Aug 2008

## 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 $W > 0$.

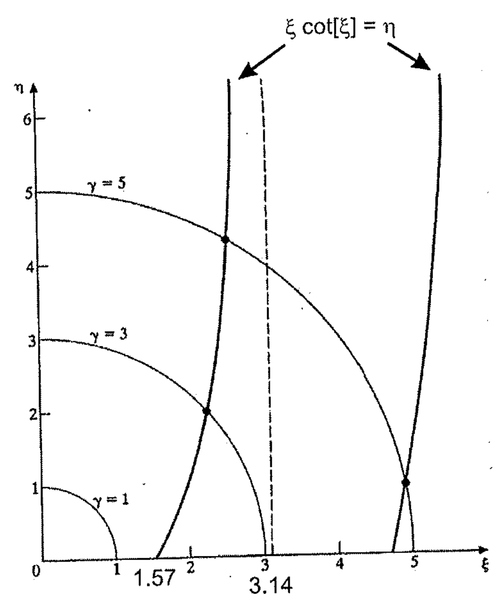
All of the following questions refer to the *zero angular momentum states* of the potential.

a. Find the form of the wave functions (i.e without matching boundary conditions), $\psi$(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$\rightarrow\infty$, 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 $\xi = \sqrt{2mE}a/2\hbar$ and $\eta = \sqrt{2m(W-E)}a/2\hbar$.**(2 Points)**

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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 $|\psi_i\rangle, i = 1,2$.

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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 $\omega$ 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 $\Psi_E$ 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)**

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# Quantum #3

a) The general form of the Schrödinger equation is: $i\hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi$

For a 1-D harmonic oscillator, the equation becomes:

$$i\hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 \Psi \quad \text{(Time Dependent)}$$

$$E\psi = \frac{-\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 \psi \quad \text{(Time Independent)}$$

b) Given: $a^+ = \sqrt{\frac{m\omega}{2\hbar}}\,x - \frac{ip}{\sqrt{2m\hbar\omega}} \Rightarrow \sqrt{2m\hbar\omega}\,a^+ = m\omega x - ip$

$a = \sqrt{\frac{m\omega}{2\hbar}}\,x + \frac{ip}{\sqrt{2m\hbar\omega}} \Rightarrow \sqrt{2m\hbar\omega}\,a = m\omega x + ip$

* Rewriting the TISE in terms of momentum will allow us later to define the Hamiltonian in terms of raising/lowering operators

TISE: $\frac{p^2}{2m}\psi + \frac{1}{2}m\omega^2 x^2 \psi = E\psi \Rightarrow H|\psi\rangle = E|\psi\rangle$

* Remember, we want to solve: $H(a^+|\psi\rangle) = A(a^+|\psi\rangle)$

$H(a|\psi\rangle) = B(a|\psi\rangle)$

$\Rightarrow$ Rewriting our Hamiltonian:

$m\omega x = \sqrt{2m\hbar\omega}\,a^+ + ip$

$\sqrt{2m\hbar\omega}\,a - ip = \sqrt{2m\hbar\omega}\,a^+ + ip$

$\sqrt{2m\hbar\omega}\,(a - a^+) = 2ip$

$-i\sqrt{\frac{m\hbar\omega}{2}}\,(a - a^+) = p$

$\sqrt{2m\hbar\omega}\,a - m\omega x = ip$

$\sqrt{2m\hbar\omega}\,a - m\omega x = m\omega x - \sqrt{2m\hbar\omega}\,a^+$

$\sqrt{2m\hbar\omega}\,(a + a^+) = 2m\omega x$

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

* Substituting into our Hamiltonian we see:

$$H = \frac{\left(-i\sqrt{\frac{m\hbar\omega}{2}}[a - a^+]\right)^2}{2m}\psi + \frac{1}{2}m\omega^2\left(\sqrt{\frac{\hbar}{2m\omega}}[a + a^+]\right)^2$$

#3 (cont.)

