

Quantum Mechanics
Qualifying Exam - August 2015

Notes and Instructions

- There are 6 problems. Read and attempt all problems, starting with problems you feel the most comfortable doing.
- Partial credit will be given so be sure to complete all parts of the questions you can. It is possible to earn points on latter parts of problems even if you have not completed earlier parts.
- Write on only one side of the paper for your solutions.
- Write your **alias** on the top of every page of your solutions.
- Number each page of your solution with the problem number and page number (e.g. Problem 3, p. 2/4 is the second of four pages for the solution to problem 3.)
- You must show your work to receive full credit.

Possibly useful formulas:

Spin Operator

$$\vec{S} = \frac{\hbar}{2}\vec{\sigma}, \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (1)$$

Angular Momentum Operators,

$$\begin{aligned} J^2 &= J_x^2 + J_y^2 + J_z^2, \quad [J_i, J_j] = i\hbar\epsilon_{ijk}J_k, \quad J_{\pm} = J_x \pm iJ_y \\ J^2|j, m\rangle &= j(j+1)\hbar^2|j, m\rangle, \quad J_z|j, m\rangle = m\hbar|j, m\rangle \\ J_{\pm}|j, m\rangle &= \hbar\sqrt{j(j+1) - m(m \pm 1)}|j, m \pm 1\rangle \end{aligned} \quad (2)$$

In spherical coordinates,

$$\nabla^2\psi = \frac{1}{r}\frac{\partial^2}{\partial r^2}r\psi + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial\psi}{\partial\theta}) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\psi. \quad (3)$$

In cylindrical coordinates,

$$\nabla^2\psi = \frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\psi}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\psi + \frac{\partial^2}{\partial z^2}\psi. \quad (4)$$

Harmonic Oscillator Operators ($\beta = \sqrt{\frac{m\omega}{\hbar}}$)

$$a = \frac{1}{\sqrt{2}}\left(\beta x + \frac{i}{\beta\hbar}p\right), \quad a^\dagger = \frac{1}{\sqrt{2}}\left(\beta x - \frac{i}{\beta\hbar}p\right), \quad [a, a^\dagger] = 1 \quad (5)$$

$$\begin{aligned} H|\Psi_n\rangle &= \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)|\Psi_n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|\Psi_n\rangle \\ \Psi_n(x) &= \frac{1}{\pi^{1/4}}\sqrt{\frac{\beta}{2^n n!}}h_n(\beta x)e^{-\beta^2 x^2/2} \\ h_0(x) &= 1, \quad h_1(x) = 2x, \quad h_2(x) = 4x^2 - 2, \quad h_3(x) = 8x^3 - 12x\ldots \end{aligned} \quad (6)$$

Problem 1: Quantum Currents

For a 1D quantum mechanical system of particles with mass m , the current in a state $\Psi(x, t)$ can be defined as:

$$j(x, t) = \frac{1}{m} \text{Re} (\Psi^*(x, t) P \Psi(x, t)) \quad (1)$$

where P is the momentum operator and Re signifies the real part.

(a) [2 pts] Consider a 1D step-potential

$$\begin{aligned} V(x) &= 0, \quad x < 0, \\ V(x) &= V_0, \quad x > 0 \end{aligned} \quad (2)$$

where $V_0 > 0$, and the 1D scattering eigenstates for the Hamiltonian for particles incident from $x < 0$

$$\begin{aligned} \Psi_E(x) &= \psi_I(x) + \psi_R(x), \quad x < 0, \\ \Psi_E(x) &= \psi_T(x), \quad x > 0, \\ H\Psi_E &= E\Psi_E \end{aligned} \quad (3)$$

where ψ_I , ψ_R , and ψ_T represent the incoming, reflected, and transmitted waves respectively.

Write down the functional form for $\Psi_E(x)$, and solve for the amplitudes of ψ_T and ψ_R in terms of the amplitude of ψ_I for $E > V_0$.

(b) [2 pts] What is the ratio of the transmitted to incoming currents,

$$\frac{j_T}{j_I}, \quad (4)$$

as a function of the energy E , for $E > V_0$? Check your result for $E \gg V_0$ and $E \rightarrow V_0$.

(c) [1 pt] What is J_T for $E < V_0$? Show your work.

(d) [2 pts] Next, consider a 1D Hamiltonian, H , that has a series of bound, non-degenerate, real eigenfunctions $\psi_n(x)$: $H\psi_n(x) = E_n\psi_n(x)$. Show that the current for these states,

$$j_n(x, t) = \frac{1}{m} \text{Re} (\Psi_n^*(x, t) P \Psi_n(x, t)) = 0 \quad (5)$$

(e) [3 pts] Now consider a bound state of H from part (c) given, at $t = 0$, by

$$\Psi(x, t = 0) = \frac{1}{\sqrt{2}} (\psi_1(x) + \psi_2(x)) \quad (6)$$

where $\psi_1(x)$ and $\psi_2(x)$ are the ground state and first excited state of H .

