Aug 2008

F-08

Problem 1: A 3-D Spherical Well(10 Points)

For this problem, consider a particle of mass m in a three-dimensional spherical potential well, $V(r)$, given as,

$$V = 0 \quad r \leq a/2$$
$$V = W \quad r > a/2.$$

with $W > 0$.

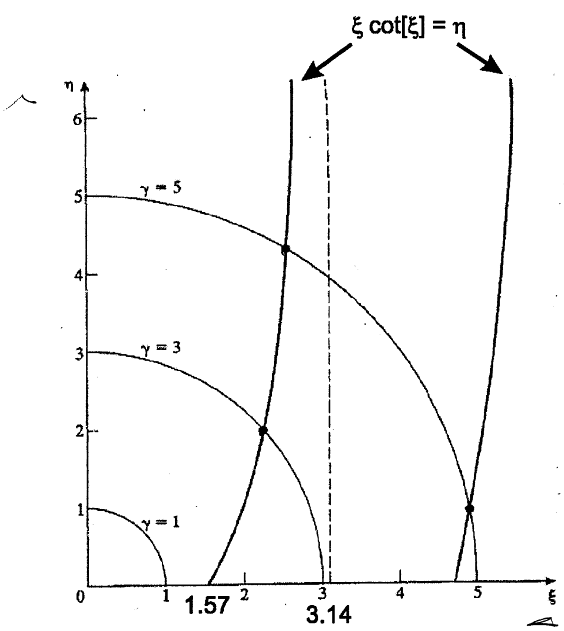
All of the following questions refer to the *zero angular momentum states* of the potential.

a. Find the form of the wave functions (i.e without matching boundary conditions), ψ(r), for this potential for an energy, E, less than the well depth, W.**(3 Points)**

b. The wave function for the one-dimensional symmetric square well has both a cosine and sine solution. Is this true for the three-dimensional spherical well potential? Explain. **(1 Point)**

c. If the potential well was infinitely deep, W$\to\infty$, what are the energies? Derive the expression using the wave functions you calculated in (a).**(2 Points)**

d. Derive the transcendental equation that determines the energies for the finite spherical well. **(2 Points)**



e. Is there always a bound state in the finite three-dimensional potential? Justify your answer to receive any credit. How does this compare to the one-dimensional finite square well? Use the figure. $\gamma^2 = \eta^2 + \xi^2$, where $\xi = \sqrt{2mEa}/2\hbar$ and $\eta = \sqrt{2m(W-E)}a/2\hbar$.**(2 Points)**

$\frac{ka}{2}$ $\frac{la}{2}$

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Problem 2: Near Degenerate Perturbation (10 Points)

Consider a system with two energy levels that are very close to each other while all others are far away. In this system, the unperturbed Hamiltonian (H_0) has two eigenstates $|\psi_1^{(0)}\rangle$ and $|\psi_2^{(0)}\rangle$ with energy eigenvalues $E_1^{(0)}$ and $E_2^{(0)}$ that are very close to each other

$$|E_1^{(0)} - E_2^{(0)}| \simeq 0\,. \tag{1}$$

We often choose a state of the form

$$|\psi\rangle = a|\psi_1^{(0)}\rangle + b|\psi_2^{(0)}\rangle \tag{2}$$

and try to diagonalize the complete Hamiltonian ($H = H_0 + H_1$) with

$$\begin{aligned} H|\psi\rangle &= E|\psi\rangle && (3)\\ H_0|\psi_i^{(0)}\rangle &= E_i^{(0)}|\psi_i^{(0)}\rangle && (4)\\ H_{ij} &= \langle\psi_i^{(0)}|H|\psi_j^{(0)}\rangle, i,j = 1,2 && (5) \end{aligned}$$

as well as

$$\tan\beta = \frac{2H_{12}}{H_{11} - H_{22}}\,. \tag{6}$$

(a) **(2 Points)** Solve the characteristic equation and find the energy eigenvalues E_1 and E_2.

(b) **(3 Points)** Show that the normalized states corresponding to the energy values E_1 and E_2 are

$$\begin{aligned} |\psi_1\rangle &= \cos(\beta/2)|\psi_1^{(0)}\rangle + \sin(\beta/2)|\psi_2^{(0)}\rangle && (7)\\ |\psi_2\rangle &= -\sin(\beta/2)|\psi_1^{(0)}\rangle + \cos(\beta/2)|\psi_2^{(0)}\rangle\,. && (8) \end{aligned}$$

In (c) and (d), consider the limit

$$|H_{11} - H_{22}| \gg |H_{12}| = |(H_1)_{12}|\,. \tag{9}$$

(c) **(3 Points)**

Find the energy eigenvalues E_1 and E_2 for the Hamiltonian H to the order of H_{12}^2 in terms of H_{11}, H_{22}, and H_{12} as well as in terms of $E_i^{(0)}$ and $|\psi_i^{(0)}\rangle, i = 1,2$.

(d) **(2 Points)** Find the eigenstates $|\psi_i\rangle, i = 1,2$.

