Griffiths Ch 2 Notes

2.1 - Stationary States

- We want to solve Schrödinger Eqn for a variety of potentials

$$\Rightarrow \quad i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi \qquad \text{where } \Psi(x,t) = \psi(x)\varphi(t)$$

- To solve Schrödinger Eqn:

$$\frac{\partial \Psi}{\partial t} = \psi \frac{\partial \varphi}{\partial t} \qquad \frac{\partial \Psi}{\partial x} = \frac{\partial \psi}{\partial x}\varphi$$

$$\Rightarrow \quad i\hbar \frac{\partial \varphi}{\partial t}\psi = \frac{-\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2}\varphi + V\psi\varphi$$

$$i\hbar \frac{1}{\varphi}\frac{\partial \varphi}{\partial t} = \frac{-\hbar^2}{2m}\frac{1}{\psi}\frac{\partial^2 \psi}{\partial x^2} + V$$

$$\rightarrow \text{ (1) } E = i\hbar \frac{1}{\varphi}\frac{\partial \varphi}{\partial t}$$

$$\text{(2) } E = \frac{-\hbar^2}{2m}\frac{1}{\psi}\frac{\partial^2 \psi}{\partial x^2}$$

> E is separation constant

- Solution of (1) always yields $\varphi(t) = e^{-iEt/\hbar}$; we now call (2) the time-independent Schrödinger Eqn, where we now must specify V to proceed
- Probability densities + expectation values constant in time due to $\psi^*\psi$ multiplication
- There is a different ψ for every allowable energy value E_i; therefore by the rules of linear algebra + differential equations, any linear combinations of solutions is also a solution

$$\Rightarrow \quad \Psi(x,t) = \sum_n c_n \psi_n(x)\exp[-iE_n t/\hbar]$$

2.2 - Infinite Square Well

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

← These boundaries can be shifted at will

- Since $E \ge V$, outside the well we know $\psi(x) = 0$
  - ↳ we want only ψ w/in the well

2.2 (cont.)

$$\Rightarrow H\psi = E\psi$$

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + 0\right)\psi = E\psi$$

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

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

* let $k \equiv \sqrt{2mE}/\hbar$

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

$$\Rightarrow \psi(x) = A\sin(kx) + B\cos(kx) \leftarrow \underline{\text{easier to solve}}$$

$$= Ae^{ikx} + Be^{-ikx}$$

* To be normalizable, generally our boundary conditions are that both ψ and $\frac{\partial \psi}{\partial x}$ are continuous, but we can ignore the second condition when $V \to \infty$.

$$\Rightarrow \psi(0) = \psi(a) = 0$$

$$0 = A\overset{0}{\cancel{\sin(kx)}} + B\cos(kx)\Big|_{x=0}$$

$\hookrightarrow B = 0$

$$0 = A\sin(ka)$$

$$\hookrightarrow k_n = \frac{n\pi}{a} \rightarrow E_n = \frac{\hbar^2 k^2}{2m} = \frac{\pi^2 n^2 \hbar^2}{2ma^2}$$

* Check normalization to solve for A

$$1 = \int_0^a \psi^*(x)\,\psi(x)\,dx$$

$$1 = |A|^2 \int_0^a \sin^2(kx)\,dx$$

$$1 = |A|^2 \frac{a}{2}$$

$\hookrightarrow A = \sqrt{\frac{2}{a}}$

* for an individual solution

$$c_n = \int \psi_n^*(x) f(x)\,dx, \quad f(x) = \sqrt{\frac{2}{a}} \sum_i c_i \sin\left(\frac{i\pi x}{a}\right)$$

5.2. The Particle in a Box

We now consider our first problem with a potential, albeit a rather artificial one:

$$\begin{aligned} V(x) &= 0, \qquad |x| < L/2 \\ &= \infty, \qquad |x| \geq L/2 \end{aligned} \tag{5.2.1}$$

This potential (Fig. 5.1a) is called the box since there is an infinite potential barrier in the way of a particle that tries to leave the region $|x| < L/2$. The eigenvalue equation in the X basis (which is the only viable choice) is

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0 \tag{5.2.2}$$

We begin by partitioning space into three regions I, II, and III (Fig. 5.1a). The solution ψ is called ψ_{I}, ψ_{II}, and ψ_{III} in regions I, II, and III, respectively.

Consider first region III, in which $V = \infty$. It is convenient to first consider the case where V is not infinite but equal to some V_0 which is greater than E. Now

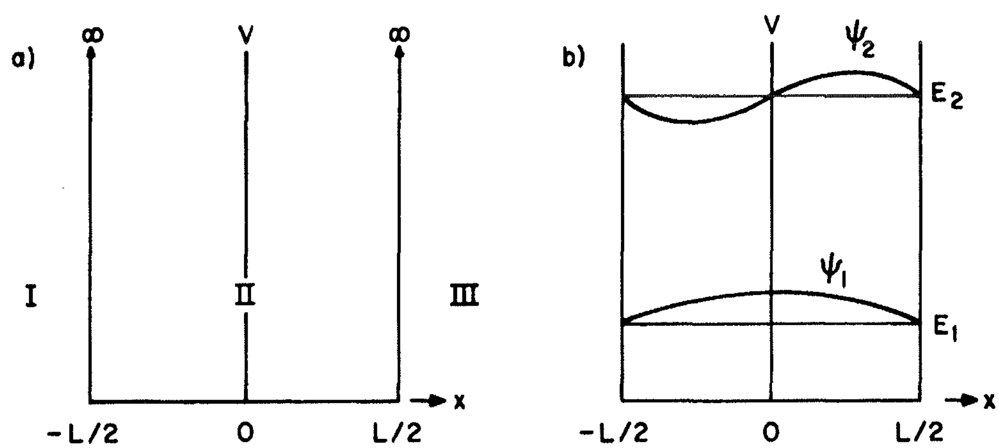


Figure 5.1. (a) The box potential. (b) The first two levels and wave functions in the box.

Eq. (5.2.2) becomes

$$\frac{d^2\psi_{\text{III}}}{dx^2}-\frac{2m(V_0-E)}{\hbar^2}\psi_{\text{III}}=0 \tag{5.2.3}$$

which is solved by

$$\psi_{\text{III}}=A\,e^{-\kappa x}+B\,e^{\kappa x} \tag{5.2.4}$$

where $\kappa=[2m(V_0-E)/\hbar^2]^{1/2}$.

Although A and B are arbitrary coefficients from a mathematical standpoint, we must set $B=0$ on physical grounds since $B\,e^{\kappa x}$ blows up exponentially as $x\to\infty$ and such functions are not members of our Hilbert space. If we now let $V\to\infty$, we see that

$$\psi_{\text{III}}\equiv 0$$

It can similarly be shown that $\psi_{\text{I}}\equiv 0$. In region II, since $V=0$, the solutions are exactly those of a free particle:

$$\psi_{\text{II}}=A\exp[i(2mE/\hbar^2)^{1/2}x]+B\exp[-i(2mE/\hbar^2)^{1/2}x] \tag{5.2.5}$$

$$=A\,e^{ikx}+B\,e^{-ikx}, \qquad k=(2mE/\hbar^2)^{1/2} \tag{5.2.6}$$

It therefore appears that the energy eigenvalues are once again continuous as in the free-particle case. This is not so, for $\psi_{\text{II}}(x)=\psi$ only in region II and not in all of space. We must require that ψ_{II} goes continuously into its counterparts ψ_{I} and ψ_{III} as we cross over to regions I and II, respectively. In other words we require that

$$\psi_{\text{I}}(-L/2)=\psi_{\text{II}}(-L/2)=0 \tag{5.2.7}$$

$$\psi_{\text{III}}(+L/2)=\psi_{\text{II}}(+L/2)=0 \tag{5.2.8}$$

(We make no such continuity demands on ψ' at the walls of the box since V jumps to infinity there.) These constraints applied to Eq. (5.2.6) take the form

$$A\,e^{-ikL/2}+B\,e^{ikL/2}=0 \tag{5.2.9a}$$

$$A\,e^{ikL/2}+B\,e^{-ikL/2}=0 \tag{5.2.9b}$$

or in matrix form

$$\begin{bmatrix} e^{-ikL/2} & e^{ikL/2} \\ e^{ikL/2} & e^{-ikL/2} \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{5.2.10}$$

Such an equation has nontrivial solutions only if the determinant vanishes:

$$e^{-ikL} - e^{ikL} = -2i \sin(kL) = 0 \tag{5.2.11}$$

that is, only if

$$k = \frac{n\pi}{L}, \qquad n = 0, \pm 1, \pm 2, \ldots \tag{5.2.12}$$

To find the corresponding eigenfunctions, we go to Eqs. (5.2.9a) and (5.2.9b). Since only one of them is independent, we study just Eq. (5.2.9a), which says

$$A\, e^{-in\pi/2} + B\, e^{in\pi/2} = 0 \tag{5.2.13}$$

Multiplying by $e^{i\pi n/2}$, we get

$$A = -e^{in\pi} B \tag{5.2.14}$$

Since $e^{in\pi} = (-1)^n$, Eq. (5.2.6) generates two families of solutions (normalized to unity):

$$\psi_n(x) = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{n\pi x}{L}\right), \qquad n \text{ even} \tag{5.2.15}$$

$$= \left(\frac{2}{L}\right)^{1/2} \cos\left(\frac{n\pi x}{L}\right), \qquad n \text{ odd} \tag{5.2.16}$$

Notice that the case $n = 0$ is uninteresting since $\psi_0 \equiv 0$. Further, since $\psi_n = \psi_{-n}$ for n odd and $\psi_n = -\psi_{-n}$ for n even, and since eigenfunctions differing by an overall factor are not considered distinct, we may restrict ourselves to positive nonzero n. In summary, we have

$$\psi_n = \left(\frac{2}{L}\right)^{1/2} \cos\left(\frac{n\pi x}{L}\right), \qquad n = 1, 3, 5, 7, \ldots \tag{5.2.17a}$$

$$= \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{n\pi x}{L}\right), \qquad n = 2, 4, 6, \ldots \tag{5.2.17b}$$

and from Eqs. (5.2.6) and (5.2.12),

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{2mL^2} \tag{5.2.17c}$$

[It is tacitly understood in Eqs. (5.2.17a) and (5.2.17b) that $|x| < L/2$.]

2.3 – Harmonic Oscillator

$$V(x) = \frac{1}{2}m\omega^2 x^2$$

$$\Rightarrow \quad H\psi = E\psi$$

$$\left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2\right)\psi = E\psi$$

* Brute force method involves power series, but we can rewrite H in terms of ladder operators to more easily achieve solution

$\Rightarrow$ Ladder Operator Method:

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

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

$$= \hbar\omega\left(a_- a_+ - \frac{1}{2}\right)$$

where $a_\pm = \frac{1}{\sqrt{2m\hbar\omega}}\left(\mp ip + m\omega x\right)$

$$= \hbar\omega\left(a_+ a_- + \frac{1}{2}\right)$$

$\Rightarrow$ Note: Applying a_- to the ground state ψ_0 yields:

$$a_-\psi_0 = 0$$

$$\frac{1}{\sqrt{2\hbar m\omega}}\left(\hbar\frac{\partial}{\partial x} + m\omega x\right)\psi_0 = 0$$

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

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

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

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

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

* Normalization yields: $A = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$

* Plugging into Schrödinger Eqn yields: $E_0 = \frac{\hbar\omega}{2}$

* Higher energy states generated by repeated application of raising operator

$$E_n = (n + 1/2)\hbar\omega$$

2.3 (cont.)

- Other facts about ladder operators include:

$$a_+ \psi_n = \sqrt{n+1}\, \psi_{n+1}$$

$$a_- \psi_n = \sqrt{n}\, \psi_n$$

$$\tilde{x} = \sqrt{\frac{\hbar}{2m\omega}}\,(a_+ + a_-)$$

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

* Normalization of previous solution requires multiplication by Gaussian to be normalizable

$$\Rightarrow \psi_n = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi)\, e^{-\xi^2/2}, \quad H_n \text{ are Hermite polynomials}$$

2.4 – Free Particle

$V = 0$ for all x

- Our solution will be of the same form as infinite square well

$$\Rightarrow \psi(x) = Ae^{ikx} + Be^{-ikx}, \quad k = \frac{\sqrt{2mE}}{\hbar}$$

$$\Psi(x,t) = A\exp\left[i\left(kx - \frac{\hbar k^2}{2m}t\right)\right], \quad k = \pm\frac{\sqrt{2mE}}{\hbar} \quad \begin{cases} k>0, & \text{travels to right} \\ k<0, & \text{travels to left} \end{cases}$$

- The velocity of the above wave is:

$$V = \frac{\hbar|k|}{2m} = \sqrt{\frac{E}{2m}}$$

$$p = \hbar k$$

* But our above solution is not normalizable on its own; we must combine these waves into a wave packet

$$\Rightarrow \Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \phi(k)\exp\left[i\left(kx - \frac{\hbar k^2}{2m}t\right)\right]dk$$

$$\hookrightarrow \phi(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \Psi(x,0)\,e^{-ikx}\,dx \quad \text{(via inverse Fourier Transform)}$$

$\Rightarrow$ But now our speeds don't match

$$V_{group} = \frac{d\omega}{dk}$$

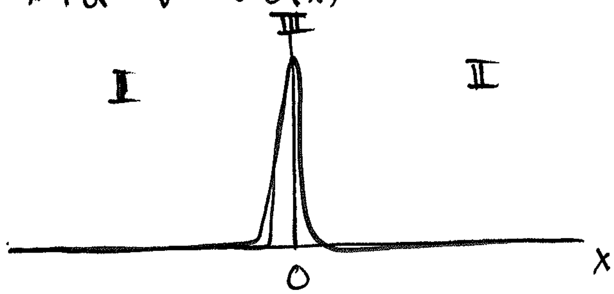
$$V_{phase} = \frac{\omega}{k}$$

2.5 - δ-Function Potential

- Potentials that do not go to infinity as $x \to \infty$ now allows to have both bound and scattered states

$$\hookrightarrow \begin{cases} E > V & \Rightarrow \text{scattering state} \\ E < V & \Rightarrow \text{bound state} \end{cases}$$

* For $V = \alpha \delta(x)$



$\Rightarrow$ If $E < 0$ (Bound States)

* In region I:

$$H\psi = E\psi$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} - \alpha \cancel{\delta(x)}^{0}\psi = E\psi$$

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

$$\Rightarrow \psi(x) = \cancel{Ae^{-kx}}^{0} + Be^{kx}, \quad k = \frac{\sqrt{-2mE}}{\hbar}$$

$$= Be^{kx}$$

* In region II:

* By same work as above

$$\psi(x) = Fe^{-kx} + \cancel{Ge^{kx}}^{0}$$

$$= Fe^{-kx}$$

* Remembering our boundary conditions:

① $\psi(x)$ is continuous

② $\frac{d\psi}{dx}$ is continuous where $V(x) \neq \infty$

2.5 (cont.)

$$\Rightarrow \psi(x) = \begin{cases} Be^{kx} & x \leq 0 \\ Be^{-kx} & x \geq 0 \end{cases}$$

* But we get no information about 2nd condition unless:

$$\frac{-\hbar^2}{2m}\int_{-\epsilon}^{\epsilon}\left(\frac{d^2\psi}{dx^2} + V(x)\psi(x)\right)dx = E\int_{-\epsilon}^{\epsilon}\psi(x)dx$$

$$\frac{-\hbar^2}{2m}\frac{d\psi}{dx}\Big|_{-\epsilon}^{\epsilon} + \int_{-\epsilon}^{\epsilon}V(x)\psi(x)dx = 0$$

$$\Delta\left(\frac{d\psi}{dx}\right) = \frac{2m}{\hbar^2}\lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon}V(x)\psi(x)dx$$

$$-2Bk = \frac{-2m\alpha}{\hbar^2}\psi(0)$$

$$\Rightarrow k = \frac{m\alpha}{\hbar^2}$$

$$E = \frac{-\hbar^2 k^2}{2m} = -\frac{m\alpha^2}{2\hbar^2}$$

* Normalization yields final form

$$\psi(x) = \frac{\sqrt{m\alpha}}{\hbar}\exp\left[-m\alpha|x|/\hbar^2\right], \quad E = \frac{-m\alpha^2}{2\hbar^2}$$

* Note: Only one bound state exists

⇒ If $E > 0$ (Scattering States)

* In region I:

$$H\psi = E\psi$$

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \alpha\delta(x)\psi = E\psi$$

$$\frac{d^2\psi}{dx^2} = \frac{-2mE}{\hbar^2}\psi$$

$$\hookrightarrow \psi(x) = Ae^{ikx} + Be^{-ikx}, \quad k = \frac{\sqrt{2mE}}{\hbar}$$

* In region II:

$$\psi(x) = Fe^{ikx} + Ge^{-ikx}$$

2.5 (cont.)

* Application of boundary conditions yields:

① $\psi(x)$ is continuous

$$\Rightarrow Ae^{ikx} + Be^{-ikx} = Fe^{ikx} + Ge^{-ikx} \Big|_{x=0}$$

$$A + B = F + G$$

② $\frac{d\psi}{dx}$ is continuous except where $V(x) = \infty$

$$\Rightarrow \Delta\left(\frac{d\psi}{dx}\right) = ik(F - G - A + B) = \frac{-2m\alpha}{\hbar^2}(A+B)$$

$$\hookrightarrow F - G = A(1 + 2i\beta) - B(1 - 2i\beta), \quad \beta = \frac{m\alpha}{\hbar^2 k}$$

⇒ Since we currently have an unsolvable system (2 eqns, 4+ unknowns) in a non-normalizable state, we rephrase the problem in terms of scattering w/ particles

↳ When combined w/ time dependent part of wavefunction:

$A \rightarrow$ Incoming wave

$B \rightarrow$ Reflected wave

$F \rightarrow$ Transmitted wave

$G \rightarrow \emptyset$

⇒ This now implies

$$B = \frac{i\beta}{1 - i\beta} A \qquad F = \frac{1}{1 - i\beta} A$$

where the reflection + transmission coefficients R & T are:

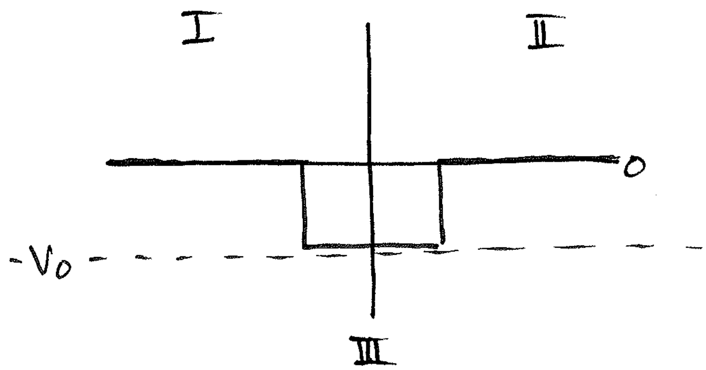
$$R = \frac{|B|^2}{|A|^2} = \frac{\beta^2}{1+\beta^2}$$

$$T = \frac{|F|^2}{|A|^2} = \frac{1}{1+\beta^2}$$

2.6 - Finite Square Well

$$V(x) = \begin{cases} 0, & |x| > a \\ -V_0, & -a < x < a \end{cases}$$

* Remember, we must consider both bound + unbound states



* For bound states $-V_0 < E < 0$ ($E < -V_0$ is not allowed)
  - In region I:

$$H\psi = E\psi$$

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

$$\frac{d^2\psi}{dx^2} = \kappa^2\psi, \quad \kappa = \frac{\sqrt{-2mE}}{\hbar}$$

$$\Rightarrow \psi(x) = \cancel{Ae^{-\kappa x}}^{\,0} + Be^{\kappa x}$$

$$= Be^{\kappa x}$$

  - In region II:
    * Similarly to above

$$\psi(x) = Fe^{-\kappa x} + \cancel{Ge^{\kappa x}}^{\,0}$$

$$= Fe^{-\kappa x}$$

  - In region III:

$$H\psi = E\psi$$

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + -V_0\psi = E\psi$$

$$\frac{d^2\psi}{dx^2} = \frac{-(E+V_0)2m}{\hbar^2}\psi$$

2.6 (cont.)

$$\Rightarrow \psi(x) = Ce^{-ikx} + De^{ikx}, \qquad k = \frac{\sqrt{2m(E+V_0)}}{\hbar}$$

$$= C\sin(kx) + D\cos(kx)$$

* Application of our boundary conditions + the fact that we have a symmetric potential informs us that solutions will either be even or odd.

$\Rightarrow$ Even Case:

$$\psi(x) = \begin{cases} Fe^{-\kappa x}, & x > a \\ D\cos(kx), & 0 < x < a \\ \psi(-x), & x < 0 \end{cases}$$

① $\psi(x)$ is continuous

$$Fe^{-\kappa a} = D\cos(ka)$$

② $\frac{d\psi}{dx}$ is continuous

$$-\kappa Fe^{-\kappa a} = -kD\sin(ka)$$

* Dividing ② by ① yields

$$+\kappa = +k\tan(ka)$$

↳ Redefining $z = ka$

$$z_0 = \frac{a}{\hbar}\sqrt{2mV_0}$$

*Notice, $k^2 + \kappa^2 = \frac{2mV_0}{\hbar^2}$

↳ $\kappa a = \sqrt{z_0^2 - z^2}$

↳ $\tan(z) = \sqrt{\frac{z_0}{z^2} - 1}$

*If we examine the limiting cases

① Wide, deep well

$$E_n + V_0 \approx \frac{\pi^2 n^2 \hbar^2}{2m(2a)^2}$$

$\Rightarrow$ Approximates infinite square well, but w/ finite energy states

② Shallow, narrow well

$\Rightarrow$ Eventually results in only one bound state

2.6 (cont.)

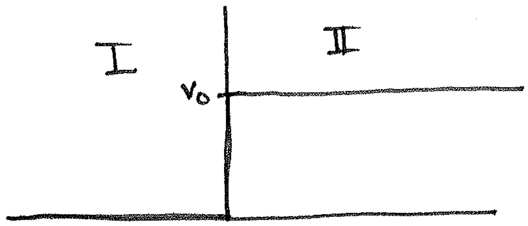
* For the scattering states ($E > 0$)
  - In region I:
    $$\psi(x) = Ae^{ikx} + Be^{-ikx}, \quad k = \frac{\sqrt{2mE}}{\hbar}$$
    * From free-particle solution
  - In region II:
    $$\psi(x) = Fe^{ikx}, \quad k = \frac{\sqrt{2mE}}{\hbar}$$
    * From free-particle solution + scattering interpretation
  - In region III:
    $$\psi(x) = C\sin(lx) + D\cos(lx), \quad l = \frac{\sqrt{2m(E+V_0)}}{\hbar}$$
    * From bound state solution
  - Applying our boundary conditions yield:
    * At $x = -a$
    $$Ae^{-ika} + Be^{ika} = -C\sin(la) + D\cos(la) \quad ①$$
    $$ik\left[Ae^{-ika} - Be^{ika}\right] = l\left[C\cos(la) + D\sin(la)\right] \quad ②$$
    * At $x = a$
    $$C\sin(la) + D\cos(la) = Fe^{ika} \quad ③$$
    $$l\left[C\cos(la) - D\sin(la)\right] = ikFe^{ika} \quad ④$$
  - Eliminating C & D yields:
    $$B = \frac{i\sin(2la)}{2kl}(l^2 - k^2)F$$
    $$F = \frac{\exp[-2ika]}{\cos(2la) - i\frac{k^2+l^2}{2kl}\sin(2la)}A$$

* Note: Perfect transmission occurs when
$$E_n + V_0 = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}$$

Step Potential

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & x > 0 \end{cases}$$

* Solutions will follow from free particle and finite well



* In region I:

$\Rightarrow$ Free particle solution

$$\psi(x) = Ae^{ikx} + Be^{-ikx}, \quad k = \frac{\sqrt{2mE}}{\hbar}$$

* In region II:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V_0\psi = E\psi$$

$$\frac{\partial^2\psi}{\partial x^2} = \frac{2m(V_0-E)}{\hbar^2}\psi$$

$$= Ce^{-\alpha x}, \quad \alpha = \frac{\sqrt{2m(V_0-E)}}{\hbar}$$

* Applying boundary conditions yields:

① ψ is continuous

$$\Rightarrow A + B = C$$

② $\frac{d\psi}{dx}$ is continuous

$$ik(A-B) = -\alpha C$$

$\Rightarrow$ Scattering states like in Finite Well

$$\delta = \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2m(V_0-E)}}$$ (skin depth, ie depth of tunnelling into barrier)

Hydrogen Atom / Central Potential

* First, we examine the Schrödinger Eqn in spherical coordinates:

$$\frac{-\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

where $\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2}{\partial\varphi^2}\right)$

$$\Rightarrow \frac{-\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2\psi}{\partial\varphi^2}\right)\right] + V\psi = E\psi$$

* Assuming a solution of the form $\psi = R(r)\,Y(\theta,\varphi)$

$$\frac{-\hbar^2}{2m}\left[\frac{Y}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + \frac{R}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{R}{r^2\sin^2\theta}\left(\frac{\partial^2 Y}{\partial\varphi^2}\right)\right] + VRY = ERY$$

* We can separate the equations by multiplying by $\frac{-2mr^2}{\hbar^2 RY}$

$$\left[\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}(V(r)-E)\right] + \frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\theta^2}\right] = 0$$

* Using the separation constant $\ell(\ell+1)$, we see:

$\Rightarrow$ Radial Eqn: $\frac{1}{R}\left(\frac{d}{dr}\left[r^2\frac{dR}{dr}\right]\right) - \frac{2mr^2}{\hbar^2}\left(V(r)-E\right) = \ell(\ell+1)$

Angular Eqn: $\frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2}\right] = -\ell(\ell+1)$

* Since there is no dependence of the angular equation on the potential, all problems in spherical coordinates will partly be composed of its solution

$$\frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{\partial^2 Y}{\partial\varphi^2}\right] = -\ell(\ell+1)$$

$$\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{\partial^2 Y}{\partial\varphi^2} = -\ell(\ell+1)\sin^2\theta\, Y$$

* Again trying separation of variables, we assume $Y(\theta,\varphi) = \Theta(\theta)\,\Phi(\varphi)$

$$\Rightarrow \sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)\Phi + \frac{\partial^2\Phi}{\partial\varphi^2}\Theta = -\ell(\ell+1)\sin^2\theta\,\Theta\Phi$$

$$\left(\frac{1}{\Theta}\left[\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)\right] + \ell(\ell+1)\sin^2\theta\right) + \frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\varphi^2} = 0$$

* Using the separation constant m^2, we see:

$$\frac{1}{\Theta}\left[\sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)\right] + \ell(\ell+1)\sin^2\theta = m^2$$

$$\frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\varphi^2} = -m^2$$

* from here it's easy to see that the solution to the Φ equation is:

$$\Phi = e^{im\varphi}$$

where m is allowed to be both positive and negative and the normalization constant is absorped into the Θ equation.

* Applying the periodic boundary condition $\Phi(\varphi) = \Phi(\varphi + 2\pi)$, we find

$$\exp[im\varphi] = \exp[im(\varphi+2\pi)]$$

$$1 = \exp[im2\pi]$$

$$\Rightarrow m \in 0, \pm 1, \pm 2, \ldots$$

* The Θ equation has the known solution of the Legendre polynomials

$$\Rightarrow \Theta = A P_\ell^m(\cos\theta), \quad P_\ell^m = (1-x^2)^{|m|/2}\left(\frac{d}{dx}\right)^{|m|} P_\ell(x)$$

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

$\Rightarrow$ Note: $\ell > 0$ and $|m| > \ell \rightarrow m \in [-\ell, \ell]$

* Multiplying the two equations together and normalizing, we obtain the <u>spherical harmonics</u>

$$Y_\ell^m(\theta,\varphi) = \epsilon\sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-|m|)!}{(\ell+|m|)!}}\, e^{im\varphi} P_\ell^m(\cos\theta)$$

$$\epsilon = \begin{cases} (-1)^m & m \geq 0 \\ 1 & m < 0 \end{cases}$$

* Returning to the radial equation, we cannot proceed any further w/o specifying a potential after a few manipulations

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

* if we substitute $u(r) = rR(r) \Rightarrow R = \frac{u}{r}$

$$\hookrightarrow \frac{-\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[V + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right]u = Eu$$

* Note: This is the 1-D Schrödinger Eqn if $V + \frac{\hbar^2}{2m}\frac{(\ell+1)\ell}{r^2} = V_{eff}$ where the extra term is called the centrifugal term, as it forces the particle further away from the origin.

The normalization condition now becomes $\int_0^\infty |u|^2 dr = 1$

ex. Spherical Well

$$V = \begin{cases} 0 & r \leq a \\ \infty & r > a \end{cases}$$

* Similar to the square well, if $r > a$, $u(r) = 0$

$$\hookrightarrow \quad \frac{-\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[V + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}\right]u = Eu$$

$$\frac{-\hbar^2}{2m}\frac{d^2u}{dr^2} + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}u = Eu$$

$$\frac{d^2u}{dr^2} + \frac{-\ell(\ell+1)}{r^2}u = \frac{-2mE}{\hbar^2}u$$

$$\frac{d^2u}{dr^2} + \frac{-\ell(\ell+1)}{r^2}u = -k^2u, \qquad k = \frac{\sqrt{2mE}}{\hbar^2}$$

* In the case where $\ell = 0$, we get our familiar square well answers

$$\frac{d^2u}{dr^2} = -k^2u \iff u(r) = A\sin(kr) + B\cos(kr)$$

$$B \to 0 \text{ since } \frac{\cos(kr)}{r} \to \infty \text{ as } r \to 0$$

$$E_{n0} = \frac{n^2\pi^2\hbar^2}{2ma^2} \qquad n \in \mathbb{Z}^+$$

$$\psi_{n00} = \frac{1}{\sqrt{2\pi a}}\,\frac{\sin(n\pi r/a)}{r}$$

* If $\ell \neq 0$, solving yields the spherical Bessel functions

$$E_{n\ell} = \frac{\hbar^2}{2ma^2}\beta_{n\ell}^2, \quad \beta_{n\ell} \text{ is } n^{th}\ 0 \text{ of } \ell^{th} \text{ spherical Bessel function}$$

$$\psi_{n\ell m} = A_{nj}\, j_\ell\!\left(\beta_{n\ell}\frac{r}{a}\right)Y_\ell^m(\theta,\phi)$$

ex. Hydrogen Atom / Central Potential

$$V(r) = \frac{-e^2}{4\pi\epsilon_0}\frac{1}{r}$$

$$\Rightarrow \frac{-\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[\frac{-e^2}{4\pi\epsilon_0}\frac{1}{r} + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}\right]u = Eu$$

$$\frac{-\hbar^2}{2mE}\frac{d^2u}{dr^2} + \frac{1}{E}\left[\frac{-e^2}{4\pi\epsilon_0}\frac{1}{r} + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}\right]u = u$$

* substituting $\kappa = \frac{\sqrt{-2mE}}{\hbar}$

$$\frac{1}{\kappa^2}\frac{d^2u}{dr^2} = u\left[1 - \frac{me^2}{2\pi\epsilon_0\hbar^2\kappa}\frac{1}{\kappa r} + \frac{\ell(\ell+1)}{(\kappa r)^2}\right]$$

* defining $p = \kappa r$, $p_0 = \frac{me^2}{2\pi\epsilon_0\hbar^2\kappa}$

$$\frac{d^2u}{dp^2} = u\left[1 - \frac{p_0}{p} + \frac{\ell(\ell+1)}{p^2}\right]$$

* Examining the limits of the equation offers clues to its solution

↳ In the limit where $p \to \infty$

$$\frac{d^2u}{dp^2} = u \quad \Leftrightarrow \quad u = Ae^{-p} + \cancel{Be^{p}}^{\,0}$$

↳ $u(p) \sim Ae^{-p}$

↳ In the limit where $p \to 0$

$$\frac{d^2u}{dp^2} = \frac{\ell(\ell+1)}{p^2}u \quad \Leftrightarrow \quad u = Cp^{\ell+1} + \cancel{Dp^{-\ell}}^{\,0}$$

↳ $u(p) \sim Cp^{\ell+1}$

* We now rewrite our general solution as: $u(p) = p^{\ell+1}e^{-p}v(p)$ and resolve the differential equation

$$\Rightarrow \frac{du}{dp} = p^{\ell}e^{-p}\left[(\ell+1-p)v + p\frac{dv}{dp}\right]$$

$$\frac{d^2u}{dp^2} = p^{\ell}e^{-p}\left[\left(-2\ell-2+p+\frac{\ell(\ell+1)}{p}\right)v + 2(\ell+1-p)\frac{dv}{dp} + p\frac{d^2v}{dp^2}\right]$$

↳ Eliminating common terms, we see:

$$p\frac{d^2v}{dp^2} + 2(\ell+1-p)\frac{dv}{dp} + [p_0 - 2(\ell+1)]v = 0$$

* Assuming we can express the solution as a power series, $v(p) = \sum' c_j p^j$ we find that:

$$\frac{dv}{dp} = \sum_{j=0}' j c_j p^{j-1} = \sum_{j=0}' (j+1) c_{j+1} p^j$$

$$\frac{d^2 v}{dp^2} = \sum_{j=0}' j(j+1) c_{j+1} p^{j-1}$$

* Plugging these into the differential equation yields the recursion relation for c_j:

$$c_{j+1} = \frac{2(j+l+1) - p_0}{(j+1)(j+2l+2)} c_j$$

$\Rightarrow$ At large j our relationship approximates: $c_{j+1} = \frac{2}{j+1} c_j$

$\hookrightarrow$ Plugging this into our differential equation yields a solution of:

$$v(p) = c_0 \sum' \frac{2^j}{j!} p^j = c_0 e^{2p} \Leftrightarrow u(p) = c_0 p^{l+1} e^p$$

Note: Since this blows up as $p \to \infty$, there must be a j_{max} such that:

$$c_{j_{max}+1} = 0$$

$$\hookrightarrow 2(j_{max} + l + 1) - p_0 = 0$$

if $n = j_{max} + l + 1$

$$p_0 = 2n \Leftrightarrow E = \frac{-\hbar^2 \kappa^2}{2m} = \frac{-me^4}{8\pi^2 \epsilon_0^2 \hbar^2 p_0^2}$$

$$\hookrightarrow E_n = -\left[\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right]\frac{1}{n^2} = \frac{E_1}{n^2} \quad n \in 1,2,3\ldots$$

* Returning to our overall solution, we know that our solution has the form:

$$\psi_{nlm} = R_{nl}(r) Y_l^m(\theta, \varphi) \; ; \; R_{nl}(r) = \frac{1}{r} p^{l+1} e^{-p} v(p)$$

Note: The derived formulas above for $v(p)$ are those of the associated Laguerre polynomials: $L_{q-p}^{p}(x) = (-1)^p \left(\frac{d}{dx}\right)^p L_q(x)$; $L_q(x) = e^x \left(\frac{d}{dx}\right)^q (e^{-x} x^q)$

6.1 - Non-degenerate Perturbation Theory

* Suppose for a system we have already solved

$$H^0 \psi_n^0 = E_n^0 \psi_n^0$$

where we have obtained a complete set of orthonormal ψ_n^0 and their corresponding E_n^0 but we have perturbed the system slightly since then. How do we find the new ψ_n and E_n?

$\Rightarrow$ We want to solve $H\psi_n = E_n \psi_n$

$\hookrightarrow$ $H = H^0 + \lambda H'$

$$\psi_n = \psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \dots$$

$$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots$$

* Note: ψ_n^1 and E_n^1 are first order corrections to wavefunction / energy

$$\Rightarrow (H^0 + \lambda H')(\psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \dots) = (E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots)(\psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \dots$$

$$H^0 \psi_n^0 + \lambda (H^0 \psi_n^1 + H' \psi_n^0) + \lambda^2 (H^0 \psi_n^2 + H' \psi_n^1) + \dots$$
$$= E_n^0 \psi_n^0 + \lambda (E_n^0 \psi_n^1 + E_n^1 \psi_n^0) + \lambda^2 (E_n^0 \psi_n^2 + E_n^1 \psi_n^1 + E_n^2 \psi_n^0) + \dots$$

* Now match orders of λ

$$\Rightarrow \lambda^0 : H^0 \psi_n^0 = E_n^0 \psi_n^0 \quad \text{(Unperturbed system)}$$

$$\lambda^1 : H^0 \psi_n^1 + H' \psi_n^0 = E_n^0 \psi_n^1 + E_n^1 \psi_n^0$$

$$\lambda^2 : H^0 \psi_n^2 + H' \psi_n^1 = E_n^0 \psi_n^2 + E_n^1 \psi_n^1 + E_n^0 \psi_n^2$$

* To determine E_n^1, take inner product w/ $\langle \psi_n^0 |$

$$\Rightarrow \langle \psi_n^0 | H^0 \psi_n^1 \rangle + \langle \psi_n^0 | H' | \psi_n^0 \rangle = \langle \psi_n^0 | E_n^0 | \psi_n^1 \rangle + \langle \psi_n^0 | E_n^1 | \psi_n^0 \rangle$$

$$\langle \psi_n^0 | E_n^0 | \psi_n^1 \rangle + \quad '' \quad = \quad \cancel{''} \quad ''$$

$$\Rightarrow E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle$$

6.1 (cont.)

* To determine ψ_n^1, we first rewrite our equation

$$\Rightarrow (H^0 - E_n^0)\psi_n^1 = -(H' - E_n^1)\psi_n^0$$

* but $\psi_n^1 = \sum_{m \neq n}' c_m^{(n)} \psi_m^0$

$$\Rightarrow \sum_{m \neq n}' (E_m^0 - E_n^0) c_m^{(n)} \psi_m^0 = -(H' - E_n^1)\psi_n^0$$

Now take inner product w/ $\langle \psi_l^0 |$

$$\sum_{m \neq n}' (E_m^0 - E_n^0) c_m^{(n)} \langle \psi_l^0 | \psi_m^0 \rangle = -\langle \psi_l^0 | H' | \psi_n^0 \rangle + E_n^1 \langle \psi_l^0 | \psi_n^0 \rangle$$

$$(E_l^0 - E_n^0) c_l^{(n)} = -\langle \psi_l^0 | H' | \psi_n^0 \rangle$$

$$c_l^{(n)} = \frac{-\langle \psi_l^0 | H' | \psi_n^0 \rangle}{E_l^0 - E_n^0} \qquad l = m$$

$$\Rightarrow \psi_n^1 = \sum_{m \neq n}' \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_m^0} \psi_m^0$$

* Following a similar procedure for the 2nd order corrections, we see:

$$E_n^2 = \sum_{m \neq n}' \frac{|\langle \psi_m^0 | H' | \psi_n^0 \rangle|^2}{E_n^0 - E_m^0}$$

6.2 - Degenerate Perturbation Theory

* Note: If our energy levels in the formulas above are degenerate, the result goes to infinity unless $\langle m | H' | n \rangle = 0$ as well

ex. Two-fold Degeneracy

Given: $H^0 \psi_a^0 = E^0 \psi_a^0$, $H^0 \psi_b^0 = E^0 \psi_b^0$ $\quad \langle \psi_a^0 | \psi_b^0 \rangle = 0$

↳ Note: $\psi^0 = \alpha \psi_a^0 + \beta \psi_b^0$ is also eigenstate w/ energy E^0

Typically, applying a perturbation H' will lift the degeneracy and allow us to write that state as a linear combination of ψ_a^0 and ψ_b^0, but we don't know the values of α and β a priori. Keeping them general, we attempt to solve: $H\psi = E\psi$

6.2 (cont.)

$$H\Psi = E\Psi \quad \text{where } H = H^0 + \lambda H'$$
$$E = E^0 + \lambda E' + \lambda^2 E^2 + \ldots$$
$$\Psi = \Psi^0 + \lambda \Psi' + \lambda^2 \Psi^2 + \ldots$$

Substituting in the expansions and collecting in powers of λ, we find:

$$H^0\Psi^0 + \lambda(H'\Psi^0 + H^0\Psi') + \ldots = E^0\Psi^0 + \lambda(E'\Psi^0 + E^0\Psi') + \ldots$$

* Ignoring terms $> \lambda^2$, we see

$$H'\Psi^0 + H^0\Psi' = E'\Psi^0 + E^0\Psi'$$

Taking the inner product with $\langle \Psi_a^0 |$ yields:

$$\langle \Psi_a^0 | H'\Psi^0 \rangle + \langle \Psi_a^0 | H_0 \Psi' \rangle = E' \langle \Psi_a^0 | \Psi^0 \rangle + E_0 \langle \Psi_a^0 | \Psi' \rangle$$

$$\langle \Psi_a^0 | H'\Psi^0 \rangle + \cancel{E^0 \langle \Psi_a^0 | \Psi' \rangle} = E' \langle \Psi_a^0 | \Psi^0 \rangle + \cancel{E_0 \langle \Psi_a^0 | \Psi' \rangle}$$

$$\langle \Psi_a^0 | H'\Psi^0 \rangle = E' \langle \Psi_a^0 | \Psi^0 \rangle$$

Remembering $\Psi^0 = \alpha \Psi_a^0 + \beta \Psi_b^0$

$$\alpha \langle \Psi_a^0 | H' | \Psi_a^0 \rangle + \beta \langle \Psi_a^0 | H' | \Psi_b^0 \rangle = \alpha E'$$

which can be rewritten as:

$$\alpha W_{aa} + \beta W_{ab} = \alpha E', \quad W_{ij} = \langle \Psi_i^0 | H' | \Psi_j^0 \rangle$$

By a similar method, the inner product w/ $\langle \Psi_b^0 |$ will yield:

$$\alpha W_{ba} + \beta W_{bb} = \beta E'$$

Notice that W_{ij} are the matrix elements of H' and should therefore be known. More importantly, if we multiply the above equation by W_{ab} we see:

$$\alpha W_{ab} W_{ba} + \beta W_{ab} W_{bb} = \beta E' W_{ab}$$
$$\beta W_{ab} = \alpha E' - \alpha W_{aa} \quad \text{from above}$$

$$\Rightarrow \alpha W_{ab} W_{ba} + W_{bb}(\alpha E' - \alpha W_{aa}) = \beta E' W_{ab}$$
$$\alpha W_{ab} W_{ba} + W_{bb} \alpha E' - \alpha W_{bb} W_{aa} = E'(\alpha E' - \alpha W_{aa})$$
$$\alpha W_{ab} W_{ba} + \alpha W_{bb} E' - \alpha W_{bb} W_{aa} = \alpha (E')^2 - \alpha W_{aa} E'$$

$$0 = \alpha\left[(E')^2 + E'(W_{aa}+W_{bb}) + (-W_{ab}W_{ba} + W_{aa}W_{bb})\right]$$

* if $\alpha \neq 0$, then solving the quadratic eqn for E' yields

$$E' = \frac{(W_{aa}+W_{bb}) \pm \sqrt{(-W_{aa}-W_{bb})^2 + 4(W_{aa}W_{bb} - W_{ab}W_{ba})}}{2}$$

$$\boxed{E' = \frac{1}{2}\left[(W_{aa}+W_{bb}) \pm \sqrt{(W_{aa}-W_{bb})^2 + 4|W_{ab}|^2}\right]}$$

* Note: There is a proff in Griffiths which states that if you can find a Hermitian operator A that commutes with H and H', then use the simultaneous eigenfunctions of A and H to use non-degenerate perturbation theory.

ex. Higher-Order Degeneracies

To see how the above procedure generalizes, we can rewrite our equations above in matrix form

$$\begin{bmatrix} W_{aa} & W_{ab} \\ W_{ba} & W_{bb} \end{bmatrix}\begin{bmatrix} \alpha \\ \beta \end{bmatrix} = E'\begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

From here, it is easy to see that the first order energy corrections are the eigenvalues of the perturbation matrix and the good eigenvectors are those of the same matrix.

In math terms, we are finding the basis in the degenerate subspace which diagonalizes the perturbation matrix.

WKB Approximation

* An equation solving technique for obtaining approximate solutions to TISE in 1-D
* A simplistic explanation follows: If we imagine a particle w/ energy E moving in a constant potential $V(x)$ where $E > V(x)$, then we know our solution to be:

$$\psi(x) = Ae^{\pm ikx} \; ; \quad k = \frac{1}{\hbar}\sqrt{2m(E-V)} \qquad \text{(Note: } \pm \text{ indicates direction of travel)}$$

$\Rightarrow$ Our solution is a oscillatory function w/ $\lambda = \frac{2\pi}{k}$ and amplitude A

If we now allow $V(x)$ to vary, but slowly in comparison to λ, we have a region over several full wavelengths where $V(x)$ is essentially constant. Thus, we can reasonably assume $\psi(x)$ stays sinusoidal in nature, with A and λ now varying w/ position.

In the situation where $E < V(x)$, our solution becomes, assuming $V \approx$ constant:

$$\psi(x) = Ae^{\pm \kappa x} \; ; \quad \kappa = \frac{1}{\hbar}\sqrt{2m(V-E)}$$

Again allowing $V(x)$ to vary; this time slowly with respect to $1/\kappa$, our solution will remain exponential in nature and A and κ will vary slowly with position.

Note: This will all fail at the "turning point" $E = V$. We will handle this later.

* We begin by examining the classical region, where $E > V$, which ensures $p(x)$ is real

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi = E(\psi) \iff \frac{d^2\psi}{dx^2} = -\frac{p^2}{\hbar^2}\psi \; ; \quad p(x) = \sqrt{2m(E-V(x))}$$

In general, we know $\psi(x)$ has the form $\psi(x) = A(x)e^{i\varphi(x)}$

$$\hookrightarrow \quad \frac{d\psi}{dx} = (A' + iA\varphi')e^{i\varphi(x)}$$

$$\frac{d^2\psi}{dx^2} = \left[A'' + 2iA'\varphi' + iA\varphi'' - A(\varphi')^2\right]e^{i\varphi(x)}$$

This separates into two equations (one real, one imaginary) when substituted into Schrödinger's equation, yielding:

$$A'' - A(\varphi')^2 = \frac{-p^2}{\hbar^2}A \iff A'' = A\left((\varphi')^2 - \frac{p^2}{\hbar^2}\right) \qquad \text{(Real)}$$

$$2A'\varphi' + A\varphi'' = 0 \iff (A^2\varphi')' = 0 \qquad \text{(Imaginary)}$$

The imaginary equation can be easily solved by:

$$A^2\varphi' = C^2 \quad \Rightarrow \quad A = \frac{C}{\sqrt{\varphi'}}, \quad C \in \mathbb{R}$$

To solve the real equation, we assume A varies slowly (A'' is ignored) such that $A''/A \ll (\varphi')^2$ and $\frac{p^2}{\hbar^2}$. Thus, our real equation becomes:

$$(\varphi')^2 = \frac{p^2}{\hbar^2} \quad \Rightarrow \quad \frac{d\varphi}{dx} = \pm \frac{p}{\hbar}$$

Therefore: $\varphi(x) = \pm \frac{1}{\hbar} \int p(x)\,dx$

This results in our overall solution becoming:

$$\psi(x) = \frac{C}{\sqrt{p(x)}} \exp\left[\pm \frac{i}{\hbar} \int p(x)\,dx\right]$$ where C has absorbed constants from the real equation and may now be complex.

Note: The true solution is a linear combination of positive and negative exponentials

ex. Potential w/ 2 vertical walls

$$V(x) = \begin{cases} V(x) & 0 < x < a \\ 0 & \text{otherwise} \end{cases}$$

We know our solution has the form $\psi(x) = \frac{1}{\sqrt{p(x)}}\left[C_+ e^{i\varphi(x)} + C_- e^{-i\varphi(x)}\right]$

$$= \frac{1}{\sqrt{p(x)}}\left[C_1 \sin[\varphi(x)] + C_2 \cos[\varphi(x)]\right]$$

where $\varphi(x) = \frac{1}{\hbar}\int_0^x p(x')\,dx'$

Since our solution must go to 0 at $x=0$, and so does $\varphi(x)$, we automatically know $C_2 = 0$. Using our other 0 at $x=a$, since $\sin(\varphi(x)) = 0$, we know that $\varphi(a) = n\pi$, $n \in \mathbb{Z}^+$

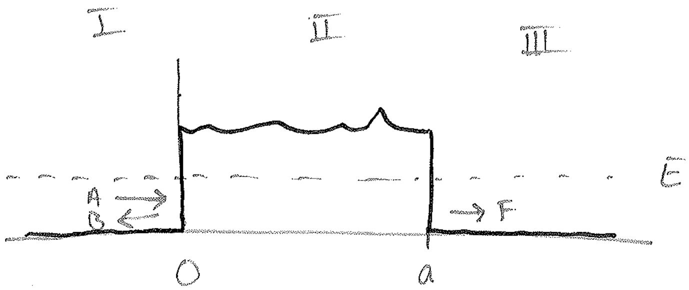
$$\hookrightarrow \int_0^a p(x)\,dx = n\pi\hbar$$

Note: For the infinite square well ($V=0$) we get $\sqrt{2mE}\,a = n\pi\hbar \Rightarrow E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$

* Now we examine the "nonclassical region" where $V(x) > E$. In this region, p is imaginary.

$$\hookrightarrow \psi(x) = \frac{C}{\sqrt{|p(x)|}} \exp\left[\pm \frac{1}{\hbar} \int |p(x)| dx\right]$$

ex. Rectangular barrier w/ uneven top



In section I : $\psi(x) = Ae^{ikx} + Be^{ikx}$, $k = \frac{1}{\hbar}\sqrt{2mE}$

III : $\psi(x) = Fe^{ikx}$, $T = |F|^2 / |A|^2$ (transmitted probability)

II : $\psi(x) = \frac{C}{\sqrt{|p(x)|}} \exp\left[\frac{1}{\hbar}\int_0^x |p(x')| dx'\right] + \frac{D}{\sqrt{|p(x)|}} \exp\left[\frac{-1}{\hbar}\int_0^x |p(x')| dx'\right]$

Quantom Exam 2 Study Guide

Basics from Exam 1

$S_i = \frac{\hbar}{2}\sigma_i$, $\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ $\sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$ $\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

$[\sigma_x, \sigma_y] = \sigma_z$ * and cyclic permutations for other commutators

$|\alpha\rangle = \sum_i c_i |a_i\rangle$ or $A|\alpha\rangle = a_i|\alpha\rangle$ (definition of a ket)

$\tilde{A} = |\beta\rangle\langle\alpha|$ (definition of an operator)

$\sum_i \Lambda_i = \sum_i |a_i\rangle\langle a_i| = 1$ (Projection operator / Completeness relation)

* All observables are represented by Hermitian operators; $A = A^{+}$ is condition for Hermitivity
* Unitary operators satisfy $UU^{+} = U^{+}U = \mathbb{I}$

$\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2$ (Schwartz Inequality)

$\langle\hat{A}\rangle = \langle\alpha|\hat{A}|\alpha\rangle$ (Definition of expectation value)

$\langle(\Delta\hat{A})^2\rangle = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2$ (RMS or avg value)

$\Delta\hat{A} = \hat{A} - \langle A\rangle\mathbb{I}$ (Dispersion operator)

$\langle(\Delta\tilde{A})^2\rangle\langle(\Delta\tilde{B})^2\rangle \geq \frac{1}{4}|\langle[A,B]\rangle|^2$ (Uncertainty relation)

Continuous Basis / Spectra

* In a continuous basis, the completeness relation is now defined as:

$$\int_a^b |x'\rangle\langle x'|\, dx' = \tilde{\mathbb{I}}$$

* Orthogonality is now defined by Dirac δ-function
* All position operators $(\tilde{x}, \tilde{y}, \tilde{z})$ commute

Translation Operators

* Allow us to see how systems evolve in time

$\tilde{T}(dx') = \mathbb{I} - \frac{i\tilde{p}\cdot d\tilde{x}}{\hbar}$ (Infinitetesimal translation operator)

⇒ Derived from the following conditions:

① Normalization unchanged ⇒ $\tilde{T}^{+}\tilde{T} = \mathbb{I}$

② Addition of successive translations ⇒ $T(dx'')T(dx') = T(dx'+dx'')$

③ Inverse is translation in opposite direction ⇒ $T^{-1}(dx) = T(-dx)$

④ Zero translation is identity operator ⇒ $T(0) = \mathbb{I}$

* Note: $[x_i, p_j] = i\hbar\,\delta_{ij}$

Wavefunctions

* We define the position space wavefunction as:

$\psi_a(x') = \langle x'|a\rangle$

$$\Rightarrow \langle\beta|\alpha\rangle = \int dx' \langle\beta|x'\rangle\langle x'|\alpha\rangle$$
$$= \int dx' \, \psi_\beta^*(x')\,\psi_\alpha(x')$$

$$\langle\beta|\hat{A}|\alpha\rangle = \int dx' \int dx'' \langle\beta|x''\rangle\langle x''|A|x'\rangle\langle x'|\alpha\rangle$$

⇒ write $\hat{A}$ in terms of position operator to solve

$$\langle\alpha|\alpha\rangle = \int dx' \langle\alpha|x'\rangle\langle x'|\alpha\rangle$$
$$= \int dx' \, |\psi_\alpha(x')|^2$$
$$= 1$$

⇒ Normalization condition + generator of PDF

* We define the momentum space wavefunction as:

$\varphi_\alpha(p') = \langle p'|\alpha\rangle$

⇒ Momentum eigenkets follow same rules as position eigenkets above

$\langle x'|\tilde{p}|p'\rangle = -i\hbar \frac{\partial}{\partial x}\langle x'|p'\rangle$ ⇒ $\tilde{p} = -i\hbar\frac{\partial}{\partial x}$ $\langle x'|p'\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp\left[\frac{ip'x'}{\hbar}\right]$

Time Evolution

* Schrödinger Picture: state vectors evolve in time; eigenkets + operators constant.

