delta L_y \geq \frac{\hbar}{2}|\langle\hat{L}_z\rangle|, \quad \Delta L_y \Delta L_z \geq \frac{\hbar}{2}|\langle\hat{L}_x\rangle|, \quad \Delta L_z \Delta L_x \geq \frac{\hbar}{2}|\langle\hat{L}_y\rangle|.$$

   Consider a particle in a normalized eigenstate of $\hat{L}^2$ and $\hat{L}_z$, $|\psi\rangle = |l, m\rangle$.

   (a) Show that in this case $\langle\hat{L}_x\rangle = \langle\hat{L}_y\rangle = 0$. Hint: use the operators $\hat{L}_+$ and $\hat{L}_-$.

   (b) Show that $\langle\hat{L}_x^2\rangle = \langle\hat{L}_y^2\rangle = \frac{\hbar^2}{2}[l(l+1) - m^2]$. Hint: use $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$.

   (c) Using your results, verify the first uncertainty relation above. Can the uncertainty in any two components of $\vec{L}$ ever vanish simultaneously?

2. **Rotation generators**

   (a) For an observable that satisfies $A^2 = I$ where I is an identity show the following holds

   $$e^{iA\theta} = I\cos\theta + iA\sin\theta$$

   (b) For $J = 1/2$ the components of angular momentum is given bellow in J_z basis

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

   Now take $\pi/2$ rotation along $\hat{x}$ axis, i.e. $R = e^{-\frac{i}{\hbar}J_x\frac{\pi}{2}}$. Show that the components of angular momentum transform as follows: $J'_x = J_x$, $J'_y = J_z$, and $J'_z = -J_y$.

3. **Products of Spin Operators**

   For $s = 1/2$ system the components of spin are given

   $$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

in S_z basis

$$|\alpha\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\beta\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

(a) Let us call a numerical operator as an operator giving the same eigenvalue for any spin state $|\chi\rangle = a|\alpha\rangle + b|\beta\rangle$, where $|a|^2 + |b|^2 = 1$. In particular, show that $S_x^2 = S_y^2 = S_z^2 = \hbar^2/4$.

(b) Anticommutator is defined as $[A, B]_+ = AB + BA$. Show that the following holds for any state $|\chi\rangle$

$$[S_x, S_y]_+ = 0, \quad [S_y, S_z]_+ = 0, \quad [S_z, S_x]_+ = 0.$$

(c) Show that the anticommutator relations in (b) together with commutation relations between the spin components result in the expressions bellow

$$S_x S_y = \frac{i\hbar}{2} S_z, \quad S_y S_z = \frac{i\hbar}{2} S_x, \quad S_z S_x = \frac{i\hbar}{2} S_y.$$

(d) These expressions are useful in simplifying products of spin components. In particular, show that

$$S_x S_y S_x = -\frac{\hbar^2}{4} S_y.$$

4. **Half Integer Spherical Harmonics Are Not Allowed**

We have seen that the commutation relations for angular momentum operators allow $l = 0, 1/2, 1, 3/2, 2, 5/2, \cdots$. However, closer inspection shows that it is not possible to formulate the quantum mechanics of orbital angular momentum consistently in the Hilbert spaces with half-integer orbital angular momentum.

(a) Assume that $l = 1/2$ is allowed. Then spherical harmonics for $l = 1/2$ should exist. Find the spherical harmonic for $l = m = 1/2$ (as we found the Y_{lm} for integer l) by using the equations:

$$\begin{aligned} L_+ |l = \frac{1}{2}, m = \frac{1}{2}\rangle &= 0 \\ L_z |l = \frac{1}{2}, m = \frac{1}{2}\rangle &= \frac{\hbar}{2} |l = \frac{1}{2}, m = \frac{1}{2}\rangle \end{aligned}$$

Your answer should be of the form:

$$Y_{\frac{1}{2},\frac{1}{2}} = N(\sin\theta)^a e^{ib\varphi}$$

Find a, b, and show that $Y_{\frac{1}{2},\frac{1}{2}}$ is normalizable.

(b) Repeat part 1. for $l = \frac{1}{2}$, $m = -\frac{1}{2}$.