P1.

$$V = 0 \quad r \leq a/2$$

$$V = W \quad r > a/2 \qquad ; W > 0$$

a) In spherical co-ordinate

$$\nabla^2 \equiv \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

$$L^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

For Spherical Co-ordinate ; central Potential $V(r)$

$$H\psi(r,\theta,\phi) = E\psi(r,\theta,\phi)$$

$$\Rightarrow \left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(r,\theta,\phi) = E\psi(r,\theta,\phi)$$

$$\Rightarrow -\frac{\hbar^2}{2mr^2}\left[\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\psi(r,\theta,\phi) + V(r) = E\psi(r,\theta,\phi)$$

$$\Rightarrow \left[-\frac{\hbar^2}{2mr^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{L^2}{2mr^2} + V(r)\right]\psi(r,\theta,\phi) = E\,\psi(r,\theta,\phi)$$

$$\psi(r,\theta,\phi) \equiv R(r)\,\Theta(\theta)\,\Phi(\phi)$$

$$= R(r)\,Y_\ell^m(\theta,\phi)$$

$$L^2\psi(r,\theta,\phi) = \hbar^2\ell(\ell+1)\,\psi(r,\theta,\phi)$$

$$\left[-\frac{\hbar^2}{2mr^2}\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right)\right]+\left[\frac{\hbar^2\, l(l+1)}{2mr^2}+V(r)\right]R(r)=ER(r)$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right)-\left[\frac{l(l+1)}{r^2}+\frac{2mV(r)}{\hbar^2}\right]R(r)=ER(r)$$

$$R_l(r)=\frac{u_l(r)}{r}$$

$$\Rightarrow\quad \frac{d}{dr}\left(r^2\frac{d}{dr}\left(\frac{u_l(r)}{r}\right)\right)=\frac{d}{dr}\left\{r^2\left[\frac{1}{r}\frac{du_l(r)}{dr}+\frac{u_l(r)}{r^2}\right]\right\}$$

$$=\frac{d}{dr}\left\{r\frac{du_l(r)}{dr}-u_l(r)\right\}$$

$$=r\frac{d^2u_l(r)}{dr^2}+\cancel{\frac{du_l(r)}{dr}}-\cancel{\frac{du_l(r)}{dr}}$$

$$\Rightarrow\quad \frac{1}{r}\frac{d^2u_l(r)}{dr^2}-\left[\frac{l(l+1)}{r^2}+\frac{2mV(r)}{\hbar^2}\right]\frac{u_l(r)}{r}=-\frac{2mE}{\hbar^2}\frac{u_l(r)}{r}$$

$$\Rightarrow\quad \left[\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}-\frac{2mV(r)}{\hbar^2}\right]u_l(r)=-\frac{2mE}{\hbar^2}u_l(r)$$

and $$Y_l^m(\theta,\phi)=\epsilon\sqrt{\frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!}}\,P_l^m(\cos\theta)\,e^{im\phi}$$

with $$\epsilon=\begin{cases}(-1)^m & \text{for } m>0\\ +1 & \text{for } m<0\end{cases}$$

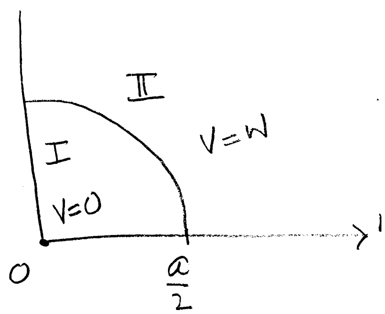
and $P_\ell^m(\cos\theta) = P_\ell^m(x) = (1-x^2)^{\frac{|m|}{2}} \dfrac{d^{|m|}}{dx^{|m|}} P_\ell(x)$

$$P_\ell(x) = \frac{1}{2^\ell \ell!}\frac{d^\ell}{dx^\ell}(x^2-1)^\ell$$

a) $\ell = 0$

$$\frac{d^2 u_0(r)}{dr^2} - \frac{2mV(r)u_0(r)}{\hbar^2} = -\frac{2mE}{\hbar^2}u_0(r)$$

$E < V(r) \Rightarrow$ bound state



• Region I $(r \leq a/2)$ $V(r) = 0$

$$\frac{d^2u_0(r)}{dr^2} = -\frac{2mE}{\hbar^2}u_0(r) \qquad K^2 = \frac{2mE}{\hbar^2}$$

$\Rightarrow u_0(r) = -K^2 u_0(r)$

$\Rightarrow u_{0,1}(r) = Ae^{+ikr} + Be^{-ikr} = A\cos k(r) + B\sin Kr$

$\Rightarrow \psi(r) = \frac{A}{r}\cos Kr + \frac{B}{r}\sin Kr$

• Region II $(r > a/2)$

$$\frac{d^2u_0(r)}{dr^2} = -\frac{2m(E-V(r))}{\hbar^2}u_0(r)$$

$$\Rightarrow \frac{d^2u_0(r)}{dr^2} = \frac{2m(W-E)}{\hbar^2}u_0(r)$$

$\Rightarrow u_{0,2}(r) = Ce^{\rho r} + De^{-\rho r} \Rightarrow \psi(r) = \frac{C}{r}e^{\rho r} + \frac{D}{r}e^{-\rho r}$

as $r \to \infty$ $e^{\rho r} \to \infty$ $\therefore$ $C = 0$ $\psi(r)_{r>\frac{a}{2}} = \frac{D}{r}e^{-\rho r}$