* Heisenberg Picture: eigenkets/operators evolve in time, state vectors constant

⇒ Time translation operator must follow these properties

1. Unitary
2. $\lim_{\delta t \to 0} \tilde{U}(t_1+\delta t, t_0) = \mathbb{I}$
3. Successive translations are also translations $\tilde{U}(t_2, t_1)\tilde{U}(t_1, t_0) = \tilde{U}(t_2, t_0)$

$$\Rightarrow \tilde{U}(t, t_0) = \mathbb{I} - i\Omega \delta t$$

* by dimensional analysis $[\Omega] = \frac{1}{t}$

$$\Rightarrow \Omega = \frac{H}{\hbar}$$

$$\rightarrow U(t, t_0) = \mathbb{I} - \frac{iHt}{\hbar}$$

* Heisenberg equations of motion:

$$i\hbar \frac{\partial A^{(H)}}{\partial t} = [A, H]$$

* Ehrenfest Theorem: $\frac{d\langle \hat{p}\rangle}{dt} = -\frac{\partial}{\partial x}\langle V(\hat{x})\rangle$

Simple Harmonic Oscillator

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

* To derive creation/annihilation operators

$$\frac{H}{\hbar\omega} = \frac{p^2}{2m\hbar\omega} + \frac{m\omega^2 x^2}{2\hbar\omega}$$

$$\Rightarrow \hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{ip}{m\omega}\right) \quad \text{(annihilation operator)}$$

$$\hat{a}^+ = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{ip}{m\omega}\right) \quad \text{(creation operator)}$$

$$\Rightarrow \hat{N} = \hat{a}^+\hat{a} \quad \text{(Number operator)}$$

$$[a, a^+] = +1 \qquad [N, a] = -\hat{a}$$

$$[a^+, a] = -1 \qquad [N, a^+] = \hat{a}^+$$

SHO (cont.)

* Acting these new operators on the energy eigenkets yields:

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

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

$$N\,|n\rangle = n\,|n\rangle$$

⇒ Hamiltonian can be rewritten as:

$$\frac{H}{\hbar\omega} = \frac{1}{2}\frac{p^2}{\sigma_p^2} + \frac{1}{2}\frac{x^2}{\sigma_x^2}\ ; \qquad \sigma_p = \sqrt{m\hbar\omega}, \quad \sigma_x = \sqrt{\hbar/m\omega}$$

Important Derivations

* See sections on Translation Operators + Time Evolution for appropriate translation operators

* Derivation of momentum operator:

$$\left(\mathbb{I} - \frac{ip\Delta x}{\hbar}\right)|\alpha\rangle = \int dx'\, T(\Delta x')\,|x'\rangle\langle x'|\alpha\rangle$$

$$= \int dx'\, |x' + \Delta x'\rangle\langle x'|\alpha\rangle$$

$$= \int dx'\, |x'\rangle\langle x' - \Delta x'|\alpha\rangle$$

* if we Taylor expand $\langle x' - \Delta x'|\alpha\rangle$

$$= \int dx'\, |x'\rangle\left(\langle x'|\alpha\rangle - \Delta x'\frac{\partial}{\partial x'}\langle x'|\alpha\rangle\right)$$

$$= |\alpha\rangle - \int dx'\left(-\Delta x'\frac{\partial}{\partial x'}\langle x'|\alpha\rangle\right)$$

$$-\frac{ip\Delta x}{\hbar} = -\int dx\left(-\Delta x'\frac{\partial}{\partial x'}\langle x'|\alpha\rangle\right.$$

$$\hat{p} = -i\hbar\int dx'\,|x'\rangle\langle x'|\alpha\rangle$$

$$\hat{p}\,|\alpha\rangle = -i\hbar\frac{\partial}{\partial x'}\,|\alpha\rangle$$

Derivations (cont.)

* Schrödinger Equation

$$\tilde{U}(t+\delta t, t_0) = U(t+\delta t, t)\,\tilde{U}(t, t_0)$$
$$= \left(\mathbb{I} - \frac{iH\delta t}{\hbar}\right)\tilde{U}(t, t_0)$$

$$\tilde{U}(t+\delta t, t_0) - U(t, t_0) = \frac{1}{i\hbar} H\, U(t, t_0)\,\delta t$$

* if $\delta t \to dt$
* Taylor expand LHS around $t - \delta t$

$$U(t+dt, t_0) - U(t, t_0) = \cancel{U(t, t_0)} + \delta t \frac{\partial}{\partial t} U(t, t_0) - \cancel{U(t, t_0)}$$

$$\delta t \frac{\partial}{\partial t} U(t, t_0) = \frac{1}{i\hbar} H\, U(t, t_0)\,\cancel{\delta t}$$

$$i\hbar \frac{\partial}{\partial t} U(t, t_0) = H\, U(t, t_0) \quad \checkmark$$

Other Important Equations

$$[\hat{x}, F(\hat{p})] = i\hbar \frac{\partial F}{\partial p}$$

$$[\hat{p}, G(\hat{x})] = -i\hbar \frac{\partial G}{\partial x}$$

$$[x_i, p_j] = -i\hbar\, \delta_{ij}$$

Quantum Exam 3 Study Guide

Basics from previous exams

$S_i = \frac{\hbar}{2}\sigma_i \Rightarrow \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

$[\sigma_i, \sigma_j] = \sigma_k$ (other relations result from cyclic permutations)

$|\alpha\rangle = \sum_i' c_i |a_i\rangle$ or $A|\alpha\rangle = a_i|\alpha\rangle$ (definition of a ket)

$\hat{A} = |a\rangle\langle b|$ (definition of an operator)

$\sum_i' \Lambda_i = \sum_i' |a_i\rangle\langle a_i| = 1$ (Projection operator / completeness relation)

*To get matrix elements:

$$A \to \sum_{m,n}' |m\rangle\underbrace{\langle m|A|n\rangle}_{\text{matrix elements}}\langle n|$$

$\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2$ (Schwartz Inequality)

$\langle\hat{A}\rangle = \langle\alpha|\hat{A}|\alpha\rangle$ (Expectation value)

$\langle(\Delta\tilde{A})^2\rangle = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2$ (RMS or avg value)

$\Rightarrow \Delta A = \hat{A} - \langle\hat{A}\rangle \mathbb{I}$ (Dispersion operator)

$\langle(\Delta A^2)\rangle\langle(\Delta B)^2\rangle \geq \frac{1}{4}|\langle[A,B]\rangle|^2$ (Uncertainty Relation)

$[x_i, x_j] = 0 = [p_i, p_j]$ (Position/Momentum operators, self commute)

* $[x_i, p_j] = i\hbar\delta_{ij}$ *

$\psi_a = \langle x'|\alpha\rangle$ (Definition of wavefunction)

$= \langle p'|\alpha\rangle$

$\langle x'|\tilde{p}|p'\rangle = -i\hbar\frac{\partial}{\partial x}\langle x'|p'\rangle \qquad \langle x'|p'\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp\left[\frac{ip'x'}{\hbar}\right]$

$\Rightarrow \hat{p} = -i\hbar\frac{\partial}{\partial x}$

Basics (cont.)

* Schrödinger Picture → state vectors time evolve; operators + eigenkets constant
* Heisenberg Picture → eigenkets + operators evolve; state vectors constant

$$\hat{U}(t, t_0) = \mathbb{I} - i\Omega\delta t$$
$$= \exp\left[\frac{-iHt}{\hbar}\right]$$

⇒ Heisenberg equations of motion: $-i\hbar \frac{\partial A}{\partial t} = [A, H]$

$$[\hat{x}, F(\hat{p})] = i\hbar \frac{\partial F}{\partial p} \qquad [\hat{p}, G(\hat{x})] = -i\hbar \frac{\partial G}{\partial x}$$

Simple Harmonic Oscillator

$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2 \Rightarrow \hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{ip}{m\omega}\right)$ annihilation operator

$\hookrightarrow E_n = (n + 1/2)\hbar\omega \qquad \hat{a}^{\dagger} = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{ip}{m\omega}\right)$ creation operator

$\hat{N} = \hat{a}^{\dagger}\hat{a}$ Number operator

$$\Rightarrow [a, \hat{a}^{\dagger}] = 1 \qquad [N, \hat{a}] = -\hat{a}$$
$$[\hat{a}^{\dagger}, \hat{a}] = -1 \qquad [N, \hat{a}^{\dagger}] = \hat{a}^{\dagger}$$

* We can rewrite position/momentum operators in terms of ladder operators as:

$$\hat{x} = \frac{\sigma_x}{\sqrt{2}}(\hat{a}^{\dagger} + \hat{a}) \qquad \sigma_x = \sqrt{\hbar/m\omega}$$
$$\hat{p} = \frac{i\sigma_p}{\sqrt{2}}(\hat{a}^{\dagger} + \hat{a}) \qquad \sigma_p = \sqrt{m\hbar\omega}$$

⇒ Uncertainty relation can be derived using these versions of $\hat{x}, \hat{p}$; result from expectation values of $\hat{x}^2, \hat{p}^2 \neq 0$

* To derive eigen function, apply annihilation operator to lowest state, switch to either position or momentum space + solve differential equation.

$$\Rightarrow U_0(x) = \frac{1}{\pi^{1/4}\sqrt{\sigma_x}} \exp[-x^2/2\sigma_x^2] \qquad \text{(position space)}$$
$$V_0(x) = \frac{1}{\pi^{1/4}\sqrt{\sigma_p}} \exp[-x^2/2\sigma_p^2] \qquad \text{(momentum space)}$$

SHO (cont.)

* Eigenfunctions can be generated from Hamiltonian by solving differential equation when written in position space using B.C. that eigenfunction must go to 0 at boundary + must be normalizable

  $\Rightarrow$ Generates Hermite polynomials (hard to recognize normally) w/ inclusion of Gaussian necessary for normalizability

* Time evolution of SHO is handled via application of Heisenberg equations of motion, yielding

$$\frac{d\tilde{p}}{dt} = -m\omega^2 \tilde{x} \qquad \frac{d\tilde{x}}{dt} = \frac{\tilde{p}}{m}$$

$\Rightarrow$ after solving for $\tilde{p}(t)$ and $\tilde{x}(t)$, time evolution of operators can be written, but rewriting ↑ equations before solving yields:

$$\frac{d\hat{a}}{dt} = \sqrt{\frac{m\omega}{2\hbar}}\left(\frac{\partial \tilde{x}}{\partial t} + \frac{i}{m\omega}\frac{d\tilde{p}}{dt}\right) = -i\omega\hat{a}$$

$$\frac{d\hat{a}^{+}}{dt} = i\omega\hat{a}^{+}$$

$\Rightarrow$ Solving above yields: $\tilde{a}(t) = \tilde{a}(0)e^{-i\omega t}$

$$\tilde{a}^{+}(t) = \tilde{a}^{+}(0)e^{i\omega t}$$

$$\tilde{x}(t) = \tilde{x}(0)\cos(\omega t) + \frac{\tilde{p}(0)}{m\omega}\sin(\omega t)$$

$$\tilde{p}(t) = -m\omega\,\tilde{x}(0)\sin(\omega t) + \tilde{p}(0)\cos(\omega t)$$

Guage Transformations

* Effectively amount to multiplying by a phase; only transformations that do not multiply everything uniformly will result in measurable difference

$\Rightarrow H = \frac{p^2}{2m} + V(\tilde{x})$ $\qquad\qquad H = \frac{p^2}{2m} + V(\tilde{x}) + V_0$

$|\alpha, t_0; t\rangle = \exp[iH\Delta t/\hbar]|\alpha, t_0\rangle$ $\qquad |\alpha, t_0; t\rangle = \exp[iV_0\Delta t/\hbar]|\alpha, t_0; t\rangle$

Guage Transforms (cont.)

* Most applicable to E+M fields

$\Rightarrow$ Maxwells Eqns

$$\nabla \cdot B = 0 \quad \Rightarrow \quad B = \nabla \times A \quad \Rightarrow \quad A \to A + \nabla \lambda$$

$$\nabla \times E = \frac{-1}{c}\frac{\partial B}{\partial t} \quad \Rightarrow \quad E = -\nabla \varphi - \frac{\partial A}{\partial t} \quad \Rightarrow \quad \varphi \to \varphi - \frac{\partial \lambda}{\partial t}$$

Rotations

* Classically, rotation about the z-axis is given by:

$$R = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} 1-\delta\varphi^2/2 & -\delta\varphi & 0 \\ \delta\varphi & 1-\delta\varphi^2/2 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

* Taylor expanded for infinitesimal rotation

$\Rightarrow$ Infinitesimal Rotation operator:

$$\mathcal{D}(\hat{n}, \delta\varphi) = \mathbb{I} - \frac{i}{\hbar}\vec{J} \cdot \hat{n}\,\delta\varphi$$

$$\lim_{N \to \infty}\left(\mathbb{I} - \frac{i}{\hbar} J_z \frac{\varphi}{N}\right)^N = \exp\left[\frac{-i}{\hbar} J_z \varphi\right] \quad \text{(finite Rotation operator)}$$

* Rotation operator must satisfy the following:

① $\mathcal{D}(R)\mathbb{I} = \mathcal{D}(R)$

② $\mathcal{D}(R_1)\mathcal{D}(R_2) = \mathcal{D}(R_3)$

③ $\mathcal{D}(R)\mathcal{D}^{-1}(R) = \mathbb{I}$

④ $[\mathcal{D}(R_1)\mathcal{D}(R_2)]\mathcal{D}(R_3) = \mathcal{D}(R_1)[\mathcal{D}(R_2)\mathcal{D}(R_3)]$

* Expanding operators yields commutator relations

$$[\tilde{J}_x, \tilde{J}_y] = i\hbar \tilde{J}_z \quad \text{(and cyclic permutations)}$$

Quantum Final Exam Study Guide

* **Basics from previous exams:**

- Definition of a ket: $|\alpha\rangle = c_i |a_i\rangle$

$$a_i|\alpha\rangle = A|\alpha\rangle$$

- Definition of an operator: $\hat{A} = |a\rangle\langle b|$

- Projection Operator/Completeness Relation: $\sum_i \Lambda_i = \sum_i |a_i\rangle\langle a_i| = 1$

  * sum to integral if a_i is continuous basis set

- To get the matrix elements of an operator: $A \rightarrow \sum_{m,n} |m\rangle\langle m|A|n\rangle\langle n|$

- Schwartz Inequality: $\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2$

- Expectation value: $\langle\hat{A}\rangle = \langle\alpha|A|\alpha\rangle$

- RMS / Avg value: $\langle(\Delta\hat{A})^2\rangle = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2$

  $\hookrightarrow \Delta\hat{A} = \hat{A} - \langle\hat{A}\rangle \mathbb{I}$ (Dispersion Operator)

- Uncertainty Relation: $\langle(\Delta\hat{A})^2\rangle\langle(\Delta\hat{B})^2\rangle \geq \frac{1}{4}|\langle[A,B]\rangle|^2$

- Important Commutation Relations include:

$[x_i, x_j] = 0 = [p_i, p_j]$

$[x_i, p_j] = i\hbar\delta_{ij}$

$S_i = \frac{\hbar}{2}\sigma_i$ $\quad \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ $\quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$

$[\sigma_i, \sigma_j] = \sigma_k$ $\quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

$[x, F(p)] = i\hbar\frac{\partial F}{\partial p}$

$[p, G(x)] = -i\hbar\frac{\partial G}{\partial x}$

$[A, H] = -i\hbar\frac{\partial A}{\partial t}$ (Heisenberg eqn of motion)

- Two pictures: Schrödinger Picture → state vectors evolve in time, operators const.

  Heisenberg Picture → eigenkets + operators evolve; state vectors cons

Bases (cont.)

* For functions of continuous variables

  - Definition of wave function: $\psi_a(x') = \langle x'|a\rangle$

$$\varphi_b(p') = \langle p'|b\rangle$$

$$\Rightarrow \langle \beta|\alpha\rangle = \int dx' \langle \beta|x'\rangle\langle x'|\alpha\rangle = \int dx'\, \psi_b^*(x')\,\psi_a(x')$$

$$= \int dp' \langle \beta|p'\rangle\langle p'|\alpha\rangle = \int dp'\, \varphi_b^*(p')\,\varphi_a(p')$$

$$\langle \beta|A|\alpha\rangle = \int dx'' \int dx' \langle \beta|x''\rangle\langle x''|A|x'\rangle\langle x'|\alpha\rangle$$

$$= \int dp'' \int dp' \langle \beta|p''\rangle\langle p''|A|p'\rangle\langle p'|\alpha\rangle$$

$\rightarrow$ rewrite $\hat{A}$ in terms of x or p to solve

$$\langle \alpha|\alpha\rangle = \int dx' \langle \alpha|x'\rangle\langle x'|\alpha\rangle$$

$$= \int dx' |\psi_a(x')|^2$$

$$= 1$$ $\rightarrow$ Normalization condition + PDF generator

$$\Rightarrow \langle x'|\hat{p}|p'\rangle = i\hbar \frac{\partial}{\partial x}\langle x'|p'\rangle \quad \Rightarrow \hat{p} = i\hbar\frac{\partial}{\partial x}$$

$$\Rightarrow \langle x'|p'\rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp\left[\frac{ip'x'}{\hbar}\right]$$

* Translation operators obey the following properties

  ① Unitary

Important Derivations

① Angular Momentum

*Remember that: $J \rightarrow$ Arbitrary angular momentum (often refers to total)

$S \rightarrow$ Spin angular momentum

$L \rightarrow$ orbital angular momentum

Total Angular momentum operator: $\tilde{J}^2 = \tilde{J} \cdot \tilde{J}$
$$= J_x^2 + J_y^2 + J_z^2$$

Commutation Relations: $[\tilde{J}^2, \tilde{J}_z] = 0$ $\qquad [\tilde{J}_i, \tilde{J}_j] = i\hbar \epsilon_{ijk} J_k$

$$[\tilde{J}^2, \tilde{J}_y] = 0$$
$$[\tilde{J}^2, \tilde{J}_x] = 0$$

*Following our approach from SHO, we define ladder operators

$$\Rightarrow J_\pm = J_x \pm i J_y$$
$$\hookrightarrow [J^2, J_\pm] = 0$$
$$[J_z, J_\pm] = \hbar J_\pm$$
$$[J_+, J_-] = 2\hbar J_z$$

$$J_\pm^n |a, b\rangle = b \pm n\hbar\, |a, b \pm n\hbar\rangle$$

*Since $\tilde{J}^2$ and $\tilde{J}_z$ commute, we right simultaneous eigenkets such

$$\tilde{J}^2 |a, b\rangle = a \quad \text{and} \quad \tilde{J}_z |a, b\rangle = b$$

$\rightarrow$ Relationship b/w $\tilde{J}^2$ and J_z implies max value for b

*Individually, $\langle a, b | J_- J_+ | a, b\rangle \geq 0$

$$\langle a, b | J_+ J_- | a, b\rangle \geq 0$$

$$\Rightarrow \langle a, b | J_+ J_- + J_- J_+ | a, b \geq 0$$

$$= \langle a, b | 2(J^2 - J_z^2) | a, b\rangle \geq 0$$

$$\hookrightarrow a \geq b^2 .$$

Derivations (cont)

* We can show that J_z is incremented in terms of $\hbar$ by:

$$J_z(J_\pm|a,b\rangle) = (J_\pm J_z + \hbar J_\pm)|a,b\rangle$$
$$= J_\pm(J_z + \hbar \mathbb{I})|a,b\rangle$$
$$= J_\pm(b+\hbar)|a,b\rangle$$
$$= (b+\hbar)(J_\pm|a,b\rangle)$$

* Note: Acting $J_\pm|a,b\rangle = c_\pm|a, b+\hbar\rangle$

Interpretation: $J_\pm$ increments eigenvalue of angular momentum

* To find extremum values, act raising/lowering operators on max/min states

$$J_+|a, b_{max}\rangle = 0$$

$$J_- J_+|a, b_{max}\rangle = 0$$

$$(J^2 - J_z^2 - \hbar J_z)|a, b_{max}\rangle = 0$$

* assuming a non-zero ket

$$a - b_{max}^2 - \hbar b_{max} = 0$$

$$a = b_{max}(b_{max} + \hbar)$$

* let $b_{max} = j\hbar$

$$a = j(j+1)\hbar^2$$

$\Rightarrow j(j+1)$ are eigenvalues of J^2

$$J_-|a, b_{min}\rangle = 0$$

$$J_+ J_-|a, b_{min}\rangle = 0$$

$$(J^2 - J_z^2 + \hbar J_z)|a, b_{min}\rangle = 0$$

$\hookrightarrow$ $a - b_{min}^2 + \hbar b_{min} = 0$

$$a = b_{min}(b_{min} - \hbar)$$

$$b_{max}(b_{max} + h) = b_{min}(b_{min} - \hbar)$$

$$\Rightarrow b_{max} = -b_{min}$$

Derivations (cont.)

$\Rightarrow$ This implies $b_{max} = b_{min} + \hbar$

$\hookrightarrow J_+^n |a, b_{min}\rangle = J_+^n |a, -b_{max}\rangle$

$\Rightarrow b_{max} = \frac{n\hbar}{2}$; since $n \in \mathbb{Z}$, b must be an integer or ½-integer

* But what about $c_\pm$?

$$\Rightarrow J_\pm |a,b\rangle = c_\pm |a, b\pm\hbar\rangle$$

$\rightarrow$ Starting w/ J_+

$$\langle a,b| J_+^\dagger J_+ |a,b\rangle = |c_+|^2 \cancel{\langle a, b+\hbar | a, b+\hbar\rangle}^{1}$$

$$\Rightarrow |c_+|^2 = \hbar^2[j(j+1)] - b^2 - \hbar b$$

*if $b = m\hbar$

$$|c_+|^2 = \hbar^2[j(j+1)] - m^2\hbar^2 - \hbar^2 m$$

$$c_+ = \hbar\sqrt{j(j+1) - m^2 - m}$$

$$= \hbar\sqrt{(j-m)(j+m+1)}$$

$\rightarrow$ Now w/ J_-

$$|c_-|^2 \cancel{\langle a, b-\hbar | a, b-\hbar\rangle}^{1} = \langle a,b| J_-^\dagger J_- |a,b\rangle$$

$$= \hbar^2[j(j+1)] - b^2 + \hbar b$$

$$= \hbar^2[j(j+1)] - m^2\hbar^2 + \hbar^2 m$$

$$c_- = \hbar\sqrt{j(j+1) - m^2 + m}$$

$$= \hbar\sqrt{(j+m)(j-m+1)}$$

Derivations (cont.)

② Orbital Angular Momentum

* We define orbital angular momentum operator $\tilde{L}$ as:

$$\tilde{L} = \tilde{\vec{X}} \times \tilde{\vec{P}} \xrightarrow{\text{via cross-product}} \begin{aligned} \tilde{L}_x &= \tilde{y}\tilde{p}_z - \tilde{z}\tilde{p}_y \\ \tilde{L}_y &= \tilde{z}\tilde{p}_x - \tilde{x}\tilde{p}_z \\ \tilde{L}_z &= \tilde{x}\tilde{p}_y - \tilde{y}\tilde{p}_x \end{aligned}$$

$$\Rightarrow [\tilde{L}_i, \tilde{L}_j] = i\hbar \tilde{L}_k$$

* Using the infinitesimal rotation operators, we can generate wavefunctions in position basis

$$\mathcal{D}(\delta\varphi, \hat{z})|x', y', z\rangle = \left(\mathbb{I} - \tfrac{i}{\hbar}\delta\varphi L_z\right)|x', y', z'\rangle$$

$$= \left(\mathbb{I} - \tfrac{i}{\hbar}\delta\varphi[xp_y - yp_x]\right)|x', y', z'\rangle$$

$$= \left(\mathbb{I} - \tfrac{i}{\hbar}\delta\varphi[p_y x - p_x y]\right)|x', y', z\rangle \quad \text{b/c } [x_i, p_j] = i\hbar\delta_{ij}$$

* But when distributed, these are translation operators

$$= |x' - y\delta\varphi, y' + x\delta\varphi, z'\rangle$$

* Note, this matches what we expect from applying rotation matrix on our position operator

* We define our wavefunction as:

$$\varphi(\vec{r}) = \langle x', y', z' | \varphi\rangle, \quad |\varphi\rangle = \left(\mathbb{I} - \tfrac{i}{\hbar}L_z\delta\varphi\right)|\alpha\rangle$$

$$= \langle r, \theta, \varphi | \varphi\rangle$$

$$= \langle r, \theta, \varphi | \mathbb{I} - \tfrac{i}{\hbar}L_z\delta\varphi|\alpha\rangle = \langle r, \theta, \varphi - \delta\varphi|\alpha\rangle$$

* Taylor expansion about $\delta\varphi = 0$ yields

$$= \langle r, \theta, \varphi|\alpha\rangle - \delta\varphi \frac{\partial}{\partial\varphi}\langle r, \theta, \varphi|\alpha\rangle$$

$$\Rightarrow -i\hbar\frac{\partial}{\partial\varphi}\langle r, \theta, \varphi|\alpha\rangle = \langle r, \theta, \varphi|\tilde{L}_z|\alpha\rangle$$

$\hookrightarrow -i\hbar\frac{\partial}{\partial\varphi} = L_z$

Derivations (cont.)

* To derive other operators in Cartesian system, apply infinitesimal rotation operator to cartesian vector, then convert to spherical using δx_i and form matching. Taylor expand $\langle r, \theta, \varphi | L_i | \alpha \rangle$ about $\delta\varphi_i = 0$ and derive form of operator

Results: $\tilde{L}_z = -i\hbar \frac{\partial}{\partial\varphi}$

$\tilde{L}_x = -i\hbar\left(-\sin\varphi \frac{\partial}{\partial\theta} - \cot\theta\cos\varphi \frac{\partial}{\partial\varphi}\right)$

$\tilde{L}_y = -i\hbar\left(\cos\varphi \frac{\partial}{\partial\theta} - \cot \sin\varphi \frac{\partial}{\partial\varphi}\right)$

* To derive Spherical Harmonics, we focus on L_z component

$\Rightarrow L_z|l, m\rangle = m\hbar |l, m\rangle$

$\langle \hat{n} | L_z | l, m\rangle = m\hbar \langle \hat{n} | l, m\rangle$

$= i\hbar \frac{\partial}{\partial\varphi} Y_l^m(\theta, \varphi) = m\hbar Y_l^m(\theta, \varphi)$

* Solving the above differential equation by separation of variables yields

$\Phi(\varphi) \propto e^{+im\varphi}$

* If we define the orbital angular momentum operators as:

$L_\pm = L_x \pm i L_y$

$= -i\hbar e^{\pm i\varphi}\left(\pm i \frac{\partial}{\partial\theta} - \cot \frac{\partial}{\partial\varphi}\right)$

then

$L_+|l, l\rangle = 0$

$\langle \hat{n} | L_+ | l, l\rangle = -i\hbar \underset{e^{i\varphi}}{\wedge} \left(i\frac{\partial}{\partial\theta} - \cot\theta \frac{\partial}{\partial\theta}\right) Y_l^l(\theta, \varphi)$

$= 0$

* Solving the above differential equation via separation of variables + $\Phi = e^{im\varphi}$

$\Rightarrow Y_l^l(\theta, \varphi) = \Theta(\theta)\Phi(\varphi) = c_l e^{im\varphi} \sin^l(\theta)$

Derivations (cont.)

* Normalization via

$$\langle l', m' | l, m \rangle = \langle l' m' | \theta, \varphi \rangle \langle \theta, \varphi | l, m \rangle$$

$$= \int_0^{2\pi} d\varphi \int_{-1}^{1} d(\cos\theta) \, |Y_l^m|^2$$

$$\Rightarrow c_l = \frac{(-1)^l}{2^l \, l!} \sqrt{\frac{(2l+1)(2l)!}{4\pi}}$$

③ Spherical Harmonic + The Rotation Operator

$\Rightarrow$ We want: $|\hat{n}\rangle = \mathcal{D}(\alpha, \beta, \gamma) |\hat{z}\rangle$

$$= \mathcal{D}(\varphi, \theta, \gamma) |\hat{z}\rangle$$

$\hookrightarrow$ $$\langle l', m' | \hat{n} \rangle = \sum_{l,m} \langle l', m' | \mathcal{D}(\varphi, \theta, \gamma) | l, m \rangle \langle l, m | \hat{z} \rangle$$

* $l = l'$ or total $\vec{L}$ changes

$$= \sum_m \langle l, m' | \mathcal{D}(\varphi, \theta, \gamma) | l, m \rangle \langle l, m | \hat{z} \rangle$$

$$= (Y_l^m)^* (\theta, \varphi) \, (Y_l^0)(\theta, \varphi)$$

$$=$$

$J_\pm = J_x \pm i J_y$

$$\Rightarrow J_- J_+ = (J_x - iJ_y)(J_x + iJ_y)$$
$$= J_x^2 - iJ_yJ_x + iJ_xJ_y - i^2 J_y$$
$$= J_x^2 + J_y^2 + i(J_xJ_y - J_yJ_x)$$
$$= J^2 - J_z^2 + i[J_x, J_y]$$
$$= J^2 - J_z^2 + i(i\hbar J_z)$$
$$= J^2 - J_z^2 - \hbar J_z$$

* To derive L_x operator form

$$\mathcal{D}(\delta\varphi, \hat{x})|x', y', z'\rangle = (\mathbb{I} - \tfrac{i}{\hbar}\delta\varphi L_x)|x', y', z'\rangle$$
$$= (\mathbb{I} - \tfrac{i}{\hbar}\delta\varphi[yp_z - zp_y])|x', y', z'\rangle$$
$$= (\mathbb{I} - \tfrac{i}{\hbar}\delta\varphi[p_zy - p_yz])|x', y', z'\rangle$$
$$= |x', y' - \delta\varphi z', z' + \delta\varphi y'\rangle$$

* In spherical: $x = r\sin\theta\cos\varphi \longrightarrow \delta x = r\cos\theta\,\delta\theta \cos\varphi + r\sin\theta\sin\varphi\,\delta\varphi$

$y = r\sin\theta\sin\varphi \longrightarrow \delta y = r\sin\theta\cos\varphi\,\delta\varphi + r\cos\theta\,\delta\theta\sin\varphi$

$z = r\cos\theta \longrightarrow \delta z = -r\sin\theta\,\delta\theta$

$$\Rightarrow y'\delta\varphi_x = r\sin\theta\sin\varphi\,\delta\varphi_x = -r\sin\theta\,\delta\theta$$
$$\hookrightarrow \delta\theta = -\sin\varphi\,\delta\varphi_x$$

$$\delta x = 0 = r\cos\theta\cos\varphi\,\delta\theta - r\sin\theta\sin\varphi\,\delta\varphi$$
$$\cos\theta\cos\varphi\,\delta\theta = \sin\theta\sin\varphi\,\delta\varphi$$
$$\cot\theta\cot\varphi\,\delta\theta = \delta\varphi$$
$$-\cot\theta\cos\varphi\,\delta\varphi_x = \delta\varphi$$

$$\Rightarrow |x', y' - \delta\varphi_x z', z' + \delta\varphi_x y'\rangle = |r, \theta + \delta\theta, \varphi - \delta\varphi\rangle$$
$$= |r, \theta + \sin\varphi\,\delta\varphi_x, \varphi - \cot\theta\cos\varphi\,\delta\varphi_x\rangle$$

* Now, Taylor expand about $\delta\varphi_x$

$$\langle r, \theta, \varphi|\mathbb{I} - \tfrac{i}{\hbar}L_x\delta\varphi_x|\alpha\rangle = \langle r, \theta + \sin\varphi\,\delta\varphi_x, \varphi - \cot\theta\cos\varphi\,\delta\varphi_x|\alpha\rangle$$

Quantum II Exam II Study Guide

Basics

$|\alpha\rangle = \sum_i' c_i |a_i\rangle$ or $A|\alpha\rangle = a_i|\alpha\rangle$ (Definition of a ket)

$A = |a\rangle\langle b|$ (Definition of an operator)

$\sum_i' \Lambda_i = \sum_i' |a_i\rangle\langle a_i| = 1$ (Projection operator / Completeness Relation)

*To get the matrix elements of an operator

$$A \rightarrow \sum_{m,n}' |m\rangle \underbrace{\langle m|A|n\rangle}_{\text{matrix element}} \langle n|$$

$\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2$ (Schwartz Inequality)

$\langle\alpha|A|\alpha\rangle = \langle A\rangle$ (Expectation Value)

$\langle(\Delta A)^2\rangle = \langle A^2\rangle - \langle A\rangle^2$ (RMS or Avg value)

$\Rightarrow \Delta A = A - \langle A\rangle \mathbb{I}$ (Dispersion Operator)

$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq \frac{1}{4}|\langle[A,B]\rangle|^2$ (Uncertainty Relation)

*Important Commutation Relations include:

$[x_i, x_j] = [p_i, p_j] = 0$

$[x_i, p_j] = i\hbar\delta_{ij}$

$[x, F(p)] = i\hbar \frac{\partial F}{\partial p}$

$[p, G(x)] = i\hbar \frac{\partial G}{\partial x}$

$[\sigma_i, \sigma_j] = \sigma_k$, $S_i = \frac{\hbar}{2}\sigma_i$

$\hookrightarrow \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$; $\sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$; $\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

$[A, H] = -i\hbar \frac{\partial A}{\partial t}$ (Heisenberg Eqn of Motion)

*For functions of continuous variables:

$\psi_a(x') = \langle x'|a\rangle$

$\varphi_b(p') = \langle p'|b\rangle$

$\langle\beta|\alpha\rangle = \int dx' \psi_b^*(x')\psi_a(x')$

$= \int dp' \varphi_b^*(p')\varphi_a(p')$

$p = i\hbar \frac{\partial}{\partial x}$

$\langle x'|p'\rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp\left[\frac{i}{\hbar} p'x'\right]$

Basics (cont.)

* Remember, when discussing angular momentum:

  $J \rightarrow$ Arbitrary Angular Momentum (often refers to total)

  $L \rightarrow$ Orbital Angular Momentum

  $S \rightarrow$ Spin Angular Momentum

* Important angular momentum formulas include:

$$J^2 = \mathbf{J} \cdot \mathbf{J} = J_x^2 + J_y^2 + J_z^2 \qquad J_\pm = J_x \pm i J_y$$

$$[J^2, J_i] = 0 \qquad [J^2, J_\pm] = 0$$

$$[J_i, J_j] = i\hbar \epsilon_{ijk} J_k \qquad [J_z, J_\pm] = \hbar J_\pm$$

$$[J_+, J_-] = 2\hbar J_z$$

$\Rightarrow$ We often write simultaneous eigenkets of J^2, J_z as $|a, b\rangle$ such that:

$$J^2 |a, b\rangle = a|a, b\rangle \qquad J_\pm^n |a, b\rangle = b \pm n\hbar |a, b \pm n\hbar\rangle$$

$$J_z |a, b\rangle = b|a, b\rangle$$

$$J_\pm |a, b\rangle = \hbar\sqrt{(j \mp m)(j \pm m + 1)}\, |a, b \pm \hbar\rangle$$

* When adding angular momentum, it is often useful to use direct product notation

$$|S_1, S_{1,z}; S_2, S_{2,z}\rangle = |S_1, S_{1z}\rangle \otimes |S_2, S_{2z}\rangle$$

$\Rightarrow$ Our total system operators now become:

$$J = J_1 + J_2 = J_1 \otimes \mathbb{I}_2 + \mathbb{I}_1 \otimes J_2$$

$$J^2 = (J_1 + J_2) \cdot (J_1 + J_2) = J_1^2 + J_2^2 + 2 J_1 \cdot J_2$$

$$= J_{1z} J_{2z} + \tfrac{1}{2}(J_{1+} J_{2-} + J_{1-} J_{2+})$$

* This flexibility allows us to use two sets of kets to describe the system

$$|j_1, j_2; m_1, m_2\rangle \Longleftrightarrow |j_1, j_2; j, m\rangle$$

$$[J_1^2, J_2^2] = 0 = [J_{1z}, J_{2z}] = [J_{1i}, J_{2k}]$$

36. CLEBSCH-GORDAN COEFFICIENTS, SPHERICAL HARMONICS, AND d FUNCTIONS

Note: A square-root sign is to be understood over *every* coefficient, *e.g.*, for −8/15 read $-\sqrt{8/15}$.

Notation:

	J	J	...
	M	M	...
m_1 m_2	Coefficients		
m_1 m_2			
. .			

1/2×1/2

	1
	+1
+1/2 +1/2	1

	1	0
	0	0
+1/2 −1/2	1/2	1/2
−1/2 +1/2	1/2	−1/2

	1
	−1
−1/2 −1/2	1

1×1/2

	3/2
	+3/2
+1 +1/2	1

	3/2	1/2
	+1/2	+1/2
+1 −1/2	1/3	2/3
0 +1/2	2/3	−1/3

	3/2	1/2
	−1/2	−1/2
0 −1/2	2/3	1/3
−1 +1/2	1/3	−2/3

	3/2
	−3/2
−1 −1/2	1

2×1

	3
	+3
+2 +1	1

	3	2
	+2	+2
+2 0	1/3	2/3
+1 +1	2/3	−1/3

	3	2	1
	+1	+1	+1
+2 −1	1/15	1/3	3/5
+1 0	8/15	1/6	−3/10
0 +1	2/5	−1/2	1/10

	3	2	1
	0	0	0
+1 −1	1/5	1/2	3/10
0 0	3/5	0	−2/5
−1 +1	1/5	−1/2	3/10

	3	2	1
	−1	−1	−1
0 −1	2/5	1/2	1/10
−1 0	8/15	−1/6	−3/10
−2 +1	1/15	−1/3	3/5

	3	2
	−2	−2
−1 −1	2/3	1/3
−2 0	1/3	−2/3

	3
	−3
−2 −1	1

1×1

	2
	+2
+1 +1	1

	2	1
	+1	+1
+1 0	1/2	1/2
0 +1	1/2	−1/2

	2	1	0
	0	0	0
+1 −1	1/6	1/2	1/3
0 0	2/3	0	−1/3
−1 +1	1/6	−1/2	1/3

	2	1
	−1	−1
0 −1	1/2	1/2
−1 0	1/2	−1/2

	2
	−2
−1 −1	1

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$$Y_1^1 = -\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\phi}$$

$$Y_2^0 = \sqrt{\frac{5}{4\pi}}\left(\frac{3}{2}\cos^2\theta - \frac{1}{2}\right)$$

$$Y_2^1 = -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{i\phi}$$

$$Y_2^2 = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta\, e^{2i\phi}$$

3/2×1

	5/2
	+5/2
+3/2 +1	1

	5/2	3/2
	+3/2	+3/2
+3/2 0	2/5	3/5
+1/2 +1	3/5	−2/5

	5/2	3/2	1/2
	+1/2	+1/2	+1/2
+3/2 −1	1/10	2/5	1/2
+1/2 0	3/5	1/15	−1/3
−1/2 +1	3/10	−8/15	1/6

	5/2	3/2	1/2
	−1/2	−1/2	−1/2
+1/2 −1	3/10	8/15	1/6
−1/2 0	3/5	−1/15	−1/3
−3/2 +1	1/10	−2/5	1/2

	5/2	3/2
	−3/2	−3/2
−1/2 −1	3/5	2/5
−3/2 0	2/5	−3/5

	5/2
	−5/2
−3/2 −1	1

2×1/2

	5/2
	+5/2
+2 +1/2	1

	5/2	3/2
	+3/2	+3/2
+2 −1/2	1/5	4/5
+1 +1/2	4/5	−1/5

	5/2	3/2
	+1/2	+1/2
+1 −1/2	2/5	3/5
0 +1/2	3/5	−2/5

	5/2	3/2
	−1/2	−1/2
0 −1/2	3/5	2/5
−1 +1/2	2/5	−3/5

	5/2	3/2
	−3/2	−3/2
−1 −1/2	4/5	1/5
−2 +1/2	1/5	−4/5

	5/2
	−5/2
−2 −1/2	1

3/2×1/2

	2
	+2
+3/2 +1/2	1

	2	1
	+1	+1
+3/2 −1/2	1/4	3/4
+1/2 +1/2	3/4	−1/4

	2	1
	0	0
+1/2 −1/2	1/2	1/2
−1/2 +1/2	1/2	−1/2

	2	1
	−1	−1
−1/2 −1/2	3/4	1/4
−3/2 +1/2	1/4	−3/4

	2
	−2
−3/2 −1/2	1

$$Y_\ell^{-m} = (-1)^m Y_\ell^{m*}$$

$$d^\ell_{m,0} = \sqrt{\frac{4\pi}{2\ell+1}}\, Y_\ell^m\, e^{-im\phi}$$

$$\langle j_1 j_2 m_1 m_2 | j_1 j_2 J M\rangle = (-1)^{J-j_1-j_2}\langle j_2 j_1 m_2 m_1 | j_2 j_1 J M\rangle$$

$$d^j_{m',m} = (-1)^{m-m'} d^j_{m,m'} = d^j_{-m,-m'}$$

$$d^1_{0,0} = \cos\theta \qquad d^{1/2}_{1/2,1/2} = \cos\frac{\theta}{2} \qquad d^1_{1,1} = \frac{1+\cos\theta}{2}$$

$$d^{1/2}_{1/2,-1/2} = -\sin\frac{\theta}{2} \qquad d^1_{1,0} = -\frac{\sin\theta}{\sqrt{2}}$$

$$d^1_{1,-1} = \frac{1-\cos\theta}{2}$$

3/2×3/2

	3
	+3
+3/2 +3/2	1

	3	2
	+2	+2
+3/2 +1/2	1/2	1/2
+1/2 +3/2	1/2	−1/2

	3	2	1
	+1	+1	+1
+3/2 −1/2	1/5	1/2	3/10
+1/2 +1/2	3/5	0	−2/5
−1/2 +3/2	1/5	−1/2	3/10

	3	2	1	0
	0	0	0	0
+3/2 −3/2	1/20	1/4	9/20	1/4
+1/2 −1/2	9/20	1/4	−1/20	−1/4
−1/2 +1/2	9/20	−1/4	−1/20	1/4
−3/2 +3/2	1/20	−1/4	9/20	−1/4

	3	2	1
	−1	−1	−1
+1/2 −3/2	1/5	1/2	3/10
−1/2 −1/2	3/5	0	−2/5
−3/2 +1/2	1/5	−1/2	3/10

	3	2
	−2	−2
−1/2 −3/2	1/2	1/2
−3/2 −1/2	1/2	−1/2

	3
	−3
−3/2 −3/2	1

2×3/2

	7/2
	+7/2
+2 +3/2	1

	7/2	5/2
	+5/2	+5/2
+2 +1/2	3/7	4/7
+1 +3/2	4/7	−3/7

	7/2	5/2	3/2
	+3/2	+3/2	+3/2
+2 −1/2	1/7	16/35	2/5
+1 +1/2	4/7	1/35	−2/5
0 +3/2	2/7	−18/35	1/5

	7/2	5/2	3/2	1/2
	+1/2	+1/2	+1/2	+1/2
+2 −3/2	1/35	6/35	2/5	2/5
+1 −1/2	12/35	5/14	0	−3/10
0 +1/2	18/35	−3/35	−1/5	1/5
−1 +3/2	4/35	−27/70	2/5	−1/10

	7/2	5/2	3/2	1/2
	−1/2	−1/2	−1/2	−1/2
+1 −3/2	4/35	27/70	2/5	1/10
0 −1/2	18/35	3/35	−1/5	−1/5
−1 +1/2	12/35	−5/14	0	3/10
−2 +3/2	1/35	−6/35	2/5	−2/5

	7/2	5/2	3/2
	−3/2	−3/2	−3/2
0 −3/2	2/7	18/35	1/5
−1 −1/2	4/7	−1/35	−2/5
−2 +1/2	1/7	−16/35	2/5

	7/2	5/2
	−5/2	−5/2
−1 −3/2	4/7	3/7
−2 −1/2	3/7	−4/7

	7/2
	−7/2
−2 −3/2	1

2×2

	4
	+4
+2 +2	1

	4	3
	+3	+3
+2 +1	1/2	1/2
+1 +2	1/2	−1/2

	4	3	2
	+2	+2	+2
+2 0	3/14	1/2	2/7
+1 +1	4/7	0	−3/7
0 +2	3/14	−1/2	2/7

	4	3	2	1
	+1	+1	+1	+1
+2 −1	1/14	3/10	3/7	1/5
+1 0	3/7	1/5	−1/14	−3/10
0 +1	3/7	−1/5	−1/14	3/10
−1 +2	1/14	−3/10	3/7	−1/5

	4	3	2	1	0
	0	0	0	0	0
+2 −2	1/70	1/10	2/7	2/5	1/5
+1 −1	8/35	2/5	1/14	−1/10	−1/5
0 0	18/35	0	−2/7	0	1/5
−1 +1	8/35	−2/5	1/14	1/10	−1/5
−2 +2	1/70	−1/10	2/7	−2/5	1/5

	4	3	2	1
	−1	−1	−1	−1
+1 −2	1/14	3/10	3/7	1/5
0 −1	3/7	1/5	−1/14	−3/10
−1 0	3/7	−1/5	−1/14	3/10
−2 +1	1/14	−3/10	3/7	−1/5

	4	3	2
	−2	−2	−2
0 −2	3/14	1/2	2/7
−1 −1	4/7	0	−3/7
−2 0	3/14	−1/2	2/7

	4	3
	−3	−3
−1 −2	1/2	1/2
−2 −1	1/2	−1/2

	4
	−4
−2 −2	1

$$d^{3/2}_{3/2,3/2} = \frac{1+\cos\theta}{2}\cos\frac{\theta}{2}$$

$$d^{3/2}_{3/2,1/2} = -\sqrt{3}\frac{1+\cos\theta}{2}\sin\frac{\theta}{2}$$

$$d^{3/2}_{3/2,-1/2} = \sqrt{3}\frac{1-\cos\theta}{2}\cos\frac{\theta}{2}$$

$$d^{3/2}_{3/2,-3/2} = -\frac{1-\cos\theta}{2}\sin\frac{\theta}{2}$$

$$d^{3/2}_{1/2,1/2} = \frac{3\cos\theta-1}{2}\cos\frac{\theta}{2}$$

$$d^{3/2}_{1/2,-1/2} = -\frac{3\cos\theta+1}{2}\sin\frac{\theta}{2}$$

$$d^2_{2,2} = \left(\frac{1+\cos\theta}{2}\right)^2$$

$$d^2_{2,1} = -\frac{1+\cos\theta}{2}\sin\theta$$

$$d^2_{2,0} = \frac{\sqrt{6}}{4}\sin^2\theta$$

$$d^2_{2,-1} = -\frac{1-\cos\theta}{2}\sin\theta$$

$$d^2_{2,-2} = \left(\frac{1-\cos\theta}{2}\right)^2$$

$$d^2_{1,1} = \frac{1+\cos\theta}{2}(2\cos\theta-1)$$

$$d^2_{1,0} = -\sqrt{\frac{3}{2}}\sin\theta\cos\theta$$

$$d^2_{1,-1} = \frac{1-\cos\theta}{2}(2\cos\theta+1) \qquad d^2_{0,0} = \left(\frac{3}{2}\cos^2\theta - \frac{1}{2}\right)$$

Figure 36.1: The sign convention is that of Wigner (*Group Theory*, Academic Press, New York, 1959), also used by Condon and Shortley (*The Theory of Atomic Spectra*, Cambridge Univ. Press, New York, 1953), Rose (*Elementary Theory of Angular Momentum*, Wiley, New York, 1957), and Cohen (*Tables of the Clebsch-Gordan Coefficients*, North American Rockwell Science Center, Thousand Oaks, Calif., 1974).

Basics (cont.)

$\Rightarrow$ Use of the Clebsh-Gordon coefficients allows us to relate the two sets of kets (see attached table)

$\rightarrow$ If calculating by hand, equate states of degenerecy 1 (ie max/min J) and use ladder operators

Tensor Operators

* For Cartesian tensors, we know they rotate as:

Rank 1 - $V_i' = R_{ij} V_j$

2 - $W = \tilde{R}'\tilde{R}\, V_i U_j$

* Remember we define our Rotation operator $R(\alpha, \beta, \gamma)$ as:

$$R(\alpha,\beta,\gamma)\,|j,m\rangle = \sum_{j'm'} |j',m'\rangle\langle j',m'|R(\alpha,\beta,\gamma)|j,m\rangle$$
$$= \mathcal{D}^{(j)}_{m,m'}\,|j',m'\rangle \quad \text{where } j=j' \text{ so } J=\text{const.}$$

$\Rightarrow$ Comparing this to our classical picture, we see:

$$\langle\alpha|V_i|\alpha\rangle \longrightarrow \langle\alpha|\mathcal{D}^{+}(R)V\mathcal{D}^{*}(R)|\alpha\rangle = \sum_{ij} R_i R_j \langle\alpha|V_j|\alpha\rangle$$
$$\text{where } \mathcal{D}(R) = \exp[\tfrac{i}{\hbar}(J\cdot\hat{n})\delta\varphi]$$

$$\hookrightarrow \sum_i R_{ij} V_j = \mathcal{D}^{+}(R)\,V_i\,\mathcal{D}(R)\,,\quad \mathcal{D}$$

* Applying our infinitesimal operator, we see

$$V_i' = V_i + \frac{\epsilon}{i\hbar}[V_i,\, J\cdot\hat{n}] = \sum_j R_{ij}(\hat{n},\epsilon)\, V_j$$

which allows us to deduce the commutation relation

$$[V_i, J_j] = i\,\epsilon_{ijk} V_k$$

Tensor Operators (cont.)

* A closer examination of rank two tensors reveals they can be decomposed as follows:

$$U_i V_j = \underbrace{\frac{U\cdot V}{3}\delta_{ij}}_{\text{scalar}} + \underbrace{\frac{U_iV_j - U_jV_i}{2}}_{\text{anti-symmetric tensor}} + \underbrace{\left(\frac{U_iV_j + U_jV_i}{2} - \frac{U\cdot V}{3}\delta_{ij}\right)}_{\text{traceless symmetric tensor}}$$

1   3   5

⇒ The circled #'s represent the number of independent per term, which happen to match the multiplicity of states for $l = 0, 1, 2$ respectively

↳ Replacing $\hat{n}$ by $\vec{V}$ in our definition of spherical tensors, we see:

$$T_q^{(k)} = Y_{l=k}^{m=q}(\vec{V})$$

ex. $$Y_1^0 = T_0^{(1)} = \sqrt{\tfrac{3}{4}}\cos\theta = \sqrt{\tfrac{3}{4}}\, V_z$$

$$Y_1^{\pm 1} = T_{\pm 1}^{(1)} = \sqrt{\tfrac{3}{8\pi}}\, e^{\pm i\varphi}\cos\theta = \sqrt{\tfrac{3}{2\pi}}\, V_x \pm i V_y$$

⇒ To derive transformation properties we return to our definition of the spherical harmonics

$$Y_l^m(\hat{n}) = \langle \hat{n} | l, m\rangle$$

* Remembering $|n'\rangle = \mathcal{D}(R)|n\rangle \Leftrightarrow \langle n'| = \langle n|\mathcal{D}(R^{-1})$, we cor ang. mom. kets will transform as:

$$\mathcal{D}(R^{-1})|l,m\rangle = \sum_{m'} |l,m'\rangle\langle l,m'|\mathcal{D}(R^{-1})|l,m\rangle$$

$$= \sum_{m'} |l,m'\rangle\, \mathcal{D}^{(l)}_{mm'}(R^{-1})$$

* Applyin $\langle n|$ to both sides of the equation

$$\langle n|\mathcal{D}(R^{-1})|l,m\rangle = \sum_{m'} \langle n|l,m'\rangle\, \mathcal{D}^{(l)}_{mm'}(R^{-1})$$

$$\langle n'|l,m\rangle = \sum_{m'} Y_l^{m'}(n)\, \mathcal{D}^{(l)}_{mm'}(R^{-1})$$

$$Y_l^m(n') = \sum_{m'} Y_l^{m'}(n)\, \mathcal{D}^{(l)}_{mm'}(R^{-1})$$

⇒

Tensor Operators (cont.)