(c) Now show that the operator L_- applied to $Y_{\frac{1}{2},\frac{1}{2}}$ does not give $Y_{-\frac{1}{2},\frac{1}{2}}$ [Since the only ingredients that went into the derivation of the relation $L_- |l,m\rangle \propto |l,m-1\rangle$ were the commutation relations of the $\hat{L}_k$ and the fact that they are Hermitian, we are forced to conclude that we cannot implement orbital angular momentum in terms of Hermitian operators on the Hilbert (sub)space spanned by $l = \frac{1}{2}$, $m = \pm\frac{1}{2}$.]

(d) Suppose you were to construct the spherical harmonic for $l = 3/2$, $m = 3/2$ in the manner of part 1. You would be led to the result,

$$Y_{3/2,3/2} = c(\sin\theta)^{3/2} e^{3i\varphi/2}$$

which satisfies $L_+ Y_{3/2,3/2} = 0$. Generate $Y_{3/2,-3/2}$ by repeated use of L_-. Show that the state you obtained does not satisfy $L_- Y_{3/2,-3/2} = 0$ and is not even normalizable.

Problem 3: Time-Independent Perturbation Theory

1. **Time independent, non-degenerate**

   (a) Calculate the correction to the ground state energy to the lowest non-vanishing order of a simple harmonic oscillator due to a anharmonic perturbation $H' = bx$.

   (b) Find the exact energy of the ground state of (a) and compare the result.

2. Calculate the first and second order energy corrections to the ground state energy of a charged particle with charge q in an infinite square well $[-a/2, a/2]$ due to a weak external electric field $H' = qEx$.

3. **Ground-State of Helium atoms** Consider the Helium atom: nuclear charge $2e$, 2 electrons with coordinates $\mathbf{r_1}$ and $\mathbf{r_2}$. Hamiltonian for this system is given by

$$H = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - \frac{2e^2}{4\pi\epsilon_0}\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + \frac{e^2}{4\pi\epsilon_0 r_{12}}$$

   where $r_{12} = |\mathbf{r_1} - \mathbf{r_2}|$.

   Consider the e-e interaction term to be a weak perturbation. Using time independent perturbation theory, obtain the 1st order correction to the ground state energy. The ground-state wavefunction for the unperturbed Hamiltonian is

$$\psi_0 = \psi_{1s}(r_1)\psi_{1s}(r_2), \quad \psi_{1s}(r_1) = \frac{1}{\sqrt{\pi}}\left(\frac{2}{a_0}\right)^{3/2} e^{-2r/a_0}, \quad a_0 = \frac{4\pi\hbar^2\epsilon_0}{me^2}.$$

4. **Time-independent, degenerate**

   Consider a two level system described by the Hamiltonian

$$H = \epsilon_0 \begin{bmatrix} 1 & \alpha \\ \alpha & 1 \end{bmatrix}$$

   where α is real and $\alpha \ll 1$.

   (a) By decomposing this Hamiltonian into $H = H_0 + H'$, find the eigenvalues and eigenvectors of the unperturbed Hamiltonian, H_0. Calculate the correction to the energy eigenvalues due to H' to the lowest non-vanishing order in α.

(b) Solve for the exact eigenvalues of the full Hamiltonian, H. Expand the eigenvalues to lowest non-vanishing order in α and compare with the perturbation results obtained in (a).

5. **Variational Methods**

   Calculate the variational ground state energy for a particle in an infinite square well $[-a, a]$ starting with a trial wave function

$$\phi(x, c) = \begin{cases} (a^2 - x^2)(1 + cx^2), & -a \leq x \leq a \\ 0, & |x| \geq a \end{cases}$$

6. (a) By varying the parameter c in the trial function

$$\phi_0(x) = \begin{cases} (c^2 - x^2)^2, & |x| < c \\ 0, & |x| \geq c \end{cases}$$

   obtain an upper bound for the ground-state energy of a linear harmonic oscillator having the Hamiltonian

$$H = \frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m\omega^2 x^2$$

   (b) Show that the function $\phi_1(x) = x\phi_0(x)$ is a suitable trial function for the first excited state, and obtain a variational estimate of the energy of this level.