Show that the current for this state will not be zero, and derive the time-dependence of the current.

Problem 2: Confined Harmonic Oscillator

Consider a particle of mass m confined in the potential

$$\begin{aligned} V(\vec{r}) &= \frac{m}{2}\omega^2 (x^2 + y^2) + V_z(z) \\ V_z(z) &= 0, \quad 0 \leq z \leq a, \quad V_z(z) = \infty, \quad z < 0, \quad z > a \end{aligned} \quad (1)$$

- (a) [2 pts] Show that the energy eigenstates for this potential can be separated into a product of three functions, each depending on a single coordinate: $X(x)$, $Y(y)$, and $Z(z)$. Using this product, determine the energy eigenvalues for the Hamiltonian, and the general form for the corresponding eigenstates. Show your work, although you don't need to solve the three 1D problems giving all the details.

- (b) [1 pt] Define the energy:

$$E_a = \frac{\pi^2 \hbar^2}{2ma^2} \quad (2)$$

What are the first four energy eigenvalues and their degeneracies for this potential in the case that $E_a = \frac{1}{2}\hbar\omega$? Give your answer in terms of the parameters in the problem.

- (c) [3 pts] Using standard cylindrical polar coordinates, ρ , ϕ , and z , where $x = \rho \cos(\phi)$ and $y = \rho \sin(\phi)$, show that the eigenstates of this potential can also be written as a product of three functions, $R(\rho)$, $F(\phi)$, and $Z(z)$. Hint: Consider the ϕ dependence of the system.

- (d) [2 pts] Show that the energy eigenstates of this Hamiltonian can be also be eigenstates of the z-component of the angular momentum, $L_z = -i\hbar \frac{\partial}{\partial \phi}$.

What is the angular dependence, $F(\phi)$, for the simultaneous eigenstates of H and L_z ?

- (e) [2 pts] The ground state you found in part (b) is an eigenstate of L_z , but the first excited states are not eigenstates of L_z . Write down two eigenstates of L_z from linear combinations of the first excited states from part (b).

What possible values of L_z can be measured for a particle in the ground state?

What possible values of L_z can be measured for a particle in the first excited states?

Problem 3: Vector Spaces and Dirac Notation

Consider a quantum system that can be described by three basis states, $|n\rangle$, $n = 1, 2, 3$, and an operator defined by its action on these three states:

$$\begin{aligned} A|1\rangle &= -i\alpha|3\rangle \\ A|2\rangle &= \alpha|2\rangle \\ A|3\rangle &= i\alpha|1\rangle \end{aligned} \tag{1}$$

where α is real.

- (a) [2 pts] Write the operator A as a matrix using these basis states:

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{2}$$

- (b) [1 pt] Show that A is Hermitian.

- (c) [3 pts] Compute the eigenvalues and corresponding eigenvectors of A .

- (d) [2 pts] In your result for part (c), you found one non-degenerate eigenstate, call it $|\gamma\rangle$, with eigenvalue γ . The other eigenstates are degenerate.

Define the projection operator $\mathcal{P}_\gamma = |\gamma\rangle\langle\gamma|$. Write the operator \mathcal{P}_γ as a matrix using the basis states $|1\rangle$, $|2\rangle$, and $|3\rangle$.

Check your results to show that this matrix form for the projection operator is correct.

- (e) [2 pts] Consider the system in the state:

$$|\phi\rangle = \frac{2}{3}|1\rangle + \frac{2}{3}|2\rangle - \frac{i}{3}|3\rangle \tag{3}$$

Write down an expression for the probability that a measurement of A would result in the value γ in terms of the projection operator \mathcal{P}_γ . Solve for this probability.

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Quantum #3

a) Using the given basis vectors, A can be written as:

$$A = \begin{bmatrix} 0 & 0 & -i\alpha \\ 0 & \alpha & 0 \\ i\alpha & 0 & 0 \end{bmatrix}$$

b) The condition for Hermiticity is that $A^\dagger A = A A^\dagger = \mathbb{I}$

$$\Rightarrow A^\dagger = \begin{bmatrix} 0 & 0 & i\alpha \\ 0 & \alpha & 0 \\ -i\alpha & 0 & 0 \end{bmatrix}$$

$$\hookrightarrow A^\dagger A = \begin{bmatrix} \alpha^2 & 0 & 0 \\ 0 & \alpha^2 & 0 \\ 0 & 0 & \alpha^2 \end{bmatrix} = \alpha^2 \mathbb{I}$$

c) Solve eigenvalue equation $\det(A - \mathbb{I}\lambda) = 0$

$$\begin{vmatrix} -\lambda & 0 & -i\alpha \\ 0 & \alpha - \lambda & 0 \\ i\alpha & 0 & -\lambda \end{vmatrix} = -\lambda[(-\lambda)(\alpha - \lambda) - 0] - 0 + -i\alpha[(0) - (i\alpha)(\alpha - \lambda)]$$

$$\begin{aligned} 0 &= \lambda^2(\alpha - \lambda) - \alpha^2(\alpha - \lambda) \\ &= (\alpha - \lambda)(\lambda^2 - \alpha^2) \\ &= (\alpha - \lambda)(\lambda + \alpha)(\lambda - \alpha) \\ \hookrightarrow \lambda &= \alpha, \alpha, -\alpha \end{aligned}$$