* Switching to operator formulations:

$$\mathcal{D}^{+}(R)\, Y_{\ell}^{m}(V)\, \mathcal{D}(R) = \sum_{m'} Y_{\ell}^{m'}(V) \left[\mathcal{D}_{mm'}^{(\ell)}(R)\right]^{*}$$

* And finally moving to tensor notation:

$$\mathcal{D}^{+}(R)\, T_{q}^{(k)}\, \mathcal{D}(R) = \sum_{q'} T_{q'}^{(k)} \left[\mathcal{D}_{qq'}^{(k)}(R)\right]^{*}$$

* Applying this equation to an infinitesimal rotation:

$$[J\cdot n, T_{q}^{(k)}] = \sum_{q'} T_{q'}^{(k)} \langle kq' | J\cdot n | kq\rangle$$

⇒ Evaluating the above in the z, and ± directions yields:

$$[J_z, T_q^{(k)}] = \hbar q\, T_q^{(k)}$$

$$[J_\pm, T_q^{(k)}] = \hbar\sqrt{(k\mp q)(k\pm q+1)}\; T_{q\pm 1}^{(k)}$$

* We have a theorem that defines spherical tensors in terms of Cartesian tensors by:

$$T_{q}^{(k)} = \sum_{q_1}\sum_{q_2} \underbrace{\langle k_1 k_2; q_1 q_2 | k_1 k_2; kq\rangle}_{\text{CG Coefficient}}\, X_{q_1}^{(k_1)} Z_{q_2}^{(k_2)}$$

← irreducible spherical tensors

⇒ To show the above transforms as a spherical tensor:

$$\mathcal{D}^{+}(R)\, T_q^{(k)}\, \mathcal{D}(R) = \sum_{q_1}\sum_{q_2} \langle k_1 k_2; q_1 q_2 | k_1 k_2; kq\rangle\, \mathcal{D}^{+}(R)\, X_{q_1}^{(k_1)}\, \mathcal{D}(R)\, \mathcal{D}^{+}(R)\, Z_{q_2}^{(k_2)}\, \mathcal{D}(R)$$

$$= \sum_{q_1}\sum_{q_2}\sum_{q_1'}\sum_{q_2'} \langle k_1 k_2; q_1 q_2 | k_1 k_2; kq\rangle\, X_{q_1'}^{(k_1)} \left[\mathcal{D}_{q_1 q_1'}^{(k_1)}(R)\right]^{*} Z_{q_2'}^{(k_2)} \left[\mathcal{D}_{q_2 q_2'}^{(k_2)}(R)\right]^{*}$$

* using $\mathcal{D}_{m_1 m_1'}^{(j_1)}(R)\, \mathcal{D}_{m_2 m_2'}^{(j_2)}(R) = \sum_{j}\sum_{m}\sum_{m'} \langle j_1 j_2; m_1 m_2 | j_1 j_2; jm\rangle \langle j_1 j_2; m_1' m_2' | j_1 j_2; jm'\rangle\, \mathcal{D}_{mm'}^{(j)}(R)$

$$= \sum_{k''}\sum_{q_1}\sum_{q_2}\sum_{q_1'}\sum_{q_2'}\sum_{q''}\sum_{q'} \langle k_1 k_2; q_1 q_2 | k_1 k_2; kq\rangle \langle k_1 k_2; q_1 q_2 | k_1 k_2; k'' q'\rangle \langle k_1 k_2; q_1 q_2 | k_1 k_2; k'', q''\rangle \left[\mathcal{D}_{q'q''}(R)\right]^{*} X_{q_1'}^{k_1} Z_{q_2'}^{k_2}$$

$$= \sum_{q'} T_{q'}^{(k)} \left[\mathcal{D}_{qq'}^{(k)}(R)\right]^{*}$$

Tensor Operators (cont.)

* We determine the matrix elements of a spherical tensor via the Wigner-Eckart Theorem

  $\Rightarrow$ Starting w/ $[J_\pm, T_q^{(k)}] = \hbar\sqrt{(k\mp q)(k\pm q+1)}\, T_{q\pm1}^{(k)}$

$$\langle \alpha', j' m' | [J_\pm, T_q^{(k)}] - \hbar\sqrt{(k\mp q)(k\pm q+1)} | \alpha, j, m\rangle = 0$$

  $\Rightarrow$ Switching to $[J_z, T_q^{(k)}] = \hbar q T_q^{(k)}$

$$\langle \alpha', j', m' | J_z T_q^{(k)} - T_q^{(k)} J_z - \hbar q T_q^{(k)} | \alpha, j, m\rangle = 0$$

$$\langle \alpha', j', m' | m' T_q^{(k)} - T_q^{(k)} m - q T_q^{(k)} | \alpha, j, m\rangle = 0$$

$\Rightarrow$ $m' = m + q$ where q is angular momentum added to system by the spherical tensor

  $\Rightarrow$ We apply the Wigner-Eckart Thm by noting $\langle \alpha', j' m' | T_q^{(k)} | \alpha, j, m\rangle$ can be written in terms of a CG coefficient and a reduced matrix element

$$\langle \alpha'; j', m' | T_q^{(k)} | \alpha; j, m\rangle = \langle j, k; m, q | j, k; j' m'\rangle \frac{1}{\sqrt{2j+1}} \langle \alpha', j' \| T_q^{(k)} | \alpha, j\rangle$$

* Our general approach is to calculate reduced matrix element in a simple case then use that # in our situation of interest

ex.

$$\langle 3, 0 | T_0^{(2)} | 1, 0\rangle = \langle 1, 2; 0 0 | 1, 2, 1, 0\rangle \langle 3 \| T^{(2)} \| 1\rangle$$

$$\int Y_3^{0}(\theta,\varphi)\, Y_2^{0}(\theta,\varphi)\, Y_1^{0}(\theta,\varphi)\, d\Omega = \langle 1, 2; 0 0 | 1, 2; 1, 0\rangle \langle 3 \| T^{(2)} \| 1\rangle$$

$$\Rightarrow \langle 3 \| T^{(2)} \| 1\rangle = \sqrt{\frac{3}{4\pi}}$$

Perturbation Theory

* We only consider time-independent, non-degenerate cases for this exam

* Perturbation theory is an approximation technique that allows us to solve non-idealized problems in quantum mechanics and other fields

* For a given Hamiltonian H, we write it as

$$H = H_0 + V \quad , \text{ where we know the solutions for } H_0 \text{ but not } V$$

$$H = E_1^{(0)} |1^{(0)}\rangle\langle 1^{(0)}| + E_2^{(0)} |2^{(0)}\rangle\langle 2^{(0)}| + \lambda V_{12} |1^{(0)}\rangle\langle 2^{(0)}| + \lambda V_{21} |2^{(0)}\rangle\langle 1^{(0)}|$$

$$\doteq \begin{bmatrix} E_1^{(0)} & \lambda V_{12} \\ \lambda V_{21} & E_2^{(0)} \end{bmatrix} ; \quad V_{21} = V_{12}, \quad V_{12}, V_{21} \in \mathbb{R} \text{ for Hermiticity}$$

$\Rightarrow$ Thru normal matrix methods we see:

$$E_1 = \frac{1}{2}(E_1 + E_2) + \sqrt{\frac{1}{4}(E_1 - E_2) + \lambda^2 V_{12}^2}$$

$$E_2 = \frac{1}{2}(E_1 + E_2) - \sqrt{\frac{1}{4}(E_1 - E_2) + \lambda^2 V_{12}^2}$$

* However, if we are unable to solve the problem exactly, we proceed as follows:

$\Rightarrow$ We know: $H_0|n\rangle = E_n^{(0)}|n\rangle$

$$(H_0 + \lambda V)|n\rangle = E_n|n\rangle$$

$\Rightarrow$ Introducing $\Delta_n = E_n - E_n^{(0)}$

$$\hookrightarrow \; E_n^{(0)} - H_0 |n\rangle = \lambda V - \Delta_n |n\rangle$$

$$\langle n^{(0)}| E_n^{(0)} - H_0 |n\rangle = \langle n^{(0)}| \lambda V - \Delta_n |n\rangle$$

$$0 = \langle n^{(0)}| \lambda V - \Delta_n |n\rangle$$

* Defining a projection operator $\varphi_n = \mathbb{I} - |n^{(0)}\rangle\langle n^{(0)}|$

$$= \sum_{k \neq n}' |k^{(0)}\rangle\langle k^{(0)}|$$

$$\Rightarrow |n\rangle = \frac{1}{E_n^{(0)} - H_0} \varphi_n (\lambda V - \Delta_n)|n\rangle$$

* but as $\lambda \to 0$, we must approach $H_0|n^{(0)}\rangle = E_n^{(0)}|n^{(0)}\rangle$

Perturbation Theory (cont.)

$\Rightarrow$ We ~~redefine~~ $|n\rangle$ as:

$$|n\rangle = c_n(\lambda)\,|n_0\rangle + \frac{1}{E_n^{(0)} - H_0}\,\varphi_n(\lambda V - \Delta_n)\,|n\rangle\,; \quad c_n(\lambda) = \langle n^0|n\rangle$$

*Note: We choose $\langle n^{(0)}|n\rangle = 1$, therefore we most always normalize $|n\rangle$ after solving for it

$$\hookrightarrow \boxed{|n\rangle = |n_0\rangle + \frac{1}{E_n^{(0)} - H_0}\,\varphi_n(\lambda V - \Delta_n)\,|n\rangle}$$

*We extract the value of Δ_n by multiplying both sides by $\langle n^{(0)}|$

$$\boxed{\Delta_n = \lambda \langle n^{(0)}|V|n\rangle}$$

* Expanding $|n\rangle$ and Δ_n as power series:

$$|n\rangle = |n^{(0)}\rangle + \lambda|n^{(1)}\rangle + \lambda^2|n^{(2)}\rangle + \ldots$$

$$\Delta_n = \lambda\Delta_n^{(1)} + \lambda^2\Delta_n^{(2)} + \ldots$$

* Substituting the above into the above boxed equations yields the corrections after matching in powers of λ:

$$\Delta_n^{(1)} = \langle n^{(0)}|V|n^{(0)}\rangle$$

$$\Delta_n^{(2)} = \langle n^{(0)}|V|n^{(1)}\rangle \quad \Rightarrow \sum_{k\neq n}{}' \frac{|V_{nk}|^2}{(E_n^{(0)} - E_k^{(0)})^2}$$

$$|n^{(1)}\rangle = \frac{1}{E_n^{(0)} - H_0}\,\varphi_n\,|n^{(0)}\rangle$$

$$= \sum_{k\neq n}{}' \frac{V_{kn}}{E_n^{(0)} - E_k^{(0)}}\,|k^{(0)}\rangle$$

Quantum II Exam III Study Guide

Basics

$|\alpha\rangle = \sum_i' c_i |a_i\rangle$ and $A|\alpha\rangle = a_i|\alpha\rangle$ (Definition of a ket)

$A = |a\rangle\langle b|$ (Definition of an operator)

$\sum_i' \Lambda_i = \sum_i' |a_i\rangle\langle a_i| = 1$ (Projection Operator/Completeness Relation)

* To get the matrix elements of an operator:

$$A \rightarrow \sum_{mn}' |m\rangle\langle m|A|n\rangle\langle n|$$

$\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2$ (Schwartz Inequality)

$\langle\alpha|A|\alpha\rangle = \langle A\rangle$ (Expectation Value)

$\Delta A = A - \langle A\rangle \mathbb{I}$ (Dispersion Operator)

$\langle(\Delta A)^2\rangle = \langle A^2\rangle - \langle A\rangle^2$ (Avg value or RMS)

$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq \frac{1}{4}|\langle[A,B]\rangle|^2$ (Uncertainty Relation)

* Important commutation relations include:

$[x_i, x_j] = [p_i, p_j] = 0$

$[x_i, p_j] = i\hbar\delta_{ij}$

$[x, F(p)] = i\hbar \frac{\partial F}{\partial p}$

$[p, G(x)] = i\hbar \frac{\partial G}{\partial x}$

$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$; $\sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$, $\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$; $S_i = \frac{\hbar}{2}\sigma_i$

$\hookrightarrow [\sigma_i, \sigma_j] = \sigma_k$

$[A, H] = -i\hbar \frac{\partial A}{\partial t}$ (Heisenberg Eqn of Motion)

* For functions of continuous variables

$\psi_a(x') = \langle x'|a\rangle$ $\quad\langle\beta|\alpha\rangle = \int dx'\, \psi_\beta^*(x')\psi_a(x')$ $\quad p = i\hbar\, \partial/\partial x$

$\varphi_b(p') = \langle p'|b\rangle$ $\quad = \int dp'\, \varphi_\beta^*(p')\varphi_a(p')$ $\quad \langle x'|p'\rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp\left[\frac{i}{\hbar}p'x'\right]$

Basics (cont.)

* Remember, for angular momentum:

$J \rightarrow$ Arbitrary Angular Momentum (usually refers to total)

$L \rightarrow$ Orbital Angular Momentum

$S \rightarrow$ Spin Angular Momentum

* Important angular momentum formulas include:

$$J^2 = J \cdot J = J_x^2 + J_y^2 + J_z^2 \qquad J_\pm = J_x \pm i J_y$$

$$[J^2, J_i] = 0 \qquad [J^2, J_\pm] = 0 = [J_z, J_\pm]$$

$$[J_i, J_j] = i\hbar \epsilon_{ijk} J_k \qquad [J_+, J_-] = 2\hbar J_z$$

$\Rightarrow$ We often write simultaneous eigenkets of J^2, J_z as $|a, b\rangle$ such that:

$$J^2 |a,b\rangle = a|a,b\rangle \qquad J_\pm |a,b\rangle = \hbar\sqrt{(j\mp m)(j\pm m+1)}\,|a, b+\hbar\rangle$$

$$J_z |a,b\rangle = b|a,b\rangle \qquad J_\pm^n |a,b\rangle = b\pm n\hbar\,|a, b+n\hbar\rangle$$

* When adding angular momentum, it is useful to use direct product notation:

$$|S_1, S_{1z}; S_2, S_{2z}\rangle = |S_1, S_{1z}\rangle \otimes |S_2, S_{2z}\rangle$$

$\Rightarrow$ Our total system operators now become:

$$J = J_1 + J_2 = J_1 \otimes \mathbb{I}_2 + \mathbb{I}_1 \otimes J_2$$

$$J^2 = (J_1 + J_2)\cdot(J_1 + J_2) = J_1^2 + J_2^2 + 2 J_1 \cdot J_2$$

$$= J_{1z} + J_{2z} + \tfrac{1}{2}(J_{1+} J_{2-} + J_{1-} J_{2+})$$

* This flexibility allows us to use two sets of kets to describe the system:

$$|j_1, j_2; m_1, m_2\rangle \Longleftrightarrow |j_1, j_2; j, m\rangle$$

$$[J_1^2, J_2^2] = 0 = [J_{1z}, J_{2z}] = [J_{1i}, J_{2k}]$$

* Use of Clebsh-Gordon coefficients allows us to relate the two sets of kets to one another (see table)

↳ If calculating by hand, equate states of degeneracy 1 (ie max or min J) and use ladder operators

Basics (cont.)

*Remember that we define tensor operators as follows:

$$T_q^{(k)} = Y_{\ell=k}^{m=q}(\vec{V}) \quad \text{where } \vec{V} \text{ is a normal cartesian vector}$$

ex. $Y_1^0 = T_0^{(1)} = \sqrt{\frac{3}{4}} \cos\Theta = \sqrt{\frac{3}{4}}\, V_z$

$$Y_1^{\pm 1} = T_{\pm 1}^{1} = \sqrt{\frac{3}{8\pi}}\, e^{\pm i\varphi} \cos\Theta = \sqrt{\frac{3}{2\pi}}\, V_x \pm iV_y$$

* Spherical Tensors / Tensor Operators have the following properties:

$$Y_\ell^m(\hat{n}) = \langle \hat{n} | \ell, m \rangle$$

$$Y_\ell^m(n') = \sum_{m'} Y_\ell^{m'}(n)\, \mathcal{D}_{mm'}^{(\ell)}(R^{-1}), \quad \text{where } R \text{ is the rotation operator}$$

$$\hookrightarrow \mathcal{D}_{mm'}^{(j)} |j', m'\rangle = \sum_{j', m'} |j', m'\rangle \langle j', m' | R(\alpha, \beta, \gamma) | j, m \rangle$$

⇒ The transformation properties are as follows:

$$\mathcal{D}^{+}(R)\, Y_\ell^m(\vec{v})\, \mathcal{D}(R) = \sum_{m'} Y_\ell^{m'}(v) [D_{mm'}^{(\ell)}(R)]^*$$

$$\mathcal{D}^{+}(R)\, T_q^{(k)}\, \mathcal{D}(R) = \sum_{q'} T_{q'}^{(k)} [D_{qq'}^{(k)}(R)]^*$$

⇒ The above properties yield the following commutators:

$$[J_z, T_q^{(k)}] = \hbar q\, T_q^{(k)}$$

$$[J_\pm, T_q^{(k)}] = \hbar \sqrt{(k \mp q)(k \pm q + 1)}\; T_{q\pm 1}^{(k)}$$

⇒ The theorem that defines spherical tensors in terms of Cartesian tensors is:

$$T_q^{(k)} = \sum_{q_1} \sum_{q_2} \langle k_1 k_2 ; q_1 q_2 | k_1 k_2 ; k, q \rangle\, X_{q_1}^{(k_1)}\, Z_{q_2}^{(k_2)}$$

irreducible spherical tensors

⇒ The matrix elements of a spherical tensor are given by the Wigner-Eckart Thm:

reduced matrix element

$$\langle \alpha'; j', m' | T_q^{(k)} | \alpha; j, m \rangle = \langle j, k; m, q | j, k; j', m' \rangle \frac{1}{\sqrt{2j+1}} \langle \alpha'; j' || T_q^{(k)} || \alpha, j \rangle$$

*for $m' = m + q$

<u>ex.</u> $\langle 3, 0 | T_0^{(2)} | 1, 0 \rangle = \langle 1, 2; 0, 0 | 1, 2; 1, 0 \rangle \langle 3 || T^{(2)} || 1 \rangle$

$$\int Y_3^0(\theta,\varphi)\, Y_2^0(\theta,\varphi)\, Y_1^0(\theta,\varphi)\, d\Omega = \langle 1, 2; 0 0 | 1, 2; 1, 0 \rangle \langle 3 || T^{(2)} || 1 \rangle$$

$$\hookrightarrow \langle 3 || T^{(2)} || 1 \rangle = \sqrt{\frac{3}{4\pi}}$$

Basics (cont.)

* For time-independent, non-degenerate perturbation theory, the key eqn's are:

$$|n\rangle = |n^{(0)}\rangle + \frac{1}{E_n^{(0)} - H_0} \varphi_n (\lambda V - \Delta_n)|n\rangle$$

$$\Delta_n = \lambda \langle n^{(0)}|V|n\rangle$$

⇒ Expanding the above as power series, we find that:

$$\Delta_n^{(1)} = \langle n^{(0)}|V|n^{(0)}\rangle$$

$$\Delta_n^{(2)} = \langle n^{(0)}|V|n^{(1)}\rangle$$

$$= \sum_{k\neq n}' \frac{|V_{nk}|^2}{(E_n^{(1)} - E_k^{(0)})}$$

$$|n^{(1)}\rangle = \frac{1}{E_n^{(0)} - H_0} \varphi_n |n^{(0)}\rangle$$

$$= \sum_{k\neq n}' \frac{V_{kn}}{E_n^{(0)} - E_k^{(0)}} |k^{(0)}\rangle$$

⇒ Remember, perturbation theory is simply an approximation schemes that cannot be easily solved exactly, but are close to a problem that can. Many problems can be easily solved by diagnolizing the Hamiltonian as normal.

Time-Independent Perturbation Theory (Degenerate Case)

* Put simply, we need to diagonalize the degenerate submatrix however we can

⇒ For our degenerate energies, our eigenkets become:

$$|\ell^{(0)}\rangle = \sum_{m\in D}' |m^{(0)}\rangle\langle m^{(0)}|\ell^{(0)}\rangle$$

⇒ To solve the eigenvalue eqn ($H = H_0 + V$)

$$(E - H_0 - V)|\ell\rangle = 0$$

↳ Isolate degenerate + non-degenerate states w/ projection operators:

$$\tilde{P}_0 = \sum_{k\in D}' |k^{(0)}\rangle\langle k^{(0)}| \qquad \tilde{P}_1 = \sum_{k\notin D}' |k^{(0)}\rangle\langle k^{(0)}| = \tilde{\mathbb{I}} - \tilde{P}_0$$

Degenerate Perturbation Theory (cont.)

⇒ Rewrite eigenvalue equation as:

$$(E-H_0-\lambda V)P_0|\ell\rangle + (E-H_0-\lambda V)P_1|\ell\rangle = 0$$

* Applying our projection operators to above yield:

① $(E-H_0-\lambda V)P_0^2|\ell\rangle + (E-H_0-\lambda V)P_0P_1|\ell\rangle = 0$

* using $P_0P_0 = P_0$ $\quad$ $P_0P_1 = 0$

$$(E-E_D^{(0)}-\lambda P_0V)P_0|\ell\rangle - \lambda P_0VP_1|\ell\rangle = 0$$

② $-\lambda P_1VP_0|\ell\rangle + (E-H_0-\lambda P_1V)P_1|\ell\rangle = 0$

* Solving the above system of equations yields:

$$|\ell\rangle = \lambda[E-H_0-\lambda P_1VP_1]^{-1}P_1VP_0|\ell\rangle$$

↳ $P_1|\ell\rangle = \tilde{P}_1 \dfrac{\lambda}{E-H_0-\lambda P_1VP_1} P_1VP_0|\ell\rangle$

* expanding $|\ell\rangle$ as a power series and $\dfrac{1}{E-H_0-\lambda P_1VP_1} \approx \dfrac{1}{E-H_0} + \dfrac{\lambda P_1VP_1}{(E-H_0)^2} + \dots$

$$\Rightarrow \boxed{P_1|\ell^{(1)}\rangle = \sum_{k\notin D} \frac{V_{k\ell}}{E_D^{(0)}-E_k^{(0)}}|k^{(0)}\rangle}$$

ex. Linear Stark Effect

* Our physical set-up is a hydrogen-like atom in a uniform $\vec{E}$-field

⇒ $V = -ezE_0$; $n = N+\ell+1$ where $n\in\mathbb{Z}^+$, $\ell\in[0,n-1]$, $N\in\{0,\mathbb{Z}^+\}$

↳ $H|n\ell m\rangle = E_n|n\ell m\rangle$

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

$L_z|n\ell m\rangle = m\hbar|n\ell m\rangle$

$\tilde{\Pi}|n\ell m\rangle = (-1)^\ell|n\ell m\rangle$ (Parity Operator)

* Remember, in terms of spherical tensors: $z = \hat{T}_0^{(1)}$

⇒ $\langle n,\ell',m'|T_0^{(1)}|n\ell m\rangle$ ⟶ $m=m'$ b/c no addition of z ang. mom

$\ell'\in[\ell+1, |\ell-1|]$

Degenerate Perturbation Theory (cont.)

* Notice that: $\Pi^{+} z \Pi = -z$

$\hookrightarrow \langle odd | z | even \rangle = \langle odd | \Pi^{+} \Pi z \Pi^{+} \Pi | even \rangle$
$= \langle odd | z | even \rangle$

$\langle odd | z | odd \rangle = -\langle odd | z | odd \rangle$
$\langle even | z | even \rangle = -\langle even | z | even \rangle$ $\Big\}$ must equal 0

* From this we see $l' = l \pm 1$ and that we can now write the interaction matrix

$\Rightarrow$ For $n = 2$, $l = 0, 1$

$$V = \begin{bmatrix} 0 & \langle 2,0,0|V|2,1,0\rangle \\ \langle 2,1,0|V|2,0,0\rangle & 0 \end{bmatrix} = \begin{bmatrix} 0 & 3ea_0E_0 \\ 3ea_0E_0 & 0 \end{bmatrix}$$

$\hookrightarrow$ via diagonalization:

$$|+\rangle = \frac{1}{\sqrt{2}}\left(|2,0,0\rangle + |2,1,0\rangle\right) \qquad \Delta_{+}^{(1)} = 3e\,a_0E_0$$

$$|-\rangle = \frac{1}{\sqrt{2}}\left(|2,0,0\rangle - |2,1,0\rangle\right) \qquad \Delta_{-}^{(1)} = -3ea_0E_0$$

$\Rightarrow$ Further corrections to the hydrogen atom from perturbation theory include:

① "Relativistic Correction"

$$E = \sqrt{(pc)^2 + m^2c^4}$$

$$T = \sqrt{(pc)^2 + m^2c^4} - m_ec^2$$

$$= mc^2\left(1 + \frac{pc^2}{m^2c^4}\right)^{1/2} - m_ec^2$$

$$\hookrightarrow T \approx \frac{p^2}{2m} - \frac{p^4}{8m_e^3c^2}$$ $\leftarrow$ becomes interaction term in perturbed Hamiltonian

$$\Rightarrow H = \frac{p^2}{2m} - \frac{e^2}{r} - \frac{p^4}{8m_e^3c^2}$$

* But notice $[L, p^2] = 0$, so we proceed via non-degenerate P.T b/c we are unable to break the degeneracy

Degenerate Perturbation Theory (cont.)

$$\Rightarrow \Delta_{n\ell}^{(1)} = \langle n\ell m | \frac{-p^4}{8m_e^3c^2} | n\ell m\rangle$$

$$* \text{but } \frac{1}{2mc^2}\left(\frac{p^2}{2m}\right)^2 = \frac{p^4}{8m_e^3c^2} = \frac{1}{2mc^2}\left(H_0 + \frac{e^2}{r}\right)^2$$

$$= \left[\langle n\ell m | \frac{e^4}{r^2} | n\ell m\rangle + 2E_n^{(0)} \langle n\ell m | \frac{e^2}{r} | n\ell m\rangle + (E_n^{(0)})^2\right] \frac{1}{2mc^2}$$

$$= \frac{-1}{2} m c^2 \alpha^4 \left(\frac{-3}{4n^2} - \frac{1}{n^3(\ell+\frac{1}{2})}\right)$$

$$= \frac{-mc^2\alpha^2}{2n^2}\left(\alpha^2\left[\frac{-3}{4} + \frac{1}{n(\ell+\frac{1}{2})}\right]\right)$$

② Spin-Orbit Coupling

$$\vec{B} = \frac{-v}{c} \times E, \quad \vec{\mu} = \frac{e\vec{S}}{m_e c} \quad (\vec{S} = \text{spin vector})$$

$$H_{LS} = -\vec{\mu}\cdot\vec{B}$$
$$= \mu \cdot \left(\frac{v}{c} \times E\right)$$
$$= \frac{eS}{m_e c}\cdot\left(\frac{v}{c} \times \frac{\vec{r}}{r}\frac{dV_c}{dr}\left(\frac{-1}{e}\right)\right) \quad * \text{Note } V_c \text{ is for central potential}$$
$$= \frac{eS}{m_e c}\cdot\left[\frac{p}{m_e c} \times \frac{\vec{r}}{r}\frac{dV}{dr}\left(\frac{-1}{e}\right)\right]$$
$$= \frac{1}{m_e^2 c^2 r}\frac{dV_c}{dr}\vec{L}\cdot\vec{S}$$

*Note: We can rewrite $L\cdot S \Rightarrow J^2 = (L+S)^2$

$\hookrightarrow L\cdot S = \frac{1}{2}(J^2 - L^2 - S^2)$

*Introducing the spin-angular functions

$$\mathcal{Y}_\ell^{j=\ell\pm 1/2} = \frac{1}{\sqrt{2\ell+1}}\begin{bmatrix} \pm\sqrt{\ell \pm m + 1/2}\; Y_\ell^{m-1/2}(\theta,\varphi) \\ \sqrt{\ell \mp m + 1/2}\; Y_\ell^{m+1/2}(\theta,\varphi)\end{bmatrix} \qquad * \text{Note: } m = m_\ell + m_s$$

$= (\;)\, Y_\ell^m \chi^+ + (\;)\, Y_\ell^m \chi^-$, where $\chi^\pm$ are spinor states

$$\Rightarrow \Delta_{n\ell}^{(1)} = \frac{1}{2m_e^2c^2}\left\langle \frac{1}{r}\frac{dV_c}{dr}\right\rangle_{n\ell} \frac{\hbar}{2}\begin{Bmatrix} \ell \\ -\ell+1 \end{Bmatrix} \begin{matrix}\text{for } j = \ell + 1/2 \\ = \ell - 1/2\end{matrix} \quad (\text{choose } |j)$$

where $\frac{1}{2}\int \mathcal{Y}^+ (J^2 - L^2 - S^2)\, \mathcal{Y}\, d\Omega = \frac{\hbar^2}{2}\left[j(j+1) - \ell(\ell+1) - s(s+1)\right](\;)$
is used in expectation value calculation

$$\Rightarrow \text{In H-atom: } V_c = \frac{e^2}{r} \Rightarrow \left\langle \frac{1}{r}\frac{dV}{dr}\right\rangle = \left\langle \frac{e^2}{r^3}\right\rangle$$

(via hyper-confluent geometric functions)

$$= \frac{-2m_e^2e^2\alpha^2}{n\,\ell(\ell+1)(\ell+\frac{1}{2})\hbar^2} E_n^{(0)}$$

Time - Dependent Perturbation Theory

* Now we assume time-dependent $H = H_0 + V(t)$
  - ⇒ Normal time evolution operator $U(t, t_0) = \exp[-\frac{i}{\hbar} H t]$ only works when H is time-independent

⇒ We must develop the <u>interaction picture</u>

$$|\alpha\rangle = \sum_n c(0)|n\rangle \;; \quad C(0) = \langle n|\alpha\rangle\big|_{t=0}$$

$$|\alpha, t_0 = 0; t\rangle = \sum_n c_n(t)\, e^{-iE_n t/\hbar}|n\rangle \rightarrow c_n(t) \text{ only associated w/ } V$$

↳ $c_n \rightarrow 0$ yields normal evolution

$$\Rightarrow |\alpha, t_0; t\rangle_I = e^{iH_0 t/\hbar}|\alpha, t_0; t\rangle_S \quad (\text{time evolve only unperturbed Hamiltonian})$$

* Operators will transform as: $\tilde{A}_I = e^{iH_0 t/\hbar} A_S e^{-iH_0 t/\hbar}$

$$\Rightarrow i\hbar \frac{\partial}{\partial t}|\alpha, t_0; t\rangle_I = i\hbar \frac{\partial}{\partial t}\left(e^{iH_0 t/\hbar}|\alpha, t_0, t\rangle_S\right)$$

$$= i\hbar \frac{H_0}{-i\hbar} e^{iH_0 t/\hbar}|\alpha, t_0; t\rangle_S + i\hbar e^{iH_0 t/\hbar}\left(\frac{\partial}{\partial t}|\alpha, t_0; t\rangle_S\right)$$

$$= \tilde{H}_0 e^{iH_0 t/\hbar}|\alpha, t_0; t\rangle_S + e^{iH_0 t/\hbar}[H_0 + V(t)]\,|\alpha, t_0, t\rangle_S$$

$$= e^{iH_0 t/\hbar} V(t) e^{-iH_0 t/\hbar} e^{iH_0 t/\hbar}|\alpha, t_0; t\rangle_S$$

$$i\hbar \frac{\partial}{\partial t}|\alpha, t_0; t\rangle = \tilde{V}_I(t)|\alpha, t_0; t\rangle_I$$

* we convert above equation to a # by multiplying both sides by $\langle n|$

$$\Rightarrow i\hbar \frac{\partial}{\partial t}\langle n|\alpha, t_0; t\rangle_I = \langle n|\, V_I(t)\,|\alpha, t_0; t\rangle_I$$

$$i\hbar \frac{\partial}{\partial t} c_n(t) = \sum_m \langle n|V_I(t)|m\rangle\langle m|\alpha, t_0, t\rangle_I$$

$$= \sum_m V_{nm}\, c_m(t)\, e^{i\omega_{nm} t}$$

* We now develop the above in terms of perturbation theory by expanding c_n such that:

$$c_n(t) = c_n^{(0)}(t) + \lambda\, c_n^{(1)}(t) + \ldots$$

Time-Dependent P.T. (cont.)

ex. Exact Solution to a 2-state problem

$$H_0 = E_1|1\rangle\langle 1| + E_2|2\rangle\langle 2|, \quad E_2 > E_1$$
$$V(t) = \gamma e^{i\omega t}|1\rangle\langle 2| + \gamma e^{-i\omega t}|2\rangle\langle 1|$$
$$> H \doteq \begin{bmatrix} E_1 & \gamma e^{i\omega t} \\ \gamma e^{-i\omega t} & E_2 \end{bmatrix}$$

* this system generates the following differential equations

$$i\hbar \frac{d}{dt}(c_1(t)) = V_{12}(t)\, e^{-i(E_2-E_1)t/\hbar} c_2(t)$$
$$i\hbar \frac{d}{dt}[c_2(t)] = V_{21}(t)\, e^{+i(E_2-E_1)t/\hbar} c_1(t)$$

* Assume $c_1(0) = 1$, $c_2(0) = 0$

⇒ we solve this set of eqns by taking a derivative of one equation + substituting it into the other equation, which yields:

$$|c_2(t)|^2 = \frac{\gamma^2/\hbar^2}{\gamma^2/\hbar^2 + (\omega - \omega_{21})^2} \sin^2\left[\left(\frac{\gamma^2}{\hbar^2} + \frac{(\omega-\omega_{21})^2}{4}\right)^{1/2} t\right]$$

$$|c_1(t)|^2 = 1 - |c_2(t)|^2$$

* But realistically, we want to develop an approximation for the above problem

$$\Rightarrow i\hbar \frac{dc_n^{(j)}}{dt} = \sum_m{}' V_{nm}\, e^{i\omega_{nm}t} c_m^{(j-1)}(t)$$

* Now we proceed to develop a proper time evolution operator

$$|\alpha, t_0, t\rangle_I = U_I(t, t_0)|\alpha, t_0; t_0\rangle_I$$

⇒ taking the time derivative yields:

$$i\hbar \frac{d}{dt}\left(U(t,t_0)|\alpha, t_0; t_0\rangle_I\right) = V_I U_I(t,t_0)|\alpha, t_0; t_0\rangle_I$$

$$i\hbar \frac{d}{dt}(U(t,t_0)) = V_I U_I(t,t_0)$$

$$\hookrightarrow U_I(t,t_0) = \mathbb{I} - \frac{i}{\hbar}\int_{t_0}^{t} V_I(t') U_I(t', t_0') dt'$$

* but since most problems aren't directly integerable, we approximate by:

$$U_I(t,t_0) = \mathbb{I} - \frac{i}{\hbar}\int_{t_0}^{t} V_I(t')dt' + \left(\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' V_I(t'') V_I(t') + \ldots$$

Time-Dependent P.T (cont.)

ex. Infinite Perturbation

$$c_n^{(0)} = \delta_{in}$$

$$c_n^{(1)}(t) = \frac{-i}{\hbar}\int_{t_0}^{t} e^{-i\omega_{ni}t'} V_{ni}(t')\,dt' \;; \quad \omega_{ni} = \omega_n - \omega_i \,, \quad E = \hbar\omega$$

⇒ Our initial state becomes

$$|i, 0; t\rangle_I \approx |i\rangle + \sum_n{}' c_n^{(1)}(t)|n\rangle \,, \qquad V = \begin{cases} 0 & t<0 \\ V & t\geq 0 \end{cases}$$

*To solve for probability:

$$P(i\to n) = |c_n^{(1)}(t)|^2$$

$$\hookrightarrow c_n^{(1)}(t) = \frac{V_{ni}}{E_n - E_i}\left(1 - e^{i\omega_{ni}t}\right)$$

$$P(i\to n) = \left|\frac{V_{ni}}{E_n - E_i}\right|^2 \left(2 - 2\cos(\omega_{ni}t)\right)$$

$$= \left|\frac{V_{ni}}{E_n - E_i}\right|^2 \sin^2\left(\frac{(E_n - E_i)t}{2\hbar}\right)$$

⇒ In the case where $E_n \approx E_i$, we see:

$$\sin\left(\frac{(E_n - E_i)t}{2\hbar}\right) \to \frac{(E_n - E_i)t}{2\hbar}$$

$$P \approx \left|\frac{V_{ni}}{E_n - E_i}\right|^2 \frac{(E_n - E_i)^2 t^2}{4\hbar^2}$$

$$\approx \frac{|V_{ni}|^2 t^2}{4\hbar^2}$$

Quantum II Final Exam Study Guide

Basics

$|\alpha\rangle = \sum_i' c_i |a_i\rangle$ and $A|\alpha\rangle = a_i|\alpha\rangle$ (Definition of a ket)

$A = |a\rangle\langle b|$ (Definition of an operator)

$\sum_i' \Lambda_i = \sum_i' |a_i\rangle\langle a_i| = 1$ (Projection Operator/Completeness Relation)

*To get the matrix elements of an operator:

$$A \rightarrow \sum_{m,n}' |m\rangle\langle m|A|n\rangle\langle n|$$

$\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2$ (Schwartz Inequality)

$\langle A\rangle = \langle\alpha|A|\alpha\rangle$ (Expectation Value)

$\Delta A = A - \langle A\rangle \mathbb{I}$ (Dispersion Operator)

$\hookrightarrow \langle(\Delta A)^2\rangle = \langle A^2\rangle - \langle A\rangle^2$ (Avg value or RMS)

$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq \frac{1}{4}|\langle[A,B]\rangle|^2$ (Uncertainty Relation)

*Important Commutation relations include:

$[x_i, x_j] = 0 = [p_i, p_j]$

$[x_i, p_j] = i\hbar\delta_{ij}$

$[x, F(p)] = i\hbar\frac{\partial F}{\partial p}$

$[p, G(x)] = i\hbar\frac{\partial G}{\partial x}$

$[\sigma_i, \sigma_j] = \sigma_k$ where:

$\sigma_x = \begin{bmatrix} 0 & 0 \\ 1 & 1 \end{bmatrix}$, $\sigma_y = \begin{bmatrix} 0 & -i \\ +i & 0 \end{bmatrix}$, $\sigma_z = \begin{bmatrix} 1 & 1 \\ 0 & -1 \end{bmatrix}$

$[A, H] = -i\hbar\frac{\partial A}{\partial t}$ (Heisenberg Eqn of Motion)

*For functions of a continuous variable:

$\psi_a(x') = \langle x'|a\rangle$

$\varphi_b(p') = \langle p'|b\rangle$

$\langle\beta|\alpha\rangle = \int dx'\, \psi_\beta^*(x')\psi_\alpha(x')$

$= \int dp'\, \varphi_\beta^*(p')\varphi_\alpha(p')$

$p = i\hbar\,\partial/\partial x$

$\langle x'|p'\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp[\frac{i}{\hbar}p'\cdot x']$

Basics (cont.)

* Remember, for angular momentum:

  $J \rightarrow$ Arbitrary Angular Momentum (usually refers to total)

  $L \rightarrow$ Orbital Angular Momentum

  $S \rightarrow$ Spin Angular Momentum

* Important angular momentum formulas include:

$$J^2 = J \cdot J = J_x^2 + J_y^2 + J_z^2 \qquad J_\pm = J_x \pm i J_y$$

$$[J^2, J_i] = 0 \qquad [J^2, J_\pm] = 0 = [J_z, J_\pm]$$

$$[J_i, J_j] = i\hbar \epsilon_{ijk} J_k \qquad [J_+, J_-] = 2\hbar J_z$$

$\Rightarrow$ We often write simultaneous eigenkets of J^2, J_z as $|a,b\rangle$ such that:

$$J^2 |a,b\rangle = a|a,b\rangle \qquad J_\pm |a,b\rangle = \sqrt{(j \pm m+1)(j \mp m)}\,\hbar\,|a, b+\hbar\rangle$$

$$J_z |a,b\rangle = b|a,b\rangle \qquad J_\pm^n |a,b\rangle = (b \pm n\hbar)|a, b \pm n\hbar\rangle$$

* When adding angular momentum, it is useful to use direct product notation:

$$|S_1, S_{1z}; S_2, S_{2z}\rangle = |S_1, S_{1z}\rangle \otimes |S_2, S_{2z}\rangle$$

$\Rightarrow$ Our total system operators now become:

$$J = J_1 + J_2 = J_1 \otimes \mathbb{I}_2 + \mathbb{I}_1 \otimes J_2$$

$$J^2 = (J_1 + J_2)\cdot(J_1 - J_2) = J_1^2 + J_2^2 + 2J_1 \cdot J_2$$

$$= J_{1z} + J_{2z} + \tfrac{1}{2}(J_{1+}J_{2-} + J_{1-}J_{2+})$$

* This flexibility allows us to use two sets of kets to describe the system:

$$|j_1, j_2; m_1, m_2\rangle \iff |j_1, j_2; j, m\rangle$$

$$[J_1^2, J_2^2] = [J_{1z}, J_{2z}] = [J_{1i}, J_{2j}] = 0$$

* Use of the Clebsh - Gordon coefficients allow us to relate the two sets of kets to one another (see table)

  $\hookrightarrow$ If calculating by hand, equate states of degeneracy 1 (ie max or min J) and use ladder operators

Tensor Operators

* For Cartesian Tensors, we know they rotate like:

Rank $1 \rightarrow \quad V_i' = R_{ij} V_j$

$2 \rightarrow \quad W = \tilde{R}' \tilde{R}\, V_i U_j$

* Remember, we defined our rotation operator $R(\alpha, \beta, \gamma)$ as:

$$R(\alpha,\beta,\gamma)|j,m\rangle = \sum_{j',m'} |j',m'\rangle\langle j',m'|R(\alpha,\beta,\gamma)|j,m\rangle$$

$$= \mathcal{D}^{(j)}_{mm'}|j',m'\rangle \quad \text{where } j=j' \text{ so } \vec{J} = \text{const.}$$

$\Rightarrow$ Comparing this to our classical picture, we see:

$$\langle\alpha|V_i|\alpha\rangle \rightarrow \langle\alpha|\mathcal{D}^{+}(R)\, V\, \mathcal{D}(R)|\alpha\rangle = \sum_{ji} R_i R_j \langle\alpha|V|\alpha\rangle$$

$$\text{where } \mathcal{D}(R) = \exp\left[\tfrac{i}{\hbar}(J\cdot\hat{n})\,\delta\varphi\right]$$

$\hookrightarrow \sum R_{ij} V_j = \mathcal{D}^{+}(R)\, V_i\, \mathcal{D}(R)$

* Applying our infinitesimal operator, we see

$$V_i' = V_i + \frac{\epsilon}{i\hbar}[V_i, \vec{J}\cdot\hat{n}] = \sum_j R_{ij}(\hat{n},\epsilon)V_j$$

which allows us to deduce the commutation relation:

$$[V_i, J_j] = i\hbar\,\epsilon_{ijk} V_k$$

* A closer examination of rank two tensors reveals they can be decomposed as follows:

$$U_i V_j = \underbrace{\frac{U\cdot V}{3}\delta_{ij}}_{\text{scalar}} + \underbrace{\frac{U_iV_j - U_jV_i}{2}}_{\text{anti-symmetric tensor}} + \underbrace{\left(\frac{U_iV_j + U_jV_i}{2} - \frac{U\cdot V}{3}\delta_{ij}\right)}_{\text{traceless symmetric tensor}}$$

1   3   5

$\Rightarrow$ The circled #'s represent the number of independent componets per term, which happen to match the multiplicity of states for $l = 0, 1, 2, \ldots$ respectively

$\hookrightarrow$ Replacing $\hat{n}$ by $\vec{v}$ in our definition of spherical tensors, we see:

$$T_q^{(k)} = Y_{l=k}^{m=q}(\vec{v})$$

ex. $\quad Y_1^0 = \sqrt{\frac{3}{4}}\cos\theta = \sqrt{\frac{3}{4}}\, V_z$

$$Y_1^{\pm1} = \sqrt{\frac{3}{8\pi}}\, e^{\pm i\varphi}\cos\theta = \sqrt{\frac{3}{2\pi}}\, V_x \pm iV_y$$

Tensor Operators (cont.)

* To derive the transformation properties, we return to our definition of the spherical harmonics

$$Y_\ell^m(\hat{n}) = \langle \hat{n} | \ell, m \rangle$$

⇒ Remembering $|n'\rangle = \mathcal{D}(R)|n\rangle \Leftrightarrow \langle n'| = \langle n|\mathcal{D}(R^{-1})$, we see our angular momentum kets transform as:

$$\mathcal{D}(R^{-1})|\ell, m\rangle = \sum_{m'} |\ell, m'\rangle\langle \ell, m'|\mathcal{D}(R^{-1})|\ell, m\rangle$$

$$= \sum_{m'} |\ell, m'\rangle \mathcal{D}_{mm'}^{(\ell)}(R^{-1})$$

* Applying $\langle n|$ to both sides of the equation

$$\langle n|\mathcal{D}(R^{-1})|\ell, m\rangle = \sum_{m'} \langle n|\ell, m'\rangle \mathcal{D}_{mm'}^{(\ell)}(R^{-1})$$

$$\langle n'|\ell, m\rangle = \sum_{m'} Y_\ell^{m'}(n)\mathcal{D}_{mm'}^{(\ell)}(R^{-1})$$

$$Y_\ell^m(n') = \sum_{m'} Y_\ell^{m'}(n)\mathcal{D}_{mm'}^{(\ell)}(R^{-1})$$

* Now switching to operator formulations:

$$\mathcal{D}^+(R)\, Y_\ell^m(v)\,\mathcal{D}(R) = \sum_{m'} Y_\ell^{m'}(v)\left[\mathcal{D}_{mm'}^{(\ell)}(R)\right]^*$$

* Finally moving to tensor notation:

$$\mathcal{D}^+(R)\, T_q^{(k)}\,\mathcal{D}(R) = \sum_{q'} T_{q'}^{(k)}\left[\mathcal{D}_{qq'}^{(k)}(R)\right]^*$$

* Applying this equation to an infinitesimal rotation:

$$[J\cdot n, T_q^{(k)}] = \sum_{q'} T_{q'}^{(k)} \langle k, q'|J\cdot n|k, q\rangle$$

⇒ Evaluating the above in the $z, \pm$ directions yields:

$$[J_z, T_q^{(k)}] = \hbar q\, T_q^{(k)}$$

$$[J_\pm, T_q^{(k)}] = \hbar\sqrt{(k\mp q)(k\pm q+1)}\; T_{q\pm 1}^{(k)}$$

* We have a theorem that defines spherical tensors in terms of Cartesian tensors:

$$T_q^{(k)} = \sum_{q_1}\sum_{q_2} \underbrace{\langle k_1, k_2; q_1, q_2 | k_1, k_2; k, q\rangle}_{\text{CG coefficient (from table)}} X_{q_1}^{(k_1)} Z_{q_2}^{(k_2)} \quad \text{(irreducable spherical tensors)}$$

Tensor Operators (cont.)

↳ To show our above formula transforms as a spherical tensor:

$$\mathcal{D}^{+}(R)T_q^{(k)}\mathcal{D}(R) = \sum_{q_1 q_2}\langle k_1 k_2; q_1 q_2 | k_1 k_2; k, q\rangle \mathcal{D}^{+}(R) X_{q_1}^{(k_1)}\mathcal{D}(R)\mathcal{D}^{+}(R) Z_{q_2}^{(k_2)}\mathcal{D}(R)$$

$$= \sum_{q_1}\sum_{q_2}\sum_{q_1'}\sum_{q_2'}\langle k_1 k_2; q_1 q_2 | k_1 k_2; k q\rangle X_{q_1'}^{(k_1)}\left[\mathcal{D}_{q_1 q_1'}^{(k_1)}(R)\right]^* Z_{q_2'}^{(k_2)}\left[\mathcal{D}_{q_2 q_2'}^{(k_2)}(R)\right]^*$$

*using $\mathcal{D}_{m_1 m_1'}^{(j_1)}(R)\,\mathcal{D}_{m_2 m_2'}^{(j_2)}(R) = \sum_{j}\sum_{m}\sum_{m'}\langle j_1 j_2, m_1 m_2 | j_1 j_2; j, m\rangle\langle j_1 j_2, m_1' m_2' | j_1 j_2, j, m'\rangle \mathcal{D}_{mm'}^{(j)}$

$$= \sum_{k''}\sum_{q_1}\sum_{q_2}\sum_{q_1'}\sum_{q_2'}\sum_{q'}\sum_{q''}\langle k_1 k_2; q_1 q_2 | k_1 k_2; k q\rangle\langle k_1 k_2, q_1 q_2 | k_1 k_2; k'' q'\rangle\langle k_1 k_2; q_1 q_2 | k_1 k_2; k'' q''\rangle \cdot \left[\mathcal{D}_{q' q''}(R)\right]^* X_{q_1'}^{(k_1)} Z_{q_2'}^{(k_2)}$$

$$= \sum_{q'} T_{q'}^{(k)}\left[\mathcal{D}_{qq'}^{(k)}(R)\right]^*$$

*We can determine the matrix elements of a spherical tensor via <u>Wigner-Eckart Theorem</u>

⇒ Starting from $[J_z, T_q^{(k)}] = \hbar q T_q^{(k)}$

$$\langle \alpha', j', m' | J_z T_q^{(k)} - T_q^{(k)} J_z - \hbar q T_q^{(k)} | \alpha, j, m\rangle = 0$$

$$\langle \alpha', j', m' | m' T_q^{(k)} - T_q^{(k)} m - q T_q^{(k)} | \alpha, j, m\rangle = 0$$

↳ $m' = m + q$ where q is the ang. momentum added by spherical tensor

⇒ We apply the Wigner-Eckart Thm by noting $\langle \alpha', j' m' | T_q^{(k)} | \alpha, j m\rangle$ can be written in terms of a CG coefficient and a reduced matrix element

$$\langle \alpha' j' m' | T_q^{(k)} | \alpha j m\rangle = \langle j k; m q | j k; j' m'\rangle \frac{1}{\sqrt{2j+1}}\langle \alpha' j' \| T_q^{(k)} \| \alpha j\rangle$$

↳ Our general approach is to calculate the reduced matrix element in a simple case then use that result in our case of interest

<u>ex.</u>

$$\langle 3, 0 | T_0^{(2)} | 1, 0\rangle = \langle 1, 2; 0, 0 | 1, 2; 1, 0\rangle\langle 3 \| T^{(2)} \| 1\rangle$$

$$\int Y_3^0(\theta,\varphi) Y_2^0(\theta,\varphi) Y_1^0(\theta,\varphi)\, d\Omega = \langle 1, 2; 0, 0 | 1, 2; 1, 0\rangle\langle 3 \| T^{(2)} \| 1\rangle$$

↳ $\langle 3 \| T^{(2)} \| 1\rangle = \sqrt{\frac{3}{4\pi}}$

Perturbation Theory

* Perturbation theory is an approximation technique that allows us to solve non-idealized problems in quantum mechanics and other fields

* In the case of time-independent, non-degenerate perturbations:

⇒ For a given Hamiltonian, we write it as:

$$H = H_0 + V, \quad \text{where the solutions to } H_0 \text{ are known, but not for } V$$

ex. Two State System

↳ $H = E_1^{(0)} |1^{(0)}\rangle\langle 1^{(0)}| + E_2^{(0)} |2^{(0)}\rangle\langle 2^{(0)}| + \lambda V_{12} |1^{(0)}\rangle\langle 2^{(0)}| + \lambda V_{21} |2^{(0)}\rangle\langle 1^{(0)}|$

$$\doteq \begin{bmatrix} E_1 & \lambda V_{12} \\ \lambda V_{21} & E_2 \end{bmatrix}; \quad V_{12} = V_{21}, \quad V_{12}, V_{21} \in \mathbb{R} \text{ for Hermiticity}$$

⇒ From normal matrix operations, we see:

$$E_1 = \tfrac{1}{2}(E_1^{(0)} + E_2^{(0)}) + \sqrt{\tfrac{1}{4}(E_1^{(0)} - E_2^{(0)}) + \lambda^2 V_{12}^2}$$

$$E_2 = \tfrac{1}{2}(E_1^{(0)} + E_2^{(0)}) - \sqrt{\tfrac{1}{4}(E_1^{(0)} - E_2^{(0)}) + \lambda^2 V_{12}^2}$$

⇒ However, if we are unable to find an exact solution, we proceed as follows:

↳ We know: $H_0 |n\rangle = E_n^{(0)} |n\rangle$

$$(H_0 + \lambda V)|n\rangle = E_n |n\rangle$$

⇒ If we define $\Delta_n = E_n - E_n^{(0)}$

↳ $E_n^{(0)} - H_0 |n\rangle = \lambda V - \Delta_n |n\rangle$

$$\langle n^{(0)}| E_n^{(0)} - H_0 |n\rangle = \langle n^{(0)} | \lambda V - \Delta_n |n\rangle$$

$$0 = \langle n^{(0)} | \lambda V - \Delta_n |n\rangle$$

* Now defining the projection operator: $\varphi_n = \mathbb{I} - |n^{(0)}\rangle\langle n^{(0)}|$

$$= \sum_{k \neq n} |k^{(0)}\rangle\langle k^{(0)}|$$

↳ $|n\rangle = \frac{1}{E_n^{(0)} - H_0} \varphi_n (\lambda V - \Delta_n)|n\rangle$

* but as $\lambda \to 0$, we must approach $H^{(0)} |n^{(0)}\rangle = E_n^{(0)} |n\rangle$

Perturbation Theory (cont.)

$\Rightarrow$ We redefine $|n\rangle$ as:

$$|n\rangle = c_n(\lambda)|n^{(0)}\rangle + \frac{1}{E_n^{(0)}-H_0}\varphi_n(\lambda V - \Delta_n)|n\rangle \,, \quad c_n(\lambda) = \langle n^{(0)}|n\rangle$$

*Note: Since we choose $\langle n^{(0)}|n\rangle = 1$, we must always normalize $|n\rangle$ after we solve for it

$\hookrightarrow$ $$\boxed{|n\rangle = |n^{(0)}\rangle + \frac{1}{E_n^{(0)}-H_0}\varphi_n(\lambda V - \Delta_n)|n\rangle}$$

*If we multiply both sides by $\langle n^{(0)}|$, we can extract Δ_n

$$\boxed{\Delta_n = \lambda\langle n^{(0)}|V|n\rangle}$$

*Now if we expand both $|n\rangle$ and Δ_n in power series:

$$|n\rangle = |n^{(0)}\rangle + \lambda|n^{(1)}\rangle + \lambda^2|n^{(2)}\rangle + \dots$$

$$\Delta_n = \lambda\Delta_n^{(1)} + \lambda^2\Delta_n^{(2)} + \dots$$

*Substituting these into our above equations + matching powers of λ:

$$\Delta_n^{(1)} = \langle n^{(0)}|V|n^{(0)}\rangle$$

$$\Delta_n^{(2)} = \langle n^{(0)}|V|n^{(1)}\rangle = \sum_{k\neq n}' \frac{|V_{nk}|^2}{(E_n^{(0)}-E_k^{(0)})^2}$$

$$|n^{(1)}\rangle = \frac{1}{E_n^{(0)}-H_0}\varphi_n|n^{(0)}\rangle = \sum_{k\neq n}' \frac{V_{kn}}{E_n^{(0)}-E_k^{(0)}}|k^{(0)}\rangle$$

*Proceeding to the <u>time-independent, degenerate</u> perturbation case:

$\Rightarrow$ Simply put we must diagonalize the degenerate submatrix however possible

$\hookrightarrow$ For our degenerate energies, our eigenkets become:

$$|l^{(0)}\rangle = \sum_{m\in D}' |m^{(0)}\rangle\langle m^{(0)}|l^{(0)}\rangle$$

$\hookrightarrow$ To solve the eigenvalue equation ($H = H_0 + V$):

$$(E - H_0 - V)|l\rangle = 0$$

$\hookrightarrow$ We isolate the degenerate/non-degenerate spaces with:

$$\tilde{P}_0 = \sum_{k\in D}' |k^{(0)}\rangle\langle k^{(0)}| \qquad \tilde{P}_1 = \sum_{k\notin D}' |k^{(0)}\rangle\langle k^{(0)}| = \tilde{\mathbb{I}} - \tilde{P}_0$$

Perturbation Theory (cont.)