Problem 4: Time-dependent Perturbation Theory

1. Consider a 2-level system described by the Hamiltonian

$$H = \begin{bmatrix} E_1^{(0)} & Ve^{i\omega t} \\ Ve^{-i\omega t} & E_2^{(0)} \end{bmatrix}$$

   where $E_1^{(0)} \neq E_2^{(0)}$, and $V \ll E_1^{(0)}, E_2^{(0)}$, i.e. treat $Ve^{i\omega t}$ as a perturbation. At $t = 0$, the system is prepared in the state

$$|\psi\rangle = \frac{1}{\sqrt{2}} \left(|\phi_1\rangle + |\phi_2\rangle\right)$$

   where $|\phi_1\rangle$ and $|\phi_2\rangle$ are the eigenstates of the unperturbed Hamiltonian. Calculate the probability of finding the system in $|\phi_1\rangle$ at any later time t within the framework of 1st order time-dependent perturbation theory.

2. Consider a particle of charge q and mass m, moving in 1D simple harmonic motion along the x-axis so that its Hamiltonian is given by

$$\hat{H}_0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega_0^2 x^2$$

   where ω_0 is the natural frequency of the oscillator. A spatially uniform, but time varying, electric field $E(t)$ directed along the x-axis is switched on at time $t = 0$, so that the system is perturbed by the interaction

$$\hat{H}'(t) = -qxE(t).$$

   $E(t)$ has the form

$$E(t) = E_0 cos(\omega t)$$

   where E_0 is the amplitude and ω is the angular frequency of the field. Assume that the oscillator is in the ground state for $t \leq 0$.

   (a) Using 1st order time-dependent perturbation theory and assuming that $\omega_0 \gg \omega$, calculate the probability of finding the system in any of the excited states at any later time t.

   (b) Why does the procedure fail when $\omega_0 \approx \omega$?

   (c) Calculate the expectation value of the position of the particle as a function of time, $\langle x\rangle(t)$, for both $t \leq 0$ and $t \geq 0$

Problem 5: Scattering

Note: Restricting attention to elastic scattering of a plane wave, one way to derive the cross section for the scattering potentials is by using the Born approximation. In the Born approximation, it is assumed that the incident wave is not substantially affected by the potential. In terms of the incident plane wave vector $\mathbf{k}$ and outgoing plane wave vector $\mathbf{k}'$, the first-order Born amplitude is given by

$$f^{(1)}(\mathbf{k}, \mathbf{k}') = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int d^3x' e^{i(\mathbf{k}-\mathbf{k}').\mathbf{x}'}V(x')$$

which corresponds physically to a single scattering at the point $\mathbf{x}'$. This simple process yields the largest contribution to the exact scattering amplitude, which means that to good approximation $f(\mathbf{k}, \mathbf{k}') \approx f^{(1)}(\mathbf{k}, \mathbf{k}')$. As quantum mechanics dictates, the probability of scattering, i.e. the differential scattering cross section, is given by the squared modulus of the amplitude

$$\frac{d\sigma}{d\Omega} = |f(\mathbf{k}, \mathbf{k}')^2|.$$

The scattering length is defined as

$$\alpha = -\lim_{k\to 0}\frac{\tan\delta_0(k)}{k}$$

which can be found in the low energy limit from the total scattering cross section

$$\sigma_{total} \xrightarrow[k\to 0]{} 4\pi\alpha^2$$

1. Particles with mass m and energy $E = \frac{\hbar^2 k^2}{2m}$ are scattered elastically by a spherically symmetrical potential

$$V(r) = A\delta(r - R), \qquad A, R > 0$$

   (a) Calculate the differential scattering cross section in the 1st Born approximation.

   (b) Use the low energy limit of the scattering amplitude to calculate the scattering length.

2. Particles with mass m and energy $E = \frac{\hbar^2 k^2}{2m}$ are scattered elastically by a spherically symmetrical potential

$$V(r) = V_0\frac{e^{-\alpha r}}{r}$$

(a) Calculate the differential scattering cross section in the 1st Born approximation.

(b) A similar-looking *classical* differential cross section is given by

$$\frac{d\sigma}{d\Omega} = \left(\frac{mZZ'e^2}{|\mathbf{p}^2|}\right) \frac{1}{(1 - \cos\theta)^2}.$$

Find the corresponding potential.

(c) Use the low energy limit of the scattering amplitude to calculate the scattering length.