b) $$H = \frac{-\frac{m\omega\hbar}{2}[a-a^\dagger]^2}{2m} + \frac{m\omega^2\hbar}{4m\omega}[a+a^\dagger]^2$$

$$= -\frac{\omega\hbar}{4}[aa - a^\dagger a - a a^\dagger + a^\dagger a^\dagger] + \frac{\hbar\omega}{4}[aa + a^\dagger a + aa^\dagger + a^\dagger a^\dagger]$$

$$= \frac{\hbar\omega}{2}[a^\dagger a + aa^\dagger]$$

* substituting $aa^\dagger = a^\dagger a + 1$ (from $[a, a^\dagger] = 1$)

$$= \hbar\omega\left(a^\dagger a + \tfrac{1}{2}\right)$$

* Using this, we can determine $[H, a^\dagger]$ and $[H, a]$ which will allow us to act $H$ on $|\psi\rangle$ while maintaining $a^\dagger|\psi\rangle$ and $a|\psi\rangle$ kets

$$[H, a^\dagger] = [\hbar\omega(a^\dagger a + 1/2), a^\dagger]$$

$$= \hbar\omega(a^\dagger a + 1/2)a^\dagger - a^\dagger(\hbar\omega[a^\dagger a + \tfrac{1}{2}])$$

$$= \hbar\omega a^\dagger a a^\dagger + \cancel{\tfrac{1}{2}\hbar\omega a^\dagger} - \hbar\omega a^\dagger a^\dagger a - \cancel{\tfrac{1}{2}\hbar\omega a^\dagger}$$

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

$$= \hbar\omega[a^\dagger(a^\dagger a + 1) - a^\dagger a^\dagger a]$$

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

$$[H, a] = [\hbar\omega(a^\dagger a + 1/2), a]$$

$$= \hbar\omega(a^\dagger a + \tfrac{1}{2})a - a(\hbar\omega[a^\dagger a + 1/2])$$

$$= \hbar\omega a^\dagger a a + \cancel{\tfrac{1}{2}\hbar\omega a} - \hbar\omega a a^\dagger a - \cancel{\tfrac{1}{2}\hbar\omega a}$$

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

$$= \hbar\omega(a^\dagger a a - (a^\dagger a + 1)a)$$

$$= \hbar\omega a$$

#3 (cont.)

b) * Applying these operators to the kets, we see:

$$H(a^\dagger|\psi\rangle) = (a^\dagger H + \hbar\omega a^\dagger)|\psi\rangle$$
$$= a^\dagger(E + \hbar\omega)|\psi\rangle$$
$$\hookrightarrow \boxed{A = E + \hbar\omega}$$

$$H(a|\psi\rangle) = (aH - \hbar\omega a)|\psi\rangle$$
$$= a(E - \hbar\omega)|\psi\rangle$$
$$\hookrightarrow \boxed{B = E - \hbar\omega}$$

c) Using the number operator $N$, where $N = a^\dagger a$ and $N|\psi_n\rangle = n|\psi_n\rangle$

$$\Rightarrow H|\psi_n\rangle = E_n|\psi_n\rangle$$
$$= \hbar\omega(a^\dagger a + 1/2)|\psi_n\rangle$$
$$= \hbar\omega(N + 1/2)|\psi_n\rangle$$
$$= \hbar\omega(n + 1/2)|\psi_n\rangle$$
$$\hookrightarrow \boxed{E_n = \hbar\omega(n + 1/2)}$$

d) To find the ground state wavefunction, we use the fact that: $a|\psi_0\rangle = 0$

$$\Rightarrow \left(\sqrt{\frac{m\omega}{2\hbar}}\, x + \frac{iP}{\sqrt{2m\hbar\omega}}\right)\psi_0 = 0$$

$$\left(\sqrt{\frac{m\omega}{2\hbar}}\, x + \frac{i(-i\hbar\, \partial/\partial x)}{\sqrt{2m\hbar\omega}}\right)\psi_0 = 0$$