$\Rightarrow$ We can now rewrite the eigenvalue equation as:

$$(E - H_0 - \lambda V) P_0 |\ell\rangle + (E - H_0 - \lambda V) P_1 |\ell\rangle = 0$$

* Applying the projection operators to the above equation yields:

① $(E - H_0 - \lambda V)\hat{P}_0^2 |\ell\rangle + (E - H_0 - \lambda V) P_0 P_1 |\ell\rangle = 0$

* using $P_0 P_0 = 1$, $P_0 P_1 = 0$

$$(E - E_D^{(0)} - \lambda P_0 V) P_0 |\ell\rangle - \lambda P_0 V P_1 |\ell\rangle = 0$$

② $-\lambda P_1 V P_0 |\ell\rangle + (E - H_0 - \lambda P_1 V) P_1 |\ell\rangle = 0$

* Solving the above system of equations yields:

$$|\ell\rangle = \lambda[E - H_0 - \lambda P_1 V P_1]^{-1} P_1 V P_0 |\ell\rangle$$

$\hookrightarrow P_1 |\ell\rangle = \tilde{P}_1 \dfrac{\lambda}{E - H_0 - \lambda P_1 V P_1} P_1 V P_0 |\ell\rangle$

* expanding $|\ell\rangle$ as a power series and $\dfrac{1}{E - H_0 - \lambda P_1 V P_1} \approx \dfrac{1}{E - H_0} + \dfrac{\lambda P_1 V P_1}{(E - H_0)^2} + \ldots$

$$\Rightarrow P_1 |\ell^{(1)}\rangle = \sum_{k \notin D} \frac{V_{k\ell}}{E_D^{(0)} - E_k^{(0)}} |k^{(0)}\rangle$$

ex. Linear Stark Effect

* Our physical set-up is a hydrogen like atom in a uniform $\vec{E}$-field

$\hookrightarrow V = -ezE_0$; $\quad n = N + \ell + 1$, where $n \in \mathbb{Z}^+$, $\ell \in [0, n-1]$, $N \in \{0, \mathbb{Z}^+\}$

$\Longrightarrow H|n\ell m\rangle = E_n |n\ell m\rangle \qquad L_z |n\ell m\rangle = m\hbar |n\ell m\rangle$

$L^2 |n\ell m\rangle = \ell(\ell+1)\hbar^2 |n\ell m\rangle \qquad \Pi |n\ell m\rangle = (-1)^\ell |n\ell m\rangle$ (Parity)

* Remember, in terms of spherical tensors: $z = \hat{T}_0^{(1)}$

$\hookrightarrow \langle n, \ell' m' | T_0^{(1)} | n\ell m\rangle \rightarrow m = m'$ b/c no addition of ang. momentum

$\ell' \in [\ell+1, |\ell-1|]$

* Notice that: $\Pi^\dagger z \Pi = -z$

$\hookrightarrow \langle \text{odd} | z | \text{even}\rangle = \langle \text{odd} | \Pi^\dagger \Pi z \Pi^\dagger \Pi | \text{even}\rangle$

$= \langle \text{odd} | z | \text{even}\rangle$

$\left.\begin{array}{l}\langle \text{odd} | z | \text{odd}\rangle = -\langle \text{odd} | z | \text{odd}\rangle \\ \langle \text{even} | z | \text{even}\rangle = -\langle \text{even} | z | \text{even}\rangle\end{array}\right\}$ must equal 0

$\Longrightarrow$ From this we see $\ell' = \ell \pm 1$ and that we can now write out the interaction matrix

Perturbation Theory (cont.)

ex. Linear Stark Effect (cont.)

$$\Rightarrow V \doteq \begin{bmatrix} 0 & \langle 200|V|210\rangle \\ \langle 210|V|200\rangle & 0 \end{bmatrix} = \begin{bmatrix} 0 & 3ea_0E_0 \\ 3ea_0E_0 & 0 \end{bmatrix} \quad \text{for } n=2,\ \ell=0,1$$

↳ via diagonalization:

$$|+\rangle = \frac{1}{\sqrt{2}}(|200\rangle + |210\rangle) \qquad \Delta_+^{(1)} = 3ea_0E_0$$

$$|-\rangle = \frac{1}{\sqrt{2}}(|200\rangle - |210\rangle) \qquad \Delta_-^{(1)} = -3ea_0E_0$$

⇒ Further corrections to H-atom from perturbation theory include:

① "Relativistic Correction"

$$E = \sqrt{(pc)^2 + m^2c^4}$$

$$T = \sqrt{(pc)^2 + m^2c^4} - m_ec^2$$

$$= mc^2\left(1 + \frac{(pc)^2}{m^2c^4}\right)^{1/2} - m_ec^2$$

$$\hookrightarrow T \approx \frac{p^2}{2m} - \frac{p^4}{8m_e^3c^2} \leftarrow \text{becomes interaction term in perturbed Hamiltonian}$$

$$\Rightarrow H = \frac{p^2}{2m} - \frac{e^2}{r} - \frac{p^4}{8m_e^3c^2}$$

* But since $[L, p^2] = 0$, we can proceed via non-degenerate P.T b/c perturbation doesn't break the degeneracy

$$\hookrightarrow \Delta_{n\ell}^{(1)} = \langle n\ell m|\frac{-p^4}{8m_e^3c^2}|n\ell m\rangle$$

$$\text{* but } \frac{1}{2mc^2}\left(\frac{p^2}{2m}\right)^2 = \frac{p^4}{8m_e^3c^2} = \frac{1}{2mc^2}\left(H_0 + \frac{e^2}{r}\right)^2$$

$$= \left[\langle n\ell m|\frac{e^4}{r^2}|n\ell m\rangle + 2E_n^{(0)}\langle n\ell m|\frac{e^2}{r}|n\ell m\rangle + \left(E_n^{(0)}\right)^2\right] \cdot \frac{1}{2mc^2}$$

$$= \frac{-1}{2}mc^2\alpha^4\left(\frac{-3}{4n^2} - \frac{1}{n^3(\ell+\frac{1}{2})}\right)$$

$$= \frac{-mc^2\alpha^2}{2n^2}\left(\alpha^2\left[\frac{-3}{4} + \frac{1}{n(\ell+\frac{1}{2})}\right]\right)$$

② Spin-Orbit Coupling

$$\vec{B} = \frac{-\vec{v}}{c} \times \vec{E}, \quad \vec{\mu} = \frac{e\vec{S}}{m_ec} \quad (\vec{S} = \text{spin vector})$$

$$H_{LS} = -\vec{\mu} \cdot B$$

$$= \frac{eS}{m_ec}\left(\frac{v}{c} \times \frac{\vec{r}}{r}\frac{dV_c}{dr}\left(\frac{-1}{e}\right)\right) \qquad \text{* } V_c = \text{central potential}$$

$$= \frac{eS}{m_ec}\left[\frac{p}{m_ec} \times \frac{\vec{r}}{r}\frac{dV_c}{dr}\left(\frac{-1}{e}\right)\right] = \frac{1}{m_e^2c^2r}\frac{dV_c}{dr}\vec{L}\cdot\vec{S}$$

Perturbation Theory (cont.)

* Rewriting $L\cdot S$ as $J^2 = (L+S)^2$

  ↳ $L\cdot S = \frac{1}{2}(J^2 - L^2 - S^2)$

* Introducing the spin-angular functions

$$\mathcal{Y}_{\ell}^{j=\ell+1/2} \equiv \frac{1}{\sqrt{2\ell+1}}\begin{bmatrix} \pm\sqrt{\ell\pm m+1/2}\; Y_{\ell}^{m-1/2}(\theta,\varphi) \\ \sqrt{\ell\mp m+1/2}\; Y_{\ell}^{m+1/2}(\theta,\varphi)\end{bmatrix}$$ * Note: $m = m_\ell + m_s$

$= (\;)Y_\ell^m \chi^+ + (\;)Y_\ell^m\chi^-$, where $\chi^\pm$ are spinor states

$\Rightarrow \Delta_{n\ell}^{(1)} = \frac{1}{2m_e^2c^2}\langle \frac{1}{r}\frac{dV_c}{dr}\rangle_{n\ell}\frac{\hbar}{2}\left\{\begin{matrix}\ell \\ -\ell+1\end{matrix}\right\}$ for $j = \ell+1/2$, $= \ell - 1/2$ (choose a j)

where $\frac{1}{2}\int \mathcal{Y}^{+}(J^2-L^2-S^2)\mathcal{Y}\,d\Omega = \frac{\hbar^2}{2}[j(j+1)-\ell(\ell+1)-s(s+1)](\;)$ is used in the expectation value calculation

$\Rightarrow$ In H-atom: $V_c = \frac{e^2}{r} \rightarrow \langle\frac{1}{r}\frac{dV}{dr}\rangle = \langle\frac{e^2}{r^3}\rangle$

$$= \frac{-2m_e^2c^2\alpha^2}{n\ell(\ell+1)(\ell+1/2)\hbar^2}$$

* Now considering a <u>time-dependent</u> perturbation such that:

$H = H_0 + V(t)$ $\Rightarrow$ Note: Our normal time evolution operator $U(t,t_0) = \exp[\frac{-i}{\hbar}Ht]$ only works when H is time independent

$\Rightarrow$ We must develop the interaction picture

$|\alpha\rangle = \sum_n' c(0)|n\rangle$; $c(0) = \langle n|\alpha\rangle|_{t=0}$

$|\alpha, t_0=0, t\rangle = \sum_n' c_n(t)\exp[-iE_nt/\hbar]|n\rangle \rightarrow c_n(t)$ only associated w/ V

↳ $c_n \rightarrow 0$ yields normal evolution

$\Rightarrow |\alpha, t_0; t\rangle_I = e^{iH_0t/\hbar}|\alpha, t_0; t\rangle_S$ (time evolve only unperturbed Hamiltonian)

* Operators now transform as: $\hat{A}_I = e^{+iH_0t/\hbar}\hat{A}_S e^{-iH_0t/\hbar}$

↳ $i\hbar\frac{\partial}{\partial t}|\alpha, t_0; t\rangle_I = i\hbar\frac{\partial}{\partial t}(e^{iH_0t/\hbar}|\alpha, t_0; t\rangle_S)$

$$= i\hbar\frac{H_0}{-i\hbar}e^{iH_0t/\hbar}|\alpha, t_0; t\rangle_S + i\hbar e^{iH_0t/\hbar}(\frac{\partial}{\partial t}|\alpha, t_0; t\rangle_S)$$

$$= -H_0 e^{iH_0t/\hbar}|\alpha, t_0; t\rangle_S + e^{iH_0t/\hbar}(H_0 + V(t))|\alpha, t_0; t\rangle_S$$

$$= e^{iH_0t/\hbar}V(t)e^{-iH_0t/\hbar}e^{iH_0t/\hbar}|\alpha, t_0; t\rangle_S$$

$$= V_I(t)|\alpha, t_0; t\rangle_I$$

Perturbation Theory (cont.)

* we convert the above equation to a # by multiplying both sides by $\langle n|$

$$\Rightarrow i\hbar \frac{\partial}{\partial t}\langle n|\alpha, t_0; t\rangle_I = \langle n|V_I|\alpha, t_0; t\rangle_I$$

$$i\hbar \frac{\partial}{\partial t} c_n(t) = \sum_m{}' \langle n|V_I|m\rangle\langle m|\alpha, t_0; t\rangle_I$$

$$= \sum_m{}' V_{nm}\, c_m(t)\, e^{i\omega_{nm}t}$$

* If we now expand c_n in a power series to develop perturbation theory

$$c_n(t) = c_n^{(0)}(t) + \lambda c_n^{(1)}(t) + \ldots$$

ex. Exact Solution to a 2 state problem

$$H_0 = E_1|1\rangle\langle 1| + E_2|2\rangle\langle 2|, \quad E_2 > E_1$$

$$V(t) = \gamma e^{i\omega t}|1\rangle\langle 2| + \gamma e^{-i\omega t}|2\rangle\langle 1| \quad > \quad H \doteq \begin{bmatrix} E_1 & \gamma e^{i\omega t} \\ \gamma e^{-i\omega t} & E_2 \end{bmatrix}$$

* From the above system we get the following differential equations:

$$i\hbar\frac{\partial}{\partial t} c_1(t) = V_{12}(t)\, e^{-i(E_2-E_1)t/\hbar} c_2(t) \qquad \text{* Assume } c_1(0) = 1$$

$$i\hbar\frac{\partial}{\partial t} c_2(t) = V_{21}(t)\, e^{+i(E_2-E_1)t/\hbar} c_1(t) \qquad c_2(0) = 0$$

$\Rightarrow$ we solve this system by taking the derivative of one equation and substituting it into the other, yielding:

$$|c_2(t)|^2 = \frac{\gamma^2/\hbar^2}{\gamma^2/\hbar^2 + (\omega-\omega_{21})^2}\sin^2\left[\left(\frac{\gamma^2}{\hbar^2} + \frac{(\omega-\omega_{21})^2}{4}\right)^{1/2} t\right]$$

$$|c_1(t)|^2 = 1 - |c_2(t)|^2$$

* But we really want an approximation technique for this problem

$$\Rightarrow i\hbar \frac{dc_n^{(j)}}{dt} = \sum_m{}' V_{nm}\, e^{i\omega_{nm}t}\, c_m^{(j-1)}(t)$$

* We now must develop a proper time evolution operator

$\hookrightarrow |\alpha, t_0; t\rangle_I = U_I(t, t_0)|\alpha, t_0; t\rangle_I$

* if we take the time derivative of the above equation:

$$i\hbar\frac{\partial}{\partial t}\left(U_I(t,t_0)|\alpha, t_0; t\rangle_I\right) = V_I\, U_I(t,t_0)|\alpha, t_0; t\rangle_I$$

$$i\hbar\frac{\partial}{\partial t} U(t,t_0) = V_I\, U_I(t,t_0)$$

$$\hookrightarrow U_I(t,t_0) = \mathbb{I} - \frac{i}{\hbar}\int_{t_0}^{t} V_I(t')\, U_I(t', t_0)\, dt'$$

* but since most problems aren't directly integerable, we approximate by

$$U_I(t,t_0) = \mathbb{I} - \frac{i}{\hbar}\int_{t_0}^{t} V_I(t')\,dt' + \left(\frac{i}{\hbar}\right)^2\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, V_I(t')\, V_I(t'') + \ldots$$

Quantom Qualifier Breakdown

January 2008
Q1: Infinite Square Well, Schrödingers Eqn, Spin 1/2 Particles
Q2: SHO, Expectation value, uncertainty relation
Q3: Variational Principle
Q4: Hermitian Operators, Probabilities,
Q5: Infinite Square Well, Perturbation Theory
Q6: Central Potential, Hydrogen Atom, Schrödingers Eqn

August 2008
Q1: 3-D Spherical Well, Schrödingers Eqn
Q2: Perturbation Theory, Degenerate Perturbation Theory
Q3: SHO; Schrödinger Eqn, Ladder Operators
Q4: Infinite Square Well, Probabilities, Perturbation Theory (Widening box)
Q5: Time Evolution, Schrödinger Eqn
Q6: Hydrogen Atom, Expectation value, Angular Momentum

January 2009
Q1: Spin 1/2 Particles, Spinors, Expectation Value, probabilities
Q2: Perturbation Theory
Q3: 2-D well, Schrödinger Eqn,
Q4: Angular Momentum, Clebsh-Gordon Coefficients, Spin Scattering?
Q5: Probabilities, Time Evolution
Q6: Hydrogen Atom, Angular Momentum

August 2009
Q1: Step Potential, Schrödingers Eqn, Probability
Q2: Variational Method, Expectation Value
Q3: Eigenvalue/Eigenvectors, Perturbation Theory
Q4: Central Potential, Angular Momentum
Q5: Infinite Square Well, Identical Particles
Q6: Spin 1/2 Particles, Time Evolution, Probabilities

January 2010

Q1: δ-Function Potential, Schrödinger Eqn, expectation value
Q2: Hydrogen Atom, Probability, Uncertainty principle
Q3: Time-Dependent Perturbation Theory,
Q4: Spin 1/2 Particles, Probability, Time Evolution
Q5: Two-level system, Coupling
Q6: Hyperfine Splitting, e^- & p^+ spin

August 2010

Q1: Step Potential, Zero-Potential, Probability
Q2: SHO, Ladder Operators, Uncertainty principle, multiple particles, degeneracy
Q3: Dirac Formalism, Matrix Mechanics
Q4: 3-D SHO, Perturbation Theory
Q5: Hydrogen Atom, Variational Method, Expectation value
Q6: Step Potential, Gamow Factor

August 2011

Q1: Completeness Relation, Probability, Time Evolution, Schrödinger Picture, Heisenberg Picture
Q2: SHO, Probability, Parity?
Q3: Angular Momentum, Probability
Q4: Spin System, Spin 1/2 Particles, Probability
Q5: Perturbation Theory, Infinite Square Well
Q6: Variational Method, SHO, Matrix Mechanics

January 2012

Q1: Stationary States, Time Evolution, Probability, Uncertainty principle
Q2: Dirac Notation, Hermitian Operators
Q3: SHO, Schrödinger Eqn, Expectation Value
Q4: Angular Momentum, Hydrogen Atom, Hyperfine splitting
Q5: Interaction Picture, Schrödinger Eqn
Q6: Perturbation Theory, SHO

August 2012

Q1: Matrix Manipulation, Time Evolution

Q2: Spin 1/2 Particles; Uncertainty Principle

Q3: Spin 1/2 Particles, Clebsh-Gordon Coefficients, Coupling

Q4: Hydrogen-like Atom, Perturbation Theory, Probability

Q5: SHO, Time-dependent Perturbation Theory

Q6: Time Evolution, Expectation Value

January 2013:

Q1: δ-Function Potential, Scattering, Schrödinger Eqn

Q2: Scattering, Born Approx,

Q3: Spin 1/2 Particles, Matrix Manipulation, Expectation value, Probability

Q4: SHO, Ladder operators

Q5: Infinite Square Well, Perturbation Theory,

Q6: 3-D Well, Schrödinger Eqn

August 2013:

Q1: Infinite Square Well, Schrödinger Eqn, Box Expansion

Q2: Angular Momentum, Ladder Operators,

Q3: Step Potential, Scattering, Schrödinger Eqn

Q4: Hydrogen Atom, Probabilities

Q5: Matrix Manipulation, Perturbation Theory

Q6: SHO, Perturbation Theory, Time Evolution, Time Dependent Perturbation Theory

January 2014:

Q1: Schrödinger Eqn, Angular Momentum, Perturbation Theory

Q2: Infinite Square Well, Schrödinger Eqn, Probability

Q3: Matrix Manipulation, Probability

Q4: Clebsh-Gordon Coefficients, Angular Momentum

Q5: Zeeman Splitting, Hydrogen Atom

Q6: SHO, Perturbation Theory

August 2014:

Q1: Schrödinger Eqn, Expectation Values, SHO, Uncertainty principle

Q2: Spin 1/2 Particles, Angular Momentum, Ladder Operators

Q3: SHO, Perturbation Theory, Probability

Q4: Identical Particles, Infinite Square Well, Spin 1/2 Particles

Q5: Angular Momentum, Expectation Value

Q6: Variational Method

January 2015:

Q1: SHO, Ladder operators

Q2: Hydrogen Atom, Angular Momentum, Time Evolution, Probability, Expectation Value

Q3: Step Potential, Schrödinger Eqn, Infinite Square Well

Q4: Matrix Manipulation, Time Evolution

Q5: Interaction Picture

Q6: 2-D Well, Perturbation Theory

August 2015:

Q1: Step Potential, Scattering, Probability Current

Q2: Confined Harmonic Oscillator, Angular Momentum

Q3: Matrix Manipulation

Q4: Infinite Square Well, Well Expansion, Probability

Q5: SHO, Perturbation Theory

Q6: Hydrogen Atom, Expectation Value, Probability

January 2016:

Q1: Clebsh-Gordon Coefficients, Spinor States, Probability

Q2: SHO, Perturbation Theory, Parity

Q3: Identical Particles, Infinite Square Well, Spin 1/2 Particles

Q4: Matrix Manipulation, Time Evolution

Q5: Spin 1/2 Particles, Spinor States, Time Evolution, Probability

Q6: Finite Square Well, Schrödinger Eqn, Scattering

Jan 2008

Problem 1: The Infinite Square Well: (10 Points)

A single particle is in a one dimensional infinitely deep potential well of width L where $V(x)$ is given by:

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

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

2. Sketch the wave functions for the first three stationary states for this potential. **(2 Points)**

3. Now, if four spin-1/2 identical particles of mass m are placed in this potential, calculate the three lowest values for the total energy of the system of particles. **(3 Points)**

4. Determine the degeneracy for each of the three energy states found in part 3. **(3 Points)**

Jan 2008

Quantum #1

a) $H\psi = E\psi$

$$\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + 0(\psi) = E\psi$$

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

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

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

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

* We know that $\psi(0) = \psi(L) = 0$

$$\hookrightarrow \; 0 = A\cancel{\sin(k\cdot 0)} + B\cos(k\cdot 0)$$

$$0 = B$$

$\Rightarrow \psi(x) = A\sin(kx)$; for this to be 0 at $x = L$, $kx = n\pi \Rightarrow k_n = \frac{n\pi}{L}$

$$\hookrightarrow \psi(x) = A\sin\left(\frac{n\pi x}{L}\right)$$

* Normalizing the wave function, we see:

$$1 = \int_{-\infty}^{\infty} \left|A\sin\left(\frac{n\pi x}{L}\right)\right|^2 dx$$

$$1 = A^2\int_0^L \sin^2\left(\frac{n\pi x}{L}\right)dx$$

$$1 = A^2\cdot\frac{L}{2}$$

$$\hookrightarrow A = \sqrt{\frac{2}{L}} \quad \Rightarrow \boxed{\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)}$$

* Returning to k_n:

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

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

$$\hookrightarrow \boxed{E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}}, \quad n \in \mathbb{Z}^+ \text{ for non-trivial solutions}$$

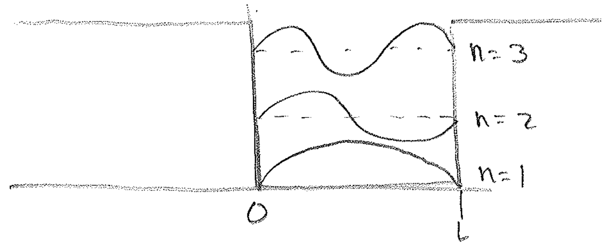
#1 (cont.)

b) $\psi_1 = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right)$

$\psi_2 = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right)$

$\psi_3 = \sqrt{\frac{2}{L}} \sin\left(\frac{3\pi x}{L}\right)$

$\infty = V(x)$



c) * Since spin-½ particles are fermions, no more than one particle can occupy a single state

↳ $E_{sys} = \dfrac{(n_1^2 + n_2^2 + n_3^2 + n_4^2)\pi^2\hbar^2}{2mL^2}$

$\Rightarrow$ our lowest energy configurations are:

$n = \{1, 2, 3, 4\}$, $E_{sys} = \dfrac{30\pi^2\hbar^2}{2mL^2}$

$n = \{1, 2, 3, 5\}$, $E_{sys} = \dfrac{39\pi^2\hbar^2}{2mL^2}$

$n = \{1, 2, 4, 5\}$ $E_{sys} = \dfrac{46\pi^2\hbar^2}{2mL^2}$

(1)(2) (4) (5)
1+4+16+25 = 46

(1) (2) (3) (6)
1 + 4 + 9 + 36 = 50

d) Each state has 4! degeneracies, 24 overall for each state

Jan 2006

Problem 2: The Harmonic Oscillator (10 Points):

The normalized wave functions for the one-dimensional quantum harmonic oscillator can be written as,

$$\Psi_n(x) = \left(\frac{\sqrt{\alpha}}{2^n n! \sqrt{\pi}}\right)^{1/2} e^{-\alpha x^2/2} H_n(\sqrt{\alpha} x),$$

where n is the principle quantum number of the oscillator, H_n is the n^{th} order Hermite polynomial, $\alpha = \omega m/\hbar$, ω is the oscillator frequency, and m is its mass. The following equations may be useful,

$$H_{n+1}(q) + 2nH_{n-1}(q) - 2qH_n(q) = 0$$

$$\frac{dH_n(q)}{dq} = 2nH_{n-1}(q)$$

and

$$\begin{aligned} \langle H_n | qH_{n+1} \rangle &= 2^n (n+1)! \sqrt{\pi} \\ \langle H_n | qH_n \rangle &= 0 \\ \langle H_n | qH_{n-1} \rangle &= 2^{n-1} n! \sqrt{\pi} \end{aligned}$$

1. Calculate the expectation value of x and x^2 for the n^{th} state of the harmonic oscillator, where x is the position. **(2 Points)**

2. Calculate the expectation value of p and p^2 for the n^{th} state of the harmonic oscillator, where p is the momentum. **(2 Points)**

3. Calculate Δx and Δp for the n^{th} state. What is the uncertainty product $(\Delta x \Delta p)$ for the oscillator? **(2 Points)**

4. Calculate the expectation value of the kinetic energy and the potential energy of the n^{th} state of the oscillator. Show that the sum of the expectation value of the kinetic and potential energies are equal to the total energy of the n^{th} state. **(2 Points)**

5. How does the uncertainty principle relate to the fact that the energy is not zero in the ground state? Explain and interpret your answer to receive credit. **(2 Points)**

Jan 2008

Quantom #2

a) Given: $\Psi_n(x) = \left(\frac{\sqrt{\alpha}}{2^n n! \sqrt{\pi}}\right)^{1/2} \exp\left[-\frac{1}{2}\alpha x^2\right] H_n(\sqrt{\alpha}\, x)$

Find: $\langle x \rangle_n$, $\langle x^2 \rangle_n$

* Using raising/lowering operators, we know:

$$x = \sqrt{\frac{\hbar}{2m\omega}}\,(a + a^+) \qquad a|\Psi_n\rangle = \sqrt{n}\,|\Psi_{n-1}\rangle \qquad \langle \Psi_n | \Psi_m \rangle = \delta_{mn}$$

$$p = -i\sqrt{\frac{\hbar m\omega}{2}}\,(a - a^+) \qquad a^+|\Psi_n\rangle = \sqrt{n+1}\,|\Psi_{n+1}\rangle$$

$$\Rightarrow \langle x \rangle_n = \langle \Psi_n | x | \Psi_n \rangle$$

$$= \langle \Psi_n | \sqrt{\frac{\hbar}{2m\omega}}\,(a + a^+) | \Psi_n \rangle$$

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

$$= \sqrt{\hbar/2m\omega}\left[\langle \Psi_n | \sqrt{n} | \Psi_{n-1} \rangle + \langle \Psi_n | \sqrt{n+1} | \Psi_{n+1} \rangle\right]$$

$$= 0$$

$$\langle x^2 \rangle_n = \langle \Psi_n | x^2 | \Psi_n \rangle$$

$$= \langle \Psi_n | \left(\frac{\hbar}{2m\omega}\right)(aa + aa^+ + a^+a + a^+a^+) | \Psi_n \rangle$$

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

$$= \frac{\hbar}{2m\omega}\left[\langle \Psi_n | \sqrt{n}\sqrt{n-1} | \Psi_{n-2} \rangle + \langle \Psi_n | \sqrt{n+1}\sqrt{n+1} | \Psi_n \rangle + \langle \Psi_n | \sqrt{n}\sqrt{n} | \Psi_n \rangle + \langle \Psi_n | \sqrt{n+1}\sqrt{n+2} | \Psi_{n+2} \rangle\right]$$

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

b) Similarly to above:

$$\langle p \rangle_n = \langle \Psi_n | p | \Psi_n \rangle$$

$$= \langle \Psi_n | -i\sqrt{\frac{\hbar m\omega}{2}}(a - a^+) | \Psi_n \rangle$$

$$= -i\sqrt{\frac{\hbar m\omega}{2}}\left[\langle \Psi_n | a | \Psi_n \rangle - \langle \Psi_n | a^+ | \Psi_n \rangle\right]$$

$$= -i\sqrt{\frac{\hbar m\omega}{2}}\left[\langle \Psi_n | \sqrt{n} | \Psi_{n-1} \rangle - \langle \Psi_n | \sqrt{n+1} | \Psi_{n+1} \rangle\right]$$

$$= 0$$

#2 (cont.)

b) $\langle p_n^2 \rangle = \langle \psi_n | p^2 | \psi_n \rangle$

$$= \langle \psi_n | -\frac{\hbar m\omega}{2}(aa - aa^\dagger - a^\dagger a + a^\dagger a^\dagger) | \psi_n \rangle$$

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

$$= -\frac{\hbar m\omega}{2}\left[\langle \psi_n | \sqrt{n-1}\sqrt{n} | \psi_{n-2} \rangle - \langle \psi_n | \sqrt{n+1}\sqrt{n+1} | \psi_n \rangle - \langle \psi_n | \sqrt{n}\sqrt{n} | \psi_n \rangle + \langle \psi_n | \sqrt{n+2}\sqrt{n+1} | \psi_{n+2} \rangle\right]$$

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

c) Generally $\Delta A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}$

$$\Rightarrow \Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\frac{\hbar}{2m\omega}[2n+1] - 0^2} = \sqrt{\frac{\hbar}{2m\omega}[2n+1]}$$

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{\frac{\hbar m\omega}{2}[2n+1] - 0^2} = \sqrt{\frac{\hbar m\omega}{2}(2n+1)}$$

$$\Rightarrow \Delta x \Delta p = \sqrt{\frac{\hbar}{2m\omega}[2n+1]}\sqrt{\frac{\hbar m\omega}{2}[2n+1]} = \frac{\hbar}{2}[2n+1]$$

d) $\langle T \rangle = \langle \psi_n | T | \psi_n \rangle = \langle \psi_n | \frac{p^2}{2m} | \psi_n \rangle = \frac{\hbar\omega}{4}[2n+1]$

$\langle U \rangle = \langle \psi_n | U | \psi_n \rangle = \langle \psi_n | \frac{1}{2}m\omega^2 x^2 | \psi_n \rangle = \frac{\hbar\omega}{4}[2n+1]$

↳ $\langle T \rangle + \langle U \rangle = \frac{\hbar\omega}{2}[2n+1]$ which matches what we know to be the energy of the n^{th} state; $E_n = \hbar\omega(n + 1/2)$

e) * From the above formula, we know $E_0 = \frac{\hbar\omega}{2}$ and that $\Delta x \Delta p = \hbar/2$

⇒ Rewriting the total energy in terms of the uncertainties, we see:

$$\Delta E = \frac{(\Delta p)^2}{2m} + \frac{1}{2}m\omega^2(\Delta x)^2$$

#2 (cont.)

e) $\quad * \text{ but } \Delta p = \frac{\hbar}{2\Delta x}$

$$\Rightarrow \Delta E = \frac{\hbar^2}{8m(\Delta x)^2} + \frac{1}{2}m\omega^2(\Delta x)^2$$

$$\frac{d(\Delta E)}{d(\Delta x)} = 0$$ will give minimum of energy

$$\Rightarrow 0 = \frac{-\hbar^2}{4m(\Delta x^3)} + m\omega^2(\Delta x)$$

$$\frac{\hbar^2}{4m(\Delta x)^3} = m\omega^2(\Delta x)$$

$$\frac{\hbar^2}{4m^2\omega^2} = \Delta x^4 \quad \Rightarrow \quad \Delta x = \sqrt{\frac{\hbar}{2m\omega}}$$

$$\Rightarrow \Delta E = \frac{\hbar^2}{8m}\left(\frac{2m\omega}{\hbar}\right) + \frac{1}{2}m\omega^2\left(\frac{\hbar}{2m\omega}\right)$$

$$= \frac{\hbar\omega}{4} + \frac{\hbar\omega}{4}$$

$$= \frac{\hbar\omega}{2}$$

$\Rightarrow$ The uncertainly principle directly implies a non-zero ground state energy

Jan 2008

Problem 3: The Variational Principle: (10 Points)

If the case where you would like to calculate the ground state energy (E_g) for a system described by the Hamiltonian H but you are unable to solve the Schrodinger equation, the variational principle will give you an upper bound for the ground state energy.

For any normalized function Ψ, the variational principle states:

$$E_g \leq \langle \Psi | H | \Psi \rangle$$

1.**(2 Points)** Prove the variational principle. i.e show that

$$E_g \leq \langle \Psi | H | \Psi \rangle$$

Hint (Write $\Psi = \Sigma_n c_n \phi_n$ where ϕ_n are the (unknown) eigenfunctions of H)

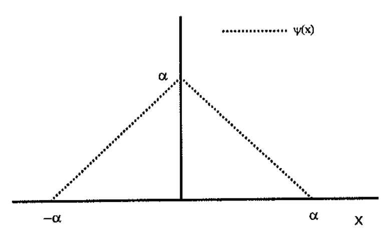
Now consider a specific case:
In the x-basis, a one-dimensional operator

$$\Omega = -\frac{d^2}{dx^2} + |x|$$

has an eigenvalue λ and an eigenfunction $\psi(x)$ with $\psi(x) \to 0$ for $|x| \to \infty$.
Let us choose an *unnormalized* trial function

$$\psi(x) = \langle x | \psi \rangle = \begin{cases} \alpha - |x|, & \text{for } |x| < \alpha \text{, and} \\ 0, & \text{for } |x| > \alpha \end{cases}$$

where α is the variational parameter.



2. **(2 Points)** Find $\langle \psi | \psi \rangle$.

3. **(3 Points)** Find the expectation value of the operator Ω.

4. **(3 Points)** Determine the **best** bound on the lowest eigenvalue (λ) of the operator Ω with the trial function $\psi(x)$. (Note your answer cannot depend on α.)

Jan 2008

Problem 4: Measurement of Hermitian Observables: (10 Points)

Consider a system with three Hermetian observables that are represented in a three-dimensional Hilbert space using the orthonormal basis $|e_1\rangle$, $|e_2\rangle$ and $|e_3\rangle$
with

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

and

$$A = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, B = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 2i \\ 0 & -2i & 1 \end{pmatrix}, C = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

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

$$|\Psi(0)\rangle = \frac{1}{\sqrt{6}}|e_1\rangle - \frac{1}{\sqrt{6}}|e_2\rangle + \sqrt{\frac{2}{3}}|e_3\rangle$$

1. Find the eigenvalues and normalized eigenvectors of B and C. **(1 Point)**
2. Find the probability of measuring B at time $t = 0$ with the eigenvalue $b = 1$, and then immediately measuring C and finding the eigenvalue $c = 1$, i.e. find $P_{|\Psi(0)\rangle}(b = 1, c = 1)$. **(2 Points)**
3. Now find the probability if these measurements are performed in reverse order at $t = 0$, i.e. find $P_{|\Psi(0)\rangle}(c = 1, b = 1)$. **(2 Points)**
4. Are the probabilities obtained in part 1. and part 2. the same or different? Explain in detail. **(2 Points)**
5. Use the Generalized Uncertainty Principle to determine a lower bound on $\Delta B \Delta C$ for the system in the initial state $|\Psi(0)\rangle$. Discuss your results. **(2 Points)**
6. Discuss in detail, the conditions that would result in obtaining a lower bound of zero when using the Generalized Uncertainty Principle. Would you expect to get zero for a particular pair of the observables, A, B, and C in this problem? Or for other conditions? **(1 Point)**

Jan 2008

Quantum #4

a) $B = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 2i \\ 0 & -2i & 1 \end{bmatrix}$

$\det(B - \lambda \mathbb{I}) = 0$

$\Rightarrow (1-\lambda)\left[(1-\lambda)^2 - (2i)(-2i)\right] = 0$

$$
\begin{aligned}
0 &= (1-\lambda)^3 - 4(1-\lambda) \\
&= \left[(1 - 2\lambda + \lambda^2) - 4\right](1-\lambda) \\
&= (\lambda^2 - 2\lambda - 3)(1-\lambda) \\
&= (1-\lambda)(\lambda - 3)(\lambda + 1)
\end{aligned}
$$

$\Rightarrow \lambda = 1, 3, -1$

$C = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

$\det(C - \lambda \mathbb{I}) = 0$

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

$\Rightarrow \lambda = 1, 1, -1$

$Bx = \lambda x$

* for $\lambda = 1$

$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 2i \\ 0 & -2i & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$

$x_1 = x_1$

$x_2 + 2i x_3 = x_2$

$-2i x_2 + x_3 = x_3$

$\Rightarrow \vec{x} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$

* for $\lambda = 3$

$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 2i \\ 0 & -2i & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = 3\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$

$x_1 = 3x_1$

$x_2 + 2i x_3 = 3x_2$

$-2i x_2 + x_3 = 3x_3$

$2i x_3 = 2x_2$

$i x_3 = x_2$

$\cancel{-2i(i x_3) + x_3 = 3x_3}$

$\cancel{-2x_3 + x_3 =}$

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

* for $\lambda = -1$

$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 2i \\ 0 & -2i & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = -1\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$

$x_1 = -x_1$

$x_2 + 2i x_3 = -x_2$

$-2i x_2 + x_3 = -x_3$

$2i x_3 = -2x_2$

$i x_3 = -x_2$

$\Rightarrow \vec{x} = \begin{bmatrix} 0 \\ -i \\ 1 \end{bmatrix} \cdot \frac{1}{\sqrt{2}}$

a) $Cx = \lambda x$

* for $\lambda = -1$

$$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = -1 \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$x_2 = -x_1$

$x_1 = -x_2$

$x_3 = -x_3$

$$\Rightarrow \vec{x} = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 1 \\ 0 \end{bmatrix}$$

* for $\lambda = 1$

$$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$x_2 = x_1$

$x_1 = x_2$

$x_3 = x_3$

$$\Rightarrow \vec{x} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \text{ or } \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$$

$|\lambda_c = 1, 2\rangle \qquad |\lambda_c = 1, 1\rangle$

b) * Convert $|\psi(0)\rangle$ into B eigenbasis

$$|\psi(0)\rangle = \begin{bmatrix} 1/\sqrt{6} \\ -1/\sqrt{6} \\ 2/\sqrt{6} \end{bmatrix} = \frac{1}{\sqrt{6}}\left(|\lambda=1\rangle + \frac{i}{2}\left[|\lambda=3\rangle - |\lambda=-1\rangle\right] + \left[|\lambda=3\rangle + |\lambda=-1\rangle\right]\right)$$

$$= \frac{1}{\sqrt{6}}\left(|\lambda=1) + \left(1+\frac{i}{2}\right)|\lambda=3\rangle + \left(1-\frac{i}{2}\right)|\lambda=-1\rangle\right)$$

* To find probability

$$\left|\langle\lambda_b=1|B|\psi(0)\rangle\right|^2 = \left|\langle\lambda_b=1|\left(\frac{1}{\sqrt{6}}\left[1|\lambda=1\rangle + 3\left(1+\frac{i}{2}\right)|\lambda=3\rangle - \left(1-\frac{i}{2}\right)|\lambda=-1\rangle\right]\right)\right|^2$$

$$= \frac{1}{6}$$

$$\left|\langle\lambda_c=1|C|\lambda_b=1\rangle\right|^2 = \left|\langle\lambda_c=1|\,C\,\middle|\frac{1}{\sqrt{2}}\left(|\lambda_c=1,1\rangle - |\lambda_c=-1\rangle\right)\right|^2$$

$$= \left|\langle\lambda_c=1,1|\frac{1}{\sqrt{2}}\left(|\lambda_c=1,1\rangle + |\lambda_c=-1\rangle\right)\right|^2$$

$$= \frac{1}{2}$$

* Note: Only need $\langle\lambda_c=1,1|$ case b/c of orthogonality of eigenkets, i.e. probability 0 in $\langle\lambda_c=1,2|$ case

Overall probability: $1/12$

#4 (cont.)

c) * Reversing the order from part b, we see:

$$|\psi(0)\rangle = \begin{bmatrix} 1/\sqrt{6} \\ -1/\sqrt{6} \\ 2/\sqrt{6} \end{bmatrix} = \frac{1}{\sqrt{6}}\left(2|\lambda_c=1,2\rangle - |\lambda_c=-1\rangle\right)$$

$$|\langle\lambda_c=1|\, C\, |\psi(0)\rangle|^2 = |\langle\lambda_c=1|\, \tfrac{1}{\sqrt{6}}\left(2|\lambda_c=1,2\rangle + |\lambda_c=-1\rangle\right)|^2$$

* only need $\langle\lambda_c=1| = \langle\lambda_c=1,2|$ case b/c of orthogonality of eigenvectors

$$= \left|\frac{2}{\sqrt{6}}\right|^2$$

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

* Converting $|\lambda_c=1,2\rangle$ to B eigenbasis: $|\lambda_c=1,2\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}}\left(|\lambda_b=3\rangle + |\lambda_b=-1\rangle\right)$

$$|\langle\lambda_b=1|\, B\, |\left(\tfrac{1}{\sqrt{2}}|\lambda_b=3\rangle + \tfrac{1}{\sqrt{2}}|\lambda_b=-1\rangle\right)|^2 = 0$$

Overall probability: 0

d) The probabilities in parts b + c are different because the two observables are not commutatable. They have different eigenbasis and therefore the system is affected in different ways depending upon which operator is acted first

e) $\langle(\Delta B)^2\rangle\, \langle(\Delta C)^2\rangle \geq \frac{1}{4}|\langle[B,C]\rangle|^2$, where $\Delta A = \langle A^2\rangle - \langle A\rangle^2$

$$~~B^2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 2i \\ 0 & -2i & 1 \end{bmatrix}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 2i \\ 0 & -2i & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 5 & -4i \\ 0 & 4i & 5 \end{bmatrix}~~$$

$$~~C^2 = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}~~$$

$$~~\langle B^2\rangle = \frac{1}{6}\begin{bmatrix} 1 & -1 & 2 \end{bmatrix}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 5 & -4i \\ 0 & 4i & 5 \end{bmatrix}\begin{bmatrix} 1 \\ -1 \\ 2 \end{bmatrix}~~$$

$$~~= \frac{1}{6}\begin{bmatrix} 1 & -1 & 2 \end{bmatrix}\begin{bmatrix} 1 \\ -5-8i \\ 10+4i \end{bmatrix} = \frac{1}{6}(1+5+20 +8i-8i) = \frac{26}{6}~~$$

$$~~\langle C^2\rangle = \frac{1}{6}\begin{bmatrix} 1 & -1 & 2 \end{bmatrix}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} 1 \\ -1 \\ 2 \end{bmatrix}~~$$

$$~~= \frac{1}{6}\begin{bmatrix} 1 & -1 & 2 \end{bmatrix}\begin{bmatrix} 1 \\ -1 \\ 2 \end{bmatrix} = \frac{1}{6}(6) = 1~~$$

#4 (cont.)

e) Taking square root of above equation yields: $(\Delta B)(\Delta C) \geq \frac{1}{2}|\langle [B,C] \rangle|$

$$\Rightarrow BC = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 2i \\ 0 & -2i & 1 \end{bmatrix}\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 2i \\ -2i & 0 & 1 \end{bmatrix}$$

$$CB = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 2i \\ 0 & -2i & 1 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 2i \\ 1 & 0 & 0 \\ 0 & -2i & 1 \end{bmatrix}$$

Jan 2008

Problem 5: Perturbation Theory: (10 Points)

A single particle is in a one dimensional infinite well of length L. The potential $V(x)$ is given by:

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

Suppose the potential energy inside the well is changed to

$$V(x) = \epsilon \sin \frac{\pi x}{L}$$

when $0 \leq x \leq L$.

Note you may use your results from Problem 1 for this problem.

1. Calculate the energy shifts for the perturbed well to first order in ϵ. **(2 Points)**
2. Which energy level is shifted the most to first order in ϵ? **(1 Point)**
3. Calculate the second order (in ϵ) correction to the ground state energy **(2 Points)**
4. Calculate the corrections to the ground state wavefunction to first order in ϵ. **(2 Points)**
5. Suppose that ϵ is larger than the energy of the first excited state. Carefully sketch the wavefunction versus x for the ground state and for the first excited state. How many nodes, maxima, and minima does the wavefunction have in each state. **(2 Points)**
6. Suppose the wavefunction is a linear combination of the ground state and the first excited state from part 5. Describe how the maximum of the probability density depends on time. **(1 Point)**

Jan 2008

Problem 6: Spherically Symmetric States: (10 Points)

Consider eigenfunctions of the Hamiltonian of a particle in a three-dimensional central potential. In particular, consider those eigenfunctions that depend only on the electron's radial coordinate r, that is $\Psi_E = \Psi_E(r)$. States represented by such eigenfunctions are called "spherically symmetric states".

1. Derive an equation for a function $\chi_E(r)$ defined by:

$$\Psi_n(r) \equiv \frac{1}{r}\chi_n(r),$$

   where n is the principle quantum number. **(2 Points)**

   The remainder of this problem concerns a hydrogen atom in the approximation that we neglect all interactions except the Coulomb interaction and treat the proton as an infinitely massive point particle at the origin.

2. Sketch $\chi_n(r)$ for the lowest three spherical bound states of the hydrogen atom. Justify the qualitative features of each function. **(2 Points)**

3. **(2 Points)**. Consider the eigenfunction for the ground state. Prove that to be physically admissible this function must decay exponentially as r becomes infinite.

$$\chi_1(r) \to e^{-\alpha r}, \text{when r} \to \infty$$

   where α is a constant, and that therefore $\chi_1(r)$ must have the form.

$$\chi_1(r) = f(r)e^{-\alpha r}.$$

4. Use $f(r) = r$. Justify why this is an appropriate choice and show that the above equation is a solution of the equation you derived for $\chi_1(r)$ and determine the corresponding eigenvalue E_1. **(2 Points)**

5. Derive an expression for the constant α in terms of fundamental constants. **(2 Points)**

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 $W > 0$.

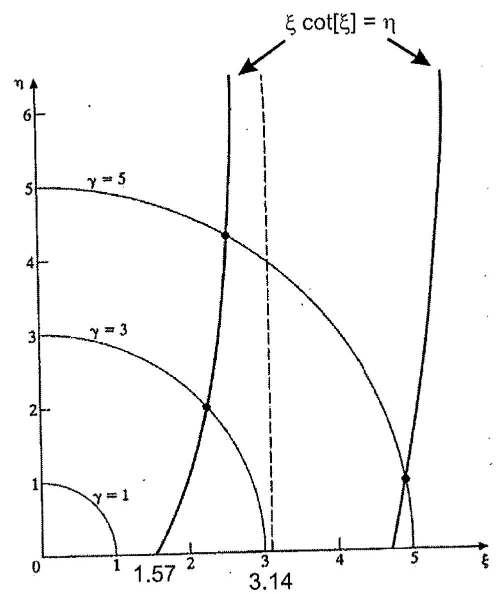
All of the following questions refer to the *zero angular momentum states* of the potential.

a. Find the form of the wave functions (i.e without matching boundary conditions), 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$\rightarrow \infty$, 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)**

Aug 2008

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

Aug 2008

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)**

Aug 2008

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: $H(a^+|\psi\rangle) = A(a^+|\psi\rangle)$

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

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

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

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

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

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

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

$$[H, a^+] = [\hbar\omega(a^+a + 1/2), a^+]$$
$$= \hbar\omega(a^+a + 1/2)a^+ - a^+(\hbar\omega[a^+a + \tfrac{1}{2}])$$
$$= \hbar\omega a^+aa^+ + \cancel{\tfrac{1}{2}\hbar\omega a^+} - \hbar\omega a^+a^+a - \cancel{\tfrac{1}{2}\hbar\omega a^+}$$
$$= \hbar\omega(a^+aa^+ - a^+a^+a)$$
$$= \hbar\omega[a^+(a^+a + 1) - a^+a^+a]$$
$$= \hbar\omega a^+$$

$$[H, a] = [\hbar\omega(a^+a + 1/2), a]$$
$$= \hbar\omega(a^+a + \tfrac{1}{2})a - a(\hbar\omega[a^+a + 1/2])$$
$$= \hbar\omega a^+aa + \cancel{\tfrac{1}{2}\hbar\omega a} - \hbar\omega aa^+a - \cancel{\tfrac{1}{2}\hbar\omega a}$$
$$= \hbar\omega(a^+aa - aa^+a)$$
$$= \hbar\omega(a^+aa - (a^+a+1)a)$$
$$= \hbar\omega a$$

#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: $V(x) = \begin{cases} \infty, & x < 0 \\ \frac{1}{2}m\omega^2x^2, & x > 0 \end{cases}$

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:

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

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

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 $V(x)$

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

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 $|L'| > |L|$

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)**

Aug 2008

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:

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

$\hookrightarrow B = 0$

$\hookrightarrow$ if n is odd:

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

$\hookrightarrow A = 0$

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

* Normalizing the above wavefunction yields

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

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

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

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

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

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

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

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

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

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

Aug 2008

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)**

Aug 2008

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 $H\vec{v} = \lambda\vec{v}$

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

* for $\lambda = 2$

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

* for $\lambda = -1$

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

* for $\lambda = 1$

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

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

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

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

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

#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 $\lambda = 2$

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

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

* 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 most 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

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

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

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

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

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

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

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

Aug 2008

Problem 6: Hydrogen Atom (10 Points)

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

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

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)**

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

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

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

* 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) $L|nlm\rangle = l(l+1)\hbar^2|nlm\rangle$

* 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.

Jan 2009

Problem 1: Spin $\frac{1}{2}$ particles (10 points)

Consider a system made up of spin 1/2 particles. If one measures the spin of the particles, one can only measure spin up or spin down. The general spin state of a spin 1/2 particle can be expressed as a two-element column matrix.

$$\chi = \begin{pmatrix} a \\ b \end{pmatrix}$$

The spin matrices are:

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

a) Can one simultaneously measure S_x, S_y and S_z? Explain your answer. (1 pt)

b) Can one simultaneously measure S^2 and S_z? Explain your answer. (1 pt)

c) Show S_z is Hermetian. (1 pt)

d) Calculate the normalized eigenvectors and eigenvalues of S_z. (2 pts)

Suppose a spin 1/2 particle is in the state

$$\chi = A\begin{pmatrix} 1+i \\ 2 \end{pmatrix}$$

e) Normalize the state in order to determine A (1 pt)

f) If one measures S_z, what is the probability of getting -$\hbar/2$? (1 pt)

g) If one measures S_x, what is the probability of getting $+\hbar/2$? (2 pts)

h) What is the expectation value of S_y (1 pt)

Jan 2009

Quantum #1

a) Simultaneous measurements can only occur if two or more operators have the same eigenbasis. Said another way, if the commutator b/w two operators is 0, then they can be simultaneously measured. It is common knowledge that for the spin operators,

$$[S_i, S_j] = i\hbar \epsilon_{ijk} S_k$$

Thus S_x, S_y, and S_z <u>cannot</u> be measured simultaneously.

b) Similarly to part a, S^2 and S_z can only be measured simultaneously if $[S^2, S_z] = 0$. Again, it is well known that $[S^2, S_i] = 0$ where $i = \{x, y, z\}$. Thus S^2 and S_z <u>can</u> be measured simultaneously.

c) The condition of Hermitivity is $A = A^+$

$$\Rightarrow S_z = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$S_z^+ = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$>$ S_z is Hermitian

d) Begin by finding eigenvalues

↳ b/c S_z is diagonalized eigenvalues are $\pm \hbar/2$

By similar logic, the corresponding eigenvectors are

$$\frac{\hbar}{2} : \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \frac{-\hbar}{2} : \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

as they would be for any diagonalized 2x2 matrix

e) Normalization Condition: $1 = \langle \chi | \chi \rangle$

$$\hookrightarrow 1 = A^2 \begin{bmatrix} 1+i & 2 \end{bmatrix} \begin{bmatrix} 1+i \\ 2 \end{bmatrix}$$

$$= A^2(1 + 1 + 4)$$

$$= 6A^2$$

$$\hookrightarrow A = \sqrt{\frac{1}{6}}$$

#1 (cont.)

f) $P(S_z = \frac{\hbar}{2}) = |\langle S_z = \frac{\hbar}{2} | \chi \rangle|^2$

$= \left| [0 \quad 1] \begin{bmatrix} 1+i \\ 2 \end{bmatrix} \cdot \frac{1}{\sqrt{6}} \right|^2$

$= \frac{1}{6} \cdot |2|^2$

$= \frac{2}{3}$

g) * We must first find eigenvectors of S_x using $S_x \vec{v} = \lambda \vec{v}$

$\begin{bmatrix} 0 & \hbar/2 \\ \hbar/2 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \hbar/2 \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$

$\Rightarrow \quad \frac{\hbar}{2} x_2 = \frac{\hbar}{2} x_1 \quad \rightarrow \quad \vec{v} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$

$\frac{\hbar}{2} x_1 = \frac{\hbar}{2} x_1$

$P(S_x = \frac{\hbar}{2}) = |\langle S_x = \frac{\hbar}{2} | \chi \rangle|^2$

$= \left| \frac{1}{\sqrt{2}} [1 \quad 1] \begin{bmatrix} 1+i \\ 2 \end{bmatrix} \frac{1}{\sqrt{6}} \right|^2$

$= \frac{1}{12} |3+i|^2$

$= \frac{1}{12} (9+1)$

$= \frac{10}{12} = \frac{5}{6}$

h) $\langle S_y \rangle = \langle \chi | S_y | \chi \rangle$

$= \frac{1}{6} [1-i \quad 2] \begin{bmatrix} 0 & -\frac{i\hbar}{2} \\ \frac{i\hbar}{2} & 0 \end{bmatrix} \begin{bmatrix} 1+i \\ 2 \end{bmatrix}$

$= \frac{1}{6} [1-i \quad 2] \begin{bmatrix} -i\hbar \\ -\frac{\hbar}{2} + \frac{i\hbar}{2} \end{bmatrix}$

$= \frac{1}{6} (-i\hbar - \hbar \quad -\hbar + i\hbar)$

$= -\hbar/3$

Jan 2009

Problem 2: A two-state system (10 points)

We can approximate the ammonia molecule NH_3 by a simple two-state system. The three H nuclei are in a plane, and the N nucleus is at a fixed distance either above or below the plane of the H's. Each is approximately a stationary state with some energy E_0. But there is a small amplitude for transition from up to down. Thus the total Hamiltonian is $H = H_0 + H_1$, where

$$H_0 = \begin{pmatrix} E_0 & 0 \\ 0 & E_0 \end{pmatrix} \quad \text{and} \quad H_1 = \begin{pmatrix} 0 & -A \\ -A & 0 \end{pmatrix}$$

with $|A| \ll |E_0|$.