Solve eigenvector equation $A\vec{v} = \lambda\vec{v}$

$$\begin{bmatrix} 0 & 0 & -i\alpha \\ 0 & \alpha & 0 \\ i\alpha & 0 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \lambda \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$$\begin{aligned} -i\alpha x_3 &= \lambda x_1 \\ \alpha x_2 &= \lambda x_2 \\ i\alpha x_1 &= \lambda x_3 \end{aligned}$$

Case: $\lambda = -\alpha$

$$\begin{aligned} -i\alpha x_3 &= -\alpha x_1 \\ -i\alpha x_3 &= -\alpha x_1 \end{aligned}$$

$$\alpha x_2 = -\alpha x_2$$

$$i\alpha x_1 = -\alpha x_3$$

$$\Rightarrow \begin{bmatrix} 1 \\ 0 \\ i \end{bmatrix} \cdot \frac{1}{\sqrt{2}}$$

Case: $\lambda = \alpha$

$$-i\alpha x_3 = \alpha x_1 \Rightarrow \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \text{ or } \begin{bmatrix} -i \\ 0 \\ 1 \end{bmatrix} \cdot \frac{1}{\sqrt{2}}$$

$$\alpha x_2 = \alpha x_2$$

$$i\alpha x_1 = \alpha x_3$$

$$d) P_\gamma = |\gamma\rangle\langle\gamma|, \text{ where } |\gamma\rangle = |2\rangle$$

$$\begin{aligned}\Rightarrow P_\gamma &= |2\rangle\langle 2| \\ &= \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 \end{bmatrix} \\ &= \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}\end{aligned}$$

$$e) |\psi\rangle = \frac{2}{3}|1\rangle + \frac{2}{3}|2\rangle - \frac{1}{3}|3\rangle$$

$$\begin{aligned}P(\lambda=\gamma) &= |\langle\gamma|A|\psi\rangle|^2 \\ &= \langle\psi|A^\dagger|\gamma\rangle\langle\gamma|A|\psi\rangle \\ &= \left[\left(\frac{2}{3}\langle 1| + \frac{2}{3}\langle 2| - \frac{1}{3}\langle 3| \right) \right]\end{aligned}$$

Problem 4: Square Well Expansion

Consider a 1D quantum particle of mass m in a square well of width a :

$$\begin{aligned} V(x) &= 0, & |x| &\leq \frac{a}{2} \\ V(x) &= \infty, & |x| &> \frac{a}{2} \end{aligned} \tag{1}$$

- (a) [1 pt] Write down the energy eigenvalues, E_n , and energy eigenstates, $\psi_n(x)$ for this well. You do not need to derive the states in all detail.

You might want to write the solutions for even and odd values of n separately.

- (b) [2 pts] The well expands very suddenly to a new width $L > a$. The expansion is uniform about $x = 0$ so that for the new well, $V(x) = 0$ for $x \leq \frac{L}{2}$.

Assuming the particle is in the state n initially, for the well of width a , write an expression for the probability for the particle to be in the state n' after the expansion, for the well of width L . You don't have to solve for this probability yet, but write this expression in as much detail as you can. Explain why, for half of the possible values of n' this probability is zero.

- (c) [2 pts] Consider the case where the particle is initially in the ground state of the well of width a . Show that the probability that the particle will end up in the ground state of the expanded well, of width L is

$$P_{11}\left(\frac{a}{L}\right) = \frac{16}{\pi^2} \frac{a}{L} \frac{\cos^2\left(\frac{\pi a}{2L}\right)}{\left(1 - \left(\frac{a}{L}\right)^2\right)^2} \tag{2}$$

- (d) [3 pts] Calculate the limiting functional form for $P_{11}(a/L)$ from part (c) for $L \gg a$, $\frac{a}{L} \rightarrow 0$. (Calculate the lowest order non-constant term in $\frac{a}{L}$.)

Calculate the limiting functional form for $P_{11}(a/L)$ from part (c) for $\frac{a}{L} \rightarrow 1$. It might be helpful to define $\frac{a}{L} = 1 - \delta$. (Calculate the lowest order non-constant term in δ .)