b) In ourcase $r \to 0$ $\frac{A}{r}\cos kr \to \infty$ $\therefore A = 0$

$$\psi(r)_{r<a} = \frac{B}{r}\sin kr$$

c) For $w \to \infty$ $\psi(r)_{r>\frac{a}{2}} = 0$

$$\Rightarrow \psi(r) = \frac{B}{a}\sin kr$$

$$\psi(r = \tfrac{a}{2}) = 0$$

$$\Rightarrow \sin\frac{ka}{2} = 0$$

$$\Rightarrow k = \frac{2n\pi}{a}$$

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{4n^2\pi^2\hbar^2}{2ma^2}$$

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

d) $\psi_I(r)\big|_{r<\frac{a}{2}} = \frac{B}{r}\sin kr$

$\psi_{II}(r)\big|_{r>\frac{a}{2}} = \frac{D}{r}e^{-\rho r}$

$$\psi_I(r=\tfrac{a}{2}) = \psi_{II}(r=\tfrac{a}{2})$$

$$\Rightarrow \frac{B}{r}\sin\frac{ka}{2} = \frac{D}{r}e^{-\rho a/2}$$

$$\Rightarrow B\sin\left(\frac{ka}{2}\right) = De^{-\rho a/2}$$

$$\Rightarrow B = \frac{De^{-\rho a/2}}{\sin\left(\frac{ka}{2}\right)}$$

$$\frac{d\psi_I}{dr}\bigg|_{r=a/2} = \frac{d\psi_{II}}{dr}\bigg|_{r=a/2}$$

$$\Rightarrow B\left(\frac{k\cos kr}{r} - \frac{\sin kr}{r^2}\right)_{r=\frac{a}{2}} = D\left(-\frac{\rho}{r}e^{-\rho r} - \frac{e^{-\rho r}}{r^2}\right)_{r=\frac{a}{2}}$$

$$\Rightarrow B\left[\frac{k2\cos(ka/2)}{a} - \frac{4\sin(ka/2)}{a^2}\right] = D\left[-\frac{2\rho}{a} - \frac{4}{a^2}\right]e^{-\rho a/2}$$

$$\Rightarrow \frac{2k}{a}\tan(ka/2) - \frac{4}{a^2} = -\frac{2\rho}{a} - \frac{4}{a^2}$$

$$\Rightarrow k\tan(ka/2) = -\rho$$

$$\Rightarrow \boxed{\cot(ka/2) = -\frac{k}{\rho}}$$

$$\underbrace{\frac{ka}{2}}_{\varepsilon}\tan\left(\frac{ka}{2}\right) = -\underbrace{\frac{\rho a}{2}}_{\eta}$$

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Problem 3: The Harmonic Oscillator(10 Points)

A one dimensional harmonic oscillator has a potential given by

$$V(x) = m\omega^2 x^2/2.$$

where ω is the oscillator frequency and m is its mass. Derive all results.

a. Write the Schrodinger equation for a single particle in a one dimensional harmonic oscillator potential. **(1 Point)**

b. Consider the raising and lowering operators

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}x - i\frac{p}{\sqrt{2m\hbar\omega}}$$

and

$$a = \sqrt{\frac{m\omega}{2\hbar}}x + i\frac{p}{\sqrt{2m\hbar\omega}},$$

respectively, where p is the momentum operator. If Ψ_E is an eigenvector of the Hamiltonian with energy eigenvalue E, find the energy eigenvalues of $a^\dagger\Psi_E$ and $a\Psi_E$. (You may need to use the fact that $[x, p] = i\hbar$). **(2 Points)**

c. Using the raising and lowering operators find the energy eigenvalues for a single particle in a one dimensional harmonic oscillator potential. **(2 Points)**

d. Find the normalized ground state wave function. **(2 Points)**

e. The harmonic oscillator models a particle attached to an ideal spring. If the spring can only be stretched, and not compressed, so that $V = \infty$ for $x < 0$, what will be the energy levels of this system? **(3 Points)**

$n = ?$

Aug - 2008

Problem 4: The Infinite Square Well: (10 Points)

A single particle is in a one dimensional infinite well whose potential $V(x)$ is given by:

$$V(x) = \begin{cases} 0, & \text{if -L} \leq \text{x} \leq \text{L} \\ \infty, & \text{otherwise} \end{cases}$$

a. Find the allowed energies (E_n) and the normalized eigenfunctions ($\Phi_n(x)$) to Schrodinger's Equation for this potential. Show all your work. **(2 Points)**

Assume the particle is in the ground state and a position measurement of the particle is made. Since any measuring apparatus has a finite resolution, the exact location of the particle cannot be detemined. We therefore only know the location of the particle within some resolution ϵ. After making the position measurement the wave function $\Psi(x)$ is:

$$\Psi(x) = \frac{1}{\sqrt{\epsilon}} \quad |x| < \frac{\epsilon}{2} \qquad -\frac{\epsilon}{2} < x < \frac{\epsilon}{2}$$

$$\Psi(x) = 0 \quad |x| > \frac{\epsilon}{2} \qquad -\frac{\epsilon}{2} > x > \frac{\epsilon}{2}$$

two wavefunc which one to use?

b. What is the probability that the particle has energy E_n? **(2 Points)**

c. If $\epsilon = 2L$, we know that the particle is somewhere in the box. What is the probability that the particle is in the ground state? **(1 Point)**

what is the ground state? $n=1$ or $n=0$

d. Before the position measurement we knew the particle was in the box and in the ground state. If after the measurement and $\epsilon = 2L$ we know that the particle is in the box, why is probability that the particle is in the ground state not 1? **(1 Point)** $\Rightarrow \Psi_0$.