$$\sqrt{\frac{m\omega}{2\hbar}}\, x\, \psi_0 + \sqrt{\frac{\hbar}{2m\omega}}\, \frac{\partial \psi_0}{\partial x} = 0$$

$$\sqrt{\frac{\hbar}{2m\omega}}\, \frac{\partial}{\partial x}\psi_0 = -\sqrt{\frac{m\omega}{2\hbar}}\, x\, \psi_0$$

$$\frac{\partial}{\partial x}\psi_0 = \frac{-m\omega}{\hbar}\, x\, \psi_0$$

$$\frac{\partial \psi_0}{\psi_0} = \frac{-m\omega}{\hbar}\, x\, \partial x$$

#3 (cont.)

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

$$\psi_0 = \exp\left[-\frac{m\omega}{2\hbar}x^2 + c\right]$$

$$\psi_0 = C\exp\left[-\frac{m\omega}{2\hbar}x^2\right]$$

* Checking the normalization

$$1 = \int_{-\infty}^{\infty} |\psi_0|^2 dx$$

$$= C^2 \int_{-\infty}^{\infty} \exp\left[-\frac{m\omega}{\hbar}x^2\right] dx$$

$$= c^2\left(\sqrt{\frac{\hbar\pi}{m\omega}}\right)$$

$$\sqrt{\frac{m\omega}{\hbar\pi}} = c^2$$

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

$\Rightarrow$ our normalized wavefunction is: $\psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left[-\frac{m\omega}{\hbar}x^2\right]$

e) * Our potential now becomes: $V(x) = \begin{cases} \infty, & x < 0 \\ \frac{1}{2}m\omega^2x^2, & x > 0 \end{cases}$

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## 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:

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

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 $\epsilon$. After making the position measurement the wave function $\Psi(x)$ is:

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

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

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)**

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)**

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

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

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

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

where $|L'| > |L|$

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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# Quantum #4

a) $H\psi = E\psi$

$$\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi = E\psi$$

$$\frac{\partial^2}{\partial x^2}\psi = \frac{-2mE}{\hbar^2}\psi$$

* let $k = \sqrt{\frac{2mE}{\hbar^2}}$

$$\frac{\partial^2}{\partial x^2}\psi = -k^2\psi$$

$\hookrightarrow \psi = A\sin(kx) + B\cos(kx)$

* Our boundary conditions are $\psi(-L) = \psi(L) = 0$

$$0 = A\sin(kL) + B\cos(kL)$$

$$0 = A\sin(-kL) + B\cos(-kL)$$

$$= -A\sin(kL) + B\cos(kL)$$

* The above equations are true when $kL = \frac{n\pi}{2} \Rightarrow k = \frac{n\pi}{2L}$

$\hookrightarrow$ if n is even:

$$0 = A\cancelto{0}{\sin(kL)} + B\cos(kL)$$

$\hookrightarrow B = 0$

$\hookrightarrow$ if n is odd:

$$0 = A\sin(kL) + \cancelto{0}{B\cos(kL)}$$

$\hookrightarrow A = 0$

$$\Rightarrow \psi(x) = \begin{cases} A\sin\left(\frac{n\pi}{2}\right) & n \text{ even} \\ B\cos\left(\frac{n\pi}{2}\right) & n \text{ odd} \end{cases}$$

* Normalizing the above wavefunction yields

$$1 = \int_{-L}^{L} A^2\sin^2(kx)\,dx$$

$$= A^2\int_{-L}^{L}\frac{1}{2}(1-\cos(2kx))\,dx$$

$$= \frac{A^2}{2}\left[x - \frac{1}{2k}\sin(2kx)\right]\Big|_{-L}^{L}$$

$$= A^2L \Rightarrow A = \frac{1}{\sqrt{L}} \text{ (same for B)}$$

#4 (cont.)

a) Therefore: $\psi(x) = \begin{cases} \sqrt{\frac{1}{L}} \sin\left(\frac{n\pi}{2}\right) & n \text{ even} \\ \sqrt{\frac{1}{L}} \cos\left(\frac{n\pi}{2}\right) & n \text{ odd} \end{cases}$