Explain physically why you would predict the two limiting values of the probability.

- (e) [2 pts] Consider the case where the particle is initially in the ground state of the well and the potential well is completely removed suddenly ($V(x) = 0$ for all x).

Write down an expression that can be solved for the probability density of the particle having a momentum p after the well disappears. Just as in part (b), provide as much detail as you can, without actually solving for the probability.

Show that this will be very similar to the result in (b) so that calculating this probability would be a simple modification of the results in part (c).

Hint: The fact that $\cos(a \pm b) = \cos a \cos b \mp \sin a \sin b$ and $\sin(a \pm b) = \sin a \cos b \pm \cos a \sin b$ might be useful.

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Quantum #4

- a) For an infinite square well w/ $V = \begin{cases} 0 & -a/2 < x < a/2 \\ \infty & \text{elsewhere} \end{cases}$

$$\hookrightarrow E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

$$\psi_n = \begin{cases} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) & n = \text{even} \\ \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi x}{a}\right) & n = \text{odd} \end{cases}$$

- b) For our expanded well with $L > a$, our solutions above are valid with $a \rightarrow L$
Therefore the probability of being in state n' after the expansion is:

$$|\langle n' | n \rangle|^2 = \left| \int_{-\infty}^{\infty} \psi_{n'}^* \psi_n dx \right|^2$$

For all values of n' even, we get an odd function, which integrates to 0 over symmetric bounds

$$c) P_{n',n} = |\langle n' | n \rangle|^2$$

$$= \left| \int_{-\infty}^{\infty} \psi_{n'}^* \psi_n dx \right|^2$$

$$= \left| \int_{-\infty}^{\infty} \sqrt{\frac{2}{L}} \cos\left(\frac{n'\pi x}{L}\right) \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi x}{a}\right) dx \right|^2$$

$$= \left| \int_{-a/2}^{a/2} \frac{2}{\sqrt{La}} \cos\left(\frac{n'\pi x}{L}\right) \cos\left(\frac{n\pi x}{a}\right) dx \right|^2$$

$$= \left| \frac{2}{\sqrt{La}} \left[\frac{\sin\left(\left(\frac{n'}{L} - \frac{n}{a}\right)x\right)}{2\left(\frac{n'}{L} - \frac{n}{a}\right)} + \frac{\sin\left(\left(\frac{n'}{L} + \frac{n}{a}\right)x\right)}{2\left(\frac{n'}{L} + \frac{n}{a}\right)} \right] \right|_{-a/2}^{a/2}$$

$$= \frac{4}{La} \left| \left(\frac{\sin\left(\left(\frac{n'}{L} - \frac{n}{a}\right)\frac{a}{2}\right)}{2\left(\frac{n'}{L} - \frac{n}{a}\right)} + \frac{\sin\left(\left(\frac{n'}{L} + \frac{n}{a}\right)\frac{a}{2}\right)}{2\left(\frac{n'}{L} + \frac{n}{a}\right)} \right) - \left(\frac{\sin\left(\left(\frac{n'}{L} - \frac{n}{a}\right)\frac{-a}{2}\right)}{2\left(\frac{n'}{L} - \frac{n}{a}\right)} + \frac{\sin\left(\left(\frac{n'}{L} + \frac{n}{a}\right)\frac{-a}{2}\right)}{2\left(\frac{n'}{L} + \frac{n}{a}\right)} \right) \right|$$

$$= \frac{4}{La} \left| \frac{\sin\left(\frac{n'a}{2L} - \frac{n}{2}\right)}{\frac{n'}{L} - \frac{n}{a}} + \frac{\sin\left(\frac{n'a}{2L} + \frac{n}{2}\right)}{\left(\frac{n'}{L} + \frac{n}{a}\right)} \right|^2$$

#4 (cont.)