(a) Find the exact eigenvalues of H. (*1 points*)

(b) Now suppose the molecule is in an electric field that distinguishes the two states. The new Hamiltonian is $H = H_0 + H_1 + H_2$, where

$$H_2 = \begin{pmatrix} \epsilon_1 & 0 \\ 0 & \epsilon_2 \end{pmatrix}$$

Find the new exact energy levels. (*1 points*)

(c) Apply perturbation theory and find the energy levels to the lowest non-vanishing order for $\epsilon_i \ll |A|$. Compare the results to the exact answer in (b). (*4 points*)

(d) Apply perturbation theory and find the energy levels to the lowest non-vanishing order for $\epsilon_i \gg |A|$. Compare the results to the exact answer in (b). (*4 points*)

Jan 2009

Quantum #2

$$H_0 = \begin{bmatrix} E_0 & 0 \\ 0 & E_0 \end{bmatrix} \qquad H_1 = \begin{bmatrix} 0 & -A \\ -A & 0 \end{bmatrix}$$

$$H = H_0 + H_1 = \begin{bmatrix} E_0 & -A \\ -A & E_0 \end{bmatrix}$$

a) Using the eigenvalue equation $\det(H - \lambda \mathbb{I}) = 0$

$$\begin{vmatrix} E_0 - \lambda & -A \\ -A & E_0 - \lambda \end{vmatrix} = 0 = (E_0 - \lambda)^2 - (-A)^2$$

$$= E_0^2 - 2\lambda E_0 + \lambda^2 - A^2$$

$$= \lambda^2 - 2E_0\lambda + (E_0^2 - A^2)$$

$$\hookrightarrow \lambda = \frac{2E_0 \pm \sqrt{4E_0^2 - 4(1)(E_0^2 - A^2)}}{2}$$

$$= \frac{2E_0 \pm \sqrt{\cancel{4E_0^2} - \cancel{4E_0^2} + 4A^2}}{2}$$

$$= E_0 \pm A$$

b) $H_2 = \begin{bmatrix} \epsilon_1 & 0 \\ 0 & \epsilon_2 \end{bmatrix}$

$$H = H_0 + H_1 + H_2 = \begin{bmatrix} E_0 + \epsilon_1 & -A \\ -A & E_0 + \epsilon_2 \end{bmatrix}$$

Again, as above:

$$\begin{vmatrix} E_0 + \epsilon_1 - \lambda & -A \\ -A & E_0 + \epsilon_2 - \lambda \end{vmatrix} = 0 = (E_0 + \epsilon_1 - \lambda)(E_0 + \epsilon_2 - \lambda) - (-A)^2$$

$$= E_0^2 + E_0\epsilon_2 - E_0\lambda + \epsilon_1 E_0 + \epsilon_1\epsilon_2 - \lambda\epsilon_1 - \lambda E_0 - \epsilon_2\lambda + \lambda^2 - A^2$$

$$= \lambda^2 - (2E_0 + \epsilon_1 + \epsilon_2)\lambda + (E_0^2 + E_0[\epsilon_1 + \epsilon_2] + \epsilon_1\epsilon_2 - A^2)$$

$$\hookrightarrow \lambda = \frac{2E_0 + \epsilon_1 + \epsilon_2 \pm \sqrt{4E_0^2 - 4(1)(E_0^2 + E_0[\epsilon_1 + \epsilon_2] + \epsilon_1\epsilon_2 - A^2)}}{2}$$

$$= \frac{2E_0 + \epsilon_1 + \epsilon_2 \pm \sqrt{4A^2 - 4E_0(\epsilon_1 + \epsilon_2) - 4\epsilon_1\epsilon_2}}{2}$$

#2 (cont.)

c) Assume H_2 is a perturbation on $H = H_0 + H_1$. Therefore, use non-degenerate perturbation theory, and we must solve for eigenvectors of $H = H_0 + H_1$

$\Rightarrow$ Using the eigenvector equation $H\vec{a} = \lambda \vec{a}$

$$\begin{bmatrix} E_0 & -A \\ -A & E_0 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \lambda \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \Rightarrow \begin{aligned} E_0 a_1 - A a_2 &= \lambda a_1 \\ -A a_1 + E_0 a_2 &= \lambda a_2 \end{aligned}$$

* for $\lambda = E_0 + A$

$$E_0 a_1 - A a_2 = E_0 a_1 + A a_1$$

$$-A a_2 = A a_1$$

$$-a_2 = a_1$$

$$\hookrightarrow \vec{a} = \begin{bmatrix} 1 \\ -1 \end{bmatrix} \cdot \frac{1}{\sqrt{2}}$$

* for $\lambda = E_0 - A$

$$E_0 a_1 - A a_2 = E_0 a_1 - A a_1$$

$$-A a_2 = -A a_1$$

$$a_2 = a_1$$

$$\vec{a} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \cdot \frac{1}{\sqrt{2}}$$

$$\Rightarrow |E_0 + A\rangle = \langle 1, -1 \rangle \cdot \frac{1}{\sqrt{2}}$$

$$|E_0 - A\rangle = \langle 1, 1 \rangle \cdot \frac{1}{\sqrt{2}}$$

* Dot product verifies orthogonality

$$\frac{1}{2}\left[(1 \cdot 1) + (1 \cdot -1)\right] = 0$$

In general $\Delta E_n^{(1)} = \langle n^{(0)} | V | n^{(0)} \rangle$

$$\hookrightarrow \Delta E_1^{(1)} = \langle E+A | H_2 | E+A \rangle$$

$$= \frac{1}{2} \begin{bmatrix} 1 & -1 \end{bmatrix} \begin{bmatrix} \epsilon_1 & 0 \\ 0 & \epsilon_2 \end{bmatrix} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

$$= \frac{1}{2} \begin{bmatrix} 1 & -1 \end{bmatrix} \begin{bmatrix} \epsilon_1 \\ -\epsilon_2 \end{bmatrix}$$

$$= \frac{1}{2}(\epsilon_1 + \epsilon_2)$$

$$\hookrightarrow \Delta E_2^{(1)} = \langle E-A | H_2 | E-A \rangle$$

$$= \frac{1}{2} \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} \epsilon_1 & 0 \\ 0 & \epsilon_2 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$= \frac{1}{2}(\epsilon_1 + \epsilon_2)$$

*If $\epsilon_i \ll A$, our exact energies are

$$E \approx \frac{2E_0 + \epsilon_1 + \epsilon_2 \pm \sqrt{4A^2 - \cancelto{0}{4E_0(\epsilon_1+\epsilon_2)} - 4\epsilon \ldots}}{2}$$

$$= E_0 \pm A + \epsilon_1 + \epsilon_2$$

which matches what we get from perturbation theory

#2 (cont.)

d) If $\epsilon_i >> |A|$, then $H = H_0 + H_2$ and H_1 is our perturbation

$\hookrightarrow \lambda = E_0 + \epsilon_1$

$\vec{a} = \langle 1, 0 \rangle$ and $\langle 0, 1 \rangle$

$\Rightarrow |E_0 + \epsilon_1\rangle = \langle 1, 0\rangle$ * Dot product verifies orthogonality

$|E_0 + \epsilon_2\rangle = \langle 0, 1\rangle$

Again as in part c

$$\Delta E_n^{(1)} = \langle n^{(0)} | V | n^{(0)} \rangle$$

$$\Delta E_1^{(1)} = \langle E_0 + \epsilon_1 | H_1 | E_0 + \epsilon_1 \rangle$$
$$= \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & -A \\ -A & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \cdot \frac{1}{2}$$
$$= \frac{1}{2} \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ -A \end{bmatrix}$$
$$= 0$$

$$\Delta E_2^{(1)} = \langle E_0 + \epsilon_2 | H_1 | E_0 + \epsilon_2 \rangle$$
$$= \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & -A \\ -A & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \cdot \frac{1}{2}$$
$$= \frac{1}{2} \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} -A \\ 0 \end{bmatrix}$$
$$= 0$$

*We must proceed to $\Delta E_n^{(2)}$ which requires $|n^{(1)}\rangle$

$$|n^{(1)}\rangle = \sum_{k \neq n}' \frac{V_{kn}}{E_n^{(0)} - E_k^{(0)}} |k^{(0)}\rangle$$

* remember that n and k refer to Energy eigen values

$$\hookrightarrow |(E_0 + \epsilon_1)^{(1)}\rangle = \frac{\langle E_0 + \epsilon_2 | H_1 | E_0 + \epsilon_1 \rangle}{(E_0 + \epsilon_1) - (E_0 + \epsilon_2)} |E_0 + \epsilon_2\rangle$$
$$= \frac{-A}{\epsilon_1 - \epsilon_2} |E_0 + \epsilon_2\rangle$$

$$\hookrightarrow |(E_0 + \epsilon_2)^{(1)}\rangle = \frac{\langle E_0 + \epsilon_1 | H_1 | E_0 + \epsilon_2 \rangle}{(E_0 + \epsilon_2) - (E_0 + \epsilon_1)} |E_0 + \epsilon_1\rangle$$
$$= \frac{-A}{\epsilon_2 - \epsilon_1} |E_0 + \epsilon_1\rangle$$

*In general, our second order correction formula is: $\Delta E_n^{(2)} = \langle n^{(0)} | V | n^{(1)} \rangle$

$$= \sum_{k \neq n}' \frac{|V_{kn}|^2}{E_n^{(0)} - E_k^{(0)}}$$

$$\Rightarrow \Delta E_1^{(2)} = \frac{A^2}{\epsilon_1 - \epsilon_2} \qquad \Delta E_2^{(2)} = \frac{A^2}{\epsilon_2 - \epsilon_1}$$

#2 (cont.)

d) This gives us energies of: $E_0 + \epsilon_1 + \frac{A^2}{\epsilon_1 - \epsilon_2} \approx E_1$

$E_0 + \epsilon_2 + \frac{A^2}{\epsilon_2 - \epsilon_1} \approx E_2$

* Returning to our exact solution

$$E_i = \frac{2E_0 + \epsilon_1 + \epsilon_2 \pm \sqrt{\cancel{4A^2}^{\approx 0} - 4E_0(\epsilon_1+\epsilon_2) - 4\epsilon_1\epsilon_2}}{2}$$

$$= E_0 + \frac{\epsilon_1+\epsilon_2}{2} \pm \sqrt{E_0(\epsilon_1+\epsilon_2) - \epsilon_1\epsilon_2}$$

$$= E_0 + \frac{\epsilon_1+\epsilon_2}{2} \mp E_0(\epsilon_1+\epsilon_2)\sqrt{1 + \frac{\epsilon_1\epsilon_2}{E_0(\epsilon_1+\epsilon_2)}}$$

$$= E_0 + \frac{\epsilon_1+\epsilon_2}{2} \mp E_0(\epsilon_1+\epsilon_2)\left[1 + \frac{1}{2}\left(\frac{\epsilon_1\epsilon_2}{E_0(\epsilon_1+\epsilon_2)}\right) - \cancel{\frac{1}{8}\left(\frac{\epsilon_1\epsilon_2}{E_0(\epsilon_1+\epsilon_2)^2}\right)}^{\text{ignore}} + \dots\right]$$

$$= E_0 + \frac{\epsilon_1+\epsilon_2}{2} \mp \left[E_0(\epsilon_1+\epsilon_2) + \frac{1}{2}\epsilon_1\epsilon_2\right]$$

↳

Jan 2009

Problem 3: 2-d potential (10 points)

A particle of mass m is confined by two impenetrable parallel walls at $x = \pm a$ to move on a two-dimensional strip defined by

$$-a < x < a$$
$$-\infty < y < \infty$$

The wave function for this system can be expressed as the product of two functions: one that depends only on the spatial co-ordinates (x and y), and one that depends only on time t.

a) Use the separation of variables technique to find the time dependent function. (2 points)

b) The part of the wave function that depends only on spatial co-ordinates can be expressed as the product of two functions: one that depends only on x and one that depends only on y. Use the separation of variables technique to find these two functions. (3 points)

c) What is the minimum energy of the particle that measurement can yield? (2 points)

d) Suppose that two additional walls are inserted at $y = \pm a$. Can a measurement of the particle's energy yield the value $3\pi^2\hbar^2/8ma^2$ Explain your answer. (3 points)

Jan 2009

Problem 4: Angular momentum (10 points)

A $|jm\rangle = |1, 0\rangle$ state scatters from a $|jm\rangle = |\frac{1}{2}, \frac{1}{2}\rangle$ state via a $|jm\rangle = |\frac{1}{2}, \frac{1}{2}\rangle$ resonance.

a) Relate the highest weight (highest possible m) states in the total j basis to the highest weight states in the direct product basis for this system of $\frac{1}{2} \otimes 1$. (1 pt)

b) Acting on the highest weight states with lowering operators, give an expansion of each total-j state in terms of direct product states and their Clebsch-Gordon co-efficients. (5 pts)
Hint: $J_\pm|jm\rangle = \hbar[(j \mp m)(j \pm m + 1)]^{1/2}|j, m \pm 1\rangle$

c) How often do the above-mentioned spin states scatter elastically, and how often do they scatter inelastically? (4 pts)

Jan 2009

Problem 5: Measurement and Probability (10 points)[5]

Consider the following two observables, H and C, whose representation in the unit basis $|e_1\rangle$, $|e_2\rangle$ and $|e_3\rangle$ is:

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

where:

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

Assume that at time t=0 the ensemble of particles is in the state:

$$|\Psi(0)\rangle = \frac{1}{\sqrt{2}}|e_1\rangle + \frac{1}{\sqrt{2}}|e_2\rangle$$

The eigenvalues of H are given by $\lambda = 2, 1, -1$ with normalized eigenvectors given by $(1,1,1)/\sqrt{3}$, $(1,0,-1)/\sqrt{2}$ and $(1,-2,1)/\sqrt{6}$ respectively.

The eigenvalues of C are given by $\lambda = 1, 1, -1$ with normalized eigenvectors given by $(1,0,-1)/\sqrt{2}$, $(0,1,0)$ and $(1,0,1)/\sqrt{2}$ respectively.

a) What is the probability of measuring H and obtaining $E = \hbar\omega$? What state is the particle in after the measurement? (2 pts)

b) If one immediately measures C after the measurement of H in part b), what is the probability of obtaining $c = 1$? (1 pt)

c) What is the probability of measuring H first and getting $E = \hbar\omega$, then measuring C and getting $c = 1$, i.e. what is $P_{|\Psi(0)\rangle}(E = \hbar\omega, c = 1)$? (1 pt)

d) If the system is allowed to evolve in time after the measurement of H and before C is measured, will your answer to part c) change? Explain your reasoning. (1 pt)

e) With the ensemble of particles all in the original state: $|\Psi(0)\rangle = \frac{1}{\sqrt{2}}|e_1\rangle + \frac{1}{\sqrt{2}}|e_2\rangle$, reverse the order of the above measurements and answer the same questions:

i) What is the probability of obtaining $c = 1$ if C is measured first? What state is the particle in after C is measured? (1 pt)

ii) If one immediately measures H after C is measured in part i), what is the probability of obtaining $E = \hbar\omega$? (1 pt) **(question continues on next page...)**

iii) What is the composite probability $P_{|\Psi(0)\rangle}(c = 1, E = \hbar\omega)$? (1 pt)

iv) If the system had been allowed to evolve in time after the measurement of C and before H is measured, would your answer to part ii) be different? Explain. (1 pt)

f) Are H and C compatible observables? Why?

Jan 2009

Quantum #5

$A^2 |\langle \psi | \varphi \rangle|^2$

Given: $H = \hbar\omega \begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix} \Rightarrow$
$|\lambda_H = 2\rangle = \frac{1}{\sqrt{3}} \langle 1, 1, 1 \rangle$
$|\lambda_H = 1\rangle = \frac{1}{\sqrt{2}} \langle 1, 0, -1 \rangle$
$|\lambda_H = -1\rangle = \frac{1}{\sqrt{6}} \langle 1, -2, 1 \rangle$

$C = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix} \Rightarrow$
$|\lambda_C = 1,1\rangle = \frac{1}{\sqrt{2}} \langle 1, 0, -1 \rangle$
$|\lambda_C = 1,2\rangle = \langle 0, 1, 0 \rangle$
$|\lambda_C = -1\rangle = \frac{1}{\sqrt{2}} \langle 1, 0, 1 \rangle$

$|\psi(t=0)\rangle = \frac{1}{\sqrt{2}} \langle 1, 1, 0 \rangle$

a) $P(H=1) = |\langle \lambda_H = 1 | H | \psi(t=0)\rangle|^2$

$= \left| \frac{1}{\sqrt{2}} \langle 1, 0, -1 \rangle \begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} \frac{1}{\sqrt{2}} \right|^2$

$= \frac{1}{4} \left| \langle 1, 0, -1 \rangle \begin{bmatrix} 2 \\ 1 \\ 1 \end{bmatrix} \right|^2$

$= \frac{1}{4} |1|^2 = \frac{1}{4}$

$\Rightarrow$ The state after measurement is
$|\lambda_H = 1\rangle = \frac{1}{\sqrt{2}} \langle 1, 0, -1 \rangle$
automatically b/c eigenvalues of H are non-degenerate

b) * From above, we know our starting state is: $|\lambda_H = 1\rangle = \frac{1}{\sqrt{2}} \langle 1, 0, -1 \rangle$

$P(C=1) = |\langle \lambda_C = 1,1 | \lambda_H = 1 \rangle|^2 + |\langle \lambda_C = 1,2 | \lambda_H = 1\rangle|^2$

$= \left| \frac{1}{\sqrt{2}} [1 \; 0 \; -1] \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} \cdot \frac{1}{\sqrt{2}} \right|^2 + \left| \cdot [0 \; 1 \; 0] \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} \cdot \frac{1}{\sqrt{2}} \right|^2$

$= \left| \frac{1}{2} \cdot 2 \right|^2 + \left| \frac{1}{\sqrt{2}} \cdot 0 \right|^2$

$= 1$

c) $P(H=1, C=1) = P(H=1) P(C=1)$

$= \frac{1}{4} \cdot 1$

$= \frac{1}{4}$

#5 (cont.)

d) Evolving the system in time after measuring H will have no impact on the measurement of C b/c the time evolution operator is a function of H and the eigenstates of H are thus stationary states

e) $P(c=1) = |\langle \lambda_c = 1,1 | \psi(0)\rangle|^2 + |\langle \lambda_c = 1,2 | \psi(0)\rangle|^2$

$$= \left|\tfrac{1}{\sqrt{2}}[1\ 0\ {-1}]\begin{bmatrix}1\\1\\0\end{bmatrix}\tfrac{1}{\sqrt{2}}\right|^2 + \left|[0\ 1\ 0]\begin{bmatrix}1\\1\\0\end{bmatrix}\tfrac{1}{\sqrt{2}}\right|^2$$

$$= \tfrac{1}{4} + \tfrac{1}{2} = \tfrac{3}{4}$$

* Our beginning state is either $|\lambda_c = 1,1\rangle$ or $|\lambda_c = 1,2\rangle$

$\Rightarrow P(H=1) = |\langle \lambda_H = 1 | \lambda_c = 1,1\rangle|^2 + |\langle \lambda_H = 1 | \lambda_c = 1,2\rangle|^2$

$$= \left|\tfrac{1}{\sqrt{2}}[1\ 0\ {-1}]\begin{bmatrix}1\\0\\-1\end{bmatrix}\tfrac{1}{\sqrt{2}}\right|^2 + \left|\tfrac{1}{\sqrt{2}}[1\ 0\ {-1}]\begin{bmatrix}0\\1\\0\end{bmatrix}\right|^2$$

$$= \left|\tfrac{1}{2}\cdot 2\right|^2 + 0^2$$

$$= 1$$

$P(c=1, H=1) = P(H=1)\,P(c=1)$

$$= 1 \cdot 3/4$$

$$= 3/4$$

* Allowing the system to evolve in time b/w measuring C and H (in that order) will result in a change in the probability of finding $E = \hbar\omega$ as the two possible eigenstates of $\lambda_c = 1$ not <u>both</u> eigenstates of H, thus they are non-stationary + will be changed after being acted upon by the time evolution operator

f) * Observables are compatible if $[A, B] = 0$, and also if they have a common, complete set of eigenvectors. Since H and C <u>do not</u> share the same eigenbasis, they are not compatible

Jan 2009

Problem 6: The hydrogen atom (10 points)

The figure below shows the radial function $R_{n,\ell}(r)$ for a stationary state of atomic hydrogen. The normalized Hamiltonian eigenfunction for this state, in atomic units, is

$$\psi_{n,\ell,m_\ell}(\boldsymbol{r}) = \frac{1}{81}\sqrt{\frac{2}{\pi}}(6-r)\;e^{-r/3}\;\cos\theta. \tag{1}$$

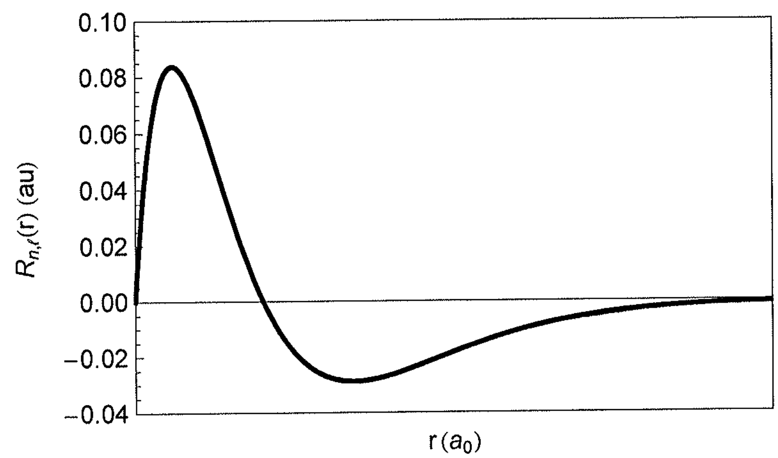


Figure 1: A radial function for a stationary state of atomic hydrogen.

1. **3 points.** What are the values of the quantum numbers n, ℓ, and m_ℓ for this state? To receive any credit, you must fully justify your answer.
2. **1 points.** What is the energy (in eV) of this state?
3. **2 points.** What are the mean value and uncertainty in r (in atomic units) for this state?
4. **2 points.** Calculate the value of r (in atomic units) at which a position measurement would be most likely to find the electron if the atom is in this state.
5. **2 points.** From Eq. 1, generate the normalized eigenfunction $\psi_{n,\ell,m_\ell+1}(\boldsymbol{r})$.

Hint:

$$\int_0^\infty e^{-2r/3} r^n \,\mathrm{d}r = n!\left(\frac{3}{2}\right)^{n+1} \tag{2}$$

Hint: *The following table gives the orbital-angular-momentum operators in Cartesian and spherical coordinates.*

Component	Cartesian coordinates	Spherical coordinates
$\widehat{L}_x$	$-\imath\hbar\left(y\dfrac{\partial}{\partial z}-z\dfrac{\partial}{\partial y}\right)$	$\imath\hbar\left(\sin\varphi\dfrac{\partial}{\partial\theta}+\cot\theta\cos\varphi\,\dfrac{\partial}{\partial\varphi}\right)$
$\widehat{L}_y$	$-\imath\hbar\left(z\dfrac{\partial}{\partial x}-x\dfrac{\partial}{\partial z}\right)$	$-\imath\hbar\left(\cos\varphi\dfrac{\partial}{\partial\theta}-\cot\theta\sin\varphi\,\dfrac{\partial}{\partial\varphi}\right)$
$\widehat{L}_z$	$-\imath\hbar\left(x\dfrac{\partial}{\partial y}-y\dfrac{\partial}{\partial x}\right)$	$-\imath\hbar\dfrac{\partial}{\partial\varphi}$
$\widehat{\boldsymbol{L}}^2$	$\widehat{L}_x^2+\widehat{L}_y^2+\widehat{L}_z^2$	$-\hbar^2\left[\dfrac{1}{\sin\theta}\dfrac{\partial}{\partial\theta}\left(\sin\theta\dfrac{\partial}{\partial\theta}\right)+\dfrac{1}{\sin^2\theta}\dfrac{\partial^2}{\partial\varphi^2}\right]$

Table 1: Components and square of the orbital angular momentum operator in Cartesian and spherical coordinates.

Aug 2009

Problem 1: Step Potential (10 points)

Consider the potential $V(x)$

$$V(x) = \begin{cases} 0, & x \leq 0 \\ -\mathrm{V}, & x > 0 \end{cases}$$

A particle of mass m and kinetic energy E approaches the step from $x < 0$.

a) Write the solution to Schrodinger's equation for $x < 0$. (1 pt)

b) Write the solution to Schrodinger's equation for $x > 0$. (1 pt)

c) Sketch the wave function for $x < 0$ as well as $x > 0$. Making sure to describe how the amplitude and frequency of the wave function changes. (1 pt)

d) What is the probability that particle will reflect back if $E = V/8$? (2 pts)

e) What is the probability that the particle will be transmitted if $E = V/8$. (2 pts) (Determine the transmission probability directly by using the flow of probability current and do not simply use $T = 1 - R$)

f) Show that $T + R = 1$. What does this mean physically? (1 pt)

g) If instead the particle approached the step from $x > 0$, how do your answers to parts a), b), d) and e) change? (2 pts)

Aug 2009

Problem 2: Variational Method (10 points) 2

Let us consider the hydrogen atom without spin. The Hamiltonian is

$$H = \frac{P^2}{2m} - \frac{C}{r} . \tag{1}$$

Since the ground state is an S state the wave function must be spherically symmetrical. Suppose you could not solve this problem exactly. Estimate the ground state wave function with a Gaussian:

$$\psi(\vec{r}) = Ne^{-r^2/b^2} .$$

a) Compute the normalization constant N so that $\psi(\vec{r})$ is correctly normalized. (2 pts)

b) Evaluate the expectation value of H in this state. (3 pts)

c) Find the best estimate for E_0 by applying the variational method. (4 pts)

d) The true ground state energy is

$$E_0 = -\frac{1}{2}(C^2 m) .$$

How much does your estimate in (c) differ from the correct answer? (1 pt)

Aug 2009

Problem 3: Artificial Atoms (10 points)

Modern techniques in nanotechnology research can create artificial atoms, man-made structures that confine electrons like real atoms but with properties that can be engineered. In this problem, consider a 2D atom (electrons tightly bound in the z-direction) with a parabolic potential in the x- and y-directions. The Hamiltonian is:

$$H_0 = \frac{p^2}{2m} + \frac{m\omega^2}{2}\left(x^2 + y^2\right). \tag{1}$$

Note: In solving this problem, you might want to use the standard operators:

$$a_x = \frac{1}{\sqrt{2}}\left(\frac{x}{\lambda} + i\frac{\lambda}{\hbar}p_x\right), \quad a_y = \frac{1}{\sqrt{2}}\left(\frac{y}{\lambda} + i\frac{\lambda}{\hbar}p_y\right) \tag{2}$$

and their Hermitian conjugates, where $\lambda = \sqrt{\frac{\hbar}{m\omega}}$.

a) What are the eigenenergies of this atom? What are the degeneracies of these energy levels? If the separation between adjacent levels is 20 meV (0.02 eV), approximately how large are the low-energy electron states in the atom (the radius)? (2 pts)

b) If the atom is put in a constant electric field, the Hamiltonian H_0 is perturbed by a potential:

$$H_1 = -eE_1 x \tag{3}$$

where E_1 is a constant (the electric field). Prove that to first order in the field, the energy levels of the atom do not change. (2 pts)

c) Next the atom is placed in a more complex field to study its properties. The new potential is:

$$H_2 = \frac{C_2}{\lambda^2}xy \tag{4}$$

To first order in C_2, what are the new eigenenergies of what were the first three energy levels of H_0? Show your work. (4 pts)

d) If a different perturbing potential:

$$H_3 = \frac{C_3}{\lambda^2}x^2 \tag{5}$$

is applied (rather than H_2), how would your answers to part (c) change? No computations should be necessary to answer this question. (2 pts)

Aug 2009

Problem 4: 3-d central-force problem (10 points)

A particle of mass m and spin $s = 0$ has a short-range potential energy $V(r)$. The particle is in a stationary state with Hamiltonian eigenfunction

$$\psi_E(\boldsymbol{r}) = N \frac{1}{r} \left(e^{-\alpha r} - e^{-\beta r} \right), \tag{6}$$

where N is a normalization constant (which you need not determine), and α and β are real numbers such that $\beta > \alpha$.

1. Is the orbital angular momentum of the particle sharp in this state? (That is, does L^2 have zero uncertainty?) If not, explain why not. If so, justify your answer and give the value of L^2 for this state. (4 pts)
2. What is the stationary-state energy of this state? (4 pts)
3. What is the potential energy $V(r)$? (2 pts)

Aug 2009

Problem 5: Quantum statistics (10 points)

1. Write down the energy eigenvalues and wave functions for a particle of mass m in an infinite square well, with $V = 0$ for $-L/2 < x < L/2$ and $V = \infty$ for $|x| > L/2$. (2 pts)

2. What is the ground state energy and wave-function if 2 identical non-interacting bosons are in the well? (4 pts)

3. What is the ground state energy and wave-function if 2 identical non-interacting spin-up fermions are in the well? (4 pts)

Aug 2009

Quantum #5

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

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

b) For bosons, there is no exclusion principle rule to follow, thus multiple bosons can occupy the same state in a system simultaneously, but the wavefunction must be symmetric

$$\Rightarrow E_{sys} = E_{1,1} + E_{2,1}$$
$$= \frac{\pi^2\hbar^2}{2m_1L^2} + \frac{\pi^2\hbar^2}{2m_2L^2}$$
$$= \frac{\pi^2\hbar^2}{mL^2}$$

$$\Rightarrow \psi_{sys} = \frac{1}{\sqrt{2}}\left(\psi_{1,1}(x_1)\psi_{2,1}(x_2) + \psi_{1,1}(x_2)\psi_{2,1}(x_1)\right)$$
$$= \frac{1}{\sqrt{2}}\left[\sqrt{\frac{2}{L}}\cos\left(\frac{\pi x_1}{L}\right)\sqrt{\frac{2}{L}}\cos\left(\frac{\pi x_2}{L}\right) + \sqrt{\frac{2}{L}}\cos\left(\frac{\pi x_2}{L}\right)\sqrt{\frac{2}{L}}\cos\left(\frac{\pi x_1}{L}\right)\right]$$
$$= \frac{4}{L\sqrt{2}}\left[\cos\left(\frac{\pi x_1}{L}\right)\cos\left(\frac{\pi x_2}{L}\right)\right]$$

* Normalizing the above wavefunction

$$1 = \frac{8}{L^2}A^2\int_{-L/2}^{L/2}dx_1\cos^2\left(\frac{\pi x_1}{L}\right)\int_{-L/2}^{L/2}dx_2\cos^2\left(\frac{\pi x_2}{L}\right)$$
$$= \frac{8A^2}{L^2}\cdot\frac{L^2}{4}$$
$$= 2A^2 \longrightarrow A = \frac{1}{\sqrt{2}}$$

$$\Rightarrow \psi_{sys} = \frac{2}{L}\cos\left(\frac{\pi x_1}{L}\right)\cos\left(\frac{\pi x_2}{L}\right)$$

c) For fermions, we must follow the exclusion principle, thus our two particles cannot occupy the same state simultaneously and the wavefunction must be antisymmetric

$$E_{sys} = E_{1,1} + E_{2,2}$$
$$= \frac{\pi^2\hbar^2}{2mL^2} + \frac{4\pi^2\hbar^2}{2mL^2}$$
$$= \frac{5\pi^2\hbar^2}{2mL^2}$$

#5 (cont.)

c) $$\psi_{sys} = \frac{1}{\sqrt{2}}\left(\psi_1(x_1)\psi_2(x_2) - \psi_1(x_2)\psi_2(x_1)\right)$$

$$= \frac{1}{\sqrt{2}}\left(\sqrt{\frac{2}{L}}^{\,2}\cos\left(\frac{\pi x_1}{L}\right)\sin\left(\frac{2\pi x_2}{L}\right) - \sqrt{\frac{2}{L}}\cos\left(\frac{\pi x_2}{L}\right)\sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x_1}{L}\right)\right]$$

$$= \frac{\sqrt{2}}{L}\left[\cos\left(\frac{\pi x_1}{L}\right)\sin\left(\frac{2\pi x_2}{L}\right) - \cos\left(\frac{\pi x_2}{L}\right)\sin\left(\frac{2\pi x_1}{L}\right)\right]$$

Aug 2009

Problem 6: Spin $\frac{1}{2}$ System (10 points)

Consider a spin $\frac{1}{2}$ particle in the state space E_s. This space can be spanned by the 2 eigenvectors of S_x, S_y, or S_z, the components of the spin operator $S = S_x\hat{i} + S_y\hat{j} + S_z\hat{k}$. The matrix representation of S_x, S_y and S_z in the eigenbasis $|+\rangle_z$, $|-\rangle_z$ of S_z are given below:

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

where $S_z|+\rangle_z = \hbar/2|+\rangle_z$ and $S_z|-\rangle_z = -\hbar/2|-\rangle_z$.

Assume that the state of the system at time $t = 0$ is: $|\Psi(0)\rangle = |-\rangle_z$.

a) If the observable S_x is measured at time $t = 0$, what results can be found and with what probabilities? (1 pt)

Now assume that a magnetic field is applied in the x **direction**: $\vec{B} = B_0\hat{i}$. The original wave function $|\Psi(0)\rangle = |-\rangle_z$ is allowed to evolve in time. The Hamiltonian governing the evolution is:

$$H_{spin} = \vec{S} \cdot \vec{B}$$

b) Set up the time evolution operator for this system, $U(t, 0)$. (1 pt)

c) Find $|\Psi(t)\rangle$, the wave function at a later time t. (1 pt)

d) At time $t > 0$ after $|\Psi(0)\rangle$ has evolved, S_x is measured. What is the probability of obtaining $+\hbar/2$? Is your answer time dependent or time independent? Explain correctly for credit. (1 pt)

e) Now let $|\Psi(0)\rangle$ evolve again and measure S_z at time t. Determine the probability of measuring S_z at time t and obtaining $-\hbar/2$. Is your answer time dependent or time independent? Explain correctly for credit. (1 pt)

f) Without explicitly finding the probabilities, discuss whether you expect the following probabilities to be equal or not. Give a brief explanation of your reasoning for any credit. The symbol $P_{|\Psi(t)\rangle}(a, c)$ represents the probability of starting with an ensemble in the state $|\Psi(t)\rangle$, measuring A first and getting eigenvalue "a" and then measuring C and getting eigenvalue "c". Assume that the eigenvalues of H_{spin} are E_+ and E_-. (1 pt)

i) Is $P_{|\Psi(0)\rangle}(+\hbar/2 \text{ for } S_y, -\hbar/2 \text{ for } S_x) = P_{|\Psi(0)\rangle>}(-\hbar/2 \text{ for } S_x, +\hbar/2 \text{ for } S_y)$? All measurements are taken at $t = 0$, i.e. the second measurement is taken immediately after the first measurement in each case. (1 pt)

ii) Is $P_{|\Psi(0)\rangle}(E_+, -\hbar/2 \text{ for } S_x) = P_{|\Psi(0)\rangle}(-\hbar/2 \text{ for } S_x,\ E_+)$? The first measurement in each case is taken at $t = 0$; the second measurement is taken immediately after the first measurement in each case. (1 pt)

iii) Is the probability $P_{|\Psi(0)\rangle}(+\hbar/2 \text{ for } S_x \text{ at } t, -\hbar/2 \text{ for } S_y \text{ at } t')$ time dependent or time independent in regards to the time t of the first measurement? Same question for the time t' of the second measurement. Discuss your reasoning in each case. (2 pts)

Aug 2009

Quantum #6

a) * To operate S_x on $|-\rangle_z$, we must rewrite S_x as:

$$S_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \left(|-\rangle_z\langle+|_z + |+\rangle_z\langle-|_z\right)\frac{\hbar}{2}$$

$$\Rightarrow S_x|-\rangle_z = \frac{\hbar}{2}\left(|-\rangle_z\langle+|_z + |+\rangle_z\langle-|_z\right)|-\rangle_z$$

$$= \frac{\hbar}{2}|+\rangle_z$$

$\hookrightarrow |+\rangle_z$ w/ $P = 1$

b) $|\psi(t)\rangle = U(t, t_0=0)\,|\psi(0)\rangle$ where $U(t,t_0=0) = \exp\left[-\frac{i}{\hbar}Ht\right]$

$$H = \vec{S}\cdot\vec{B} = S_x B_0$$

$$= \frac{B_0\hbar}{2}\left(|-\rangle_z\langle+|_z + |+\rangle_z\langle-|_z\right)$$

c) $\hookrightarrow |\psi(t)\rangle = e^{-iB_0t/2}\,|+\rangle_z$

d) $S_x|\psi(t)\rangle = S_x\left(e^{-iB_0t/2}|+\rangle_z\right)$

$$= e^{-iB_0t/2}\,|-\rangle_z \qquad \text{w/ probability } P=1$$

The answer is time independent b/c there is only one allowed state. Alternatively, $|c_n|^2$ determines the probability of that state. $|e^{-iB_0t/2}|^2 = 1$

e) $S_z|\psi(t)\rangle = \left(|+\rangle_z\langle+|_z - |-\rangle_z\langle-|_z\right)e^{-iB_0t/2}\,|+\rangle_z$

$$= e^{-iB_0t/2}\,|+\rangle_z$$

$P(S_z = -\hbar/2) = 0$ By same logic as above

f) i – $S_y = \frac{\hbar}{2}\left(-i|-\rangle\langle+| + i|+\rangle\langle-|\right)$

$\hookrightarrow$ No, $[S_x, S_y] \neq 0$, therefore they are not compatible observables

ii – yes, b/c H is simply a multiple of S_x, therefore $[S_x, H] = 0$ and the observables are compatible.

#6 (cont.)

f) iii - Both probabilities are time dependent

Quantum Mechanics
Qualifying Exam–January 2010

Notes and Instructions:

- There are **6** problems and **7** pages.
- Be sure to write your alias at the top of every page.
- Number each page with the problem number, and page number of your solution (e.g. "Problem 3, p. 1/4" is the first page of a four page solution to problem 3).
- **You must show all your work.**

Possibly useful formulas:

Pauli spin matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

One-dimensional simple harmonic oscillator operators:

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

$$P = -i\sqrt{\frac{\hbar m\omega}{2}}(a - a^\dagger)$$

Spherical Harmonics:

$$Y_0^0(\theta,\varphi) = \frac{1}{\sqrt{4\pi}}$$

$$Y_2^2(\theta,\varphi) = \frac{5}{\sqrt{96\pi}}\,3\sin^2\theta\, e^{2i\varphi}$$

$$Y_2^1(\theta,\varphi) = -\frac{5}{\sqrt{24\pi}}\,3\sin\theta\cos\theta\, e^{i\varphi}$$

$$Y_1^1(\theta,\varphi) = -\frac{3}{\sqrt{8\pi}}\sin\theta\, e^{i\varphi} \qquad Y_2^0(\theta,\varphi) = \frac{5}{\sqrt{4\pi}}\left(\tfrac{3}{2}\cos^2\theta - \tfrac{1}{2}\right)$$

$$Y_1^0(\theta,\varphi) = \frac{3}{\sqrt{4\pi}}\cos\theta \qquad Y_2^{-1}(\theta,\varphi) = \frac{5}{\sqrt{24\pi}}\,3\sin\theta\cos\theta\, e^{-i\varphi}$$

$$Y_1^{-1}(\theta,\varphi) = \frac{3}{\sqrt{8\pi}}\sin\theta\, e^{-i\varphi} \qquad Y_2^{-2}(\theta,\varphi) = \frac{5}{\sqrt{96\pi}}\,3\sin^2\theta\, e^{-2i\varphi}$$

Angular momentum raising and lowering operators:

$$\hat{L}_\pm = (\hat{L}_x \pm i\,\hat{L}_y)$$

PROBLEM 1: The Delta-Function Potential

Let us consider a single particle of mass m moving in one dimension with the Hamiltonian

$$H = T + V(x) \, ,$$

where the kinetic energy is

$$T = \frac{P^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \, ,$$

the potential energy is

$$V(x) = -V_0 \, \delta(x) \, ,$$

and $\delta(x)$ is the Dirac delta function.

(a) [2 points] Find an expression for the discontinuity of the derivative of the wave function at $x = 0$.

(b) [3 points] Find the ground state wave function.

(c) [2 points] Find the ground state energy.

(d) [3 points] Find the expectation value for the kinetic energy, $\langle T \rangle$.

PROBLEM 2: Hydrogenic Atoms with One Electron

In terms of the first Bohr radius, $a_0 \equiv \hbar/(c\alpha m_e)$, where α is the fine-structure constant, the ground-state eigenfunction of a hydrogen atom is

$$\psi_{1,0,0}(r,\theta,\varphi) = \frac{1}{\sqrt{\pi a_0^3}}\, e^{-r/a_0}.$$

(a) [3 points] Evaluate the probability of finding an electron in the ground-state of a hydrogen atom in the classically forbidden region. The classically forbidden region is the region of space where the classical kinetic energy is negative.

(b) [4 points] For the ground state, evaluate the uncertainty in the Cartesian coordinate x and the uncertainty in the corresponding component of the linear momentum, p_x. *Hint: You need not use the explicit form of the operator for the linear momentum to evaluate* Δp_x.

(c) [3 points] Show explicitly that the product of your uncertainties, $\Delta x\, \Delta p_x$, is consistent with the Heisenberg uncertainty principle.

PROBLEM 3: Time-Dependent Perturbation Theory

Consider a non-relativistic particle of mass m and charge q with the potential energy:

$$V(x) = \frac{1}{2}\, k\, X^2$$

A homogeneous electric field $\mathcal{E}(t)$ directed along the x-axis is switched on at time $t = 0$. This causes a perturbation of the form

$$H' = -q\, X\, \mathcal{E}(t)$$

where $\mathcal{E}(t)$ has the form

$$\mathcal{E}(t) = \mathcal{E}_o e^{-t/\tau}$$

where $\mathcal{E}_o$ and τ are constants.

The particle is in the ground state at time $t \leq 0$. This problem will deal with calculating the probability that it will be found in an excited state as $t \longrightarrow \infty$.

The probability that the particle makes a transition from an initial state i to a final state f is given by:

$$P_{fi}(t, t_o) = \frac{1}{\hbar^2} \left| \int_{t_o}^{t} dt' \, \langle \phi_f | H'(t') | \phi_i \rangle \, e^{i\omega_{fi} t'} \right|^2 .$$

where the particle originally is in state ϕ_i and finally in state ϕ_f.

(a) [2 points] In terms of known quantities, what is the value of ω_{fi} ?

(b) [2 points] How many excited states can the particle make a transition to?

(c) [6 points] Derive an expression for the probability that the particle will be found in any allowed excited state as $t \longrightarrow \infty$.

PROBLEM 4: Spin Physics

Spin-1/2 objects generally have magnetic moments that affect their energy levels and dynamics in magnetic fields. The interaction between the magnetic moment and a magnetic field, $\vec{B}$ can be written as:

$$H = -\mu \vec{S} \cdot \vec{B} \tag{1}$$

where $\vec{S}$ is the spin of the particle

$$\vec{S} = \frac{\hbar}{2}\vec{\sigma} \tag{2}$$

where the σ_i's are Pauli matrices.

In this problem we'll be using as our basis the eigenstates of S_z,

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \ |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{3}$$

with eigenvalues $\pm\frac{\hbar}{2}$.

(a) [1 point] If a particle is in the spin state $|+\rangle$, compute the expectation values of S_x, S_y, and S_z.

(b) [1 point] If a particle is in the spin state $|+\rangle$, what are the uncertainties of S_x, S_y, and S_z? ($\Delta S_i^2 = \langle S_i^2 \rangle - \langle S_i \rangle^2$.) Explain the physics of your results in terms of the eigenvalues and measurement probabilities of the spin in the x, y, and z directions.

(c) [3 points] A large ensemble of particles are all prepared to be in the spin state $|+\rangle$ at time $t = 0$ when a magnetic field in the x-direction is switched on, $\vec{B} = B_0 \hat{e}_x$. Solve for the time-dependent probabilities, $P_\pm(t)$, of measuring S_z to be $\pm\hbar/2$.

(d) [2 points] For the experiment described in part (c), what are the probabilities for measuring S_x to be $\pm\hbar/2$? Explain the differences between the results for S_z and S_x.

(e) [3 points] Consider the case where the magnetic field is $\vec{B} = \frac{B_0}{\sqrt{2}}(\hat{e}_x + \hat{e}_z)$. In this case what is the time-dependent probability of measuring S_z to be $+\hbar/2$?

Jan 2010

Quantum #4

a) $S_x = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ $\quad S_y = \frac{\hbar}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$ $\quad S_z = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

$$\langle S_x \rangle = {}_z\langle + | S_x | + \rangle_z = \begin{bmatrix} 1 & 0 \end{bmatrix}\begin{bmatrix} 0 & \hbar/2 \\ \hbar/2 & 0 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = 0$$

$$\langle S_y \rangle = {}_z\langle + | S_y | + \rangle_z = \begin{bmatrix} 1 & 0 \end{bmatrix}\begin{bmatrix} 0 & -\frac{i\hbar}{2} \\ \frac{i\hbar}{2} & 0 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = 0$$

$$\langle S_z \rangle = {}_z\langle + | S_z | + \rangle_z = \begin{bmatrix} 1 & 0 \end{bmatrix}\begin{bmatrix} \hbar/2 & 0 \\ 0 & -\hbar/2 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \hbar/2$$

b) $\Delta S_i^2 = \langle S_i^2 \rangle - \langle S_i \rangle^2$

$$\langle S_x^2 \rangle = \begin{bmatrix} 1 & 0 \end{bmatrix}\begin{bmatrix} \hbar/2 & 0 \\ 0 & -\hbar/2 \end{bmatrix}\begin{bmatrix} \hbar/2 & 0 \\ 0 & -\hbar/2 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \end{bmatrix}\begin{bmatrix} \hbar^2/4 & 0 \\ 0 & \hbar^2/4 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \hbar^2/4$$

$$\langle S_y^2 \rangle = \begin{bmatrix} 1 & 0 \end{bmatrix}\begin{bmatrix} 0 & -\frac{i\hbar}{2} \\ \frac{i\hbar}{2} & 0 \end{bmatrix}\begin{bmatrix} 0 & -\frac{i\hbar}{2} \\ \frac{i\hbar}{2} & 0 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \end{bmatrix}\begin{bmatrix} \hbar^2/4 & 0 \\ 0 & \hbar^2/4 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \hbar^2/4$$

$$\langle S_z^2 \rangle = \begin{bmatrix} 1 & 0 \end{bmatrix}\begin{bmatrix} \hbar/2 & 0 \\ 0 & -\hbar/2 \end{bmatrix}\begin{bmatrix} \hbar/2 & 0 \\ 0 & -\hbar/2 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \end{bmatrix}\begin{bmatrix} \hbar^2/4 & 0 \\ 0 & \hbar^2/4 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \hbar^2/4$$

$$\Rightarrow \Delta S_x^2 = \frac{\hbar^2}{4} - (0)^2 = \hbar^2/4$$
$$\Delta S_y^2 = \frac{\hbar^2}{4} - (0)^2 = \frac{\hbar^2}{4}$$
$$\Delta S_z^2 = \frac{\hbar^2}{4} - \left(\frac{\hbar}{2}\right)^2 = 0$$

* Because we are working in the S_z basis, there is no uncertainty b/c we know the state of the particle. However, the S_x and S_z eigenstates are linear combinations of the S_z states, thus there is some uncertainty as to which eigenvalue is preferred.

#4 (cont.)

c) $H = -\mu \vec{S} \cdot \vec{B}$ $\qquad |\psi(t=0)\rangle = |+\rangle_z$

$= -\mu (S_x B_0)$

* To act time evolution operator, convert to S_x basis

$|+\rangle_x = \frac{1}{\sqrt{2}}(|+\rangle_z + |-\rangle_z)$

$|-\rangle_x = \frac{1}{\sqrt{2}}(|+\rangle_z - |-\rangle_z)$ $\quad > \quad |+\rangle_z = \frac{1}{\sqrt{2}}(|+\rangle_x + |-\rangle_x)$

$|\psi(t)\rangle = U(t, t_0 = 0)|\psi(t=0)\rangle$

$= e^{-iHt/\hbar}\left(\frac{1}{\sqrt{2}}[|+\rangle_x + |-\rangle_x]\right)$ $\qquad E_\pm = \pm\frac{\mu_0 B\hbar}{2}$

$= \frac{1}{\sqrt{2}}\left(e^{-iE_+t/\hbar}|+\rangle_x + e^{-iE_-t/\hbar}|-\rangle_x\right)$

$P(S_z = +\hbar/2) = |{}_z\langle + |\psi(t)\rangle|^2$

$= \left|\frac{1}{\sqrt{2}}[\langle +|_x + \langle -|_x]\frac{1}{\sqrt{2}}\, e^{-iE_+t/\hbar}|+\rangle_x + e^{-iE_-t/\hbar}|-\rangle_x\right.$

$= \frac{1}{4}\left|e^{iE_+t/\hbar} + e^{-iE_-t/\hbar}\right|^2$

$= \frac{1}{4}\left(2 + e^{-i(E_+ - E_-)t/\hbar} + e^{+i(E_+ - E_-)t/\hbar}\right)$

$= \frac{1}{4}\left(2 + 2\cos\left(\frac{\Delta E t}{\hbar}\right)\right)$, $\Delta E = E_+ - E_-$

$= \frac{1}{2}\left(1 + \cos\left(\frac{\Delta E t}{\hbar}\right)\right)$

$P(S_z = -\hbar/2) = 1 - P(S_z = \hbar/2)$

$= 1 - \frac{1}{2}\left(1 + \cos\left(\frac{\Delta E t}{\hbar}\right)\right)$

$= \frac{1}{2}\left(1 - \cos\left(\frac{\Delta E t}{\hbar}\right)\right)$

#4 (cont.)

d) * utilizing work done in part c;

$$P(S_x = \hbar/2) = |{}_x\langle + | \psi(t)\rangle|^2$$

$$= |{}_x\langle + | \left(\tfrac{1}{\sqrt{2}}\left[e^{-iE_+t/\hbar}|+\rangle_x + e^{-iE_-t/\hbar}|-\rangle_x\right]\right)|^2$$

$$= \tfrac{1}{2}|e^{-iE_+t/\hbar}|^2$$

$$= \tfrac{1}{2}$$

$$P(S_x = -\hbar/2) = 1 - P(S_x = \hbar/2)$$

$$= \tfrac{1}{2}$$

* In this case, our final states are in the same eigenbasis as our original state, which is a linear combination of the two states where the coefficients evolve in time in a coupled manner. But since we are operating in only 1 eigenbasis, we must have time independent probabilities, as the basis states are stationary states.

e) With $\vec{B} = \frac{B_0}{\sqrt{2}}(\hat{e}_x + \hat{e}_z)$, our Hamiltonian now becomes $-\frac{\mu B_0 \hbar}{2\sqrt{2}}(S_x + S_z)$

* if $A = \frac{-\mu B_0 \hbar}{2\sqrt{2}}$

$$\Rightarrow H = A\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

* Determining eigenvalues + eigenvectors

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

$$= -1 + \cancel{\lambda} - \cancel{\lambda} + \lambda^2 - 1$$

$$= \lambda^2 - 2$$

$$\hookrightarrow \lambda = \pm\sqrt{2}$$

$$H\vec{v} = \lambda\vec{v} \rightarrow \quad x_1 + x_2 = \lambda x_1$$
$$x_1 - x_2 = \lambda x_2$$

* if $\lambda = +\sqrt{2}$

$$x_1 + x_2 = \sqrt{2}\, x_1$$
$$x_1 - x_2 = \sqrt{2}\, x_2$$
$$\hookrightarrow x_1 = 1+\sqrt{2}, \ x_2 = 1$$
$$\vec{v}_1 = \begin{bmatrix} 1+\sqrt{2} \\ 1 \end{bmatrix} = |+\rangle_{xz}$$

* if $\lambda = -\sqrt{2}$

$$x_1 + x_2 = -\sqrt{2}\, x_1$$
$$x_1 - x_2 = -\sqrt{2}\, x_2$$
$$\hookrightarrow x_1 = 1-\sqrt{2}, \ x_2 = 1$$
$$\vec{v}_2 = \begin{bmatrix} 1-\sqrt{2} \\ 1 \end{bmatrix} = |-\rangle_{xz}$$

$$A^2[(1+\sqrt{2})^2 + 1] = 1$$

$$A^2(1 + 2\sqrt{2} + 2 + 1) = 1$$

$$A^2 = \frac{1}{4+2\sqrt{2}}\left(\frac{4-2\sqrt{2}}{4-2\sqrt{2}}\right)$$

$$A^2 = \frac{4-2\sqrt{2}}{16+4(2)} = \frac{4-2\sqrt{2}}{24} = \left(\frac{2-\sqrt{2}}{12}\right)^{1/2}$$

$$A^2[(1-\sqrt{2})^2 + 1] = 1$$

$$A^2[1 - 2\sqrt{2} + 2 + 1] = 1$$

$$A^2 = \frac{1}{[4-2\sqrt{2}]}$$

$$A^2 = \frac{4+2\sqrt{2}}{16-4(2)}$$

$$A^2 = \frac{2+2\sqrt{2}}{4}$$

$$A = \left(\frac{2+2\sqrt{2}}{4}\right)^{1/2}$$

#4 (cont.)

e) * To act time evolution operator, convert $|\Psi(t=0)\rangle$ to H-basis

$$|\Psi(t=0)\rangle = |+\rangle_z = \left(\left(\frac{1}{4+2\sqrt{2}}\right)^{1/2} |+\rangle_{xz} + \left(\frac{1}{4-2\sqrt{2}}\right)^{1/2} |-\rangle_{xz} \right)$$

* Not worth time + effort

PROBLEM 5: Two Level System

Consider a quantum system that can be accurately approximated as having two energy levels $|+\rangle$ and $|-\rangle$ such that

$$H_0|\pm\rangle = \pm\epsilon|\pm\rangle\,,$$

where ϵ is energy.