* Returning to the energy

$$k = \sqrt{\frac{2mE}{\hbar^2}} = \frac{n\pi}{2L}$$

$$\frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{4L^2}$$

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

b) $P = \left| \int_{-\epsilon/2}^{\epsilon/2} \sqrt{\frac{1}{L}} \cos\left(\frac{n\pi x}{2L}\right) \frac{1}{\sqrt{\epsilon}} \, dx \right|^2$

$$= \frac{1}{\epsilon L} \left| \int_{-\epsilon/2}^{\epsilon/2} \cos\left(\frac{n\pi x}{2L}\right) dx \right|^2$$

$$= \frac{1}{\epsilon L} \left| \frac{2L}{n\pi} \sin\left(\frac{n\pi x}{2L}\right) \Big|_{-\epsilon/2}^{\epsilon/2} \right|^2$$

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

$$= \frac{16L}{\epsilon n^2\pi^2} \sin^2\left(\frac{n\pi\epsilon}{4L}\right)$$

c) If $\epsilon = 2L$, $n=1$:

$$P = \frac{8}{\pi^2}$$

d) The act of measuring the particle has perturbed the system, thus altering the state of the system

e) After expansion, our wavefunction becomes

$$\psi_n(x) = \begin{cases} \sqrt{1/L'} \sin\left(\frac{n\pi x}{2L'}\right) & n' \text{ even} \\ \sqrt{1/L'} \cos\left(\frac{n\pi x}{2L'}\right) & n' \text{ odd} \end{cases}$$

$$\Rightarrow P = \left| \int_{-L'}^{L'} \sqrt{\frac{1}{L'}} \cos\left(\frac{n\pi x}{2L'}\right) \sqrt{\frac{1}{L}} \cos\left(\frac{n\pi x}{2L}\right) dx \right|^2$$

#4 (cont.)

f) The eigenstates of the infinite square well are stationary states, thus $|\Psi(x,t)|^2$ has no time dependence

g) See part f

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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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# Quantum #5

a) Starting w/ $H = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$

$\Rightarrow$ find the eigenvalues from: $\det(H - \lambda \mathbb{I}) = 0$

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

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

$\hookrightarrow \lambda = 2, -1, 1$

$\Rightarrow$ find eigenvectors from $H\vec{v} = \lambda\vec{v}$

$$\begin{bmatrix} 2 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \lambda\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \quad \Rightarrow \quad \begin{aligned} 2x_1 &= \lambda x_1 \\ x_3 &= \lambda x_2 \\ x_2 &= \lambda x_3 \end{aligned}$$

* for $\lambda = 2$

$$\begin{aligned} 2x_1 &= 2x_1 \\ x_3 &= 2x_2 \\ x_2 &= 2x_3 \end{aligned} \quad \Rightarrow \vec{V} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

* for $\lambda = -1$

$$\begin{aligned} 2x_1 &= -x_1 \\ x_3 &= -x_2 \\ x_2 &= -x_3 \end{aligned} \quad \Rightarrow \vec{V} = \begin{bmatrix} 0 \\ 1 \\ -1 \end{bmatrix} \cdot \frac{1}{\sqrt{2}}$$

* for $\lambda = 1$

$$\begin{aligned} 2x_1 &= x_1 \\ x_3 &= x_2 \\ x_2 &= x_3 \end{aligned} \quad \Rightarrow V = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix}$$

* Similiarly for $B = \begin{bmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{bmatrix}$

$$\begin{vmatrix} 1-\lambda & 0 & -1 \\ 0 & 2-\lambda & 0 \\ -1 & 0 & 1-\lambda \end{vmatrix} = (1-\lambda)\left[(2-\lambda)(1-\lambda) - 0\right] - 1\left(0 + (2-\lambda)\right) = 0$$

$$\begin{aligned} \Rightarrow \quad 0 &= (2-\lambda)(1-\lambda)^2 - (2-\lambda) \\ &= (2-\lambda)\left[(1-\lambda)^2 - 1\right] \\ &= (2-\lambda)\left[(1-\lambda)+1\right]\left[(1-\lambda)-1\right] \end{aligned}$$