$$\begin{aligned}
 c) \quad P_{1,1} &= \frac{4}{La} \left| \left(\frac{1}{\frac{\pi^2}{L^2} - \frac{\pi^2}{a^2}} \right) \left[\left(\frac{\pi}{L} + \frac{\pi}{a} \right) \sin \left(\frac{\pi a}{2L} - \frac{\pi}{2} \right) + \left(\frac{\pi}{L} - \frac{\pi}{a} \right) \sin \left(\frac{\pi a}{2L} + \frac{\pi}{2} \right) \right] \right|^2 \\
 &= \frac{4}{La} \left| \frac{1}{\frac{\pi^2}{L^2} - \frac{\pi^2}{a^2}} \left[\left(\frac{\pi}{L} + \frac{\pi}{a} \right) \sin \left(\frac{\pi a}{2L} - \frac{\pi}{2} \right) - \left(\frac{\pi}{L} - \frac{\pi}{a} \right) \sin \left(\frac{\pi a}{2L} - \frac{\pi}{2} \right) \right] \right|^2 \\
 &= \frac{4}{La} \left| \frac{1}{\frac{\pi^2}{L^2} - \frac{\pi^2}{a^2}} \cdot \frac{2\pi}{a} \sin \left(\frac{\pi a}{2L} - \frac{\pi}{2} \right) \right|^2 \\
 &= \frac{16\pi^2}{La^2} \sin^2 \left(\frac{\pi a}{2L} - \frac{\pi}{2} \right) \cdot \left(\frac{1}{\frac{\pi^2}{L^2} - \frac{\pi^2}{a^2}} \right)^2 \\
 &= \frac{16\pi^2}{La^2} \cos^2 \left(\frac{\pi a}{2L} \right) \cdot \left(\frac{1}{\frac{\pi^2}{L^2} - \frac{\pi^2}{a^2}} \right)^2 \\
 &= \frac{16 \cos^2 \left(\frac{\pi a}{2L} \right)}{\pi^2 L a^2 \left(\frac{1}{L^2} - \frac{1}{a^2} \right)^2} \\
 &= \frac{16 \cos^2 \left(\frac{\pi a}{2L} \right)}{\pi^2 L \left(a^2 \left(1 - \left(\frac{a}{L} \right)^2 \right)^2 \right)} a^6 \quad \text{off by factor } a^2 ??
 \end{aligned}$$

d) Using $P_{1,1} = \frac{16a \cos^2 \left(\frac{\pi a}{2L} \right)}{\pi^2 L \left(1 - \left(\frac{a}{L} \right)^2 \right)^2}$, if $L \gg a$, $\frac{a}{L} \rightarrow 0$

$$P_{1,1} = \frac{16 \cos^2 \left(\frac{\pi a}{2L} \right)}{\pi^2} \cdot \left(\frac{a}{L} \right) \quad \left(1 - \left(\frac{a}{L} \right)^2 \right)^2 \rightarrow 1$$

Problem 5: Simple Harmonic Oscillator with External Perturbations

Consider a one-dimensional simple harmonic oscillator of mass m with a natural angular frequency ω . If there is no external perturbation, the Hamiltonian for this system is

$$H_0 = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{m}{2} \omega^2 x^2, \quad H_0 |n\rangle = \hbar\omega \left(n + \frac{1}{2} \right) |n\rangle \quad (1)$$

- (a) [2 pts] Consider the case where there is an external potential on the oscillator of the form $V_1(x) = \gamma_1 x$. Calculate the exact eigenenergies of $H_0 + V_1$.

Describe the difference between the new eigenstates of this total Hamiltonian and the eigenstates of H_0 .

(Hint: The new Hamiltonian can be transformed back into a harmonic oscillator of frequency ω plus an extra term).

- (b) [4 pts] Using perturbation theory to the first non-zero order, calculate the perturbed eigenenergies of $H_0 + V_1$. How do these compare with the exact solutions from (a)?
- (c) [1 pts] Now consider the case where there is an external potential on the oscillator of the form $V_2(x) = \gamma_2 x^2$. Calculate the exact eigenenergies of $H_0 + V_2$.

Describe the new eigenstates of this total Hamiltonian, comparing them with the eigenstates of H_0 .

- (d) [3 pts] Using perturbation theory to the first non-zero order, calculate the perturbed eigenenergies of $H_0 + V_2$. How do these compare with the exact solutions from (c)?

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Quantum #5

a) Adding the potential $V_1(x) = \gamma_1 x$ to the SHO yields

$$H_0 + V_1 = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{m\omega^2}{2} x^2 + \gamma_1 x$$

* To rewrite this as a version of SHO, we shift variables such that

$$x = y - \frac{\gamma_1}{m\omega^2}, \quad \frac{d}{dx} = \frac{dy}{dx} \frac{d}{dy}, \quad \frac{dy}{dx} = 1 \Rightarrow \frac{d^2}{dx^2} = \frac{d^2}{dy^2}$$

$$\begin{aligned} \hookrightarrow H_0 + V_1 &= \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial y^2} + \frac{m\omega^2}{2} \left(y - \frac{\gamma_1}{m\omega^2} \right)^2 + \gamma_1 \left(y - \frac{\gamma_1}{m\omega^2} \right) \\ &= \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial y^2} + \frac{m\omega^2}{2} \left(y^2 - \frac{2\gamma_1 y}{m\omega^2} + \frac{\gamma_1^2}{m^2\omega^4} \right) + \gamma_1 y - \frac{\gamma_1^2}{m\omega^2} \\ &= \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial y^2} + \frac{m\omega^2 y^2}{2} - \cancel{\gamma_1 y} + \frac{\gamma_1^2}{2m\omega^2} + \cancel{\gamma_1 y} - \frac{\gamma_1^2}{m\omega^2} \\ &= \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial y^2} + \frac{m\omega^2 y^2}{2} - \frac{\gamma_1^2}{2m\omega^2} \end{aligned}$$