For parts e), f) and g) now assume that the particle is in the potential $V(x)$

$$V(x) = \begin{cases} 0, & \text{if -L} \leq \text{x} \leq \text{L} \\ \infty, & \text{otherwise} \end{cases}$$

and in the ground state. The position of the walls are quickly increased to

$$V(x) = \begin{cases} 0, & \text{if -L'} \leq \text{x} \leq \text{L'} \\ \infty, & \text{otherwise} \end{cases}$$

where $|L'| > |L|$

$\psi_0 = \frac{1}{\sqrt{L}} \cos\left(\frac{\pi}{2L}\right) x$

e. After the expansion, what is the probability that the particle has energy E_n? You do not need to solve the integral. **(2 Points)**

f. Before the walls of the potential are increased, does $|\Psi(x,t)|^2$ (where $\Psi(x,t)$ is a solution to Schrodinger's equation before the expansion) have any time dependance? Explain **(1 Point)**

g. After the position of the walls are increased to L', does $|\Psi(x,t)|^2$ (where $\Psi(x,t)$ is a solution to Schrodinger's equation after the expansion) have any time dependance? Explain. **(1 Point)**

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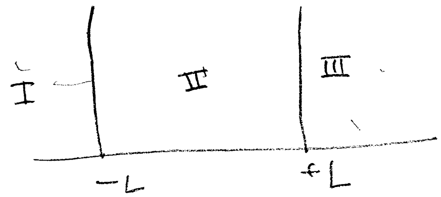
P4

$$V(x) = \begin{cases} 0 & -L \leq x \leq L \\ \infty & \text{otherwise} \end{cases}$$



a) $-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}(x)}{dx^2} = E\,\psi_{II}(x)$

$\Rightarrow \frac{d^2\psi_{II}(x)}{dx^2} = -k^2 \qquad k^2 = \frac{2mE}{\hbar^2}$

$\Rightarrow \psi_{II}(x) = A\cos kx + B\sin kx$

$\psi_{I}(x) = 0 \quad \psi_{III}(x) = 0$

$\psi_{II}(x=-L) = \psi_{I}(x=-L) = 0$ | $\psi_{II}(x=L) = \psi_{III}(x=L) = 0$

$\Rightarrow A\cos kL - B\sin kL = 0 \;(1)$ | $\Rightarrow A\cos kL + B\sin kL = 0 \;(2)$

/* $\begin{vmatrix} \cos kL & -\sin kL \\ \cos kL & \sin kL \end{vmatrix} = 0 \Rightarrow 2\sin kL\cos kL = 0$

$\Rightarrow \sin 2kL = 0 \Rightarrow 2kL = n\pi$

$\Rightarrow k = \frac{n\pi}{2L}$ $\underline{n\text{ even}}$

$E_n = \frac{\hbar^2 k^2}{2m} = \frac{n^2\pi^2\hbar^2}{8mL^2}$

*/

$(1)+(2) = \underline{\underline{2A\cos kL = 0}} \Rightarrow kL = \frac{n\pi}{2}$, ~~n odd~~

$\Rightarrow k = \frac{n\pi}{2L}$, n odd

$(1)-(2) = 2B\sin kL = 0$

$kL = m\pi$, $m = 1, 2, 3 \ldots$

$\Rightarrow k = \frac{m\pi}{L}$

$\psi_n = \frac{1}{\sqrt{L}}\cos\left(\frac{n\pi}{2L}\right)x$ n odd

$\psi_n(x) = \frac{1}{\sqrt{L}}\sin\left(\frac{n\pi}{2L}\right)x$ n even

b. $P(E_n) = \dfrac{|\langle \psi_n | \Psi \rangle|^2}{\langle \Psi | \Psi \rangle}$

$$= \left| \int_{-\epsilon/2}^{+\epsilon/2} \psi_n^*(x)\, \Psi(x)\, dx \right|^2$$

$$= \int_{-\epsilon/2}^{+\epsilon/2} \frac{1}{\sqrt{L}} \cos\left(\frac{n\pi}{2L}x\right) \frac{\epsilon}{2}\, dx \qquad \cancel{n \text{ odd}}$$

$$= \frac{\epsilon}{2\sqrt{L}} \sin\left(\frac{n\pi}{2L}x\right)\Bigg|_{-\epsilon/2}^{+\epsilon/2} \frac{2L}{n\pi}$$

$$= \frac{\epsilon\sqrt{L}}{n\pi}\left[\sin\left(\frac{n\pi\epsilon}{4L}\right) + \sin\left(\frac{n\pi\epsilon}{4L}\right)\right]$$

$$= \left|\frac{2\epsilon\sqrt{L}}{n\pi} \sin\left(\frac{n\pi\epsilon}{4L}\right)\right|^2$$

$$= \frac{4\epsilon^2 L}{n^2\pi^2} \sin^2\left(\frac{n\pi\epsilon}{4L}\right)$$

~~n even~~ n,

$$\langle \psi_n | \Psi \rangle = \int_{-\epsilon/2}^{+\epsilon/2} \frac{1}{\sqrt{L}}\ \psi_n^*(x)\Psi(x)\,dx = 0$$

c. $\psi_0(x) = \frac{1}{\sqrt{L}} \cos$

P3

a) $H|\psi\rangle = E|\psi\rangle$

$\left[\frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2\right]\psi(x) = E\psi(x) \rightarrow -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi(x) = E\psi(x)$