When placed in an external field, the eigenstates of H_0 are mixed by another term in the total Hamiltonian

$$V|\pm\rangle = \delta|\mp\rangle\,.$$

For simplicity, we choose ϵ to be real.

(a) [1 points] Using the states $|+\rangle$ and $|-\rangle$ as your basis states, write down the matrix representations for the operators H_0 and V.

(b) [3 points] What will be the possible results if a measurement is made of the energy for the full Hamiltonian $H = H_0 + V$?

(c) [2 points] Experiments are performed that measure the transition energies between eigenstates. Without the external field ($\delta = 0$) it is found that the transition energy is 4 eV and with the external field ($\delta \neq 0$) the transition energy is 6 eV. What is the coupling between the states $|\pm\rangle$, δ, in this case?

(d) [2 points] We can write the eigenstates of the total Hamiltonian in terms of two energy levels $|\pm\rangle$ as

$$\begin{aligned} |1\rangle &= \cos(\theta_1)|+\rangle + \sin(\theta_1)|-\rangle \\ |2\rangle &= \cos(\theta_2)|+\rangle + \sin(\theta_2)|-\rangle\,. \end{aligned}$$

Letting $\delta/\epsilon = C$, solve for the angles θ_1 and θ_2 in terms of C.

(e) [2 points] Consider an experiment where the two-level system starts in the eigenstate of H_0 with eigenvalue $-\epsilon$. A very weak field is turned on so that $C \ll 1$. To the lowest order in C, what is the probability of measuring a positive energy for the system when $\delta \neq 0$?

PROBLEM 6: Hyperfine Splitting

The hyperfine splitting in hydrogen comes from a spin-spin interaction between the electron and the proton. The total Hamiltonian can be written as

$$H = \frac{P_p^2}{2m_p} + \frac{P_e^2}{2m_e} - \frac{e^2}{r} + H_{HF}$$

where $H_{HF} = A\vec{S}_e \cdot \vec{S}_p$, and A is a real constant.

(a) [1 points] What are the spin quantum numbers s and m_s of the electron?

(b) [1 points] What are the spin quantum numbers s and m_s of the proton?

(c) [1 points] What are the spin quantum numbers s and m_s of the combined electron-proton system?

(d) [5 points] Diagonalize H_{HF} in the total $\vec{S} = \vec{S}_e + \vec{S}_p$ basis and compute the energy eigenvalues.

(e) [2 points] Write an expression for the energy of a photon that would be emitted from a hyperfine transition in terms of A, $\hbar$, and any other relevant constants.

Quantum Mechanics
Qualifying Exam–August 2010

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- **You must show all your work.**

Possibly useful formulas:

Pauli spin matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

One-dimensional simple harmonic oscillator operators:

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

$$P = -i\sqrt{\frac{\hbar m\omega}{2}}(a - a^\dagger)$$

Spherical Harmonics:

$$Y_0^0(\theta,\varphi) = \frac{1}{\sqrt{4\pi}} \qquad Y_2^2(\theta,\varphi) = \frac{5}{\sqrt{96\pi}}\, 3\sin^2\theta\, e^{2i\varphi}$$

$$Y_2^1(\theta,\varphi) = -\frac{5}{\sqrt{24\pi}}\, 3\sin\theta\cos\theta\, e^{i\varphi}$$

$$Y_1^1(\theta,\varphi) = -\frac{3}{\sqrt{8\pi}}\sin\theta\, e^{i\varphi} \qquad Y_2^0(\theta,\varphi) = \frac{5}{\sqrt{4\pi}}\left(\frac{3}{2}\cos^2\theta - \frac{1}{2}\right)$$

$$Y_1^0(\theta,\varphi) = \frac{3}{\sqrt{4\pi}}\cos\theta \qquad Y_2^{-1}(\theta,\varphi) = \frac{5}{\sqrt{24\pi}}\, 3\sin\theta\cos\theta\, e^{-i\varphi}$$

$$Y_1^{-1}(\theta,\varphi) = \frac{3}{\sqrt{8\pi}}\sin\theta\, e^{-i\varphi} \qquad Y_2^{-2}(\theta,\varphi) = \frac{5}{\sqrt{96\pi}}\, 3\sin^2\theta\, e^{-2i\varphi}$$

In spherical coordinates, the Laplacian is

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

PROBLEM 1: Motion of a Particle in One Dimension

Consider a particle of mass m moving along the $+x$ direction in free space.

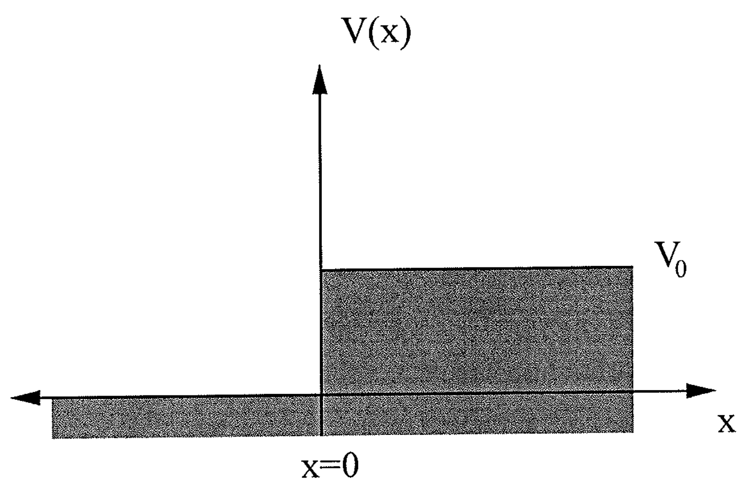
(a) [2 points] Suppose the particle is in a momentum eigenstate where the particles momentum is known precisely to be p_0. Write a wavefunction $\Psi(x,t)$ that describes such a state.

(b) [2 points] Suppose the particle is in a state where it is equally probable for the particle to have any momentum between $p_0 - \Delta p/2$ and $p_0 + \Delta p/2$ at time $t = 0$. Construct a wavefunction $\Psi(x,t)$ that describes such a state.

(c) [2 points] Suppose a beam of particles, each in the state described in part (a), encounters an abrupt step in potential energy at $x = 0$. The step height V_0 is less than the particles total energy E. Construct the wavefunction, $\Psi(x,t)$ with $-\infty \le x \le \infty$, that describes this situation.

(d) [2 points] Calculate the probability that a particle is reflected by the potential energy step described in part (c).

(e) [2 points] Consider the situation described in part (c), except with V_0 greater than E. Compare the probability of finding a particle at a distance x inside the barrier to the probability of finding a particle at $x = 0$.



PROBLEM 2: Harmonic Oscillator with Two Particles

Consider a Hamiltonian for two non-interacting particles:

$$\begin{aligned} H(1,2) &= \frac{P_1^2}{2m} + \frac{1}{2}m\omega_1^2 X_1^2 + \frac{P_2^2}{2m} + \frac{1}{2}m\omega_2^2 X_2^2 \\ &= H_1 + H_2 \end{aligned}$$

where $\omega_2 = 2\omega_1 = 2\omega$.

Defining the raising and lowering operators:

$$\begin{aligned} a_n &= \frac{1}{\sqrt{2}}(\bar{X}_n + i\bar{P}_n) \\ a_n^\dagger &= \frac{1}{\sqrt{2}}(\bar{X}_n - i\bar{P}_n) \end{aligned}$$

where $n = 1, 2$ and

$$\begin{aligned} \bar{X}_n &= \left(\frac{m\omega_n}{\hbar}\right)^{1/2} X_n \\ \bar{P}_n &= \left(\frac{1}{\hbar m\omega_n}\right)^{1/2} P_n \end{aligned}$$

such that $[a_m, a_n^\dagger] = \delta_{mn}, m, n = 1, 2$.

Answer the following questions:

(a) [2 points] Write the Hamiltonian in terms of raising and lowering operators.

(b) [2 points] Write the eigenvector $|\psi_{n_1,n_2}\rangle$ in terms of the ground state $\psi_{0,0}\rangle = |\phi_{n_1=0}\rangle|\phi_{n_2=0}\rangle$ where $|\phi_{n_1}\rangle$ is the eigenvector for particle 1, i.e.,

$$H_1|\phi_{n_1}\rangle = \left(n_1 + \frac{1}{2}\right)\hbar\omega_1|\phi_{n_1}\rangle$$

and similarly for particle 2.

(c) [1 points] Write a formula for the energy levels of this oscillator, E_n with n defined in terms of n_1 and n_2.

(d) [1 points] Determine a formula for the degeneracy, g_n , of an energy level E_n.

(e) [2 points] Using your results from part (d) determine the degeneracy g_n for the energy, $E = 15/2\hbar\omega$ and list all the eigenfunctions $|\psi_{n_1,n_2}\rangle$ that have this energy.

(f) [2 points] Determine ΔX_1, the uncertainty in X_1 for the state $|\psi_{n_1=1,n_2=2}\rangle$ using raising and lowering operators. Discuss the dependence of ΔX_1, on the frequency ω_1 and explain why it makes sense physically.

Aug 2010

Quantum #2

a) Given $H(1,2) = \frac{P_1^2}{2m} + \frac{1}{2}m\omega_1^2 X_1^2 + \frac{P_2^2}{2m} + \frac{1}{2}m\omega_2^2 X_2^2$

$$\bar{X}_n = \sqrt{\frac{m\omega_n}{\hbar}}\, X_n \qquad \bar{P}_n = \sqrt{\frac{1}{\hbar m\omega_n}}\, P_n$$

$$a_n = \frac{1}{\sqrt{2}}(\bar{X}_n + i\bar{P}_n) \qquad a_n^+ = \frac{1}{\sqrt{2}}(\bar{X}_n - i\bar{P}_n)$$

$$\Rightarrow H(1,2) = \frac{(\sqrt{\hbar m\omega_1}\,\bar{P}_1)^2}{2m} + \frac{1}{2}m\omega_1^2\left(\sqrt{\frac{\hbar}{m\omega_1}}\,\bar{X}_1\right)^2 + \frac{(\sqrt{\hbar m\omega_2}\,\bar{P}_2)^2}{2m} + \frac{1}{2}m\omega_2^2\left(\sqrt{\frac{\hbar}{m\omega_2}}\,\bar{X}_2\right)^2$$

$$= \frac{\hbar\omega_1\bar{P}_1^2}{2} + \frac{1}{2}\hbar\omega_1\bar{X}_1^2 + \frac{\hbar\omega_2\bar{P}_2}{2} + \frac{1}{2}\hbar\omega_2\bar{X}_2^2$$

$$= \frac{1}{2}\hbar\omega_1(\bar{X}_1^2 + \bar{P}_1^2) + \frac{1}{2}\hbar\omega_2(\bar{X}_2^2 + \bar{P}_2^2)$$

*Notice: $(a_n + a_n^+)\frac{1}{\sqrt{2}} = \bar{X}_n$

$\frac{-i}{\sqrt{2}}(a_n - a_n^+) = \bar{P}_n$

$$= \frac{1}{2}\hbar\omega_1\left[\frac{1}{2}(a_1+a_1^+)^2 - \frac{1}{2}(a_1-a_1^+)^2\right] + \frac{1}{2}\hbar\omega_2\left[\frac{1}{2}(a_2+a_2^+)^2 - \frac{1}{2}(a_2-a_2^+)^2\right]$$

$$= \frac{1}{4}\hbar\omega_1\left[a_1a_1 + a_1a_1^+ + a_1^+a_1 + a_1^+a_1^+ - a_1a_1 + a_1a_1^+ + a_1^+a_1 - a_1^+a_1^+\right]$$

$$+ \frac{1}{4}\hbar\omega_2\left[a_2a_2 + a_2a_2^+ + a_2^+a_2 + a_2^+a_2^+ - a_2a_2 + a_2a_2^+ + a_2^+a_2 - a_2^+a_2^+\right]$$

$$= \frac{1}{2}\hbar\omega_1(a_1a_1^+ + a_1^+a_1) + \frac{1}{2}\hbar\omega_2(a_2a_2^+ + a_2^+a_2)$$

$$= \frac{1}{2}\hbar\omega_1(2a_1^+a_1 + 1) + \frac{1}{2}\hbar\omega_2(2a_2^+a_2 + 1)$$

$$= \hbar\omega_1(N_1 + 1) + \hbar\omega_2(N_2 + 1), \quad N_n = a_n^+a$$

b) We know: $|\psi_n\rangle = \frac{(a^+)^n}{\sqrt{n!}}|\psi_0\rangle$

$$\hookrightarrow |\psi_{n_1,n_2}\rangle = \frac{(a_1^+)^{n_1}(a_2^+)^{n_2}}{\sqrt{n_1!\,n_2!}}|\psi_{n_1=0}\rangle|\psi_{n_2=0}\rangle$$

$$= \frac{(a_1^+)^{n_1}(a_2^+)^{n_2}}{\sqrt{n_1!\,n_2!}}|\psi_{00}\rangle$$

#2 (cont.)

c) $E_{sys} = E_1 + E_2$

$= \hbar\omega_1(n_1 + 1/2) + \hbar\omega_2(n_2 + 1/2)$

$= \hbar\omega_1(n_1 + 2n_2 + 3/2)$

$= \hbar\omega_1(N + 3/2)$, $N = n_1 + 2n_2$

d) $E_{11} = \frac{9\hbar\omega_1}{2}$ $g =$ $a = n_1 + 2n_2 + 3/2$

$E_{21} = \frac{11\hbar\omega}{2}$ $g =$

$E_{12} = \frac{13\hbar\omega}{2}$ $g =$ $\boxed{g = \frac{a - 3/2}{2} + 1}$

$E_{22} = \frac{15\hbar\omega}{2}$

e) $E_{n_1 n_2} = \frac{15\hbar\omega}{2}$

$\frac{15}{2} = n_1 + 2n_2 + 3/2$

$6 = n_1 + 2n_2 \longrightarrow (n_1, n_2) = \{(0,3); (6,0); (2,2), (4,1)\}$

$g = 4$

f)

PROBLEM 3: Dirac formulation of quantum mechanics

Let $\mathcal{E}_3$ be a three-dimensional Hilbert space that is spanned by the orthonormal basis $\{|u_1\rangle, |u_2\rangle, |u_3\rangle\}$. The operator Ω acts in $\mathcal{E}_3$ as follows:

$$\Omega|u_1\rangle = 3|u_1\rangle \tag{1}$$
$$\Omega|u_2\rangle = 2|u_2\rangle - |u_3\rangle \tag{2}$$
$$\Omega|u_3\rangle = -|u_2\rangle + 2|u_3\rangle \tag{3}$$

(a) [5 pt] Prove that Ω is Hermitian. Find its eigenvalues, ω_1, ω_2, and ω_3, and write down each of the corresponding eigenvectors in the $\{|u_1\rangle, |u_2\rangle, |u_3\rangle\}$ basis.

(b) [1 pt] Does $\{\Omega\}$ constitute a complete set of commuting operators for $\mathcal{E}_3$? Why or why not?

(c) [2 pt] According to Eq. (1), $\mathcal{E}_3$ can be partitioned into eigensubspaces by letting $\mathcal{E}_a$ be the subspace spanned by $\{|u_1\rangle\}$ and $\mathcal{E}_b$ be its orthogonal supplement. Construct an orthonormal basis $\{|t_2\rangle, |t_3\rangle\}$ of $\mathcal{E}_b$, and write each basis vector in $\{|u_1\rangle, |u_2\rangle, |u_3\rangle\}$ basis. (Choose $|t_3\rangle$ to correspond to the *smallest* eigenvalue of Ω.)

(d) [2 pt] With $|t_1\rangle = |u_1\rangle$, the set $\{|t_1\rangle, |t_2\rangle, |t_3\rangle\}$ constitutes an alternate basis of $\mathcal{E}_3$. Find the matrix S, with elements $S_{i,k} = \langle u_i \mid t_k\rangle$, that transforms between $\{|u_1\rangle, |u_2\rangle, |u_3\rangle\}$ and $\{|t_1\rangle, |t_2\rangle, |t_3\rangle\}$.

Aug 2010

Quantum #3

a) * Based on the given info, we can determine Ω has the form

$$\Omega = \begin{array}{c c} & \begin{array}{ccc} |u_1\rangle & |u_2\rangle & |u_3\rangle \end{array} \\ \begin{array}{c} \langle u_1| \\ \langle u_2| \\ \langle u_3| \end{array} & \begin{bmatrix} 3 & 0 & 0 \\ 0 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix} \end{array}$$

The condition for Hermitivity is that $A^+ = A$

$$\Rightarrow \Omega^+ = \begin{bmatrix} 3 & 0 & 0 \\ 0 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix} = \Omega \checkmark$$

* To solve for eigenvalues

$$|\Omega - \lambda \mathbb{I}| = 0$$

$$\hookrightarrow \; 0 = (3-\lambda)[(2-\lambda)^2 - 1]$$

$$= (3-\lambda)[2-\lambda+1][2-\lambda-1]$$

$$\hookrightarrow \; \lambda = 3, 3, 1$$

* To solve for eigenvectors

$$\Omega \vec{v} = \lambda \vec{v} \;\Rightarrow\; \begin{aligned} 3x_1 &= \lambda x_1 \\ 2x_2 - x_3 &= \lambda x_2 \\ -x_2 + 2x_3 &= \lambda x_3 \end{aligned}$$

$\Rightarrow$ if $\lambda = 3$

$$3x_1 = 3x_1$$
$$2x_2 - x_3 = 3x_2$$
$$-x_2 + 2x_3 = 3x_3$$

$$\Rightarrow |u_1\rangle = \langle 1, 0, 0\rangle$$
$$|u_2\rangle = \langle 0, 1, -1\rangle \cdot \tfrac{1}{\sqrt{2}}$$

$\Rightarrow$ if $\lambda = 1$

$$3x_1 = x_1$$
$$2x_2 - x_3 = x_2$$
$$-x_2 + 2x_3 = x_3$$

$$|u_3\rangle = \langle 0, 1, 1\rangle \cdot \tfrac{1}{\sqrt{2}}$$

#3 (cont.)

b) Because Ω has degenerate eigenvalues, it cannot by definition be a complete set of commuting operators

c)

PROBLEM 4: Stationary Perturbation Theory

Consider a non-relativistic particle of mass m moving in the three dimensional potential:

$$V(x) = \frac{1}{2}k(x^2 + y^2 + z^2)\,.$$

(a) [1 point] What is the ground state energy and first excited state energy for this potential?

Now there is a perturbation applied so the potential becomes

$$V(x) = \frac{1}{2}k(x^2 + y^2 + z^2) + \lambda xy$$

where λ is a small parameter.

(b) [1 point] Calculate the ground state energy to first order in λ.

(c) [4 point] Calculate the ground state energy to second order in λ.

(d) [4 point] Calculate the first excited state energies to first order in λ.

PROBLEM 5: Variational Method

In the x-basis, the Hamiltonian for a hydrogen atom is

$$\begin{aligned} H &= \frac{P^2}{2m} - \frac{e^2}{r} \\ &= -\frac{\hbar^2}{2m}\nabla^2 - \frac{e}{r}. \end{aligned}$$

Let us choose

$$\psi_\alpha(r) = e^{-\alpha r^2}, \quad \alpha > 0$$

as a trial wave function for the ground state.

(a) [2 points] Find $\langle \psi_\alpha | \psi_\alpha \rangle$. (**N.B.** This wave function is not normalized.)

(b) [4 points] Find the expectation value of the Hamiltonian $\langle H \rangle$.

(c) [4 points] Determine the best bound on the energy for the ground state of this system using the variational method and the trial wave function given above.

PROBLEM 6: Radioactive Decay

In this problem you will calculate the transmission and reflection coefficients for a simple potential step. Then you will use this result to estimate the tunneling probability through an arbitrary potential. This evaluated tunneling probability is called the Gamow Factor. Finally, you will use the Gamow Factor to explain radioactive decay by calculating the decay probability for an α-particle being emitted from a radioactive nuclei and the mean lifetime for that process.

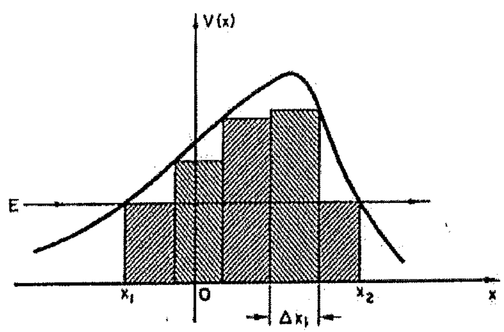
(a) [4 points] **Potential Step:** Calculate the transmission and reflection coefficients for a particle with total energy E interacting with a potential barrier that is a simple potential step ($V_0 > 0$):

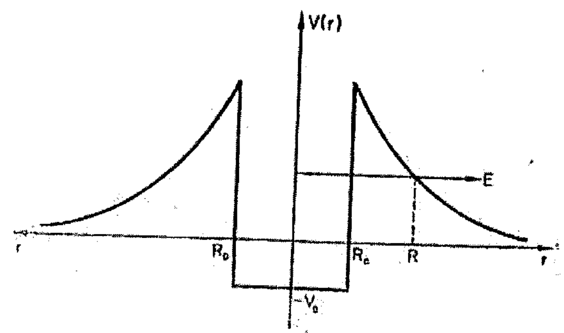
$$V(x) = \begin{cases} 0, & \text{if } x < 0 \\ V_0, & \text{if } 0 < x < a \\ 0, & \text{if } x > a. \end{cases}$$

(b) [3 points] **Arbitrary Potential:** A particle of total energy E interacts with an arbitrary potential barrier $V = V(x)$. The classical turning points are $x = x_1$ and $x = x_2$. Assume the potential curve $V(x)$ is sufficiently smooth, then divide the interval $[x_1, x_2]$ into intervals of length Δx_i, large compared with the relative penetration depth $d_i = \hbar\,[8m(v(x_i) - E)]^{-1/2}$ of a particle in the rectangular barriers. Find an expression for the transmission coefficient T (the Gamow Factor) in this approximate way for the barrier $V = V(x)$, knowing that

$$T_i \approx e^{\left[-\frac{1}{\hbar}\sqrt{8m(V(x_i)-E)}\right]}$$

for the *ith* rectangular barrier.





(c) [3 points] **α-emission of radioactive nuclei:** Now show that α-particles with energies of a few MeV can leave potential wells with depths of tens of MeV. Use a simplified model potential, *i.e.* let $V(r) = -V_0$ if $r < R_0$, and $V(r) = \frac{e_1 e_2}{r}$ if $r > R_0$. Now calculate Gamow's factor for this barrier, *i.e.* the decay probability for emission of α-particles of energy E through the barrier. Express the result in terms of the final velocity of the α-particle, and estimate the mean lifetime of an α-emitting nucleus.

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In spherical coordinates, the Laplacian is

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

PROBLEM 1: Postulates of Quantum Mechanics

A physical system consists of three distinct physical states. For this system, an operator Λ has eigenvalues λ_1, λ_2 and λ_3.

(a) Write down the completeness relation for this system. [2 points]

(b) Apply the completeness relation, then write down the expansion of a general state $|\psi\rangle$ in terms of eigenvectors of Λ [1 point]

(c) What is the probability that a measurement Λ of the state $|\psi\rangle$ yields the value λ_1? [2 points]

(d) A measurement of Λ on the state $|\psi\rangle$ is found to give a value λ_2. What is the state of the system immediately after the measurement? [1 point]

(e) A second measurement of Λ on the system is immediately performed. What is the probability of finding $\langle\Lambda\rangle = \lambda_1$? What is the probability of finding $\langle\Lambda\rangle = \lambda_2$? [2 points]

(f) Let us assume that the Hamiltonian H is time independent. Write down an equation that determines the time evolution of the state $|\psi(t)\rangle$ in the Schrödinger picture. Write down an equation that determines the time evolution of $\Lambda(t)$ in the Heisenberg picture. [2 points]

Aug 2011

Quantum #1

a) The completeness relation for any system is such that

$$1 = \sum_i |\lambda_i\rangle\langle\lambda_i|$$

$\Rightarrow$ For this system where we define the kets as $|\lambda_1\rangle, |\lambda_2\rangle, |\lambda_3\rangle$ (in Λ-basis)

$$1 = |\lambda_1\rangle\langle\lambda_1| + |\lambda_2\rangle\langle\lambda_2| + |\lambda_3\rangle\langle\lambda_3|$$

b) To expand the state, we use the projection operator $\tilde{P} = 1$

$\hookrightarrow$ $P|\psi\rangle = \langle\lambda_1|\psi\rangle|\lambda_1\rangle + \langle\lambda_2|\psi\rangle|\lambda_2\rangle + \langle\lambda_3|\psi\rangle|\lambda_3\rangle$

c) $|\langle\lambda_1|1|\psi\rangle|^2$

d) Assuming the system is defined in the Λ eigenbasis, we would expect to find $|\psi\rangle = |\lambda_2\rangle$ immediately after measurement

e) λ_1: $|\langle\lambda_1|\Lambda|\lambda_2\rangle| = 0$

λ_2 $|\langle\lambda_2|\Lambda|\lambda_2\rangle| = |\lambda_2|^2$

f) $|\psi(t)\rangle = \exp[iHt/\hbar]|\psi\rangle$

$\Lambda(t) = e^{+iHt/\hbar}\,\Lambda\, e^{-iHt/\hbar}$

PROBLEM 2: Harmonic Oscillator

A particle of mass m is confined to one dimension. Its potential energy is

$$V(x) = \frac{1}{2} m \, \omega^2 x^2,$$

where $\omega > 0$ is a real parameter. At time $t = 0$, the state of the particle is represented by the real wave function

$$\Psi(x, 0) = \frac{1}{\sqrt{2}} \left(1 - \frac{x}{|x|} \right) \phi(x),$$

where $\phi(x)$ is a normalized function of odd parity.

On each question, to receive *any* credit you must fully justify your answer.

(a) At $t = 0$, what is value of the *position probability density* $\mathcal{P}(x, 0)$ at the origin, $x = 0$? [2 points]

(b) **Describe** the *parity* of the wave function at $t = 0$ and at any $t > 0$. [2 points]

(c) The *region probability* $\mathcal{P}\big([a, b], t \big)$ denotes the probability that a position measurement at time t would detect the particle in the finite region $x \in [a, b]$. What are the *initial values* of this quantity for the left and right halves of the x axis: $\mathcal{P}\big((-\infty, 0\,], 0 \big)$ and $\mathcal{P}\big([0, \infty), t \big)$? [2 points]

(d) At what time $t_{\text{right}} > 0$, *if any*, is $\mathcal{P}\big([0, \infty), t_{\text{right}} \big) = 1$? [1 point]

(e) At what time $t_{\text{left}} > 0$, *if any*, is $\mathcal{P}\big((-\infty, 0\,], t_{\text{left}} \big) = 1$? [1 point]

(f) At what time $t_{\text{same}} > 0$, *if any*, are the two region probabilities equal:
$\mathcal{P}\big((-\infty, 0\,], t_{\text{same}} \big) = \mathcal{P}\big([0, \infty), t_{\text{same}} \big)$? [2 points]

PROBLEM 3: Angular Momentum Operators

Consider a state space formed from the direct sum of the two subspaces: $\mathcal{E}$(j=0) spanned by $|j=0, m_y=0\rangle$ and $\mathcal{E}$(j=1) spanned by $|j=1, m_y=1\rangle, |j=1, m_y=0\rangle$, and $|j=1, m_y=-1\rangle$,: i.e.

$$\mathcal{E} = \mathcal{E}(\mathrm{j}=1) \oplus \mathcal{E}(\mathrm{j}=0)$$

where

$$J^2|j, m_y\rangle = j(j+1)\hbar^2|j, m_y\rangle$$
$$J_y|j, m_y\rangle = m_y\hbar|j, m_y\rangle$$

Let

$$|\Psi\rangle = \frac{1}{\sqrt{5}}|j=1, m_y=1\rangle + \frac{\sqrt{3}}{\sqrt{10}}|j=1, m_y=0\rangle - \frac{1}{\sqrt{2}}|j=0, m_y=0\rangle$$

(a) Consider the measurement of the two observables J^2 and J_y. Do these observables commute? Demonstrate explicitly the value of the commutator of J^2 and J_y. **(2 points]**

(b) Determine the probability of measuring J^2 and getting $2\hbar^2$, i.e. determine $P_{|\Psi\rangle}(2\hbar^2 \text{ for } \mathrm{J}^2)$. What is the resulting normalized state vector, $|\Psi'\rangle$ after this measurement? **(2 points]**

(c) If J_y is then measured after the measurement in part (b), what is the probability of obtaining $m_y = 0$, i.e. what is $P_{|\Psi'\rangle}(0 \text{ for } \mathrm{J_y})$? What is the resulting normalized state vector after this measurement? [2 points]

(d) What is the composite probability of measuring J^2 and getting $2\hbar^2$ and then measuring J_y and getting zero, i.e. what is $P_{|\Psi\rangle}(2\hbar^2 \text{ for } \mathrm{J}^2, 0 \text{ for } \mathrm{J_y})$? **(1 point)**

(e) Now starting with the original $|\Psi\rangle$ reverse the measurements, measuring J_y first and getting zero, and then measuring J^2 and getting $2\hbar^2$. Determine four quantities: 1) $P_{|\Psi\rangle}(0 \text{ for } \mathrm{J_y})$; 2) the resulting normalized state $|\Psi''\rangle$; 3) $P_{|\Psi''\rangle}(2\hbar^2 \text{ for } \mathrm{J}^2)$; and 4) the final normalized state after both measurements have been taken. [2 points]

(f) What is the new composite probability when the measurements are reversed, i.e. what is: $P_{|\Psi\rangle}(0 \text{ for } \mathrm{J_y}, 2\hbar^2 \text{ for } \mathrm{J}^2)$? Are your two composite probabilities the same or different? Discuss in detail. [1 point]

PROBLEM 4: Spin Angular Momentum

A Stern-Gerlach experiment is set up with the axis of the inhomogeneous magnetic field in the $x-y$ plane, at an angle θ relative to the x−axis. Let us call this direction $\hat{r} = \cos\theta\hat{x} + \sin\theta\hat{y}$. Then the spin operator in the $\hat{r}$ direction is $S_r = \cos\theta S_x + \sin\theta S_y$. Let us describe the common eigenvectors for S^2 and S_i as $|s, m_i\rangle$, e.g. $|s, m_x\rangle$ or $|s, m_z\rangle$.

(a) For a spin−1/2 particle, calculate the matrix corresponding to S_r. [1 point]

(b) Evaluate the eigenvalues of S_r. [1 point]

(c) Find the normalized eigenvectors of S_r. [2 points]

(d) Suppose a measurement of the spin of the particle in the $\hat{r}$ direction is made and it is determined that the spin is in the positive $\hat{r}$ direction, i.e. $S_r|\psi\rangle = (+\hbar/2)|\psi\rangle$. Now a second measurement is made to determine m_x (the component of the spin in the x direction). What is the probability that $m_x = -1/2$? [3 points]

(e) Suppose that the particle has spin in the positive $\hat{r}$ direction as in part (d). The z component of the spin is measured and it is discovered that $m_z = +1/2$. Now a third measurement is made to determine m_x. What is the probability that $m_x = -1/2$? [3 points]

PROBLEM 5: Stationary Perturbation Theory

Consider a particle of mass m confined in a 2D infinite square well:

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

with energy eigenfunctions

$$\psi_{n_x,n_y}(x,y) = \frac{2}{L} \sin\left(\frac{n_x \pi}{L} x\right) \sin\left(\frac{n_y \pi}{L} y\right) .$$

(a) What are the energies and degeneracies of the first four energy levels (eigenenergies) of the particle? Explain your answer. [1 point]

Impurities in the well will shift these energy levels. Assume we can model the effect of an impurity through a local potential:

$$W(x,y) = -V_0 \; L \; \delta(x - x_0)\delta(y - y_0)$$

where the point (x_0, y_0) is the position of the impurity.

(b) For the case where $x_0 = y_0 = L/2$, what are the energy shifts (including splitting of energy levels) to first order in V_0 for the first two energy levels of the particle? Show your work. [3 points]

Which of the energy eigenstates will not be changed by this impurity? Explain. (You should not have to do any calculations to answer this second question.)

(c) Again for $x_0 = y_0 = L/2$, what is the shift in the ground state energy that is second order in V_0? You should write your result in terms of sums, and approximate the result by summing over the largest terms. [3 points]

(d) For the case where $x_0 = L/3$ and $y_0 = L/4$, what are the energy shifts (including splitting of energy levels) to first order in V_0 for the first two energy levels of the particle? Show your work. [3 points]

PROBLEM 6: Variational Method

Consider a Hamiltonian H that may or may not be solved exactly. The variational theorem states that the expectation value of energy obtained from a trial wavefunction will always be greater than or equal to the ground state energy.

Consider a trial wave function ϕ consisting of two basis wavefunctions Ψ_1 and Ψ_2 such that

$$\phi = c_1\Psi_1 + c_2\Psi_2$$

where c_1 and c_2 are constants.

(a) Find the expectation value of the energy for this system. [1 point]

(b) Now assume $\langle\Psi_1|\Psi_2\rangle = \langle\Psi_2|\Psi_1\rangle = 0$, $\langle\Psi_1|H|\Psi_2\rangle = \langle\Psi_2|H|\Psi_1\rangle$ and c_1 and c_2 are real. Determine a 2x2 matrix relationship for the best bound on the energy. [3 points]

(c) Now also assume Ψ_1 and Ψ_2 are orthonormal. Solve the matrix relationship you found in part (b) to determine 2 solutions for the best bound energy. [2 points]

(d) Note that there are 2 solutions to the best bound energy found in part (c). What additional constraint can you apply to remove one of the solutions? [2 points]

(e) Confirm your answer to part (c) by using a Simple Harmonic Oscillator Hamiltonian and setting Ψ_1 to be the ground state eigenfunction and Ψ_2 to be the first excited state eigenfunction of the Simple Harmonic Oscillator [2 points]

Quantum Mechanics
Qualifying Exam–January 2012

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Possibly useful formulas:

Pauli spin matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

One-dimensional simple harmonic oscillator operators:

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

$$P = -i\sqrt{\frac{\hbar m\omega}{2}}(a - a^\dagger)$$

Spherical Harmonics:

$$Y_0^0(\theta,\varphi) = \tfrac{1}{\sqrt{4\pi}} \qquad Y_2^2(\theta,\varphi) = \tfrac{5}{\sqrt{96\pi}}\, 3\sin^2\theta\, e^{2i\varphi}$$

$$Y_2^1(\theta,\varphi) = -\tfrac{5}{\sqrt{24\pi}}\, 3\sin\theta\cos\theta\, e^{i\varphi}$$

$$Y_1^1(\theta,\varphi) = -\tfrac{3}{\sqrt{8\pi}}\sin\theta\, e^{i\varphi} \qquad Y_2^0(\theta,\varphi) = \tfrac{5}{\sqrt{4\pi}}\left(\tfrac{3}{2}\cos^2\theta - \tfrac{1}{2}\right)$$

$$Y_1^0(\theta,\varphi) = \tfrac{3}{\sqrt{4\pi}}\cos\theta \qquad Y_2^{-1}(\theta,\varphi) = \tfrac{5}{\sqrt{24\pi}}\, 3\sin\theta\cos\theta\, e^{-i\varphi}$$

$$Y_1^{-1}(\theta,\varphi) = \tfrac{3}{\sqrt{8\pi}}\sin\theta\, e^{-i\varphi} \qquad Y_2^{-2}(\theta,\varphi) = \tfrac{5}{\sqrt{96\pi}}\, 3\sin^2\theta\, e^{-2i\varphi}$$

In spherical coordinates, the Laplacian is

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

PROBLEM 1: Stationary States

For a quantum system with a time independent Hamiltonian ($\mathbf{H}$), the wave function ($\Psi(x,t)$) is a linear combination of stationary state solutions ($\Psi_n(x,t)$) to the Schrödinger equation:

$$\Psi_n(x,t) = u_n(x)\exp\left(-iE_n t/\hbar\right)$$

where $u_n(x)$ are eigenfunctions of the Hamiltonian

$$\mathbf{H}u_n(x) = E_n u_n(x)$$

and they form a complete orthonormal basis.

(a) Evaluate the uncertainty in the energy for a system in a stationary state with the wave function $\Psi(x,t) = \Psi_n(x,t)$. [Show all work.] (2 Points)

(b) Derive the time evolution operator $\mathbf{U}(t,t_0)$ in terms of the Hamiltonian ($\mathbf{H}$), and apply it to a stationary state $\Psi_n(x, t_0 = 0)$. Describe the change in the stationary state. (2 Points)

Now consider a particle that starts out in a normalized wave function

$$\Psi(x,0) = c_1u_1(x) + c_2u_2(x)$$

where the $u_n(x)$ are real eigenfunctions of the Hamiltonian and c_n are real.

(c) Determine an expression for the wave function $\Psi(x,t)$ at subsequent times. (2 Points)

(d) Evaluate the probability density and describe its motion in time. (3 Points)

(e) Determine the uncertainty in the energy ΔE with $\Delta t = \tau$ that is the period of oscillation in (d). (1 Points)

PROBLEM 2: Dirac Notation in Quantum Mechanics

Consider the kets $|a_n\rangle$ as the eigenstates of an observable operator $\mathbf{A}$

$$\mathbf{A}|a_n\rangle = a_n|a_n\rangle\,.$$

Assume that $|a_n\rangle$ form a discrete orthonormal basis in the vector space. Define an operator $U(m,n)$ as

$$U(m,n) = |a_m\rangle\langle a_n|.$$

(a) Show that $U(m,n)$ is an Hermitian operator. Calculate the commutator $[A, U(m,n)]$. [2 Points]

(b) For a generic operator with matrix elements $B_{mn} = \langle a_m|B|a_n\rangle$, show that

$$B = \sum_{mn} B_{mn} U(m,n).$$

[2 Points]

(c) Assume the Hamiltonian of a three-level system

$$\mathbf{H} = H_{12}U(1,2) + H_{21}U(2,1) + H_{23}U(2,3) + H_{32}U(3,2)$$

where $H_{12} = H_{23}$, and $H_{21} = H_{32}$ are complex numbers with dimension of energy. Find the eigenvectors and the eigenvalues of the Hamiltonian in the $|a_n\rangle$ basis. [4 Points]

(d) Assuming the Hamiltonian above, and $n = 1, 2, 3$, find the condition where the observable operator A is time independent. [2 Points]

Jan 2012

Quantum #2

a) * The condition for Hermiticity is $A^{\dagger} = A$

$$U(m,n)^{\dagger} = \left[|a_m\rangle\langle a_n| \right]^{\dagger}$$

$$= |a_m\rangle^{\dagger} \langle a_n|^{\dagger}$$

$$= |a_n\rangle\langle a_m|$$

$$= U(n,m) \quad \text{as expected}$$

* To evaluate the commutator, we act it upon the state $|a_n\rangle$

$$\Rightarrow [A, U(m,n)]|a_n\rangle = AU(m,n) - U(m,n)A\, |a_n\rangle$$

$$= AU(m,n)|a_n\rangle - U(m,n)A|a_n\rangle$$

$$= A\, |a_m\rangle\langle a_n|a_n\rangle - |a_m\rangle\langle a_n|A|a_n\rangle$$

$$= A\, |a_m\rangle - a_n |a_m\rangle\langle a_n|a_n\rangle$$

$$= a_m|a_m\rangle - a_n|a_m\rangle$$

$$= (a_n - a_m)|a_n\rangle \quad \text{(indexes arbitrary, so we switch order)}$$

$$\hookrightarrow [A, U(m,n)] = a_n - a_m$$

b) We want to show: $B = \sum_{mn}' B_{mn} U(m,n)$ where $B_{mn} = \langle a_m|B|a_n\rangle$

$$\hookrightarrow \sum_{mn}' B_{mn} U(m,n) = \sum_{mn}' \langle a_m|B|a_n\rangle |a_m\rangle\langle a_n|$$

* To determine matrix elements of B, we use completeness relation

$$B = \sum_{m,n}' |a_m\rangle\langle a_m|B|a_n\rangle\langle a_n|$$

$$= \sum_{m,n}' \langle a_m|B|a_n\rangle |a_m\rangle\langle a_n|$$

$$\Rightarrow B = \sum_{mn}' B_{mn} U(m,n)$$

#2 (cont.)

c) Given $H = H_{12}\,U(1,2) + H_{21}\,U(2,1) + H_{23}\,U(2,3) + H_{32}\,U(3,2)$, we can rewrite H as:

$$H \doteq \begin{array}{c} \begin{matrix} |a_1\rangle & |a_2\rangle & |a_3\rangle \end{matrix} \\ \begin{bmatrix} 0 & H_{12} & 0 \\ H_{21} & 0 & H_{23} \\ 0 & H_{32} & 0 \end{bmatrix} \end{array}$$

$$0 = \begin{vmatrix} -\lambda & H_{12} & 0 \\ H_{21} & -\lambda & H_{23} \\ 0 & H_{32} & -\lambda \end{vmatrix}.$$

$$0 = -\lambda(\lambda^2 - H_{23}H_{32}) - H_{12}(-H_{21}\lambda)$$
$$= -\lambda^3 + H_{23}H_{32}\lambda + H_{12}H_{21}\lambda$$
$$= -\lambda^3 + 2H_{12}H_{21}\lambda$$
$$= -\lambda(\lambda^2 - 2H_{12}H_{21})$$

$\hookrightarrow \lambda = 0,\ +\sqrt{2H_{12}H_{21}},\ -\sqrt{2H_{12}H_{21}}$

* To find eigenvectors:

$H\vec{v} = \lambda\vec{v}$

$$\begin{bmatrix} 0 & H_{12} & 0 \\ H_{21} & 0 & H_{12} \\ 0 & H_{21} & 0 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \lambda\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \Rightarrow \begin{aligned} H_{12}x_2 &= \lambda x_1 \\ H_{21}x_1 + H_{12}x_3 &= \lambda x_2 \\ H_{21}x_2 &= \lambda x_3 \end{aligned}$$

* for $\lambda = 0$

$H_{12}x_2 = 0$

$H_{21}x_1 + H_{12}x_3 = 0$

$H_{21}x_2 = 0$

* for $\lambda = \sqrt{2H_{12}H_{21}}$

$H_{12}x_2 = \sqrt{2H_{12}H_{21}}\,x_1$

$H_{21}x_1 + H_{12}x_3 = \sqrt{2H_{12}H_{21}}\,x_2$

$H_{21}x_2 = \sqrt{2H_{12}H_{21}}\,x_3$

* for $\lambda = -\sqrt{2H_{12}H_{21}}$

$H_{12}x_2 = -\sqrt{2H_{12}H_{21}}\,x_1$

$H_{21}x_1 + H_{12}x_3 = -\sqrt{2H_{12}H_{21}}\,x_2$

$H_{21}x_2 = -\sqrt{2H_{12}H_{21}}\,x_3$

$$\Rightarrow \vec{v} = \begin{bmatrix} H_{12} \\ 0 \\ H_{21} \end{bmatrix}\frac{1}{\sqrt{H_{12}H_{21}}}$$

$$= \frac{1}{\sqrt{H_{12}H_{21}}}\left(H_{12}|a_1\rangle + H_{21}|a_3\rangle\right)$$

PROBLEM 3: Harmonic Oscillator

A particle of mass m is under the influence of the following potential

$$V(x) = V_0\sqrt{A^2 + x^2}$$

where V_0 and A are constants. For small displacements $x \ll A$ this potential can be approximated by a simple harmonic oscillator.

(a) Determine the lowest energy this particle can have in terms of $\hbar$, m, V_0 and a for $x \ll A$. (2 Points)

Now consider the Hamiltonian describing the true one-dimensional harmonic oscillator

$$\mathbf{H} = \frac{\mathbf{P}^2}{2m} + \frac{1}{2}k\mathbf{X}^2$$

with eigenstates

$$\mathbf{H}|n\rangle = E_n|n\rangle \quad n = 0, 1, 2, \cdots .$$

(b) Using commutation relations, calculate the equations of motion for $\mathbf{P}$ and $\mathbf{X}$ in the Heisenberg picture. (Find $\dot{X}$ and $\dot{P}$.) (2 Points)

(c) Solve for $P(t)$ and $X(t)$ in terms of $P(0)$ and $X(0)$ and show that $[X(t), X(0)] \neq 0$ for $t \neq 0$. (2 Points)

A harmonic oscillator system is known to be in the state

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |3\rangle)$$

where $|0\rangle$ and $|3\rangle$ are the normalized ground state and the third excited state of the harmonic oscillator respectively.

(d) What is the value of $n > 0$ for the first non-zero value of $\langle X^n\rangle$ with the state vector $|psi\rangle$? (2 Points)

(e) What is the expectation value $\langle X^3\rangle$ with the state vector $|\psi\rangle$? (2 Points)

PROBLEM 4: Angular Momentum

The hydrogen atom including hyperfine splitting can be described by a Hamiltonian

$$\mathbf{H} = \frac{\mathbf{P}_p^2}{2m_p} + \frac{\mathbf{P}_e^2}{2m_e} - \frac{e^2}{r} + \mathbf{H}_{HF}$$

where $\mathbf{H}_{HF} = A\vec{S}_p \cdot \vec{S}_e$ describes the spin-spin or hyperfine interaction and the total spin angular momentum is given by $\vec{S} = \vec{S}_p + \vec{S}_e$. The subscripts ($p$ and e) refer to proton and electron, respectively

(a) Write down the form of the spin-spin direct product state vectors. What are the "good", *i.e.* diagonal operators for this set of state vectors? [2 points]

(b) Write down the form of the "total-s" state vectors. What are the "good", *i.e.* diagonal operators for this set of state vectors? [2 points]

(c) Choosing an appropriate set of state vectors, calculate the H_{HF} energy eigenvalues, and the energy splitting due to the hyperfine interaction. [5 points]

(d) If the photon wavelength (λ) is 21 cm from the hyperfine transition, evaluate the constant A in H_{HF}. *Hint:* $\hbar c = 1.97 \times 10^{-5}$ $eV{\cdot}cm$. [1 point]

PROBLEM 5: Interaction Picture

There is a 3rd 'picture' in quantum mechanics in addition to the Schrödinger and Heisenberg pictures that is often used. This picture is called the interaction picture. The interaction picture is related to the Schrödinger picture through the following unitary transformation for a Hamiltonian, $H = H_0 + V$.

$$\Psi_I(x,t) = \mathbf{U}_0^{-1}\Psi_S(x,t)$$

where

$$\mathbf{U}_0 = e^{-\frac{i}{\hbar}(t-t_0)H_0}\,.$$

The Hamiltonian $\mathbf{H}_0$ is assumed to be time independent, V is considered to be small in comparison to $\mathbf{H}_0$, I denotes interaction picture and S denotes Schrödinger picture, t_0 is the time when the two pictures coincide (you can take this to be $t_0 = 0$) and t is the time from when the two pictures coincide.

(a) Use this information to find the equation, analogous to the Schrödinger equation, that gives the time evolution for Ψ_I. To receive full credit justify all steps. (4 Points)

(b) How are operators in the interaction picture ($\mathbf{\Omega}_I$) and the Schrödinger picture ($\mathbf{\Omega}_S$) related? (2 Points)

(c) These 2 pictures are related to each other through a unitary transformation. In general, what is a unitary transformation and what are the important quantities that a unitary transformation preserves? (3 Points)

(d) Why do you think this is called the interaction picture? Why is it useful? To receive credit you must explain how the name relates to the dynamics. (1 Points)

PROBLEM 6: Stationary Perturbation Theory

Let us consider the Hamiltonian $\mathbf{H}$ for a harmonic oscillator with a charged particle in a constant electric field (E):

$$\begin{aligned} \mathbf{H} &= \mathbf{H}_0 + \mathbf{H}_1 \\ \mathbf{H}_0 &= \frac{\mathbf{P}^2}{2m} + \frac{1}{2}k\mathbf{X}^2 \quad \text{and} \\ \mathbf{H}_1 &= \lambda \mathbf{X} \end{aligned}$$

where $\lambda = qE$ and q is the electric charge.