* If we move our extra term to other side, and call $E + \frac{\gamma_1^2}{2m\omega^2} = E'$ we return our expected SHO

$$\hookrightarrow E'_n = \hbar\omega(n + 1/2) + \frac{\gamma_1^2}{2m\omega^2}$$

* Our eigenstates will be shifted along the x axis by $+\frac{\gamma_1}{m\omega^2}$

b) Our first order energy corrections are determined by:

$$\Delta E^{(1)} = \langle n^{(0)} | V_1 | n^{(0)} \rangle$$

$$\begin{aligned} V_1 &= \gamma_1 x \\ &= \gamma_1 \sqrt{\frac{\hbar}{2m\omega}} (a^\dagger + a) \end{aligned}$$

$$a^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle$$

$$a |n\rangle = \sqrt{n} |n-1\rangle$$

$$= \langle n | \gamma_1 \sqrt{\frac{\hbar}{2m\omega}} (a^\dagger + a) | n \rangle$$

$$= 0 \text{ by the orthogonality of } |n\rangle \text{ states } (\langle m | n \rangle = \delta_{mn})$$

#5 (cont.)

b) Our second order energy corrections are determined by:

$$\begin{aligned}
 \Delta E^{(2)} &= \sum_{k \neq n} \frac{|\langle k | V_1 | n \rangle|^2}{E_n^{(0)} - E_k^{(0)}} \\
 &= \sum_{k \neq n} \frac{|\langle k | \gamma_1 \sqrt{\frac{\hbar}{2m\omega}} (a^\dagger + a) | n \rangle|^2}{\hbar\omega(n-k)} \\
 &= \frac{\gamma_1^2 \hbar}{2m\omega} \cdot \frac{1}{\hbar\omega} \sum_{k \neq n} |\langle k | a^\dagger | n \rangle + \langle k | a | n \rangle|^2 / (n-k) \\
 &= \frac{\gamma_1^2}{2m\omega^2} \sum_{k \neq n} |\sqrt{n+1} \langle k | n+1 \rangle + \sqrt{n} \langle k | n-1 \rangle|^2 / (n-k) \\
 &= \frac{\gamma_1^2}{2m\omega^2} \left[\frac{n+1}{n-(n+1)} + \frac{n}{n-(n-1)} \right] \\
 &= \frac{\gamma_1^2}{2m\omega^2} [- (n+1) + n] \\
 &= -\frac{\gamma_1^2}{2m\omega^2}
 \end{aligned}$$

$$\boxed{E_n = E_n' - \frac{\gamma_1^2}{2m\omega^2}} \Rightarrow \text{Matches our exact solution}$$

c) For $V_2 = \gamma_2 x^2$, our Hamiltonian becomes

$$H_0 + V_2 = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{m}{2} x^2 \left(\omega^2 + \frac{2\gamma_2}{m} \right)$$

$$= \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} m \omega_1^2 x^2$$

$$\hookrightarrow E_n'' = \hbar\omega_1 \left(n + \frac{1}{2} \right)$$

$$= \hbar \left(n + \frac{1}{2} \right) \left(\omega^2 + \frac{2\gamma_2}{m} \right)^{1/2}$$

$$= \hbar\omega \left(n + \frac{1}{2} \right) \left(1 + \frac{2\gamma_2}{m\omega^2} \right)^{1/2} \quad \text{if } \gamma_2/\omega^2 \ll 1$$

$$= \hbar\omega \left(n + \frac{1}{2} \right) \left(1 + \frac{\gamma_2}{m\omega^2} \right)$$

#5 (cont.)

d) Again, our first order energy corrections are:

$$\Delta E^{(1)} = \langle n^{(0)} | V_2 | n^{(0)} \rangle$$

$$= \langle n | \frac{1}{2} x^2 | n \rangle$$

$$x^2 = \frac{\hbar}{2m\omega} (a^\dagger a^\dagger + a^\dagger a + a a^\dagger + a a)$$

$$= \frac{\hbar}{2m\omega} \left[\langle n | \cancel{a^\dagger a^\dagger} | n \rangle + \langle n | a^\dagger a | n \rangle + \langle n | a a^\dagger | n \rangle + \langle n | \cancel{a a} | n \rangle \right]$$

$$= \frac{\hbar}{2m\omega} [n + n+1]$$

$$= \frac{\hbar}{m\omega} (n + 1/2) \quad * \text{Matches exact solution}$$

Problem 6: Hydrogen Atom Measurements

Consider a hydrogen atom, ignoring the spin of the electron, with the usual eigenstates of H , L^2 , and L_z written as $|n, \ell, m_z\rangle$.