$\hookrightarrow \lambda = 2, 2, 0$

#5 (cont.)

a) $B\vec{v} = \lambda \vec{v}$

$$\begin{bmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \lambda \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \Rightarrow \begin{aligned} x_1 - x_3 &= \lambda x_1 \\ 2x_2 &= \lambda x_2 \\ -x_1 + x_3 &= \lambda x_3 \end{aligned}$$

* for $\lambda = 2$

$$\begin{aligned} x_1 - x_3 &= 2x_1 \\ 2x_2 &= 2x_2 \\ -x_1 + x_3 &= 2x_3 \end{aligned} \Rightarrow \vec{v} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \text{ or } \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} \cdot \frac{1}{\sqrt{2}}$$

$|\lambda_B = 2, 1\rangle \quad |\lambda_B = 2, 2\rangle$

* for $\lambda = 0$

$$\begin{aligned} x_1 - x_3 &= 0 \\ 2x_2 &= 0 \\ -x_1 + x_3 &= 0 \end{aligned} \Rightarrow \vec{v} = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} \cdot \frac{1}{\sqrt{2}}$$

b) Given $|\psi(0)\rangle = \langle 0, 1, 0\rangle$, we must first convert this to H basis before acting time-evolution operator

$$\Rightarrow |\psi(0)\rangle = \frac{1}{\sqrt{2}}\left(|\lambda_H = -1\rangle + |\lambda_H = 1\rangle\right)$$

$$|\psi(t)\rangle = U(t, t_0 = 0)|\psi(0)\rangle, \text{ where } U(t, t_0 = 0) = e^{-iHt/\hbar}$$

$$= e^{-iHt/\hbar}\left(\frac{1}{\sqrt{2}}\left[|\lambda_H = -1\rangle + |\lambda_H = 1\rangle\right)\right.$$

$$= \frac{1}{\sqrt{2}}\left(e^{-it\omega}|\lambda_H = 1\rangle + e^{it\omega}|\lambda_H = -1\rangle\right)$$

c) $P(b = 2) = |\langle \lambda_b = 2, 1|\psi(t)\rangle|^2 + |\langle \lambda_b = 2, 2|\psi(t)\rangle|^2$

*convert kets from B basis to H basis

$$|\lambda_b = 2, 1\rangle = \frac{1}{\sqrt{2}}\left(|\lambda_H = -1\rangle + |\lambda_H = 1\rangle\right)$$

$$|\lambda_b = 2, 2\rangle = \frac{1}{\sqrt{3}}\left(|\lambda_H = 2\rangle + \sqrt{2}|\lambda_H = -1\rangle - \sqrt{2}|\lambda_H = 1\rangle\right) = \begin{bmatrix} 1 \\ \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ \sqrt{2} \end{bmatrix}$$

$$P(b = 2) = \left|\frac{1}{\sqrt{2}}\left(\langle \lambda_H = -1| + \langle \lambda_H = 1|\right)\left(\frac{1}{\sqrt{3}}e^{-it\omega}|\lambda_H = 1\rangle + e^{it\omega}|\lambda_H = -1\rangle\right)\right|^2 + \ldots$$

$$= \left|\frac{1}{2}\left(e^{it\omega} + e^{-it\omega}\right)\right|^2 + \left|\frac{2}{3}\left(e^{it\omega} - e^{-it\omega}\right)\right|^2$$

$$= \left(\frac{1}{2}\left(e^{-it\omega} + e^{it\omega}\right)\left(e^{it\omega} + e^{-it\omega}\right) + \frac{2}{3}\left(e^{-it\omega} - e^{it\omega}\right)\left(e^{it\omega} - e^{-it\omega}\right)\right)$$