$H = \hbar\omega(a^\dagger a + \frac{1}{2})$

b) $H|\Psi_E\rangle = E|\Psi_E\rangle$

$[a^\dagger, H] = \hbar\omega[a^\dagger, a^\dagger a]$

$= -\hbar\omega a^\dagger$

$\Rightarrow a^\dagger H - Ha^\dagger = -\hbar\omega a^\dagger$

$\Rightarrow a^\dagger H + \hbar\omega a^\dagger = Ha^\dagger$

$\Rightarrow a^\dagger H - [a^\dagger, H] = Ha^\dagger$

$[a, H] = \hbar\omega[a, a^\dagger]a$

$= \hbar\omega a$

$\Rightarrow H(a^\dagger|\psi_E\rangle)$

$= (a^\dagger H + \hbar\omega a^\dagger)|\psi_E\rangle$

$= a^\dagger H|\psi_E\rangle + \hbar\omega a^\dagger|\psi_E\rangle$

$= (E + \hbar\omega) a^\dagger|\psi_E\rangle$

$H(a|\psi_E\rangle)$

$= (aH - \hbar\omega a)|\psi_E\rangle$

$= aH|\psi_E\rangle - \hbar\omega a|\psi_E\rangle$

$= (E - \hbar\omega) a|\psi_E\rangle$

c) $H|\Psi_n\rangle = (\hbar\omega a^\dagger a + \frac{1}{2})|\Psi_n\rangle = \hbar\omega((\sqrt{n})^2 + \frac{1}{2})|\Psi_n\rangle$

$= \hbar\omega(n + \frac{1}{2})|\psi_n\rangle$

d) $a|\psi_0\rangle = 0$

$\Rightarrow \left(\sqrt{\frac{m\omega}{2\hbar}}\hat{x} + i\frac{\hat{p}}{\sqrt{2m\hbar\omega}}\right)|\psi_0\rangle = 0$

$\Rightarrow \int\sqrt{\frac{m}{2\hbar}}|x\rangle\langle x|\hat{x}|\psi_0\rangle\, dx = -\frac{i}{\sqrt{2m\hbar\omega}}\int|x\rangle\langle x| -i\hbar\frac{d}{dx}|\psi_0\rangle\, dx$

$\Rightarrow$ equating the co-eff of $|x\rangle$

$$\Rightarrow \sqrt{\frac{m\omega}{2\hbar}} \int x\, \psi_0(x)\, dx = -\frac{i}{\sqrt{2m\hbar\omega}} \int (-i\hbar) \frac{d\psi_0(x)}{dx} dx$$

$$\Rightarrow \sqrt{\frac{m\omega}{2\hbar}} \int x\, dx = -\sqrt{\frac{\hbar}{2m\omega}} \int \frac{d\psi_0(x)}{\psi_0(x)}$$

ask

$$\Rightarrow \sqrt{\frac{m\omega}{2\hbar}} \frac{x^2}{2} \times \left(-\sqrt{\frac{2m\omega}{\hbar}}\right) = \ln \psi_0(x)$$

$$a|\psi_0\rangle = 0$$

$$\langle x| a|\psi_0\rangle = 0$$

$$\int \langle x|a|y\rangle \langle y|\psi_0\rangle\, dy = 0$$

$$\Rightarrow \int \langle x| \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + i\frac{\hat{p}}{\sqrt{2m\hbar\omega}} |y\rangle\, \psi_0(y)\, dy = 0$$

$$\Rightarrow \langle x|\hat{x}|y\rangle = x\,\delta(x-y)$$

$$\Rightarrow \langle x|\hat{p}|y\rangle = -i\hbar \frac{d}{dx}\delta(x-y)$$

$$\Rightarrow \sqrt{\frac{m\omega}{2\hbar}} \int x\,\delta(x-y)\psi_0(y)\,dy + \sqrt{\frac{\hbar}{2m\omega}} \int \frac{d}{dx}\delta(x-y)\,\psi_0(y)\,dy = 0$$

$$\Rightarrow \sqrt{\frac{m\omega}{2\hbar}}\, x\,\psi_0(x) + \sqrt{\frac{\hbar}{2m\omega}} \frac{d\psi_0(x)}{dx} = 0$$

$$\Rightarrow \frac{d\psi_0(x)}{dx} + \frac{m\omega}{\hbar} x\, \psi_0(x) = 0$$

$$\Rightarrow \int \frac{d\psi_0(x)}{\psi_0(x)} = \int -\frac{m\omega}{\hbar} x\, dx$$

$$\Rightarrow \ln \psi_0(x) = -\frac{m\omega}{\hbar}\frac{x^2}{2}$$

$$\Rightarrow \psi_0(x) = A e^{-\left(\frac{m\omega}{2\hbar}\right)x^2}$$

$$\int_{-\infty}^{+\infty} |\psi_0(x)|^2 dx = 1$$

$$\Rightarrow |A|^2 \int_{-\infty}^{+\infty} e^{-\left(\frac{m\omega}{\hbar}\right)x^2} dx = 1$$

$$\Rightarrow |A|^2 \sqrt{\frac{\pi\hbar}{m\omega}} = 1$$

$$\Rightarrow A = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$$

$$\Rightarrow \psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\left(\frac{m\omega}{2\hbar}\right)x^2}$$

e) For, $x < 0$ $V = \infty$ $\therefore \psi_0(x=0) = 0$ as the wave func should go to zero at the boundary

Hence, n has to be odd

$E_n = (n+\frac{1}{2})\hbar\omega$; n odd $V(x) \neq V(-x)$ so odd

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Problem 5: Time Evolution (10 Points)

Consider the Hamiltonian and a second observable, B, for a system that can be represented in a 3-dimensional Hilbert space using the orthonormal basis: $|e_1\rangle$, $|e_2\rangle$ and $|e_3\rangle$ with

$$|e_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |e_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, |e_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

as:

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

The system at time t=0 is in the state:

$$|\Psi(0)\rangle = |e_2\rangle$$

a) Calculate the eigenvalues and normalized eigenvectors of H and B. **(2 Point)**

b) Determine $|\Psi(t)\rangle$, the wavefunction at a later time. **(1 Point)**

c) Determine $P_{|\Psi(t)\rangle}(b = 2)$, the probability of obtaining $b = 2$ if b is measured at an arbitrary time. **(1 Points)**

d) Is your probability in part c) time-dependent or time-independent? Discuss in detail. **(1 Point)**

e) Derive an expression for $\frac{\partial}{\partial t}\langle B\rangle$ where $\langle B\rangle = \langle\Psi(t)|B|\Psi(t)\rangle$ by explicit differentiation using the Time-Dependent Schrodinger Equation. **(2 Points)**

f) Use your expression in part b) to find $\frac{\partial}{\partial t}\langle B\rangle$ for this system using the $|\Psi(t)\rangle$ you found in part a). **(2 Points)**

g) Without doing further calculations describe what result you would expect for $\frac{\partial}{\partial t}\langle B\rangle$ if the initial wavefunction $|\Psi(0)\rangle = |e_2\rangle$ changes to:

$$|\Psi(0)\rangle = |e_1\rangle$$

Explain your answer in detail. **(1 Point)**

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Problem 6: Hydrogen Atom (10 Points)

The spatial component of the ground state wavefunction for the hydrogen atom is

ψ not radial

$$\longrightarrow \quad \phi(r,\theta,\phi) = Ae^{-\left(\frac{r}{a_o}\right)}$$

where A and a_o (the Bohr radius) are constants.

a) Find A by normalizing the wavefunction. Express your answer in terms of a_o. **(2 Points)**

b) Calculate the expectation value of the potential energy. **(2 Points)**

c) Calculate the expectation value of r and the most probable value for r. **(2 Points)**

d) What is the expectation value for L, the magnitude of the angular momentum? How does this value compare to the prediction of the Bohr model? **(2 Points)**

e) Many solutions to the Schrodinger equation for the hydrogen atom are related to a z-axis despite the fact that the potential energy is spherically symmetric. What defines the z-axis? Explain your answer. **(2 Points)**

P5.

a) $H = \underline{\hbar\omega} \begin{pmatrix} 2 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$

$$\begin{vmatrix} 2-\lambda & 0 & 0 \\ 0 & -\lambda & 1 \\ 0 & 1 & -\lambda \end{vmatrix} = 0 \Rightarrow (2-\lambda)(\lambda^2 - 1) = 0$$

$$\Rightarrow \lambda = 2, \pm 1$$

• $\underline{\lambda = 1}$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 1 \\ 0 & 1 & -1 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = 0 \quad \begin{array}{l} \Rightarrow a_1 = 0 \\ \left.\begin{array}{l} \Rightarrow -a_2 + a_3 = 0 \\ \Rightarrow a_2 - a_3 = 0 \end{array}\right\} a_2 = a_3 \end{array}$$

$|\lambda = 1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$ $\qquad |E = \hbar\omega\rangle = \frac{1}{\sqrt{2}}\left[|e_2\rangle + |e_3\rangle\right]$

• $\underline{\lambda = -1}$

$$\begin{pmatrix} 3 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = 0 \quad \begin{array}{l} \Rightarrow b_1 = 0 \\ \Rightarrow b_3 = -b_2 \end{array}$$

$|\lambda = -1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}$ $\qquad \Rightarrow |E = -\hbar\omega\rangle = \frac{1}{\sqrt{2}}\left[|e_2\rangle - |e_3\rangle\right]$

$\Rightarrow \sqrt{2}|e_2\rangle = |E = \hbar\omega\rangle + |E = -\hbar\omega\rangle$

$\Rightarrow |e_2\rangle = \frac{1}{\sqrt{2}}\left[|E = \hbar\omega\rangle + |E = -\hbar\omega\rangle\right]$

• $\underline{\lambda = 2}$

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & -2 & 1 \\ 0 & 1 & -2 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = 0 \quad \begin{array}{l} \Rightarrow c_1 \text{ arbitary} \\ \left.\begin{array}{l} \Rightarrow -2c_2 + c_3 = 0 \\ \Rightarrow c_2 - 2c_3 = 0 \end{array}\right\} c_2 = c_3 = 0 \end{array}$$

$|\lambda = 2\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$ $\qquad |E = 2\hbar\omega\rangle = |e_1\rangle$

$$B = \begin{pmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{pmatrix} \qquad \begin{vmatrix} 1-\lambda & 0 & -1 \\ 0 & 2-\lambda & 0 \\ -1 & 0 & 1-\lambda \end{vmatrix} = 0$$

$$\Rightarrow (1-\lambda)\{(2-\lambda)(1-\lambda)\} + 1(2-\lambda) = 0$$

$$\Rightarrow (2-\lambda)\{(1-\lambda)^2 - 1\} = 0$$

$$\Rightarrow (2-\lambda)(1-\lambda-1)(1-\lambda+1) = 0$$

$$\Rightarrow \lambda(2-\lambda)(2-\lambda) = 0 \qquad \lambda = 0, 2, 2$$

- $\underline{\lambda = 0}$

$$\begin{pmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = 0 \quad \begin{aligned} &\Rightarrow a_1 - a_3 = 0 \Rightarrow a_1 = a_3 \\ &\Rightarrow 2a_2 = 0 \Rightarrow a_2 = 0 \\ &\Rightarrow -a_1 + a_3 = 0 \end{aligned}$$

$$|\lambda = 0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$$

- $\underline{\lambda = 2}$

$$\begin{pmatrix} -1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & -1 \end{pmatrix}\begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = 0 \quad \begin{aligned} &\Rightarrow -b_1 - b_3 = 0 \; \} \Rightarrow b_3 = -b_1 \\ &\Rightarrow 0 = 0 \; \} \; b_2 \\ &\Rightarrow -b_1 - b_3 = 0 \end{aligned}$$

$$|\lambda = 2\rangle = \frac{1}{\sqrt{2|b_1|^2 + |b_2|^2}}\begin{pmatrix} b_1 \\ b_2 \\ -b_1 \end{pmatrix}$$

$$|\lambda = 2, 1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

$$\langle \lambda = 2, 2 | \lambda = 2, 1\rangle = 0$$

$$\begin{pmatrix} b_1 & b_2 & -b_1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \Rightarrow b_1 + b_1 = 0$$

$$\Rightarrow b_1 = 0$$

$$|\lambda = 2, 2\rangle = b\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

b) $|\psi(0)\rangle = |e_2\rangle = \frac{1}{\sqrt{2}}\left[|E=\hbar\omega\rangle + |E=\hbar\omega\rangle\right]$