- (a) [2 pts] If the hydrogen atom is in its ground state, $|1, 0, 0\rangle$, what is $\langle r \rangle$, the average distance of the electron from the proton?
- (b) [3 pts] If the hydrogen atom is in its ground state, $|1, 0, 0\rangle$, what is the probability of measuring the electron's position to be in the classically forbidden region of space?
The forbidden region is where the energy of the atom is less than the potential energy, $V(r)$, corresponding to a negative value for the classical kinetic energy.
- (c) [2 pts] Consider the first excited states of the atom with $\ell = 1$, $|2, 1, m\rangle$. Calculate the expectation value $\langle z \rangle$ for these states (where $z = r \cos \theta$ using standard spherical coordinates).
- (d) [3 pts] The state $|2, l, 0\rangle$ has a rather different shape from the states $|2, 1, \pm 1\rangle$. This can be seen by considering the spread in z , $\Delta z = \sqrt{\langle z^2 \rangle - \langle z \rangle^2}$, or the expectation value $\langle z^2 \rangle$.
Compute the ratio of $\langle z^2 \rangle$ in the state $|2, 1, 0\rangle$ to that in the state $|2, 1, 1\rangle$,

$$\frac{\langle z^2 \rangle_{2,1,0}}{\langle z^2 \rangle_{2,1,1}} \quad (1)$$

Hydrogen Atom States:

$$V(r) = -\frac{e^2}{r}, \quad a_0 = \frac{\hbar^2}{me^2}, \quad Ryd = \frac{e^2}{2a_0}, \quad \alpha = \frac{e^2}{\hbar c} \quad (2)$$

The spatial representation of the Hydrogen Atom energy eigenstates can be written:

$$\psi_{n,\ell,m}(r) = R_{n,\ell}(r)Y_{\ell,m}(\theta, \phi), \quad E_n = -\frac{Ryd}{n^2}$$

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}}, \quad Y_{1,0} = \sqrt{\frac{3}{4\pi}} \cos \theta, \quad Y_{1,\pm 1} = \mp \sqrt{\frac{3}{8\pi}} \sin \theta e^{\pm i\phi}$$

$$R_{10} = \frac{2}{(a_0)^{3/2}} e^{-r/a_0}, \quad R_{20} = \frac{2}{(2a_0)^{3/2}} \left(1 - \frac{r}{2a_0}\right) e^{-r/2a_0}, \quad R_{21} = \frac{1}{(2a_0)^{3/2}} \frac{r}{\sqrt{3}a_0} e^{-r/2a_0}$$

A possibly useful integral:

$$\int_x^\infty t^n e^{-\alpha t} dt = \frac{n!}{\alpha^{n+1}} e^{-\alpha x} \sum_{k=0}^n \frac{(\alpha x)^k}{k!}$$

where α is real and positive.

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Quantum #6

$$\begin{aligned}
 a) \langle r \rangle &= \langle 1,0,0 | r | 1,0,0 \rangle \\
 &= \int_0^\infty r^2 dr \int_0^{2\pi} d\phi \int_0^\pi \sin\theta d\theta \cdot r \left(\frac{1}{\sqrt{4\pi}}\right)^2 \left(\frac{2}{a_0^{3/2}}\right)^2 e^{-2r/a_0} \\
 &= \int_0^\infty \frac{4}{a_0^3} r^3 e^{-2r/a_0} dr \\
 &= \frac{4}{a_0^3} \left(\frac{3!}{(2/a_0)^4} \right) \\
 &= \frac{a_0 \cdot 3 \cdot 2}{2^4} \\
 &= \frac{3a_0}{2}
 \end{aligned}$$

b) We must determine what the forbidden region is

$$\begin{aligned}
 E &< V(r) \\
 \frac{-e^2/a_0}{n^2} &< \frac{-e^2}{r} \\
 r &> 2a_0 n^2
 \end{aligned}$$

\Rightarrow Our problem is the same as above except $r \in [0, \infty)$ now is $r \in [2a_0, \infty)$

$$\begin{aligned}
 \hookrightarrow P &= \int_{2a_0}^\infty \frac{4}{a_0^3} r^2 e^{-2r/a_0} dr \\
 &= \frac{4}{a_0^3} \int_{2a_0}^\infty r^2 e^{-2r/a_0} dr \\
 &= \frac{4}{a_0^3} \left(\frac{2!}{(2/a_0)^3} e^{-2/a_0 \cdot 2a_0} \sum_{k=0}^2 \frac{(2/a_0 \cdot 2a_0)^k}{k!} \right) \\
 &= e^{-4} \left[\frac{1}{0!} + \frac{4}{1!} + \frac{16}{2!} \right] \\
 &\quad \quad \quad 1 \quad + \quad 4 \quad + \quad 8 \\
 &= 13e^{-4}
 \end{aligned}$$

#6(cont.)