$$= \left(\frac{1}{2}\left(1 + e^{-2it\omega} + e^{2i\omega t} + 1\right) + \frac{2}{3}\left(1 - e^{2i\omega t} - e^{-2i\omega t} + 1\right)\right)$$

$$= 1 + \frac{4}{3}$$

Aug 2008

## Problem 6: Hydrogen Atom (10 Points)

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

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

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)**

Aug 2008

# Quantum #6

a) $\psi(r,\theta,\varphi) = A e^{-(r/a_0)}$

$$1 = A^2 \int_0^\infty r^2 dr \int_0^{2\pi} d\varphi \int_0^\pi \sin\theta \, d\theta \; e^{-(2r/a_0)}$$

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

$$\text{* but} \int_0^\infty x^n e^{-ax} dx = \frac{\Gamma(n+1)}{a^{n+1}} \qquad \begin{matrix} x = r \\ n = 2 \end{matrix} \qquad a = 2/a_0$$

$$1 = 4\pi \, \Gamma(3) \, a_0^3 \cdot \tfrac{1}{8} A^2 \qquad (\Gamma(3) = 2)$$

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

b) For the hydrogen atom: $V = \dfrac{-e^2}{4\pi\epsilon_0 r}$

$$\langle\psi|V|\psi\rangle = \int d\vec{r}^{\,3} \, \psi^* V \psi$$

$$= \int_0^\infty r^2 dr \int_0^{2\pi} d\varphi \int_0^\pi \sin\theta \, d\theta \; \frac{-e^2}{4\pi\epsilon_0 r} e^{-2r/a_0} \cdot \frac{1}{\pi a_0^3}$$

$$= 4\pi \cdot \frac{-e^2}{4\pi\epsilon_0} \int_0^\infty r \, e^{-2r/a_0} dr \qquad \begin{matrix} x = r \\ n = 1 \end{matrix} \qquad a = 2/a_0$$

$$= \frac{-e^2}{\epsilon_0} \frac{\Gamma(2)}{(2/a_0)^2} \cdot \frac{1}{\pi a_0^3}$$

$$= \frac{-e^2 a_0^2}{4\epsilon_0} \cancel{\Gamma(2)}^{\,1} \cdot \frac{1}{\pi a_0^3}$$

$$= \frac{-e^2}{4\pi\epsilon_0 a_0}$$

c) $$\langle r\rangle = \int_0^\infty r^2 dr \int_0^{2\pi} d\varphi \int_0^\pi \sin\theta \, d\theta \; r \, e^{-2r/a_0} \cdot \frac{1}{\pi a_0^3}$$

$$= \frac{4}{a_0^3} \int_0^\infty r^3 e^{-2r/a_0} \qquad \begin{matrix} x = r \\ n = 3 \end{matrix} \qquad a = 2/a_0$$

$$= \frac{4}{a_0^3} \frac{\Gamma(4)}{(2/a_0)^4}$$

$$= \frac{4a_0}{16} 3!$$

$$= \frac{6a_0}{4} = \frac{3a_0}{2}$$

#6 (cont.)

c) $\langle \psi | \psi \rangle = \int_0^\infty 4\pi r^2 e^{-2r/a_0} \, dr = 1?$

$\frac{dP}{dr} = 0 = \frac{4}{a_0^3} r^2 e^{-2r/a_0}$

$\frac{d^2P}{dr^2} = \frac{4}{a_0^3}\left[2re^{-2r/a_0} + r^2 \frac{-2}{a_0} e^{-2r/a_0}\right] = 0$

* 2nd derivative gives inflection points

$$2r + r^2 \frac{-2}{a_0} = 0$$

$$2 + r\frac{-2}{a_0} = 0$$

$$\frac{-2r}{a_0} = 2$$

$$r = a_0$$

d) $L|n l m\rangle = l(l+1)\hbar^2 |n l m\rangle$

* since ground state $|\psi\rangle = |1,0,0\rangle$

$L|1,0,0\rangle = 0$

e) z-axis is defined by the line $\perp$ to the plane in which the ground state electron orbits the central nucleus.