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}} e^{-i\omega t}|E=\hbar\omega\rangle - \frac{1}{\sqrt{2}} e^{i\omega t}|E=-\hbar\omega\rangle$$

$$= \frac{1}{\sqrt{2}}\left[e^{-i\omega t}|E=\hbar\omega\rangle - e^{i\omega t}|E=-\hbar\omega\rangle\right]$$

c) $P(b=2)_{|\Psi(t)\rangle} = \frac{|\langle b=2|\Psi(t)\rangle|^2}{\langle\Psi(t)|\Psi(t)\rangle} =$

$$|b=2\rangle_E = \sum_E |E\rangle\langle E|\,|b=2\rangle$$

$$|b=2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\-1\end{pmatrix} = \frac{1}{\sqrt{2}}\left[|e_1\rangle - |e_3\rangle\right]$$

$$= \frac{1}{\sqrt{2}}|E=2\hbar\omega\rangle - \frac{1}{2}\left[|E=\hbar\omega\rangle - |E=-\hbar\omega\rangle\right]$$

$$|b=2,2\rangle = \begin{pmatrix}0\\1\\0\end{pmatrix} = |e_3\rangle = \frac{1}{\sqrt{2}}\left[|E=\hbar\omega\rangle - |E=-\hbar\omega\rangle\right]$$

$$P(b=2)_{|\psi(t)\rangle} = |\langle b=2,1|\Psi(t)\rangle|^2 + |\langle b=2,2|\Psi(t)\rangle|^2$$

$$= \left|-\frac{1}{2\sqrt{2}}e^{-i\omega t} + \frac{1}{2\sqrt{2}}e^{i\omega t}\right|^2 + \left|\frac{e^{-i\omega t}}{2} + \frac{e^{i\omega t}}{2}\right|^2$$

$$= \left|\frac{1}{\sqrt{2}}\, i \sin\omega t\right|^2 + |\cos\omega t|^2 = \cos^2\omega t + \frac{1}{2}\sin^2\omega t$$

d) Since, $[B, H] \neq 0$ so, B is not a const. of motion, so $P(b=1)$ is time dependent

e) $$\frac{\partial}{\partial t}\langle B\rangle = \frac{\partial}{\partial t}\langle \Psi(t)|B|\Psi(t)\rangle$$

$$= \left\langle \frac{\partial \Psi}{\partial t}\right|B|\Psi(t)\rangle + \left\langle \Psi(t)\left|\frac{\partial B}{\partial t}\right|\Psi(t)\right\rangle$$

$$+$$

P6 $\Phi(r,\theta,\phi) = A\, e^{-(r/a_0)}$

$$\int_0^\infty \int_0^\pi \int_0^{2\pi} |A|^2 e^{-2r/a_0} r^2 dr \sin\theta d\theta d\phi = 1$$

$$\Rightarrow |A|^2 4\pi \int_0^\infty r^2 e^{-2r/a_0} dr = 1$$

$$\Rightarrow |A|^2 4\pi \left[-\frac{r^2 a_0}{\cancel{2}} e^{-2r/a_0} \Big|_0^\infty + \int_0^\infty a_0 r\, e^{-2r/a_0} \right] = 1$$

$$\Rightarrow |A|^2 4\pi a_0 \int_0^\infty r\, e^{-2r/a_0} = 1$$

$$\Rightarrow |A|^2 \frac{4\pi a_0^2}{2} \int_0^\infty e^{-2r/a_0} = 1$$

$$\Rightarrow |A|^2 4\pi a_0^2 \left(-\frac{a_0}{2} e^{-2r/a_0} \right)_0^\infty = 1$$

$$\Rightarrow |A|^2 \pi a_0^3 = 1$$

$$\Rightarrow A = \frac{1}{\sqrt{\pi a_0^3}}$$

$$\langle V \rangle = \frac{e^2}{\pi a_0^3} \int_0^\infty e^{-r/a_0} \frac{1}{r} e^{-r/a_0} r^2 \, dr \, d\Omega$$

$$= \frac{e^2 4\pi}{\pi a_0^3} \int_0^\infty r e^{-2r/a_0} \, dr$$

$$= \frac{4e^2}{a_0^3} \left[\overset{0}{\cancel{-\frac{r a_0 e^{-2r/a_0}}{2} \Big|_0^\infty}} + \int_0^\infty \frac{a_0}{2} e^{-2r/a_0} \, dr \right]$$

$$\Rightarrow \frac{2e^2}{a_0^2} \left[-\frac{a_0}{2} e^{-2r/a_0} \right]_0^\infty$$

$$\Rightarrow -\frac{e^2}{a_0}$$

c) $\langle r \rangle = \int \phi^*(r,\theta,\phi)\ r\ \phi(r,\theta,\phi)\ dr\,d\Omega$

$$= \frac{1}{\pi a_0^3} \int_{0,0,0}^{\infty,\pi,2\pi} e^{-r/a_0}\ r\ e^{-r/a_0}\ r^2\, dr\ \cancel{d\Omega}\ \sin\theta\, d\theta\, d\phi$$