c) Our first excited states are $|2, 1, m\rangle$

$$\hookrightarrow |2, 1, 0\rangle = \frac{1}{(2a_0)^{3/2}} \frac{r}{\sqrt{3}a_0} e^{-r/2a_0} \sqrt{\frac{3}{4\pi}} \cos\theta$$

$$|2, 1, 1\rangle = \frac{-1}{(2a_0)^{3/2}} \frac{r}{\sqrt{3}a_0} e^{-r/2a_0} \sqrt{\frac{3}{8\pi}} \sin\theta e^{i\varphi}$$

$$|2, 1, -1\rangle = \frac{1}{(2a_0)^{3/2}} \frac{r}{\sqrt{3}a_0} e^{-r/2a_0} \sqrt{\frac{3}{8\pi}} \sin\theta e^{-i\varphi}$$

* For the $|2, 1, 0\rangle$ state:

$$\begin{aligned}\langle z \rangle &= \int_0^\infty r^2 dr \int_0^{2\pi} d\varphi \int_0^\pi \sin\theta d\theta \cdot r \cos\theta \cdot \frac{1}{(2a_0)^3} \frac{r^2}{3a_0^2} e^{-r/a_0} \frac{3}{4\pi} \cos^2\theta \\&= \int_0^\infty \frac{1}{32\pi a_0^5} r^4 e^{-r/a_0} \int_0^{2\pi} d\varphi \int_0^\pi \cos^3\theta \sin\theta d\theta \\&= \int_0^\infty dr \frac{1}{16a_0^5} r^4 e^{-r/a_0} \int_0^\pi -\cos^3\theta d(\cos\theta) \\&= \int_0^\infty dr \frac{1}{16a_0^5} r^4 e^{-r/a_0} \left[-\frac{1}{4} \cos^4\theta \right]_0^\pi \\&= \int_0^\infty \frac{1}{16a_0^5} r^4 e^{-r/a_0} dr \left[-\frac{1}{4} \Big|_0^\pi \right] \\&= 0\end{aligned}$$

* For the $|2, 1, 1\rangle$ state:

$$\begin{aligned}\langle z \rangle &= \int_0^\infty r^2 dr \int_0^{2\pi} d\varphi \int_0^\pi \sin\theta d\theta \cdot r \cos\theta \cdot \left(\frac{-1}{(2a_0)^3} \right) \frac{r^2}{3a_0^2} e^{-r/a_0} \frac{3}{8\pi} \sin^2\theta e^{i\varphi} \\&= \int_0^\infty \frac{-1}{64\pi a_0^5} r^4 e^{-r/a_0} dr \int_0^{2\pi} e^{i\varphi} d\varphi \int_0^\pi \sin^3\theta \cos\theta d\theta \\&= \quad \quad \quad \cdot 0 \\&= 0\end{aligned}$$

* The θ is the same in the $|2, 1, -1\rangle$ state

$$\hookrightarrow \langle z \rangle_{2,1,-1} = 0$$

#6(cont.)

d) * Repeating part c now for $\langle z^2 \rangle$

* For the $|2, 1, 0\rangle$ state, r and θ integrals change

$$\begin{aligned}\langle z^2 \rangle &= \int_0^\infty \frac{1}{16a_0^5} r^5 e^{-r/a_0} dr \int_0^\pi \cos^4(\theta) \sin\theta d\theta \\&= \int_0^\infty \frac{1}{16a_0^5} r^5 e^{-r/a_0} dr \left[\frac{1}{5} \cos^5(\theta) \right]_0^\pi \\&= \int_0^\infty \frac{1}{16a_0^5} r^5 e^{-r/a_0} dr \cdot \left(\frac{1}{5}(-1)^5 - \frac{1}{5}(1)^5 \right) \\&= \frac{2}{80a_0^5} \int_0^\infty r^5 e^{-r/a_0} dr \\&= \frac{1}{40a_0^5} \left[\frac{5!}{(r/a_0)^6} \right] \\&= \frac{3a_0}{2^6}\end{aligned}$$

* For the $|2, 1, 1\rangle$ state, r, θ integrals change, same as $|2, 1, -1\rangle$ state

$$\begin{aligned}\langle z^2 \rangle &= \int_0^\infty \frac{1}{64\pi a_0^5} r^5 e^{-r/a_0} dr \int_0^{2\pi} e^{i\varphi} e^{-i\varphi} d\varphi \int_0^\pi \sin^3\theta \cos^2\theta d\theta \\&= \frac{1}{32a_0^5} \left[\frac{5!}{(r/a_0)^6} \right] \int_0^\pi \sin^3\theta \cos^2\theta d\theta \\&= \frac{1}{32a_0^5} \left(\frac{120a_0^6}{2^6} \right) \cdot \frac{4}{15} \text{ (from mathematica)} \\&= \frac{a_0}{64}\end{aligned}$$