The non-perturbed Hamiltonian has the following eigenvalue equation

$$\mathbf{H}_0|n\rangle = E_n^{(0)}|n^{(0)}\rangle\,, \quad E_n^{(0)} = \hbar\omega(n+\frac{1}{2}) \quad \text{and} \quad \omega = \sqrt{k/m}\,.$$

(a) Apply perturbation theory and determine the first order energy $E_n^{(1)}$. [2 Points]

(b) Apply perturbation theory and evaluate the second order energy $E_n^{(2)}$. [3 Points]

(c) Solve this problem exactly and find the energy E_n. [3 Points]

(d) Determine the eigenvector to the first order $|n\rangle = |n^{(0)}\rangle + |n^{(1)}\rangle$. [2 Points]

Quantum Mechanics
Qualifying Exam–August 2012

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Pauli spin matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

One-dimensional simple harmonic oscillator operators:

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

$$P = -i\sqrt{\frac{\hbar m\omega}{2}}(a - a^\dagger)$$

Spherical Harmonics:

$$Y_0^0(\theta,\varphi) = \frac{1}{\sqrt{4\pi}} \qquad Y_2^2(\theta,\varphi) = \frac{5}{\sqrt{96\pi}}\, 3\sin^2\theta\, e^{2i\varphi}$$

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$$Y_1^0(\theta,\varphi) = \frac{3}{\sqrt{4\pi}}\cos\theta \qquad Y_2^{-1}(\theta,\varphi) = \frac{5}{\sqrt{24\pi}}\, 3\sin\theta\cos\theta\, e^{-i\varphi}$$

$$Y_1^{-1}(\theta,\varphi) = \frac{3}{\sqrt{8\pi}}\sin\theta\, e^{-i\varphi} \qquad Y_2^{-2}(\theta,\varphi) = \frac{5}{\sqrt{96\pi}}\, 3\sin^2\theta\, e^{-2i\varphi}$$

In spherical coordinates, the Laplacian is

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

PROBLEM 1: Eigenvalue Equation and Time Evolution

The Hamiltonian for a certain three-level system is represented by the matrix

$$H = \begin{pmatrix} a & 0 & b \\ 0 & c & 0 \\ b & 0 & a \end{pmatrix},$$

where a, b, and c are real numbers and $a - c \neq \pm b$. $\Rightarrow$ $c \neq a \mp b$

(a) Find the eigenvalues E_n and normalized eigenvectors $|E_n\rangle, n = 1, 2, 3$ of H. [4 points]

(b) If the system starts out in the state

$$|\psi(0)\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix},$$

what is $|\psi(t)\rangle$? [3 points]

(c) If the system starts out in the state

$$|\psi(0)\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix},$$

what is $|\psi(t)\rangle$? [3 points]

Aug 2012

Quantum #1

a) $H = \begin{bmatrix} a & 0 & b \\ 0 & c & 0 \\ b & 0 & a \end{bmatrix}$

* To find eigenvalues, we solve characteristic equation

$\det(H - \lambda \mathbb{I}) = 0$

$$\begin{vmatrix} a-\lambda & 0 & b \\ 0 & c-\lambda & 0 \\ b & 0 & a-\lambda \end{vmatrix} = a-\lambda\left[(c-\lambda)(a-\lambda) - 0\right] - 0\left[0(a-\lambda) - 0(b)\right] + b\left[0 - b(c-\lambda)\right]$$

$$= (a-\lambda)^2(c-\lambda) - b^2(c-\lambda)$$

$$= (c-\lambda)\left[(a-\lambda^2) - b^2\right]$$

$$= (c-\lambda)(a-\lambda+b)(a-\lambda-b)$$

$\hookrightarrow \boxed{\lambda = c,\ a-b,\ a+b}$

* To find eigenvectors, we solve $H\vec{v} = \lambda\vec{v}$

$$\Rightarrow \begin{bmatrix} a & 0 & b \\ 0 & c & 0 \\ b & 0 & a \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} ax_1 + bx_3 \\ cx_2 \\ bx_1 + ax_3 \end{bmatrix}$$

* Case $\lambda = c$

$ax_1 + bx_3 = cx_1$

$cx_2 = cx_2$

$bx_1 + ax_3 = cx_3$

$\hookrightarrow b = 0$

$c = 1 \neq a$

$\Rightarrow V_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$

Case $\lambda = a-b$

$ax_1 + bx_3 = (a-b)x_1$

$cx_2 = (a-b)x_2$

$bx_1 + ax_3 = (a-b)x_3$

$b = 0,\ c \neq a$

$\hookrightarrow x_2 = 0$

$bx_3 = -bx_1$

$bx_1 = -bx_3$

$V_1 = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$

Case $\lambda = a+b$

$ax_1 + bx_3 = (a+b)x_1$

$cx_2 = a+b\,x_2$

$bx_1 + ax_3 = (a+b)x_3$

$b = 0,\ c \neq a$

$\hookrightarrow x_2 = 0$

$bx_3 = bx_1$

$bx_1 = bx_3$

$V_3 = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 0 \\ +1 \end{bmatrix}$

#1 (cont)

b) $U(t,0) = \exp\left[-\frac{i}{\hbar} Ht\right]$

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

$*$ substituting $|\psi(0)\rangle = |c\rangle = c\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$

$$= e^{-iHt/\hbar} |c\rangle$$
$$= e^{-ict/\hbar} |c\rangle$$ (after taylor expansion to act out operator)

c) $|\psi(0)\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = \sqrt{2}\left(|a+b\rangle - |a-b\rangle\right)$ where $|a+b\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}$, $|a-b\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$

$= \sqrt{2}$

$$\hookrightarrow |\psi(t)\rangle = U(t,0)|\psi(0)\rangle$$
$$= e^{-iHt/\hbar}\left(\sqrt{2}|a+b\rangle - \sqrt{2}|a-b\rangle\right)$$
$$= \sqrt{2}\left[e^{-i(a+b)t/\hbar}|a+b\rangle - e^{-i(a-b)t/\hbar}|a-b\rangle\right]$$ (taylor expand exponential to act operator as above)

PROBLEM 2: Generalized Uncertainty Principle

Consider the spin 1/2 operator

$$\mathbf{S} = \frac{\hbar}{2}\vec{\sigma},$$

where $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is a vector of Pauli matrices, which are defined in the basis of the S_z operator eigenvectors,

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

(a) Compute the commutator $[S_i, S_j]$, with $i, j = x, y, z$. [2 Points]

(b) Compute the expectation values $\langle(\delta S_x)^2\rangle$ and $\langle(\delta S_y)^2\rangle$ for the state

$$|\alpha\rangle = \cos(\alpha)|+\rangle + \sin(\alpha)|-\rangle,$$

where $\delta\mathbf{S} = \mathbf{S} - \langle\mathbf{S}\rangle$. Show explicitly that the relation

$$\langle(\delta S_x)^2\rangle\langle(\delta S_y)^2\rangle \geq \frac{1}{4}\,|\langle[S_x, S_y]\rangle|^2$$

is satisfied. What does it physically mean? [4 Points]

(c) Find the states that maximize and minimize the product $\langle(\delta S_x)^2\rangle\langle(\delta S_y)^2\rangle$. Interpret the results. [2 Points]

(d) Suppose one performs an experiment which filters the $+\hbar/2$ eigenstate of the S_z operator from the initially prepared state $|\alpha\rangle$. Then the S_x component of the spin is measured. Compute the expectation value of this measurement in the state $|\alpha\rangle$. [2 Points]

Aug 2012

Quantum #2

a) It is well known that $[S_i, S_j] = i\hbar S_k$

$$\Rightarrow S_x = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad S_y = \frac{\hbar}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad S_y = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Proof! $[S_x, S_y] = S_x S_y - S_y S_x$

* Continues as such for other pairs and can be proved quickly on exam

$$= \left(\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} - \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\right)\frac{\hbar^2}{4}$$

$$= \left(\begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix} - \begin{bmatrix} -i & 0 \\ 0 & i \end{bmatrix}\right)\frac{\hbar^2}{4}$$

$$= \frac{\hbar^2}{4}\begin{bmatrix} 2i & 0 \\ 0 & -2i \end{bmatrix}$$

$$= \frac{i\hbar^2}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$= i\hbar S_z$$

b) Using $|\alpha\rangle = \cos(\alpha)|+\rangle + \sin(\alpha)|-\rangle$, find $\langle(\delta S_x)^2\rangle \langle(\delta S_y)^2\rangle$

* Note! $\langle(\delta A)^2\rangle = \langle A^2\rangle - \langle A\rangle^2$

$$\Rightarrow \langle(\delta S_x)^2\rangle = \langle S_x^2\rangle - \langle S_x\rangle^2$$

$$= [\cos(\alpha)\ \sin(\alpha)]\begin{bmatrix} \hbar^2/4 & 0 \\ 0 & \hbar^2/4 \end{bmatrix}\begin{bmatrix} \cos(\alpha) \\ \sin\alpha \end{bmatrix} - \left([\cos(\alpha)\ \sin(\alpha)]\begin{bmatrix} 0 & \hbar/2 \\ \hbar/2 & 0 \end{bmatrix}\begin{bmatrix} \cos\alpha \\ \sin\alpha \end{bmatrix}\right)^2$$

$$= [\cos\alpha\ \sin\alpha]\begin{bmatrix} \hbar^2/4 \cos\alpha \\ \hbar^2/4 \sin\alpha \end{bmatrix} - \left([\cos\alpha\ \sin\alpha]\begin{bmatrix} \hbar/2 \sin\alpha \\ \hbar/2 \cos\alpha \end{bmatrix}\right)^2$$

$$= \hbar^2/4 - (\cdot\,\hbar \sin\alpha \cos\alpha)^2$$

$$= \hbar^2\left(\frac{1}{4} - \sin^2\alpha \cos^2\alpha\right)$$

$$= \frac{\hbar^2}{4}\left(1 - \frac{1-\cos(4\alpha)}{2}\right)$$

$$= \frac{\hbar^2}{4}\left(\frac{1}{2} - \cos(4\alpha)\right)$$

$$= \frac{\hbar^2}{8}(1 - \cos(4\alpha))$$

#2 (cont.)

b) $\langle(\delta S_y)^2\rangle = \langle S_y^2\rangle - \langle S_y\rangle^2$

$$= \hbar^2/4 - \left(\begin{bmatrix}\cos\alpha & \sin\alpha\end{bmatrix}\begin{bmatrix}0 & -\frac{i\hbar}{2}\\ \frac{i\hbar}{2} & 0\end{bmatrix}\begin{bmatrix}\cos\alpha\\ \sin\alpha\end{bmatrix}\right)^2$$

$$= \frac{\hbar^2}{4} - \left(\begin{bmatrix}\cos\alpha & \sin\alpha\end{bmatrix}\begin{bmatrix}-\frac{i\hbar}{2}\sin\alpha\\ \frac{i\hbar}{2}\cos\alpha\end{bmatrix}\right)^2$$

$$= \frac{\hbar^2}{4} - \left(-\frac{i\hbar}{2}\sin\alpha\cos\alpha + \frac{i\hbar}{2}\cos\alpha\sin\alpha\right)^2$$

$$= \frac{\hbar^2}{4}$$

$$\frac{1}{4}|\langle[S_x, S_y]\rangle|^2 = \frac{1}{4}|\langle S_z\rangle|^2$$

$$= \frac{1}{4}\left|\begin{bmatrix}\cos\alpha & \sin\alpha\end{bmatrix}\begin{bmatrix}\hbar/2 & 0\\ 0 & -\hbar/2\end{bmatrix}\begin{bmatrix}\cos\alpha\\ \sin\alpha\end{bmatrix}\right|^2$$

$$= \frac{1}{4}\left|\begin{bmatrix}\cos\alpha & \sin\alpha\end{bmatrix}\begin{bmatrix}\hbar/2\cos\alpha\\ -\hbar/2\sin\alpha\end{bmatrix}\right|^2$$

$$= \frac{1}{4}\left|\frac{\hbar}{2}(\cos^2\alpha - \sin^2\alpha)\right|^2$$

$$= \frac{\hbar^2}{16}(\cos^4\alpha - 2\cos^2\alpha\sin^2\alpha + \sin^4\alpha)$$

$$\Rightarrow \langle(\delta S_x)^2\rangle\langle(\delta S_y)^2\rangle \overset{?}{\geq} \frac{1}{4}|\langle[S_x, S_y]\rangle|^2$$

$$\frac{\hbar^2}{4}\left(\frac{\hbar^2}{4} - \hbar^2\sin^2\alpha\cos^2\alpha\right) \overset{?}{\geq} \frac{\hbar^2}{16}(\cos^4\alpha - 2\cos^2\alpha\sin^2\alpha + \sin^4\alpha)$$

$$\frac{\hbar^4}{16} - \frac{\hbar^4}{4}\sin^2\alpha\cos^2\alpha \overset{?}{\geq} \frac{\hbar^2}{16}(\cos^4\alpha + \sin^4\alpha) - \frac{\hbar^2}{8}\cos^2\alpha\sin^2\alpha$$

#2 (cont.)

c) $A = \langle(\delta S_x)^2\rangle\langle(\delta S_y)^2\rangle \Rightarrow$ max/min @ $\frac{dA}{d\alpha} = 0$

$$\Rightarrow \quad 0 = \frac{dA}{d\alpha} = \frac{d}{d\alpha}\left(\frac{\hbar^4}{16} - \frac{\hbar^4}{4}\sin^2\alpha\cos^2\alpha\right)$$

$$0 = -\frac{\hbar^4}{4}\left(2\sin\alpha\cos^3\alpha - 2\cos\alpha\sin^3\alpha\right) \quad \Rightarrow$$ any multiple of $\pi/2$ also zero's function

$$0 = \frac{-\hbar^2}{2}\sin\alpha\cos^3\alpha + \frac{\hbar^2}{2}\cos\alpha\sin^3\alpha$$

$$\sin\alpha\cos^3\alpha = \cos^\alpha\sin^3\alpha$$

$$\cos^2\alpha = \sin^2\alpha$$

$$1 - \sin^2\alpha = \sin^2\alpha$$

$$1 = 2\sin^2\alpha$$

$$\frac{1}{2} = \sin^2\alpha$$

$$\pm\frac{1}{\sqrt{2}} = \sin\alpha$$

$$\sin^{-1}\left(\frac{\sqrt{2}}{2}\right) = \alpha = n\frac{\pi}{4}, \quad n = 1, 3, 5 \ldots$$

$\Rightarrow$ minimums at multiples of $n\pi/2$, maximums at multiples of $n\pi/4$

↳ Minimal states: $|\alpha\rangle = |+\rangle$
$= |-\rangle$

↳ Maximal states: $|\alpha\rangle = \frac{1}{\sqrt{2}}\left(|+\rangle + |-\rangle\right)$
$= \frac{1}{\sqrt{2}}\left(|+\rangle - |-\rangle\right)$
$= \frac{1}{\sqrt{2}}\left(-|+\rangle + |-\rangle\right)$
$= \frac{1}{\sqrt{2}}\left(-|+\rangle - |-\rangle\right)$

d) $|\alpha\rangle = |+\rangle$ by virtue of the experiment

$$\Rightarrow \langle S_x\rangle = \langle +|S_x|+\rangle$$

$$= \begin{bmatrix}1 & 0\end{bmatrix}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}\begin{bmatrix}1\\ 0\end{bmatrix}$$

$$= 0$$

PROBLEM 3: Clebsch-Gordan Coefficients

Consider a system of 2 spin 1/2 particles, i.e. $s_1 = \frac{1}{2}, s_2 = \frac{1}{2}$ where:

$$S_{1z}|s_1, m_{s1}\rangle = m_{s1}\hbar|s_1, m_{s1}\rangle$$

$$S_1^2|s_1, m_{s1}\rangle = s_1(s_1+1)\hbar^2|s_1, m_{s1}\rangle = 3/4\hbar^2|s_1, m_{s1}\rangle$$

and similarly for S_{2z} and S_2^2.

Initially, the 2 spin particles are uncoupled and subject to a Hamiltonian:

$$H_0 = \omega_1 S_{1z} + \omega_2 S_{2z}$$

The eigenvectors $|s_1, s_2; m_{s1}, m_{s2}\rangle$, for this Hamiltonian can be written in compact notation as: $|++\rangle, |+-\rangle, |-+\rangle, |--\rangle$ where the $+$ and $-$ denote the sign of m_{s1} and m_{s2} respectively.

Answer the following questions:

(a) Set up the matrix representation for H_0 in this uncoupled basis. [1 point]

Now add an interaction term: $A\vec{S}_1 \cdot \vec{S}_2$ to H_0:

$$H = H_0 + A\vec{S}_1 \cdot \vec{S}_2$$

(b) Determine the commutator : $[H, S_{1z}]$. Will the uncoupled basis be an eigenbasis for H? Explain. [2 points]

(c) Determine a coupled basis for this system: $|S, M\rangle$ where S is the value of the total spin $\vec{S} = \vec{S}_1 + \vec{S}_2$ and M is its component, i.e.

$$S^2|S, M\rangle = S(S+1)\hbar^2|S, M\rangle, \; S_z|S, M\rangle = M\hbar|S, M\rangle.$$

by setting up the matrix for $S^2 = (\vec{S}_1 + \vec{S}_2)^2$ in the uncoupled basis and diagonalizing it. List the eigenvectors of S^2 with the correct values of S and M i.e. as $|S, M\rangle$ states. [3 points]

(d) Identify the Clebsch-Gordan coefficients: $\langle s_1, s_2, m_{s1}, m_{s2}|S, M\rangle$ from the expansions you found in part c). Fill in values for all the quantum numbers in the Dirac braket for each Clebsch-Gordan coefficient and give the numerical value for all the Clebsch-Gordan coefficients you have found. There should be 6 Clebsch-Gordan coefficients. [4 points]

PROBLEM 4: Stationary Perturbation Theory

Suppose an electron is in orbit in the ground state about a tritium nucleus. The tritium nucleus suddenly undergoes beta decay, so that ${}^3_1H \rightarrow {}^3_2 He^+ + e^- + \bar{\nu}_e$.

(a) What are the orbital quantum numbers of the still-bound electron after the beta emission and why? [2 points]

(b) Estimate the probability that the orbital electron remains in the ground state after the beta emission. [6 points]

(c) What is the probability that the orbital electron is in an excited state after the beta emission? [2 points]

Helpful information: the radial wavefunction of the still-bound electron in the ground state is $R_{10} = 2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$, *which is similar to the wavefunction of the hydrogen atom.*

PROBLEM 5: Time Dependent Perturbation Theory

A particle of charge q, undergoing simple harmonic motion along the x-axis (1-D), is acted on by a time-dependent homogeneous electric field,

$$\vec{E}(t) = E_0 e^{-t^2/\tau^2}\hat{x}$$

where E_0 and τ are constants.

(a) What is the new interaction term in the Hamiltonian for the simple harmonic motion due to the specified electric field? [1 Point]

(b) If the oscillator is in its ground state at $t = -\infty$, find the probability that it will be in an excited state at $t = \infty$. Assume the interaction can be treated as a time-dependent perturbation. [3 Points]

(c) Consider the same charged particle linear harmonic oscillator as in (a). Assuming that dE/dt is small, and that at $t = -\infty$ the oscillator is in the ground state, use the adiabatic approximation to obtain the probability that the oscillator will be found in an excited state as $t \rightarrow \infty$. Compare your result with the one you obtained in (b). [3 Points]

(d) Again consider the charged particle harmonic oscillator but with a slightly different perturbation. For $t < 0$

$$H_0 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}kx^2 .$$

For $t > 0$

$$H(t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}k(x-a)^2 - ka^2$$

with

$$a = \frac{qE_0}{m\omega^2},$$

where $\omega = \sqrt{k/m}$. Show that in the weak coupling limit for $t > 0$ that the only *eigenstate of* H_0 which will be excited with any sizable probability is the first excited state, $\psi_1(x)$, and that the corresponding transition probability is

$$P_{10}(t) = \frac{2q^2E_0^2}{m\hbar\omega^3}\sin^2(\omega t/2).$$

Assume the perturbation is turned on suddenly (fast). [3 Points]

PROBLEM 6: Neutron Evolution

A polarized beam of neutrons with energy E_0 and spin projection along the positive z-axis enters abruptly at $t = 0$ a region where there is a uniform magnetic field $\vec{B}$. If we ignore the spatial degrees of freedom the Hamiltonian for the neutron interacting with the magnetic field is

$$H = -\vec{B} \cdot \vec{\mu}_n = 2\omega \hat{n} \cdot \vec{S}$$

where $\hat{n}$ is a unit vector in the direction of the magnetic field and $\omega = B\mu_n/\hbar$.

(a) **Hamiltonian:** Express $\hat{n}$ in spherical coordinates $\{\theta, \phi\}$ and then find an expression for $\hat{n} \cdot \vec{S}$. [2 points]

(b) **Time Evolution Operator:** Write down an explicit expression for the time-evolution operator in terms of $\{\theta, \phi, t\}$. [3 points]

(c) **Evolved State:** Find the state of the time evolved system for any time $t > 0$. [2 points]

(d) **Expectations:** Find the expectation value of the spin $\vec{S}$. [2 points]

(d) **A Special Case:** Determine and describe the motion for a system where $\vec{B} = B\hat{x}$ [1 point]

Quantum Mechanics
Qualifying Exam - January 2013

Notes and Instructions

- There are 6 problems. Attempt them all as partial credit will be given.
- 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

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

In spherical coordinates,

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

Problem 1: Bound States and Scattering for a Delta-Function Well

Consider a delta-fuction for a 1-D system,

$$V(x) = -g\ \delta(x) \tag{1}$$

where $g > 0$. We will consider the states of a particle of mass m interacting with this potential for both $E < 0$ and $E > 0$.

This potential has a single bound state $E_b < 0$.

(a) [1 pt] Explain why the bound state wavefunction for the particle will have the form $\Psi(x) = ce^{-|x|/\lambda}$. (You don't need to solve for anything to answer this question.)

(b) [2 pts] Derive the boundary conditions for $\Psi(x)$ and $\partial_x \Psi(x)$ at $x = 0$.

(c) [1 pt] Using the boundary conditions at $x = 0$, determine the value of λ.

(d) [1 pts] What is the energy of the bound state, E_b? What is the normalization constant c?

(e) [2 pts] What is the uncertainty in position, Δx for the particle in this bound state?

(f) [2 pts] Next consider a scattering state for this particle with energy $E > 0$

$$\begin{aligned} \Psi(x) &= e^{ikx} + ae^{-ikx}, \quad x < 0 \\ &= be^{ikx}, \quad x > 0 \end{aligned} \tag{2}$$

For this state, $E = \frac{\hbar^2 k^2}{2m}$

Using the boundary conditions you found in part (b), determine a and b, and the transmission and reflection coefficients for this scattering state.

Problem 2: Born Approximation

In the Born approximation, the scattering amplitude for a particle of mass m elastically scattering from a potential $V(\vec{r})$ is given by

$$f(\theta,\phi) \simeq -\frac{m}{2\pi\hbar^2}\int e^{i(\vec{k}-\vec{k}')\cdot\vec{r}}V(\vec{r})d^3r \tag{1}$$

and where $\hbar\vec{k}$ is the incoming momentum, $\hbar\vec{k}'$ is outgoing momentum, θ is the scattering angle measured from the incoming momentum, and ϕ is an azimuthal angle about the incoming momentum.

The scattering cross section is given by

$$\frac{d\sigma}{d\Omega} = |f(\theta,\phi)|^2. \tag{2}$$

(a) [2 pts] Define $\vec{\kappa} \equiv \vec{k}' - \vec{k}$. Show that the magnitude $|\vec{\kappa}| = 2k\sin(\theta/2)$ for elastic scattering.

(b) [6 pts] Find $\frac{d\sigma}{d\Omega}$ for the Yukawa potential: $V(r) = \beta\frac{e^{-\mu r}}{r}$

(c) [2 pts] Why does the cross section get larger as μ gets smaller? What is the scattering cross section the limit as $\mu \to 0$? What physical problem does this correspond to in the $\mu \to 0$ limit?

Problem 3: Spin Measurements and Uncertainty

Define the operator $S_\alpha = \vec{S} \cdot \hat{n}_\alpha$ where $\vec{S}$ is the vector spin operator and $\hat{n}_\alpha$ is a unit vector in the $x - z$ plane that makes an angle α with the z-axis. So $\hat{n}_\alpha = \hat{z}$ for $\alpha = 0$ and $\hat{n}_\alpha = \hat{x}$ for $\alpha = \pi/2$.

Consider a spin 1/2 system initially prepared to be in the eigenstate of S_α with eigenvalue $+\hbar/2$,

$$S_\alpha|\alpha, +\rangle = \frac{\hbar}{2}|\alpha, +\rangle \tag{1}$$

(a) [3 pts] Compute the eigenstates of S_α in the basis of the S_z operator, $|0, \pm\rangle \equiv |\pm\rangle$.

(b) [2 pts] If the spin is in the state $|\alpha, +\rangle$ and S_x is measured, what is the probability of measuring $-\hbar/2$?

(c) [3 pts] Compute the expectation value $\langle(\delta S_x)^2\rangle$ for the state $|\alpha, +\rangle$, where $\delta S_x = S_x - \langle S_x\rangle$.

If one measures S_x, what are the values of α that minimize the uncertainty of the measurement for the state $|\alpha, +\rangle$? Interpret the physical meaning of those states.

(d) [2 pts] Finally, define $\mathcal{P}_{x,+}$ to be the projection operator for the spin 1/2 state of S_x, $|\pi/2, +\rangle$. Compute the matrix element $\mathcal{P}_{x,+}$ in the initial state, $\langle +, \alpha|\mathcal{P}_{x,+}|\alpha, +\rangle$. Explain the behavior of the resultant expression as a function of the angle α.

Problem 4: Operator Solutions to the Harmonic Oscillator

Consider the Harmonic Oscillator Hamiltonian in one dimension:

$$H_{ho} = \frac{P^2}{2m} + \frac{m\omega^2}{2}X^2 \tag{1}$$

To simplify this problem, define the new observables:

$$p = \sqrt{\frac{1}{m\hbar\omega}}P\ , \quad q = \sqrt{\frac{m\omega}{\hbar}}X \tag{2}$$

This gives the dimensionless Hamiltonian,

$$H = \frac{1}{\hbar\omega}H_{ho} = \frac{1}{2}\left(p^2 + q^2\right) \tag{3}$$

(a) [1 pt] Calculate the commutation relation for these new variables, $[q, p]$. Be sure to show your work.

(b) [1 pt] Define the non-Hermitian operators $a = \frac{1}{\sqrt{2}}(q + ip)\ , \quad a^\dagger = \frac{1}{\sqrt{2}}(q - ip)$ and the Hermitian operator $n = a^\dagger a$. Compute $[a, a^\dagger]$, $[n, a^\dagger]$, and $[n, a]$

(c) [1 pt] Write the dimensionless Hamiltonian H in terms of a and $a^\dagger$. Write the dimensionless Hamiltonian H in terms of n.

(d) [3 pts] Define the eigenvalues and eigenvectors of n as:

$$n|\lambda\rangle = \lambda|\lambda\rangle. \tag{4}$$

and assume that these eigenvectors form a complete set.

Show that

$$\begin{aligned} a^\dagger|\lambda\rangle &= A|\lambda + 1\rangle \\ a|\lambda\rangle &= B|\lambda - 1\rangle \end{aligned} \tag{5}$$

Determine the normalization constants A and B.

(e) [2 pts.] Show that $n = a^\dagger a$ must have non-negative eigenvalues, $\lambda \geq 0$. Explain why this implies that there must be a state where $a|0\rangle = 0$ and that the eigenvalues of n must be non-negative integers.

(f) [2 pts.] Write the definition for the state $|0\rangle$

$$a|0\rangle = 0 \tag{6}$$

as a differential equation, in q, for the ground state wavefunction of H. Solve this expression for the normalized ground state wavefunction.

Jan 2013

Quantum #4

a) * Remember $[x_i, p_j] = i\hbar \delta_{ij}$

$$\Rightarrow [q,p] = qp - pq$$
$$= \sqrt{\frac{m\omega}{\hbar}} x \sqrt{\frac{1}{m\hbar\omega}} p - \sqrt{\frac{1}{m\hbar\omega}} p \sqrt{\frac{m\omega}{\hbar}} x$$
$$= \frac{1}{\hbar}(xp - px)$$
$$= \frac{1}{\hbar}[x,p]$$
$$= \frac{1}{\hbar} i\hbar$$
$$= i$$

b) $[a, a^\dagger] = aa^\dagger - a^\dagger a$
$$= \frac{1}{\sqrt{2}}(q+ip)\frac{1}{\sqrt{2}}(q-ip) - \frac{1}{\sqrt{2}}(q-ip)\frac{1}{\sqrt{2}}(q+ip)$$
$$= \frac{1}{2}(q^2 + ipq - iqp + p^2) - \frac{1}{2}(q^2 - ipq + iqp + p^2)$$
$$= \frac{i}{2}(pq - qp) - \frac{i}{2}(qp - pq)$$
$$= -i(pq + qp)$$
$$= -i([q,p])$$
$$= -i(i)$$
$$= 1$$

$$[n, a^\dagger] = [a^\dagger a, a^\dagger]$$
$$= a^\dagger a a^\dagger - a^\dagger a^\dagger a$$
$$= a^\dagger [aa^\dagger - a^\dagger a]$$
$$= a^\dagger [a, a^\dagger]$$
$$= a^\dagger$$

$$[n, a] = [a^\dagger a, a]$$
$$= a^\dagger a a - a a^\dagger a$$
$$= [a^\dagger a - a a^\dagger] a$$
$$= [a^\dagger, a] a$$
$$= -[a, a^\dagger] a$$
$$= -a$$

#4 (cont.)

c) We want to rewrite $H = \frac{1}{2}(p^2 + q^2)$ in terms of a and a^+

$$\Rightarrow \sqrt{2}\, a = q + ip$$

$$\sqrt{2}\, a^+ = q - ip$$

$$\sqrt{2}(a + a^+) = 2q \qquad \sqrt{2}(a - a^+) = 2ip$$

$$\frac{1}{\sqrt{2}}(a + a^+) = q \qquad \frac{-i}{\sqrt{2}}(a - a^+) = p$$

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

$$= \frac{1}{2}\left[\frac{-1}{2}\left(aa - a^+a - aa^+ + a^+a^+\right) + \frac{1}{2}\left(aa + a^+a + aa^+ + a^+a^+\right)\right]$$

$$= \frac{1}{2}\left(a^+a + aa^+\right)$$

$$= \frac{1}{2}\left(n + aa^+\right)$$

$$= \frac{1}{2}\left(n + 1 + a^+a\right) \quad (\text{from } [a, a^+] = 1)$$

$$= \frac{1}{2}(2n + 1)$$

$$= n + 1/2$$

d) * We must use the n-operator and its commutation relations to solve this problem

$$\Rightarrow a^+|\lambda\rangle = A|\lambda + 1\rangle$$

$$\hookrightarrow n a^+|\lambda\rangle = a^+n + a^+|\lambda\rangle$$

$$= (a^+\lambda + a^+)|\lambda\rangle$$

$$= a^+(\lambda + 1)|\lambda\rangle$$

$$= (\lambda + 1)|\lambda\rangle$$

$$\Rightarrow \langle\lambda|a a^+|\lambda\rangle = A^2\langle\lambda + 1|\lambda + 1\rangle$$

$$\langle\lambda|a^+a + 1|\lambda\rangle = A^2$$

$$\langle\lambda|n + 1|\lambda\rangle = A^2$$

$$\lambda + 1 = A^2 \Rightarrow \boxed{A = \sqrt{\lambda + 1}}$$

#4 (cont.)

d) Similiarly,

$$n(a|\lambda\rangle) = an - a\,|\lambda\rangle$$
$$= a(n-1)\,|\lambda\rangle$$
$$= a(\lambda-1)|\lambda\rangle$$
$$= (\lambda-1)(a|\lambda\rangle)$$

$$\Rightarrow \langle\lambda|a^{\dagger}a|\lambda\rangle = B^2\langle\lambda-1|\lambda-1\rangle$$
$$\langle\lambda|n|\lambda\rangle = B^2$$
$$\lambda = B^2 \rightarrow \boxed{\sqrt{\lambda} = B}$$

e)

#4 (cont.)

f) Given $a|0\rangle = 0$, where $a = \frac{1}{\sqrt{2}}(q + ip)$

$$\frac{1}{\sqrt{2}}(q+ip)|0\rangle = 0$$

$$\frac{1}{\sqrt{2}}\left(q + i\left(-i\hbar \frac{\partial}{\partial q}\right)\right)|0\rangle = 0$$

$$\frac{1}{\sqrt{2}}\left(q - \hbar \frac{\partial}{\partial q}\right)\psi_0 = 0$$

$$q\psi_0 - \hbar\frac{\partial \psi_0}{\partial q} = 0$$

$$\Rightarrow \frac{\partial \psi_0}{\partial q} = \frac{q}{\hbar}\psi_0$$

$$\int \frac{\partial \psi_0}{\psi_0} = \int \frac{q}{\hbar}\partial q$$

$$\ln(\psi_0) = -\frac{1}{2\hbar}q^2 + C$$

$$\psi_0 = \exp\left[\frac{-1}{2\hbar}q^2 + C\right]$$

$$= C\exp\left[\frac{-q^2}{2\hbar}\right]$$

*Checking our normalization

$$1 = C^2\int_{-\infty}^{\infty}\left|\exp\left[\frac{-q^2}{2\hbar}\right]\right|^2 dq$$

$$1 = C^2\int_{-\infty}^{\infty}\exp\left[-\frac{q^2}{\hbar}\right]dq$$

$$1 = C^2\sqrt{\pi\hbar}$$

$$\frac{1}{\sqrt{\pi\hbar}} = C^2$$

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

$$\Rightarrow \psi_0 = \left(\frac{1}{\pi\hbar}\right)^{1/4}\exp\left[\frac{-q^2}{2\hbar}\right]$$

Problem 5: Perturbing a Square Well

Consider a particle of mass m in a 1D infinite square well of width a,

$$V(x) = 0, \quad 0 \leq x \leq a \qquad V(x) = \infty, \quad x < 0, \quad x > a. \tag{1}$$

(a) [2 pts] Derive the eigenfunctions and eigenenergies of the particle in this potential. Be sure to normalize the states.

(b) [2 pts] Show that if the well is perturbed by a potential $V'(x) = \alpha\, x$, the energy of all the unperturbed states shift by the same amount to first order in α. Find an expression for this energy shift. Give a physical explanation for why this perturbation results in an equal first-order energy shift for all states.

(c) [3 pts] Next, instead of the perturbing potential from part (b), the well is perturbed by a potential

$$V'(x) = V_0, \quad \frac{a}{2} - \delta \leq x \leq \frac{a}{2} + \delta \qquad V'(x) = 0, \quad x < \frac{a}{2} - \delta, \quad x > \frac{a}{2} + \delta \tag{2}$$

Compute the energy shift to first order in α for the unperturbed energy eigenstates $\psi_n(x)$. Explain the limit of this result as n, the unperturbed energy level, gets large.

(d) [2 pts.] What is the energy shift of the states $\psi_n(x)$ to first order in δ as $\delta \to 0$? (V_0 is constant.) Give a physical explanation of this result. Note: You should be able to answer this question even if you did not get a solution to part (c).

(e) [1 pt] What is the energy shift of the states $\psi_n(x)$ as $\delta \to \frac{a}{2}$? (V_0 is constant.) Give a physical explanation of this result. Note: You should again be able to answer this question even if you did not get a solution to part (c).

Problem 6: Spherical Square Well

Consider a spin 0 particle of mass m moving in a 3D square well, given by the potential

$$V(\vec{r}) = -V_0 \quad 0 \le |\vec{r}| \le a_0 \ , \qquad V(\vec{r}) = 0 \quad |\vec{r}| > a_0 \qquad (V_0 > 0). \tag{1}$$

In this problem we will only consider the bound states of this well, so that $-V_0 < E < 0$.

(a) [1 pt] Explain why we can write the eigenstates of this potential as

$$\Psi_{k,l,m} = f_{k,l}(r) Y_l{}^m(\theta, \phi). \tag{2}$$

(b) [2 pts] Defining the function $u_{k,l}(r) = r f_{k,l}(r)$, write the radial Schrödinger equation for $u_{k,l}(r)$.

(c) [2 pts] For $l = 0$, write the form for the function $u_{k,0}(r)$ in the regions $0 \le r \le a_0$ and $r \ge a_0$. Define any constants that you use.

(d) [3 pts] Using the boundary conditions on the function $u_{k,0}(r)$, derive an equation that gives the bound state energies for the $l = 0$ states. Hint: Considering that $f(r) = u(r)/r$, what is the boundary condition on u as $r \to 0$?

(e) [2 pts] For a fixed radius for the potential, a_0, calculate the minimum depth, $V_0 = V_{min}$, for the potential to have a bound state.

Quantum Mechanics
Qualifying Exam - August 2013
Notes and Instructions

- There are 6 problems. Attempt them all as partial credit will be given.
- Write your alias, the name you selected at the start of this test, on the top of every page of your solutions. *DO NOT* put your own name on your answer sheets.
- 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 Operators

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

Angular momentum operators in 3D obey

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k \tag{2}$$

In spherical coordinates,

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

In cylindrical coordinates,

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

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

$$\begin{aligned} \psi_n(x) &= \left(\frac{\beta^2}{\pi}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}e^{-\beta^2x^2/2}H_n(\beta x) \\ H_0(x) = 1, \quad H_1(x) &= 2x, \quad H_2(x) = 4x^2 - 2, \quad H_3(x) = 8x^3 - 12x \end{aligned} \tag{5}$$

Spherical Harmonics,

$$Y_0^0(\theta,\phi) = \frac{1}{\sqrt{4\pi}}, \quad Y_1^0(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta, \quad Y_1^{\pm1}(\theta,\phi) = \mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\phi} \tag{6}$$

Hydrogen Atom States (a_0 is the Bohr Radius),

$$\begin{aligned} \Psi_{n,\ell,m}(\vec{r}) &= R_{n,\ell}(r)Y_{\ell,m}(\theta,\phi) \\ R_{1,0}(r) &= \frac{2}{(a_0)^{3/2}}e^{-r/a_0} \\ R_{2,0}(r) &= \frac{2}{(2a_0)^{3/2}}\left(1 - \frac{r}{2a_0}\right)e^{-r/2a_0} \\ R_{2,1}(r) &= \frac{1}{(2a_0)^{3/2}}\frac{r}{\sqrt{3}a_0}e^{-r/2a_0} \end{aligned} \tag{7}$$

Problem 1: 1D Square Wells

(a) [1 pt] Consider an electron confined to an infinitely deep 1D well with walls at $x = 0$ and $x = L$. In the ground state, the electron has an energy of 2.5 eV (the bottom of the well is defined as $V = 0$). What is the width of the well?

(b) [1 pt] A proton is confined to an infinite 1D square well of width 10 fm. What is the wavelength (or frequency) of a photon emitted when the proton undergoes a transition from the first excited state to the ground state of the well?

(c) [2 pt] Sketch the probability density as a function of x for the first 3 energy eigenstates for an electron in an infinite well of width L. Describe qualitatively (or draw) how the probability densities for these states will differ (from the infinite well case) for a square well with an infinite potential barrier at $x = 0$ and a finite potential barrier at $x = L$.

(d) [2 pt] Consider an electron in the nth energy eigenstate of an infinitely deep well with walls at $x = 0$ and $x = L$. Calculate the probability that the electron will be measured between $x = 0$ and $x = \epsilon\ L$, with $0 < \epsilon < 1$. Your answer should be a function of both n and ϵ.

Give a physical explanation for your solution as $n \to \infty$.

(e) [2 pt] The electron is in the ground state of the infinite well when the wall at $x = L$ is very suddenly moved to $x = 2L$. What is the probability that the electron will be found in the ground state of the expanded box?

(f) [1 pt] What energy eigenstate in the expanded box will have the highest probability of being occupied by the electron? What is this probability? Hint: You should be able to determine this result without doing an integral, but you should explain your answer.

(g) [1 pt] Suppose the electron is in the ground state of the infinitely deep well when the walls are suddenly removed completely. Write down an expression for the probability distribution for the momentum of the freed electron. Setup but do not solve the integral.

Problem 2: Quantum Operators

In this problem you will work with the ladder operators for angular momentum:

$$L_+ = L_x + iL_y, \quad L_- = L_x - iL_y \tag{1}$$

where

$$\begin{aligned} L^2 &= L_x^2 + L_y^2 + L_z^2 \\ L^2|\ell, m\rangle &= \ell(\ell+1)\hbar^2|\ell, m\rangle \\ L_z|\ell m\rangle &= m\hbar|\ell, m\rangle \end{aligned} \tag{2}$$

(a) [1 pt] Show that the eigenvalues of any Hermitian operator are real.

(b) [2 pt] Is the the operator L_+L_-, the product of the angular momentum ladder operators, Hermitian? Show your work to justify your answer.

(c) [4 pt] Determine the results of the operations: $\hat{L}_+|\ell, m\rangle$ and $\hat{L}_-|\ell, m\rangle$. Show all of your work and make sure you determine all constants correctly.

Hint: The commutation relation $[L_z, L_\pm]$ and the matrix elements $\langle \ell, m|L_\pm L_\mp|\ell, m\rangle$ might be useful.

(d) [3 pt] Using the results from part (c), prove that $-\ell \leq m \leq +\ell$. Explain the physics of this result in terms of the operators L^2 and L_z.

Aug 2013

Quantum #2

a) The condition for Hermiticity is $A = A^\dagger$ for an operator A

Using: $A|\lambda\rangle = a|\lambda\rangle$, it must be true that $\langle\lambda|A^\dagger = a^*\langle\lambda|$
$= \langle\lambda|A$

$$\Rightarrow \langle\lambda|A|\lambda\rangle = a^*\langle\lambda|\lambda\rangle$$

$$a\langle\lambda|\lambda\rangle = a^*\langle\lambda|\lambda\rangle$$

$a = a^*$, which is only true if $a \in \mathbb{R}$

b) $L_+ = L_x + iL_y$
$L_- = L_x - iL_y$ $\Bigg\rangle$ We want $L_+L_- = (L_+L_-)^\dagger = L_-^\dagger L_+^\dagger$

$$
\begin{aligned}
L_+L_- &= (L_x + iL_y)(L_x - iL_y) \\
&= (L_x^2 + iL_yL_x - iL_xL_y + L_y^2) \\
&= (L_x^2 + L_y^2 - i[L_x, L_y]) \\
&= (L_x^2 + L_y^2 - i(i\hbar L_z) \\
&= (L_x^2 + L_y^2 + \hbar L_z) \\
&= (L^2 - L_z^2 + \hbar L_z)
\end{aligned}
$$

$$
\begin{aligned}
L_-^\dagger L_+^\dagger &= (L_x - iL_y)^\dagger(L_x + iL_y)^\dagger \\
&= (L_x^\dagger + iL_y^\dagger)(L_x^\dagger - iL_y^\dagger)
\end{aligned}
$$

* but $L_x^\dagger = L_x$, $L_y^\dagger = L_y$ by their status as observables

$$
\begin{aligned}
&= (L_x + iL_y)(L_x - iL_y) \\
&= L^2 - L_z^2 + \hbar L_z
\end{aligned}
$$

c) We must first determine $L_\pm|\ell, m\rangle$

$$
\begin{aligned}
L_z(L_\pm|\ell, m\rangle) &= (L_\pm L_z \pm \hbar L_\pm)|\ell, m\rangle \\
&= L_\pm(L_z \pm \hbar)|\ell, m\rangle \\
&= (m \pm \hbar)(L_\pm|\ell, m\rangle)
\end{aligned}
$$

$\hookrightarrow$ $L_\pm$ increments the z-states of angular momentum

#2 (cont.)

c) Given the above, we know: $J_{\pm}|l,m\rangle = c_{\pm}|l, m\pm\hbar\rangle$

$$\Rightarrow \langle l,m|L_+^{\dagger}L_+|l,m\rangle = |c_+|^2 \langle l,m\cancel{\pm\hbar}|\cancel{l},m\pm\hbar\rangle^{1}$$

$$\langle l,m|L^2 - L_z^2 - \hbar L_z|l,m\rangle = |c_+|^2$$ (see part b for work)

$$\hbar^2 l(l+1) - \hbar^2 m^2 - \hbar^2 m \langle l,\cancel{m|l},m\rangle^{1} = |c_+|^2$$

$$\hookrightarrow |c_+|^2 = \hbar^2[l(l+1) - m^2 - m]$$

$$c_+ = \hbar\sqrt{(l-m)(l+m+1)}$$

Similarly for J_-

$$\Rightarrow \langle l,m|J_-^{\dagger}J_-|l,m\rangle = |c_-|^2\langle l,m\cancel{-\hbar}|\cancel{l},m-\hbar\rangle^{1}$$

$$\langle l,m|L^2 - L_z^2 + \hbar L_z|l,m\rangle = |c_-|^2$$

$$\hbar^2 l(l+1) - \hbar^2 m^2 + \hbar^2 m\langle l,m|l,m\rangle = |c_-|^2$$

$$\hookrightarrow |c_-|^2 = \hbar^2[l(l+1) - m^2 + m]$$

$$= \hbar\sqrt{(l+m)(l-m+1)}$$

$$\Rightarrow L_{\pm}|l,m\rangle = \hbar\sqrt{(l\mp m)(l\pm m+1)}\,|l, m\pm 1\rangle$$

d) This part of the problem is effectively asking us to find the extremum values therefore we act upon the max/min states

$$\Rightarrow L_+|l, m_{max}\rangle = 0$$

$$L_- L_+|l, m_{max}\rangle = 0$$

$$L^2 - L_z^2 - \hbar L_z|l, m_{max}\rangle = 0$$

$$\hbar^2 l(l+1) - \hbar^2 m^2 - \hbar^2 m|l, m_{max}\rangle = 0$$

* assuming a non-zero ket

$$l(l+1) = m(m+1) \Rightarrow m_{max} = l$$

#2 (cont.)

d) $L_- |l, m_{min}\rangle = 0$

$L_+ L_- |l, m_{min}\rangle = 0$

$L^2 - L_z^2 + \hbar L_z |l, m_{min}\rangle = 0$

$\hbar^2(l+1)l - \hbar^2 m_{min}^2 + \hbar^2 m_{min} |l, m_{min}\rangle = 0$

* assuming a non-zero ket

$l(l+1) = m_{min}(m_{min} - 1)$

$m_{max}(m_{max} + 1) = m_{min}(m_{min} - 1)$

$\hookrightarrow m_{max} = -m_{min}$

$\hookrightarrow m_{min} = -l$

$\Rightarrow m \in [-l, l]$

Physically, the z-state of angular momentum can only contain as much angular momentum as the overall angular momentum of the whole system

Problem 3: Barrier Scattering

Consider a particle of mass m in one dimension scattering off of a square barrier of width L:

$$\begin{aligned} V(x) &= 0, \quad x < 0 \\ V(x) &= V, \quad 0 < x < L, \quad V > 0 \\ V(x) &= 0, \quad x > L \end{aligned} \tag{1}$$

Assume the particle has an energy $E > V$ and is incoming from the left ($x < 0$).

Define the usual wavenumbers for this problem:

$$\frac{\hbar^2 k^2}{2m} = E, \quad \frac{\hbar^2 k'^2}{2m} = E - V \tag{2}$$

(a) [1 pt] Write down general expressions for the scattering wave function, the un-normalized eigenfunction of the scattering Hamiltonian, in the three regions, $x < 0$, $0 < x < L$, and $x > L$.

(b) [1 pt] Using the expressions from part (a), write down the boundary conditions on the scattering wave function. Explain the physics of each of these boundary conditions.

(c) [2 pt] Using your boundary conditions from part (b), show that

$$\frac{A}{E} = e^{ikL}\left(\cos k'L) - i\frac{k^2 + k'^2}{2kk'}\sin(k'L)\right) \tag{3}$$

where A is the amplitude of the incoming wave (from $x = -\infty$) and E is the amplitude of the outgoing wave (to $x = \infty$). Hint: We're not interested in the amplitude of the reflected wave.

(d) [3 pt] Solve for the transmission coefficient, T, for the barrier scattering. You may express this in terms of k, k', and L, but it will be useful for later parts of the question to write it in terms of E, V, L, and constants in the problem.

(e) [1 pt] What is the limit for the transmission coefficient T in the limit that $E \gg V$? Show your work and explain the physics of this result.

(f) [1 pt] There are energies where $T = 1$. What are these energies and the wavelength of the particle wave function? Give a physical argument of why the transmission coefficient is a maximum for these energies.

(g) [1 pt] What is the value for the transmission coefficient, T, in the limit that $E \to V$? Hint: To solve this you might define $\delta = E - V$.

Problem 4: Properties of the Hydrogen Atom

The wavefunctions for the ground state and first excited states of the hydrogen atom are given on the first page of this test.

(a) [2 pt] For the ground state of the hydrogen atom, determine the expectation value for the radial position of the electron, $\langle 1,0,0|r|1,0,0\rangle$.

(b) [3 pt] Define the radial probably density for the electron in a hydrogenic eigenstate: $P_{n,\ell,m}(r)dr$ as the probability of the electron being measured in the spherical shell between r and $r+dr$.

Write down expressions for $P_{1,0,0}(r)$ and $P_{2,1,1}(r)$, and sketch these as functions of r.

Hint: Remember that the integral of the probability density over r must be equal to one,

$$\int_0^\infty P_{n,\ell,m}(r)dr = 1 \tag{1}$$

(c) [3 pt] For the ground state of the hydrogen atom, determine the most probable radius for the electron. Compare your result to part (a) and explain the similarities and differences.

(d) [1 pt] What is the functional form for $P_{1,0,0}(r)$ in the limit as $r \to 0$? Explain your result considering that the ground state wavefunction is non-zero at $r=0$.

(e) [1 pt] What are the functional forms of $P_{1,0,0}(r)$, $P_{2,1,1}(r)$, and $P_{200}(r)$ as $r \to 0$? Explain the similarities and differences.

Aug 2013

Quantum #4

a) $\psi_{n\ell m} = R_{n,r}(r)\, Y_\ell^m(\theta,\varphi)$

$$\psi_{100} = \frac{2}{\sqrt{a_0^3}} e^{-r/a_0} \frac{1}{\sqrt{4\pi}}$$

$$= \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

$$\langle r \rangle = \int dr^3 \frac{r}{\pi a_0^3} e^{-2r/a_0}$$

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

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

$$= \frac{4 \cdot 3!\, a_0^4}{2^4 a_0^3}$$

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

b) $P_{n\ell m}(r)\, dr = \int_r^{r+dr} \psi^*_{n\ell m} \psi_{n\ell m} \cdot 4\pi r^2 dr$

$$P_{100}(r)\, dr = \int_r^{r+dr} \frac{4}{a_0^3} e^{-2r/a_0} r^2 dr$$

$$\psi_{211} = \frac{1}{\sqrt{8a_0^3}} \frac{r}{\sqrt{3}\, a_0} e^{-r/2a_0} \cdot -\sqrt{\frac{3}{8\pi}} \sin\theta\, e^{i\varphi}$$

$$= -\frac{r}{8\sqrt{\pi a_0^5}} e^{-r/2a_0} e^{i\varphi} \sin\theta$$

$$P_{211} = \int_r^{r+dr} \int_0^{\pi} \frac{r^4 \cdot 2\pi}{64\pi a_0^5} e^{-r/a_0} \sin^4\theta\, dr\, d\theta$$

*Modified version of Sakurai 5.11

Problem 5: Two Level Systems

Consider the Hamiltonian for a two-state system:

$$H = \begin{pmatrix} \epsilon & \lambda\Delta \\ \lambda\Delta & -\epsilon \end{pmatrix} \tag{1}$$

where λ (a unitless parameter) determines the strength of the perturbation on the two-level system and ϵ and Δ are constants with the unit of energy.

The energy eigenvectors for the unperturbed Hamiltonian ($\lambda = 0$) are

$$\psi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \psi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{2}$$

(a) [2 pt] Solve for the energy eigenvalues E_1 and E_2 for the full Hamiltonian (for any λ). What is the functional form of the eigenenergies in the limits $\lambda \to 0$ and $\lambda \to \infty$?

(b) [2 pt] For the case that $\lambda|\Delta| \ll \epsilon$, solve for the energy eigenvalues to first order and second order in λ.

Compare these results with the exact results obtained in part (a) and show that they are in agreement.

(c) [1 pt] For the case that $\lambda|\Delta| \ll \epsilon$, what is the change in the unperturbed eigenstate ψ_+ to first order in λ?

(d) [2 pt] For the case that the unperturbed Hamiltonian is nearly degenerate, $\epsilon \ll \lambda|\Delta|$ show that the exact results obtained in part (a) agree with the results of applying first order degenerate perturbation theory with $\epsilon = 0$.

(e) [3 pts] For the case that $\epsilon \ll \lambda|\Delta|$, it would advantageous to use a different set of basis states to describe the system. Using basis states that are approximately eigenstates of the Hamiltonian for small ϵ, determine the Hamiltonian matrix in this new basis. Show that the exact solutions for the eigenenergies are the same as in part (a) in this basis.

Aug 2013

Quantum # 5

a) Given $H = \begin{bmatrix} \epsilon & \lambda\Delta \\ \lambda\Delta & -\epsilon \end{bmatrix}$ we want the energy eigenvalues

Using the eigenvalue equation $\det(H - a\mathbb{I}) = 0$

$$\begin{vmatrix} \epsilon - a & \lambda\Delta \\ \lambda\Delta & -\epsilon - a \end{vmatrix} = 0 = (\epsilon - a)(-\epsilon - a) - \lambda^2\Delta^2$$
$$= -\epsilon^2 + a^2 - \lambda^2\Delta^2$$

$$\hookrightarrow 0 = a^2 - [\lambda^2\Delta^2 + \epsilon^2]$$
$$0 = (a + \sqrt{\lambda^2\Delta^2 + \epsilon^2})(a - \sqrt{\lambda^2\Delta^2 + \epsilon^2})$$
$$\hookrightarrow E = \pm\sqrt{\lambda^2\Delta^2 + \epsilon^2}$$

* in the limit $\lambda \to 0$, $E = \pm\epsilon$

$\lambda \to \infty$ $E = \pm\lambda\Delta$ (assumes $\lambda^2\Delta^2 \gg \epsilon^2$)

b) Note $|\psi_+\rangle = \langle 1, 0\rangle$ $E_+ = \epsilon$

$|\psi_-\rangle = \langle 0, 1\rangle$ $E_- = -\epsilon$

$$\Delta E_\pm^{(1)} = \langle\psi_\pm|V|\psi_\pm\rangle \quad \text{where } V = \begin{bmatrix} 0 & \lambda\Delta \\ \lambda\Delta & 0 \end{bmatrix}$$

$$\Delta E_+^{(1)} = [1\ 0]\begin{bmatrix} 0 & \lambda\Delta \\ \lambda\Delta & 0 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = 0$$

$$\hookrightarrow E_+ \approx \epsilon + \cancel{\lambda\Delta}$$

$$\Delta E_- = [0\ 1]\begin{bmatrix} 0 & \lambda\Delta \\ \lambda\Delta & 0 \end{bmatrix}\begin{bmatrix} 0 \\ 1 \end{bmatrix} = 0$$

$$\hookrightarrow E_- \approx -\epsilon + \cancel{\lambda\Delta}$$

$$\Delta E_\pm^{(2)} = \frac{|V_{kn}|^2}{E_n - E_k} = \frac{\Delta^2\lambda^2}{\pm 2\epsilon}$$

5 (cont.)

c) * Assuming $\lambda|\Delta| \ll \epsilon$

$$|\psi_+^{(1)}\rangle = \sum_{k\neq n}' \frac{V_{kn}}{E_n^{(0)} - E_k^{(0)}} |\psi_k\rangle$$

$$= \frac{\Delta\lambda}{2\epsilon} |\psi_-^{(0)}\rangle$$

d)

Problem 6: Harmonic Oscillators in 1D

A quantum harmonic oscillator is described by the Hamiltonian

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

where p is momentum, x is position, m is mass, and ω is the oscillation frequency.

The Hamiltonian has the usual eigenstates and energies:

$$H|n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|n\rangle, \quad n = 0, 1, 2, ... \tag{2}$$

Let the system be perturbed by a potential in the form $V = Ax^2$ where A is a real constant.

(a) [2 pt] What is the change in the energy of the unperturbed eigenstates $|n\rangle$ to first order in A? Show your work.

(b) [2 pt] If the perturbation is time-dependent, $V(t) = A(t)x^2$, it can cause transitions between the harmonic oscillator states. To study these transitions, it is helpful to use the time-dependent expansion:

$$|\psi(t)\rangle = \sum_{n'} c_{n'}(t) e^{-\frac{i}{\hbar}E_{n'}t}|n'\rangle \tag{3}$$

The $c_{n'}(t)$ are time-dependent probability amplitudes for the states $|n'\rangle$ and the energies $E_{n'}$ are the unperturbed eigenenergies. Use the Schroedinger equation to show that the expansion amplitudes satisfy a set of coupled equations:

$$i\hbar\frac{\partial}{\partial t}c_n(t) = \sum_{n'} c_{n'}(t) e^{-\frac{i}{\hbar}(E_{n'}-E_n)t}\langle n|V(t)|n'\rangle \tag{4}$$

(c) [3 pt] Consider the case where the oscillator starts at time $t = 0$ in the ground state, $c_n(t = 0) = \delta_{n,0}$. Use the result from (b) to write down the time dependence of the excited state probability amplitudes to first order in V, $c_n^{(1)}(t)$, $n > 0$. This will be an integral equation, as we have not yet defined $A(t)$.

Show that, to first order, there is a transition only to the $n = 2$ excited state.