$dv = e^{-2r/a_0} dr$

$\Rightarrow v = -\frac{a_0}{2} e^{-2r/a_0}$

$u = r^3$

$du = 3r^2$

$$= \frac{1}{\cancel{\pi} a_0^3} 4\cancel{\pi} \int_0^\infty r^3 e^{-2r/a_0}\, dr$$

$$= \frac{1}{\cancel{\pi} a_0^3} 4\pi \left[\cancel{-\frac{r^3 a_0}{2} e^{-2r/a_0}}\Big|_0^\infty \xrightarrow{} 0 + \int_0^\infty \frac{3a_0}{2} r^2 e^{-2r/a_0}\, dr \right]$$

$$= \frac{4\pi \cdot 3}{2 \cancel{\pi} a_0^{\cancel{3}2}} \int_0^\infty r^2 e^{-2r/a_0}\, dr$$

$$= \frac{\cancel{12\pi}\ 6}{a_0^2} \left[-\frac{r^2 a_0}{2} e^{\cancel{-2r/a_0}}\Big|_0^\infty \xrightarrow{} 0 + \int_0^\infty \frac{a_0}{\cancel{2}} r\, e^{-2r/a_0}\, dr \right]$$

$$= \frac{\cancel{12\pi a_0}\ 6}{a_0} \int_0^\infty r\, e^{-2r/a_0}\, dr$$

$$= \cancel{12\pi a_0}\ 6/a_0 \left[-r \frac{a_0}{2} e^{\cancel{-2r/a_0}}\Big|_0^\infty \xrightarrow{} 0 + \frac{a_0}{2} \int_0^\infty e^{-2r/a_0}\, dr \right]$$

$$= \frac{\cancel{12\pi a_0}}{3\ \cancel{\pi a_0}} \left[-\frac{a_0}{2} e^{-2r/a_0} \right]_0^\infty$$

$$= \cancel{6\pi a_0^3}\ \frac{3}{\cancel{\ \ }} \left(\frac{a_0}{2} \right)$$

$$= \frac{3}{2} a_0$$

$$P(r) = \int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi} \phi^*(r,\theta,\phi)\,\phi(r,\theta,\phi)\, r^2 \sin\theta\, d\theta\, d\phi$$

$$= \frac{4\pi}{\pi a_0^3} r^2 e^{-2r/a_0}$$

$$\frac{dP(r)}{dr} = \frac{4}{a_0^3}\left[2r\, e^{-2r/a_0} - \frac{2}{a_0} r^2 e^{-2r/a_0}\right] = 0$$

$$\Rightarrow \quad \left(1 - \frac{r}{a_0}\right) = 0$$

$$\Rightarrow \quad \underline{r = a_0}$$

d) $L = rp\sin\theta = -i\hbar r \nabla \sin\theta$

$$\nabla \equiv \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial\theta} + \hat{\phi}\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}$$

blah blah!

$$\nabla_r = \hat{r}\frac{\partial}{\partial r}$$

$$\langle L \rangle = \frac{1}{\pi a_0^3}\int e^{-r/a_0}(-i\hbar)\, r\frac{\partial}{\partial r}\sin\theta\, e^{-r/a}\, r^2\, dr\, \sin\theta\, d\theta\, d\phi$$

$$= -\frac{i\hbar}{\pi a_0^3}\int e^{-r/a_0}\, r\sin\theta\left(-\frac{r^2}{a} e^{-r/a} + 2r e^{-r/a}\right) dr\, \sin\theta\, d\theta\, d\phi$$

$$= -\frac{i\hbar}{\pi a_0^3}\int e^{-2r/a_0}\, r\left(2r - \frac{r^2}{a}\right) dr \underbrace{\int_0^{\pi}\sin^2\theta\, d\theta}_{\frac{\pi}{2}} \underbrace{\int_0^{2\pi} d\phi}_{2\pi}$$

$$= -\frac{i\pi\hbar}{a_0^3}\int\left[2r^2 e^{-2r/a_0} - \frac{1}{a} r^3 e^{-2r/a_0}\right] dr$$

$$= -\frac{2i\pi\hbar}{a_0^3}\int r^2 e^{-2r/a_0} + \frac{i\pi\hbar}{a_0^4}\int r^3 e^{-2r/a_0}$$

$$= -\frac{2i\pi\hbar}{a_0^3}\left[2!\left(\frac{a_0}{2}\right)^3\right] + \frac{i\pi\hbar}{a_0^4}\left[3!\left(\frac{a_0}{2}\right)^4\right]$$

$$= -\frac{i\pi\hbar}{2} + \frac{3i\pi\hbar}{8}$$

$$= i\pi\hbar\left(\frac{-4+3}{8}\right)$$

$$\psi(r,\theta,\phi) = R(r)\, Y_l^m(\theta,\phi)$$

$m=0$ $\quad = R(r)\, P_l(\cos\theta)$

$l=0$ $\quad P_0(\cos\theta) = 1$

$$= R(r)$$

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

$$L|nlm\rangle = \hbar\sqrt{l(l-1)}\,|nlm\rangle$$

$$= 0$$

$\langle L\rangle = 0$

$L = n\hbar$ $\quad n=1$

Bohr model $\quad \langle L\rangle = \hbar$

e) $[L_z, L^2] = 0$