(d) [3 pt] Finally, consider a time dependent perturbation with $A(t)$ of the form

$$A(t) = Ae^{-i\Omega t}e^{-\Gamma t} \tag{5}$$

Ω and Γ being real and positive.

Compute the probability that the $n = 2$ state is populated for $t \to \infty$, and explain the dependence of your result on Ω and Γ.

Note: In this problem, it is useful to use

$$a^\dagger = \frac{1}{\sqrt{2}}\left(\frac{x}{\lambda} - i\frac{\lambda}{\hbar}p\right), \quad a = \frac{1}{\sqrt{2}}\left(\frac{x}{\lambda} + i\frac{\lambda}{\hbar}p\right) \tag{6}$$

where $\lambda = \sqrt{\frac{\hbar}{m\omega}}$ is the length scale in the problem.

You do not need to derive the properties of these two operators, but you should state the results you are using.

Aug 2013

Quantum #6

$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$ $\qquad V' = Ax^2, \; A \in \mathbb{R}$

$H|n\rangle = \hbar\omega(n+1/2)|n\rangle$

a) $V' = Ax^2$

* but we know the raising/lowering operators

$$a^+ = \frac{1}{\sqrt{2}}\left(\frac{x}{\lambda} - \frac{i\lambda}{\hbar}p\right)$$

$$a = \frac{1}{\sqrt{2}}\left(\frac{x}{\lambda} + \frac{i\lambda}{\hbar}p\right)$$

$$a + a^+ = \frac{2x}{\sqrt{2}\lambda} \rightarrow x^2 = \frac{\lambda^2}{2}(a+a^+)^2$$

$$\Delta E_n^{(1)} = \langle n^{(0)}|V'|n^{(0)}\rangle$$

$$= A\langle n|\frac{\lambda^2}{2}(aa + aa^+ + a^+a + a^+a^+)|n\rangle$$

$$= \frac{A\lambda^2}{2}\left[\underbrace{\cancel{\langle n|\sqrt{n(n-1)}|n-2\rangle}}_{0} + \langle n|(n+1)|n\rangle + \langle n|n|n\rangle + \underbrace{\cancel{\langle n|\sqrt{(n+1)(n+2)}|n+2\rangle}}_{0}\right]$$

$$= \frac{A\lambda^2}{2}(2n+1)$$

$$= \frac{A\hbar}{2m\omega}(2n+1)$$

b)

Quantum Mechanics
Qualifying Exam - January 2014

Notes and Instructions

- There are 6 problems. Attempt them all as partial credit will be given.
- Write your alias (not your name) 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, Page 2 of 4, is the second of four pages for the solution to problem 3.)
- You must show all your work to receive full credit.

Possibly useful formulas:

Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Laplacian in spherical coordinates

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

One dimensional simple harmonic oscillator operators:

$$X = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger), \qquad P = -i\sqrt{\frac{\hbar m\omega}{2}}(a - a^\dagger)$$

Spherical Harmonics:

$$\begin{aligned}
Y_0^0(\theta,\phi) &= \frac{1}{\sqrt{4\pi}} \\
Y_1^0(\theta,\phi) &= \sqrt{\frac{3}{4\pi}}\cos\theta \\
Y_1^{\pm1}(\theta,\phi) &= \mp\sqrt{\frac{3}{8\pi}}\sin\theta\mathrm{e}^{\pm i\phi} \\
Y_2^0(\theta,\phi) &= \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1) \\
Y_2^{\pm1}(\theta,\phi) &= \mp\sqrt{\frac{15}{8\pi}}(\sin\theta\cos\theta)\,\mathrm{e}^{\pm i\phi} \\
Y_2^{\pm2}(\theta,\phi) &= \sqrt{\frac{15}{32\pi}}\sin^2\theta\,\mathrm{e}^{\pm 2i\phi}
\end{aligned}$$

PROBLEM 1: Rigid Rotator

A free molecule of NaCl can be approximated as a dumbell, or rigid rotator. Attach a reference frame to its center of mass, with z-axis oriented in an arbitrary direction. The Hamiltonian can be taken to be $H = \frac{L^2}{2I}$ where $\vec{L}$ is angular momentum and I is the (fixed) moment of inertia.

a) Write the Schroedinger equation for the molecule. (1 Point)

b) What are the energy eigenvalues? (2 points)

c) What are the steady-state eigenfunctions? (2 points)

d) Sketch an energy level diagram for the rotator. Note any possible degeneracies. (2 points)

e) The rotator, with electric dipole moment $\vec{D}$ oriented along the dumbell symmetry axis, is placed in an electric field $\vec{E} = E\hat{z}$. The dipole interaction is $H_D = -\vec{D} \cdot \vec{E}$. What is the first order perturbative correction to the lowest energy level? (3 points)

PROBLEM 2: Particle in a Box

A particle of mass m is in the ground state of a one dimension box of length L. At $t = 0$, the box suddenly expands *symmetrically* to *three* times its size, leaving the wavefunction of the particle undisturbed. Assume the particle was in the ground state before the expansion.

a) Solve the Schrodinger equation and calculate the eigenenergies and eigenfunctions in the box before and *after* the expansion (show all your work). (3 Points)

b) What is the probability of finding the particle in the ground state immediately after the expansion? (4 Points)

c) Compute the wave function of the particle $\psi(x, t)$ for $t \geq 0$. Hint: express your answer as a superposition of eigenstates. (3 Points)

Hint: $\int_{-\pi/2}^{\pi/2} \mathrm{d}\theta \, \cos\theta \cos(q\theta) = \frac{2}{1-q^2} \cos\left(q\frac{\pi}{2}\right)$,

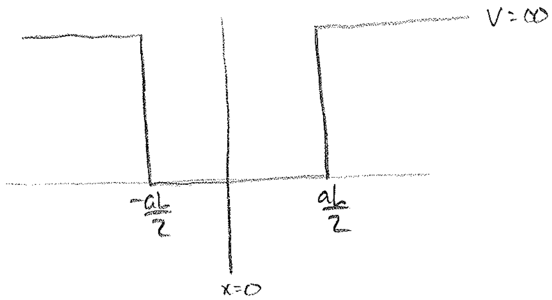
$\int_{-\pi/2}^{\pi/2} \mathrm{d}\theta \, \cos\theta \sin(q\theta) = 0.$

Jan 2014

Quantum #2

* Due to symmetric expansion, we choose our edges to by symmetric about $x=0$

a)



$H\psi = E\psi$

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

$$\frac{d^2\psi}{dx^2} = -k^2\psi, \quad k = \frac{\sqrt{2mE}}{\hbar}$$

$$= Ae^{ikx} + Be^{-ikx}$$

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

* Solving for our boundary conditions, we know $\psi(\frac{-aL}{2}) = 0 = \psi(\frac{aL}{2})$

$$\pm\frac{kaL}{2} = \frac{n\pi}{2} \quad \Rightarrow \quad k = \frac{n\pi}{aL}$$

↳ if $n =$ even, $\sin(kL) = 0 \rightarrow B = 0$

$n =$ odd, $\cos(kL) = 0 \rightarrow A = 0$

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

* Checking normalization

$$1 = A^2\int_{-\frac{aL}{2}}^{aL/2} \sin^2\left(\frac{n\pi x}{aL}\right)dx$$

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

$$= \frac{A^2}{2}\left[x - \frac{aL}{2n\pi}\sin\left(\frac{2n\pi x}{aL}\right)\right]\Big|_{-aL/2}^{aL/2}$$

#2 (cont.)

a) $1 = \frac{A^2}{2}(aL - 0)$ b/c n = even, sin → 0

$A^2 = \frac{2}{aL} \rightarrow A = \sqrt{\frac{2}{aL}}$

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

$1 = \frac{B^2}{2} \int_{-aL/2}^{aL/2} \left(1 + \cos\left(\frac{2n\pi x}{aL}\right)\right) dx$

$1 = \frac{B^2}{2} \left[x + \sin\left(\frac{2n\pi x}{aL}\right) \cdot \frac{La}{2n\pi} \right] \Big|_{-aL/2}^{aL/2}$

$1 = \frac{B^2}{2}[aL + 0]$ b/c n = odd, cos → 0

$B^2 = \frac{2}{aL} \rightarrow B = \sqrt{\frac{2}{aL}}$

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

* To determine energies

$$\frac{\sqrt{2mE}}{\hbar} = \frac{n\pi}{aL} \Rightarrow E = \frac{n^2\pi^2\hbar^2}{2ma^2L^2}$$

* Pre-expansion, $a = 1$

$$\hookrightarrow \psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) & n = \text{even} \\ \sqrt{2/L} \cos\left(\frac{n\pi x}{L}\right) & n = \text{odd} \end{cases} \qquad E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

* Post-expansion, $a = 3$

$$\hookrightarrow \psi_m(x) = \begin{cases} \sqrt{2/3L} \sin\left(\frac{n\pi x}{3L}\right) & n = \text{even} \\ \sqrt{2/3L} \cos\left(\frac{n\pi x}{3L}\right) & n = \text{odd} \end{cases} \qquad E_m = \frac{m^2\pi^2\hbar^2}{18mL^2}$$

#2 (cont.)

b) * Both before and after expansion, the ground state corresponds to n=1

$$P = \left| \langle \psi_{m=1} | \psi_{n=1} \rangle \right|^2$$

$$= \left| \int \psi^*_{m=1} \psi_{n=1} \, dx \right|^2$$

$$= \left| \int_{-L/2}^{L/2} \cos\left(\frac{\pi x}{3L}\right) \cos\left(\frac{\pi x}{L}\right) dx \cdot \frac{2}{L\sqrt{3}} \right.$$

$$= \left| \frac{1}{L\sqrt{3}} \int_{-L/2}^{L/2} \cos\left(\frac{\pi x}{3L} - \frac{\pi x}{L}\right) + \cos\left(\frac{\pi x}{3L} + \frac{\pi x}{L}\right) dx \right|^2$$

$$= \left| \frac{1}{L\sqrt{3}} \int_{-L/2}^{L/2} \cos\left(-\frac{2\pi x}{3L}\right) + \cos\left(\frac{4\pi x}{3L}\right) dx \right|^2$$

$$= \left| \frac{1}{L\sqrt{3}} \left[\frac{3L}{-2\pi} \sin\left(\frac{-2\pi x}{3L}\right) + \frac{3L}{4\pi} \sin\left(\frac{4\pi x}{3L}\right) \right] \Big|_{-L/2}^{L/2} \right|^2$$

$$= \left| \frac{\sqrt{3}}{\pi} \left[-\frac{1}{2}\left(\sin\left(-\frac{\pi}{3}\right) - \sin\left(\frac{\pi}{3}\right)\right) + \frac{1}{4}\left(\sin\left(\frac{2\pi}{3}\right) - \sin\left(\frac{-2\pi}{3}\right)\right) \right] \right|^2$$

$$= \left| \frac{\sqrt{3}}{\pi} \left[\sin(\pi/3) + \frac{1}{2}\sin(2\pi/3) \right] \right|^2$$

$$= \left| \frac{\sqrt{3}}{\pi} \left(\frac{\sqrt{3}}{2} + \frac{1}{2}\left(\frac{\sqrt{3}}{2}\right) \right) \right|^2$$

$$= \left| \frac{\sqrt{3}}{\pi} \left(\frac{3\sqrt{3}}{4} \right) \right|^2$$

$$= \left| \frac{9}{4\pi} \right|^2$$

$$= \frac{81}{16\pi^2}$$

#2 (cont.)

c) $|\psi_n(t)\rangle = e^{-iHt/\hbar}|\psi_n\rangle$

* to write this as an expansion of eigenstates

$$\sum_m' |\psi_m\rangle\langle\psi_m|\psi_n\rangle = \sum_m' c_m |\psi_m\rangle$$

In integral form

$$C_m = \int \psi_m^* \psi_n \, dx$$

$$\hookrightarrow \psi_n = \sum_m' \left(\int \psi_m^* \psi_n \, dx\right) \psi_m(x)$$

$$\psi_n(t) = \sum_m' \int \psi_m^* \psi_n \, dx \, e^{-iHt/\hbar} \psi_m(x)$$

$$= \sum_m' \int \psi_m^* \psi_n \, dx \, e^{-iE_m t/\hbar} \psi_m(x)$$

PROBLEM 3: Matrix Mechanics

Let A, B and C be three ensembles that are represented in the orthonormal basis $|e_1\rangle$, $|e_2\rangle$ and $|e_3\rangle$,

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

by

$$A = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad B = \begin{pmatrix} 1 & -3 & 0 \\ -3 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}, \qquad C = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The eigenvalues of A are doubly degenerated, $a = 1,\ 1,\ -1$, with eigenvectors

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

The eigenvalues of C are also doubly degenerate, $c = 2,\ 1,\ 1$, with eigenvectors:

$$|c=2\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |c=1,1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad |c=1,2\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

Assume that all particles in the ensemble are in the state $|\psi\rangle$,

$$|\psi\rangle = \frac{1}{2}|e_1\rangle - \frac{1}{2}|e_2\rangle + \frac{1}{\sqrt{2}}|e_3\rangle.$$

Answer the following questions:

a) Find the probability of measuring C and obtaining a value $c = 2$; then immediately measuring A and getting $a = 1$, *i.e.* find $P_{|\psi\rangle}(c = 2, a = 1)$. Identify the intermediate state $|\psi'\rangle$ after C is measured. (2 Points)

b) Now find the probability if those measurements are performed in the reverse order, *i.e.*, find $P_{|\psi\rangle}(a = 1, c = 2)$. Identify the intermediate state $|\psi''\rangle$ after A is measured. (2 Points)

c) Compare the results of parts a) and b) and explain why this happened. (1 Point)

d) If you are told that the eigenvalues of B are $b = -2, -2, 4$, justify whether or not the following 2 probabilities $P_{|\psi\rangle}(a = -1, b = 4)$ and $P_{|\psi\rangle}(b = 4, a = -1)$ will be equal (do NOT explicitly calculate the probabilities). Will the final states be the same or different? Explain. (2 Points)

e) Does $\{A, B\}$ constitute a complete set of commuting observables? Demonstrate explicitly. (3 Points)

Jan 2014

Quantum #3

a) * With the initial state $|\psi\rangle = \frac{1}{2}|e_1\rangle - \frac{1}{2}|e_2\rangle + \frac{1}{\sqrt{2}}|e_3\rangle$

$\Rightarrow$ Probability of measuring $C=2$

$\hookrightarrow$ $|\langle c=2|C|\psi\rangle|^2$

$\Rightarrow$ Immediately after, probability of measuring

$\hookrightarrow$ $|\langle a=1,1|A|c=2\rangle|^2 + |\langle a=1,2|A|c=2\rangle|$

* State is $|c=2\rangle$ immediately after first measurement, need both terms above b/c $a=1$ is doubly degenerate eigenvalue

$\Rightarrow$ $P_{|\psi\rangle}(c=2, a=1) = \left(|\langle a=1,1|A|c=2\rangle|^2 + |\langle a=1,2|A|c=2\rangle|\right)^2 |\langle c=2|C|\psi\rangle|^2$

$$= \left[\left(\frac{1}{\sqrt{2}}[1\,1\,0]\begin{bmatrix}0&1&0\\1&0&0\\0&0&1\end{bmatrix}\begin{bmatrix}1\\0\\0\end{bmatrix}\right)^2 + \left([0\,0\,1]\begin{bmatrix}0&1&0\\1&0&0\\0&0&1\end{bmatrix}\begin{bmatrix}1\\0\\0\end{bmatrix}\right)^2\right]\left([1\,0\,0]\begin{bmatrix}2&0&0\\0&1&0\\0&0&1\end{bmatrix}\begin{bmatrix}1/2\\-1/2\\1/\sqrt{2}\end{bmatrix}\right)$$

$$= \left[\left(\frac{1}{\sqrt{2}}[1\,1\,0]\begin{bmatrix}0\\1\\0\end{bmatrix}\right)^2 + \left([0\,0\,1]\begin{bmatrix}0\\1\\0\end{bmatrix}\right)^2\right]\left([1\,0\,0]\begin{bmatrix}1\\-1/2\\1/\sqrt{2}\end{bmatrix}\right)^2$$

$$= \left(\frac{1}{2} + 0\right)(1)$$

$$= \frac{1}{2}$$

b) * Proceeding in a similar manner as above:

$P_{|\psi\rangle}(a=1, c=2) = \left(|\langle c=2|C|a=1,1\rangle|^2 + \langle a=1,1|A|\psi\rangle|^2\right) + \left(|\langle c=2|C|a=1,2\rangle|^2 \, |\langle a=1,2|A|\psi\rangle|^2\right.$

$$= \left[\left([1\,0\,0]\begin{bmatrix}2&0&0\\0&1&0\\0&0&1\end{bmatrix}\begin{bmatrix}1\\1\\0\end{bmatrix}\frac{1}{\sqrt{2}}\right)^2\left([1\,1\,0]\begin{bmatrix}0&1&0\\1&0&0\\0&0&1\end{bmatrix}\begin{bmatrix}1\\0\\0\end{bmatrix}1/\sqrt{2}\right)^2\right] + \left[\left([1\,0\,0]\begin{bmatrix}2&0&0\\0&1&0\\0&0&1\end{bmatrix}\begin{bmatrix}0\\0\\1\end{bmatrix}\right)^2\left([0\,0\,1]\begin{bmatrix}0&1&0\\1&0&0\\0&0&1\end{bmatrix}\right.\right.$$

$$= \left[\left(\frac{1}{2}\right)\left(\frac{1}{2}\right) + (0)(0)\right]$$

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

c) $$\begin{bmatrix}0&1&0\\1&0&0\\0&0&1\end{bmatrix}\begin{bmatrix}2&0&0\\0&1&0\\0&0&1\end{bmatrix} - \begin{bmatrix}2&0&0\\0&1&0\\0&0&1\end{bmatrix}\begin{bmatrix}0&1&0\\1&0&0\\0&0&1\end{bmatrix} = \begin{bmatrix}0&1&0\\2&0&0\\0&0&1\end{bmatrix} - \begin{bmatrix}0&2&0\\1&0&0\\0&0&1\end{bmatrix} = \begin{bmatrix}0&-1&0\\1&0&0\\0&0&0\end{bmatrix}$$

$\hookrightarrow$ non-commuting observables, thus order of observation matters

#1 (cont.)

d) Solving for the eigenvectors of B we see:

$B\vec{x} = \lambda\vec{x}$

Case $\lambda = 4$

$x_1 - 3x_2 = 4x_1 \rightarrow -x_2 = x_1$

$-3x_1 + x_2 = 4x_2 \rightarrow -x_1 = x_2$

$-2x_3 = 4x_3$

$\Rightarrow x_3 = 0$

$\vec{x} = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix} \cdot \frac{1}{\sqrt{2}}$

Case $\lambda = -2$

$x_1 - 3x_2 = -2x_1$

$-3x_1 + x_2 = -2x_2$

$-2x_3 = -2x_3$

$\vec{x} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$ or $\begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} \cdot \frac{1}{\sqrt{2}}$

$\Rightarrow$ Same set of eigenvectors indicates commuting observables, and since both states under consideration have the same corresponding eigenvector, the eigenvalues are simultaneous. This will result in no difference in probability based on the order of observation and in both cases the particle will be in the same final state.

e) The criteria for $\{A, B\}$ to be a complete set of commuting observables is:

① All the observables commute in pairs

② If we specify the eigenvalues of all operators in the set, we identify a unique eigenvector in the Hilbert space

$[A,B] = AB - BA$

$= \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} 1 & -3 & 0 \\ -3 & 1 & 0 \\ 0 & 0 & -2 \end{bmatrix} - \begin{bmatrix} 1 & -3 & 0 \\ -3 & 1 & 0 \\ 0 & 0 & -2 \end{bmatrix}\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

$= \begin{bmatrix} -3 & 1 & 0 \\ 1 & -3 & 0 \\ 0 & 0 & -2 \end{bmatrix} - \begin{bmatrix} -3 & 1 & 0 \\ 1 & -3 & 0 \\ 0 & 0 & -2 \end{bmatrix}$

$= 0$ ✓ (Condition 1 statisfied)

$\vec{x} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = |a=1, b=-2\rangle$ $\quad \vec{x} = \begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \\ 0 \end{bmatrix} = |a=-1, b=4\rangle$ $\quad \vec{x} = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{bmatrix} = |a=-1, b=-2\rangle$

↳ Condition 2 statisfied

Problem 4: Clebsh-Gordon Coefficients

Consider a system with two distinguishable spinless particles with angular momentum $j_1 = 1$ and $j_2 = 1$. Suppose the system is prepared in a state with total angular momentum $j = 2$ and total angular momentum projection $m = m_1 + m_2 = 0$. The state in the total j basis $|j_1, j_2; j, m\rangle$ is

$$|\psi\rangle \equiv |1, 1; j = 2, m = 0\rangle.$$

a) Express $|\psi\rangle$ in terms of products of single particle states, namely in the direct product basis $|j_1 = 1, m_1\rangle|j_2 = 1, m_2\rangle$. (4 Points).

b) If the angular momentum projection of particle 1 is measured along the z direction, what is the probability of finding a non-zero result? (2 Points)

c) If $\mathbf{J}_i$ is the angular momentum operator of each particle ($i = 1, 2$), compute the expectation value of $\mathbf{J}_1 \cdot \mathbf{J}_2$ in the $|\psi\rangle$ state. (2 Points)

d) If the $|\psi\rangle$ state is rotated by an infinitesimal angle $\delta\theta$ around the x direction, compute the probability of measuring the $|1, 1; j = 2, m = 1\rangle$ state in leading order in $\delta\theta$. (2 Points)

Raising and lowering angular momentum operators:

$$J_{\pm}|j, m\rangle = \hbar\sqrt{(j \mp m)(j \pm m + 1)}|j, m \pm 1\rangle$$

Jan 2014

Quantum #4

* Two distinguishable spinless particles,

a) with both particles having $j_i = 1$, $m_i = \{-1, 0, 1\}$

$$\hookrightarrow |1,1, j=2, m=0\rangle = A|1, m_1=0\rangle \otimes |1, m_2=0\rangle + B|1, m_1=1\rangle \otimes |1, m_1=-1\rangle + C|1, m_1=-1\rangle \otimes |1, m_2=1\rangle$$

* To determine the values of A, B, C (the Clebsh-Gordon) coefficients, we must start in either the highest or lowest state for two distinguishable spinless particles and use raising/lowering operators to reach our known state

$$J_- = J_{1,-} + J_{2,-} = J_{1,-} \otimes \mathbb{I}_2 + \mathbb{I}_1 \otimes J_{2,-}$$

$$J_- |a,b\rangle = \hbar\sqrt{(j+m)(j-m+1)}\,|a, b-\hbar\rangle$$

* Our maximum state is: $|1,1,2,2\rangle = |1,1\rangle \otimes |1,1\rangle$, $\hbar = 1$

$$J_- |1,1;2,2\rangle = |1,1;2,1\rangle \cdot \sqrt{(2+2)(2-2+1)}$$

$$= 2|1,1;2,1\rangle$$

$$J_- |1,1\rangle \otimes |1,1\rangle = \sqrt{2}\,\hbar|1,0\rangle \otimes |1,1\rangle + \sqrt{2}\,|1,1\rangle \otimes |1,0\rangle$$

$$\Rightarrow |1,1;2,1\rangle = \frac{1}{\sqrt{2}}\left[|1,0\rangle \otimes |1,1\rangle\right] + \frac{1}{\sqrt{2}}\left[|1,1\rangle \otimes |1,0\rangle\right]$$

* Repeating

$$J_- |1,1;2,1\rangle = \sqrt{(2+1)(2-1+1)}\,|1,1;2,0\rangle$$

$$= \sqrt{6}\,|1,1;2,0\rangle$$

$$J_-\left[\frac{1}{\sqrt{2}}(|1,0\rangle \otimes |1,1\rangle) + \frac{1}{\sqrt{2}}(|1,1\rangle \otimes |1,0\rangle)\right] = \frac{1}{\sqrt{2}}\Big(\sqrt{(1+0)(1-0+1)}\,|1,-1\rangle \otimes |1,1\rangle$$
$$+ \sqrt{(1+1)(1-1+1)}\,|1,0\rangle \otimes |1,0\rangle$$
$$+ \sqrt{(1+1)(1-1+1)}\,|1,0\rangle \otimes |1,0\rangle$$
$$+ \sqrt{(1+0)(1-0+1)}\,|1,1\rangle \otimes |1,-1\rangle\Big)$$

$$= \frac{1}{\sqrt{2}}\left(\sqrt{2}\,|1,-1\rangle \otimes |1,1\rangle + 2\sqrt{2}\,|1,0\rangle \otimes |1,0\rangle + \sqrt{2}\,|1,1\rangle \otimes |1,-1\rangle\right)$$

#4 (cont.)

a) $\Rightarrow \; |1,1;2,0\rangle = \frac{1}{\sqrt{6}}|1,-1\rangle \otimes |1,1\rangle + \sqrt{\frac{2}{3}}\,|1,0\rangle \otimes |1,0\rangle + \frac{1}{\sqrt{6}}|1,1\rangle \otimes |1,1\rangle$

b) $J_{z,1}|1,1;2,0\rangle = J_{z,1}\left[\frac{1}{\sqrt{6}}|1,-1\rangle \otimes |1,1\rangle + \sqrt{\frac{2}{3}}|1,0\rangle \otimes \overset{|1,0\rangle}{} + \frac{1}{\sqrt{6}}|1,1\rangle \otimes |1,1\rangle\right]$

$\underline{P}(J_{z,1} \neq 0) = \langle 1,1;2,0| J_{z,1} | 1,1;2,0\rangle$

$= \sum |c_n|^2$

$= \frac{1}{6}(-1) + \frac{1}{6}(1) + \frac{2}{3}(0)$

$\hookrightarrow \frac{1}{3}$ overall, $\frac{1}{6}$ each for $J_{z,1} = \pm 1$

c) $J_1 \cdot J_2 = (J^2 - J_1^2 + J_2^2) \cdot \frac{1}{2}$

$\hookrightarrow$ From $J^2 = (J_1 + J_2) \cdot (J_1 + J_2)$

$J^2 = J_1^2 + 2 J_1 \cdot J_2 + J_2^2$

$\langle J_1 \cdot J_2 \rangle = \langle 1,1;2,0| J_1 \cdot J_2 |1,1;2,0\rangle$

$= \langle 1,1;2,0| \frac{1}{2}(J^2 - J_1^2 - J_2^2) |1,1;2,0\rangle$

$= \frac{1}{2}(2^2 - 1^2 - 1^2)$

$= \frac{1}{2}(4 - 1 - 1)$

$= 1$

d)

PROBLEM 5: Zeeman Field

Consider the eight $n = 2$ states of Hydrogen. This problem is on the *strong* field Zeeman effect with spin-orbit interaction. Assume that the constant magnetic field B lies along the z-direction. The spin orbit coupling term is

$$H_{SO} = \frac{1}{2m_l^2c^2}\frac{1}{r}\frac{\mathrm{d}V}{\mathrm{d}r}\mathbf{L}\cdot\mathbf{S},$$

where $V(r)$ is the Coulomb potential, c is the speed of light and m_l is the angular momentum projection quantum number. Remember:

$$\langle n, l, m_l|\frac{1}{r^3}|n, l, m_l\rangle = \frac{1}{a_0^3n^3l(l+\frac{1}{2})(l+1)}$$

for $l \neq 0$.

a) Find a general expression for the energy due to the spin-orbit term in the physical limit of strong magnetic field, where the strong field Zeeman splitting expressions are valid. Express your answer in terms of the good quantum numbers in this problem. Recall that because of the strong magnetic field, the good quantum numbers in this regime are n, l, m_l and m_s and not j and m_j. (Hint: compute $\langle H_{SO}\rangle$ in the proper basis) (3 Points)

b) Explicitly write down the quantum numbers for all eight $n = 2$ states. Find the energy of each state under strong field Zeeman splitting. Express the energy of each state as the sum of 3 terms: the Bohr energy, the spin-orbit interaction, and the Zeeman contribution. (4 Points)

c) If you ignore the spin-orbit interaction, how many distinct energy levels are there and what are their degeneracies? (3 Points)

* Modified version of Sakurai 5.4

Problem 6: Perturbation Theory

An isotropic Harmonic oscillator in two dimensions has the Hamiltonian

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

where x and y are position operators in Cartesian coordinates x and y.

a) What is the energy of the *three* lowest energy levels and their respective degeneracies? (2 Points)

b) Consider a perturbative potential of the form:

$$V(x, y) = Am\omega^2 xy.$$

Compute the energy correction of the lowest level in the lowest order in perturbation theory where the result is non-zero. (3 Points)

c) Compute the energy splitting of the first excited energy level (which is degenerate), due to the perturbation. Compute the split ket states in terms of the original unperturbed kets. (3 Points)

d) Suppose that there are three indistinguishable spin 1/2 particles in the system. Compute the total energy of the ground state in first order in perturbation theory. (2 Points)

Jan 2014

Quantum #6

a) The energies of the isotropic oscillator are the sum of 2 1-D harmonic oscillators as the differential equation will be seperable by $\psi = X(x)\,Y(y)$

$\hookrightarrow$ $E_n = (n + 1/2)\hbar\omega$ in 1-D SHO

$\Rightarrow$ $E_n = (n_x + n_y + 1/2)\hbar\omega$ in 2-D isotropic HO

Our 3 lowest levels are: $\frac{1}{2}\hbar\omega$ - $n_x = n_y = 0$

$\frac{3}{2}\hbar\omega$ - $(n_x = 1,\ n_y = 0),\ (n_x = 0,\ n_y = 1)$

$\frac{5}{2}\hbar\omega$ - $(n_x = 2,\ n_y = 0),\ (n_x = 1,\ n_y = 1),\ (n_x = 0, n_y = 2)$

b) $V'(x) = Am\omega^2 xy$

* We want lowest level $(n_x = n_y = 0)$, non-zero energy perturbation

$\hookrightarrow$ $\Delta E_{0,0}^{(1)} = \langle \psi_{00} | V' | \psi_{00} \rangle$

$= \langle 0,0 | Am\omega^2 xy | 0,0 \rangle$

$= Am\omega^2 \langle 0,0 | xy | 0,0 \rangle$

* Note that x, y can be written in terms of raising/lowering operators where:

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

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

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

$= Am\omega^2 \cdot \frac{\hbar}{2m\omega} \langle 0,0 | (a_x + a_x^{+})(a_y + a_y^{+}) | 0,0 \rangle$

$= \frac{A\hbar\omega}{2} \langle 0,0 | a_x a_y + a_x^{+} a_y + a_x a_y^{+} + a_x^{+} a_y^{+} | 0,0 \rangle$

$= \frac{A\hbar\omega}{2} \left[0 \cancelto{0}{\langle 0,0 | 0,-1 \rangle} + 0 \cancelto{0}{\langle 0,0 | 1,-1 \rangle} + 0 \cancelto{0}{\langle 0,0 | -1,1 \rangle} + 1 \cancelto{0}{\langle 0,0 | 1,1 \rangle} \right]$

* Note: First 3 terms physically impossible

$= 0$

#6 (cont.)

b) $$\Delta E^{(2)}_{0,0} = \sum_{k\neq n}' \frac{|\langle k|V'|n\rangle|^2}{E_n^{(0)} - E_k^{(0)}}$$

$$= \sum_{k\neq n}' \frac{|\langle k_x k_y | \frac{A\hbar\omega}{2} a_x^\dagger a_y^\dagger |0,0\rangle|^2}{\frac{1}{2}\hbar\omega - E_k^{(0)}}$$

$$= \sum_{k\neq n}' \frac{|\langle k_x k_y | \frac{A\hbar\omega}{2} |1,1\rangle|^2}{\frac{1}{2}\hbar\omega - E_k^{(0)}}$$

* Numerator $\neq 0$ only if $k_x = k_y = 1$ by orthogonality

$$= \frac{A^2\hbar^2\omega^2/4}{\frac{1}{2}\hbar\omega - \frac{3}{2}\hbar\omega}$$

$$= -\frac{A^2\hbar\omega}{8}$$

c) This problem can be achieved by diagonalizing the perturbation matrix for the first excited state

* Remember $E_1 = \frac{3}{2}\hbar\omega$, $(n_x = 1, n_y = 0)$ or $(n_x = 0, n_y = 1)$

$$xy = a_x a_y + a_x^\dagger a_y + a_x a_y^\dagger + a_x^\dagger a_y^\dagger$$

$$V' = \begin{array}{c c} & \begin{array}{cc} |1,0\rangle & |0,1\rangle \end{array} \\ \begin{array}{c} |1,0\rangle \\ |0,1\rangle \end{array} & \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \end{array} \cdot \frac{A\hbar\omega}{2}$$

* To find the energy corrections, we find the eigenvalues

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

$$\hookrightarrow \lambda = \pm 1$$

* To find the states that correspond to these energy corrections, we find the eigenvectors by $V\vec{a} = \lambda\vec{a}$

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \lambda\begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \Rightarrow \begin{array}{l} a_2 = \lambda a_1 \\ a_1 = \lambda a_2 \end{array}$$

#6 (cont.)

c) $*$ for $\lambda = 1$

$$\left.\begin{array}{l} a_2 = a_1 \\ a_1 = a_2 \end{array}\right\rangle \vec{a} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \frac{1}{\sqrt{2}}$$

$*$ for $\lambda = -1$

$$\left.\begin{array}{l} a_2 = -a_1 \\ a_1 = -a_2 \end{array}\right\rangle \vec{a} = \begin{bmatrix} 1 \\ -1 \end{bmatrix} \frac{1}{\sqrt{2}}$$

Orthogonality check: $\vec{a}_1 \circ \vec{a}_{-1} = 1 + -1 = 0$ ✓

$\hookrightarrow$ $\Delta E_1^{(1)} = \frac{A\hbar\omega}{2}$, $\quad |\psi\rangle = \frac{1}{\sqrt{2}}|1,0\rangle + \frac{1}{\sqrt{2}}|0,1\rangle$

$\Delta E_2^{(1)} = -\frac{A\hbar\omega}{2}$, $\quad |\psi\rangle = \frac{1}{\sqrt{2}}|1,0\rangle - \frac{1}{\sqrt{2}}|0,1\rangle$

d)

Quantum Mechanics
Qualifying Exam - August 2014

Notes and Instructions

- There are 6 problems. Attempt them all as partial credit will be given.
- 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 all your work to receive full credit.

Possibly useful formulas:

Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Laplacian in spherical coordinates

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

One dimensional simple harmonic oscillator operators:

$$X = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger), \qquad P = -i\sqrt{\frac{\hbar m\omega}{2}}(a - a^\dagger)$$

Spherical Harmonics:

$$\begin{aligned}
Y_0^0(\theta,\phi) &= \frac{1}{\sqrt{4\pi}} \\
Y_1^0(\theta,\phi) &= \sqrt{\frac{3}{4\pi}}\cos\theta \\
Y_1^{\pm 1}(\theta,\phi) &= \mp\sqrt{\frac{3}{8\pi}}\sin\theta \mathrm{e}^{\pm i\phi} \\
Y_2^0(\theta,\phi) &= \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1) \\
Y_2^{\pm 1}(\theta,\phi) &= \mp\sqrt{\frac{15}{8\pi}}(\sin\theta\cos\theta)\,\mathrm{e}^{\pm i\phi} \\
Y_2^{\pm 2}(\theta,\phi) &= \sqrt{\frac{15}{32\pi}}\sin^2\theta\,\mathrm{e}^{\pm 2i\phi}
\end{aligned}$$

PROBLEM 1: Stationary and Non-Statonary States

Consider a quantum system whose particles are in the following state:

$$\Psi(x,t) = \frac{1}{\sqrt{8}}\psi_1(x)\mathrm{e}^{-iE_1t/\hbar} - i\sqrt{\frac{3}{8}}\psi_3(x)\mathrm{e}^{-iE_3t/\hbar} + \frac{1}{\sqrt{2}}\psi_5(x)\mathrm{e}^{-iE_5t/\hbar}, \tag{1}$$

where $\psi_n(x)$, $n = 1, 2, 3\ldots$ are stationary states of the Hamiltonian governing the system,

$$H\psi_n(x) = E_n\psi(x).$$

Answer the following questions:

a) Do you expect $\langle x\rangle$, $\langle x^2\rangle$ and $\langle E\rangle$ to be time dependent or time independent? Discuss briefly, but do not calculate. (2 Points)

b) Is the uncertainty ΔE positive, negative or zero? Is ΔE time dependent or time independent? Again, discuss briefly but do not calculate. (2 Points)

c) Is $\Psi(t)$ above a solution of the time dependent Schroedinger equation? Demonstrate. (2 Points)

d) If the stationary states $\psi_1(x)$, $\psi_3(x)$ and $\psi_5(x)$ are eigenstates of the harmonic oscillator, will any of your answers to part a) change? Justify. (2 Points)

e) Now assume the particles are in the state

$$\Psi(x,t) = \psi_3(x)\mathrm{e}^{-iE_3t/\hbar}.$$

Answer parts a) and b) for this state. (2 Points)

Aug 2014

Quantum #1

a) Operators that commute with the Hamiltonian will be time independent. Since in general $[H, x] \neq 0$, $[H, x^2] \neq 0$, and $[H, E] = 0$, we would expect $\langle x \rangle$ and $\langle x^2 \rangle$ to vary with time while $\langle E \rangle$ will not

b) $\Delta E = \sqrt{\langle E^2 \rangle - \langle E \rangle^2}$

* From this equation, we know ΔE cannot be negative and there is no reason to expect $\langle E^2 \rangle = \langle E \rangle$, thus our answer should not be 0. ΔE should be time independent as $[E^2, E] = 0$ and thus $[H, E^2] = 0$

c) The time-dependent Schrödinger eqn is:

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = H|\psi\rangle \quad \text{where } H|\psi_n\rangle = E_n|\psi\rangle$$

$$|\psi\rangle = \frac{1}{\sqrt{8}} e^{-iE_1 t/\hbar}|\psi_1\rangle - i\sqrt{3/8}\, e^{-iE_3 t/\hbar}|\psi_3\rangle + \frac{1}{\sqrt{2}} e^{-iE_5 t/\hbar}|\psi_5\rangle$$

$$\Rightarrow H|\psi\rangle = \frac{E_1}{\sqrt{8}} e^{-iE_1 t/\hbar}|\psi_1\rangle - E_3 i\sqrt{3/8}\, e^{-iE_3 t/\hbar}|\psi_3\rangle + \frac{E_5}{\sqrt{2}} e^{-iE_5 t/\hbar}|\psi_5\rangle$$

$$i\hbar \frac{\partial}{\partial t}|\psi\rangle = i\hbar\left[\frac{-iE_1/\hbar}{\sqrt{8}} e^{-iE_1 t/\hbar}|\psi_1\rangle + \frac{i^2 E_3}{\hbar}\sqrt{3/8}\, e^{-iE_3 t/\hbar}|\psi_3\rangle + \frac{-iE_5}{\hbar}\sqrt{\frac{1}{2}}\, e^{-iE_5 t/\hbar}|\psi_5\rangle\right.$$

$$= \frac{E_1}{\sqrt{8}} e^{-iE_1 t/\hbar}|\psi_1\rangle - iE_3\sqrt{3/8}\, e^{-iE_3 t/\hbar}|\psi_3\rangle + \frac{E_5}{\sqrt{2}} e^{-iE_5 t/\hbar}|\psi_5\rangle$$

$\therefore$ $|\psi\rangle$ is a solution to time dependent Schrödinger Eqn

d) If we now specify that $|\psi_n\rangle$ are the states of the SHO, the only answer that changes from part a is $\langle x \rangle$ should now be time independent since $\langle x \rangle = 0$

e) If $|\psi\rangle = e^{-iE_3 t/\hbar}|\psi_3\rangle$, All our answers in part a will be time independent b/c $|\psi_3\rangle$ is a stationary state and the time dependences will cancel out ($e^{iE_3 t/\hbar} \cdot e^{-iE_3 t/\hbar} = 1$) Additionally, since we now definitively know E $\langle E \rangle^2 = \langle E^2 \rangle$ which means $\Delta E = 0$

PROBLEM 2: Oscillator Model of Angular Momentum

Arbitrary angular momentum can be constructed from spin-1/2. The latter can be described in terms of the Pauli matrices

$$\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}.$$

The construction of a general angular momentum can be done by introducing two sets of independent harmonic oscillators, in terms of creation ($a_\zeta^\dagger$) and annihilation (a_ζ) operators,

$$[a_+, a_-] = 0, \quad [a_+^\dagger, a_-^\dagger] = 0, \quad [a_\zeta, a_{\zeta'}^\dagger] = \delta_{\zeta,\zeta'},$$

with $\zeta, \zeta' = \pm$ indexing oscillators of type $\pm$. Now define

$$\mathbf{J} = \frac{\hbar}{2} a^\dagger \boldsymbol{\sigma} a,$$

where a is a two component operator,

$$a = \begin{pmatrix} a_+ \\ a_- \end{pmatrix}.$$

a) Given the form of the Pauli matrices, give the explicit form for J_x, J_y, J_z in terms of $a_\zeta^\dagger$ and a_ζ operators (2 Points).

b) Show that $J_\pm = J_x \pm iJ_y$ have particularly simple forms in terms of a_ζ and $a_\zeta^\dagger$ operators (1 Point).

c) Compute the commutator $[J_x, J_y]$. How is this generalized for the other components? (2 Points)

d) Show that

$$J^2 = J_z^2 + J_+J_- + i[J_x, J_y],$$

and then write this in terms of the number operators for the two harmonic oscillators,

$$n_+ = a_+^\dagger a_+, \quad n_- = a_-^\dagger a_-.$$

Show that this implies that the eigenvalues of J^2 are $j(j+1)\hbar^2$, where j is an integer or an integer plus $\frac{1}{2}$ (Hint: apply the J^2 operator in the two harmonic oscillator state $|n_+, n_-\rangle$) (3 Points).

e) Using the properties of the harmonic oscillators, show that the state in which J^2 has the eigenvalue $j(j+1)\hbar$ and $J_z = m\hbar$ can be constructed from the state in which both n_+ and n_- have the value zero, $|0\rangle$, by

$$|jm\rangle = \frac{(a_+^\dagger)^{j+m}}{\sqrt{(j+m)!}} \frac{(a_-^\dagger)^{j-m}}{\sqrt{(j-m)!}} |0\rangle.$$

(2 Points)

Aug 2014

Quantom #2

a) Given $\vec{J} = \frac{\hbar}{2} a^{\dagger} \vec{\sigma} a$ where $a = \langle a_+, a_- \rangle$

$$J_x = \frac{\hbar}{2} a^{\dagger} \sigma_x a$$
$$= \frac{\hbar}{2} \begin{bmatrix} a_+^{\dagger} & a_-^{\dagger} \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} a_+ \\ a_- \end{bmatrix}$$
$$= \frac{\hbar}{2} \begin{bmatrix} a_+^{\dagger} & a_-^{\dagger} \end{bmatrix} \begin{bmatrix} a_- \\ a_+ \end{bmatrix}$$
$$= \frac{\hbar}{2} (a_+^{\dagger} a_- + a_-^{\dagger} a_+)$$

$$J_y = \frac{\hbar}{2} a^{\dagger} \sigma_y a$$
$$= \frac{\hbar}{2} \begin{bmatrix} a_+^{\dagger} & a_-^{\dagger} \end{bmatrix} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \begin{bmatrix} a_+ \\ a_- \end{bmatrix}$$
$$= \frac{\hbar}{2} \begin{bmatrix} a_+^{\dagger} & a_-^{\dagger} \end{bmatrix} \begin{bmatrix} -i a_- \\ i a_+ \end{bmatrix}$$
$$= \frac{\hbar}{2} (-i a_+^{\dagger} a_- + i a_-^{\dagger} a_+)$$

$$J_z = \frac{\hbar}{2} \begin{bmatrix} a_+^{\dagger} & a_-^{\dagger} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} a_+ \\ a_- \end{bmatrix}$$
$$= \frac{\hbar}{2} \begin{bmatrix} a_+^{\dagger} & a_-^{\dagger} \end{bmatrix} \begin{bmatrix} a_+ \\ -a_- \end{bmatrix}$$
$$= \frac{\hbar}{2} [a_+^{\dagger} a_+ - a_-^{\dagger} a_-]$$

b) $J_{\pm} = J_x \pm i J_y$

$$\hookrightarrow J_+ = \frac{\hbar}{2} [a_+^{\dagger} a_- + a_-^{\dagger} a_+] + i \left(\frac{-i\hbar}{2} [a_+^{\dagger} a_- + a_-^{\dagger} a_+] \right)$$
$$= \frac{\hbar}{2} [a_+^{\dagger} a_- + a_-^{\dagger} a_+] + \frac{\hbar}{2} [a_+^{\dagger} a_- - a_-^{\dagger} a_+]$$
$$= \hbar [a_+^{\dagger} a_-]$$

$$\hookrightarrow J_- = \frac{\hbar}{2} [a_+^{\dagger} a_- + a_-^{\dagger} a_+] - i \left(\frac{-i\hbar}{2} [a_+^{\dagger} a_- - a_-^{\dagger} a_+] \right)$$
$$= \frac{\hbar}{2} [a_+^{\dagger} a_- + a_-^{\dagger} a_+] - \frac{\hbar}{2} [a_+^{\dagger} a_- - a_-^{\dagger} a_+]$$
$$= \hbar [a_-^{\dagger} a_+]$$

c) $[J_x, J_y] = J_x J_y - J_y J_x$

$$= \frac{i\hbar^2}{4} \left([a_+^{\dagger} a_- + a_-^{\dagger} a_+][a_-^{\dagger} a_+ - a_+^{\dagger} a_-] - [a_-^{\dagger} a_+ - a_+^{\dagger} a_-][a_+^{\dagger} a_- + a_-^{\dagger} a_+] \right)$$
$$= \frac{i\hbar^2}{4} \Big(a_+^{\dagger} a_- a_-^{\dagger} a_+ + \cancel{a_-^{\dagger} a_+ a_-^{\dagger} a_+} - a_+^{\dagger} \cancel{a_- a_+^{\dagger} a_-} - a_-^{\dagger} a_+ a_+^{\dagger} a_- - a_-^{\dagger} a_+ a_+^{\dagger} a_-$$
$$- \cancel{a_-^{\dagger} a_+ a_-^{\dagger} a_+} + a_+^{\dagger} \cancel{a_- a_+^{\dagger}} a_- + a_+^{\dagger} a_- a_-^{\dagger} a_+ \Big)$$
$$= \frac{i\hbar^2}{4} (2 a_+^{\dagger} a_- a_-^{\dagger} a_+ - 2 a_-^{\dagger} a_+ a_+^{\dagger} a_-)$$

#2 (cont.)

c) $$[J_x, J_y] = \frac{i\hbar^2}{2}\left(a_+^\dagger \cancelto{1}{a_- a_-^\dagger} a_+ - a_-^\dagger \cancelto{1}{a_+ a_+^\dagger} a_-\right)$$

$$= \frac{i\hbar^2}{2}\left(a_+^\dagger a_+ - a_-^\dagger a_-\right)$$

$$= i\hbar J_z$$

$\Rightarrow$ Angular momentum operators will generalize as $[J_i, J_j] = i\hbar \epsilon_{ijk} J_k$

d) $$J^2 = J_x^2 + J_y^2 + J_z^2$$

$$= J_z^2 + (J_x^2 + J_y^2)$$

$$= J_z^2 + (J_x + iJ_y)(J_x - iJ_y) \underline{- iJ_yJ_x + iJ_xJ_y}$$

$$= J_z^2 + J_+J_- + i[J_x, J_y]$$

eliminate cross terms in expansion

* Rewriting this in terms of the oscillators

$$= \frac{\hbar^2}{4}[a_+^\dagger a_+ - a_-^\dagger a_-]^2 + \hbar^2 a_+^\dagger a_- a_-^\dagger a_+ + i(i\hbar J_z)$$

$$= \frac{\hbar^2}{4}[a_+^\dagger a_+ a_+^\dagger a_+ - a_+^\dagger a_+ a_-^\dagger a_- - a_-^\dagger a_- a_+^\dagger a_+ + a_-^\dagger a_- a_-^\dagger a_-] + \hbar^2 a_+^\dagger a_- a_-^\dagger a_+$$
$$- \frac{\hbar^2}{2}[a_+^\dagger a_+ - a_-^\dagger a_-]$$

$$= \frac{\hbar^2}{4}[a_+^\dagger a_+ - a_+^\dagger a_+ a_-^\dagger a_- - a_-^\dagger a_- a_+^\dagger a_+ + a_-^\dagger a_-] + \hbar^2 a_+^\dagger a_+ - \frac{\hbar^2}{2}[a_+^\dagger a_+ - a_-^\dagger a_-]$$

$$= \frac{\hbar^2}{4}[n_+ - n_+n_- - n_-n_+ + n_-] + \hbar^2 n_+ - \frac{\hbar^2}{2}[n_+ - n_-]$$

$$= \frac{\hbar^2}{4}[3n_+ - n_+n_- - n_-n_+ - n_-]$$

$= \ldots$??

PROBLEM 3: Perturbation Theory

Consider a particle of mass m trapped inside a 1D parabolic potential

$$V(x) = \frac{1}{2} m\omega^2 x^2,$$

where ω sets the frequency of oscillation inside the potential.

a) If the particle is perturbed by a *static* potential

$$V_I = \alpha x,$$

with α small, compute energy correction of the energy levels in the lowest order where the result is non-zero. (3 Points)

b) What is the pertubed ket in the ground state? Compute the expectation value $\langle x \rangle$ in this state. Interpret the sign of $\langle x \rangle$. (3 Points)

c) Assume from now on that $\alpha = 0$. Imagine that the particle is charged and sits in the ground state at $t = -\infty$. Suppose an electric field is gradually tuned on, increases to a maximum at $t = 0$ and then slowly dies away,

$$V_I'(t) = -e|\mathbf{E}| x \, \mathrm{e}^{-t^2/\tau^2},$$

where e is the electric charge, and $\mathbf{E}$ is the electric field . Write down the general expression for the amplitude of transition from a generic level i to level f. (Do not solve the integral yet) (2 Points).

d) Evaluate the probability of having the particle in the first excited state at $t = +\infty$. (2 Points).

Hint: $\int_{-\infty}^{\infty} \mathrm{d}t \, \mathrm{e}^{-t^2/\tau^2} \mathrm{e}^{i\omega t} = \sqrt{\pi}\tau \, \mathrm{e}^{-\omega^2\tau^2/4}$

Aug 2014

Quantum #3

a) In general, our first order energy correction is $\Delta E^{(1)} = \langle n^{(0)} | V' | n^{(0)} \rangle$

$\hookrightarrow V = \frac{1}{2} m\omega^2 x^2 \rightarrow$ SHO

$V' = \alpha x = \alpha \left(\sqrt{\frac{\hbar}{2m\omega}} [a^\dagger + a] \right)$

$$\Rightarrow \Delta E^{(1)} = \langle n | \alpha \sqrt{\frac{\hbar}{2m\omega}} (a^\dagger + a) | n \rangle$$

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

$$= \alpha \sqrt{\frac{\hbar}{2m\omega}} \left[\cancel{\langle n | a^\dagger | n \rangle}^{0} + \cancel{\langle n | a | n \rangle}^{0} \right]$$

* results will go to 0 by orthogonality $\langle n | m \rangle = \delta_{nm}$

Our second order correction is generally: $\Delta E^{(2)} = \sum\limits_{k \neq n}' \frac{|V_{kn}|^2}{E_n^{(0)} - E_k^{(0)}}$

$$\Rightarrow \Delta E^{(2)} = \sum_{k \neq n}' \frac{|\langle k | V' | n \rangle|^2}{\hbar\omega [(n + 1/2) - (k + 1/2)]}$$

$$= \sum_{k \neq n}' \frac{|\langle k | \alpha \sqrt{\frac{\hbar}{2m\omega}} (a^\dagger + a) | n \rangle|^2}{\hbar\omega (n - k)}$$

$$= \frac{\alpha^2 \hbar}{2m\omega} \cdot \frac{1}{\hbar\omega} \sum_{k \neq n}' \frac{|\langle k | a^\dagger a | n \rangle|^2}{(n - k)}$$

$$= \frac{\alpha^2}{2m\omega^2} \sum_{k \neq n}' \frac{|\langle k | n+1 \rangle \sqrt{n+1} + \langle k | n-1 \rangle \sqrt{n}|^2}{n - k}$$

$$= \frac{\alpha^2}{2m\omega^2} \sum_{k \neq n}' \frac{|\sqrt{n+1}\, \delta_{k,n+1} + \sqrt{n}\, \delta_{k,n-1}|^2}{n - k}$$

$$= \frac{\alpha^2}{2m\omega} \left[\frac{n+1}{n - (n+1)} + \frac{n}{n - (n-1)} \right]$$

$$= \frac{\alpha^2}{2m\omega} \left[-(n+1) + n \right]$$

$$= \frac{-\alpha^2}{2m\omega}$$

#3 (cont.)

b) The formula for the first order correction to the wave function is:

$$|n^{(1)}\rangle = \sum_{k\neq n}' \frac{\langle k|V'|n\rangle}{E_n - E_k} |k^{(0)}\rangle$$

$$= \sum_{k\neq n}' \frac{\alpha\sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n+1}\,\delta_{k,n+1} + \sqrt{n}\,\delta_{k,n-1}\right)}{\hbar\omega(n-k)} |k^{(0)}\rangle$$

$$= \left(\frac{\alpha^2}{2m\hbar\omega^3}\right)^{1/2} \left(\frac{\sqrt{n+1}}{n-(n+1)}|n+1\rangle + \frac{\sqrt{n}}{n-(n-1)}|n-1\rangle\right)$$

$$= \left(\frac{\alpha^2}{2m\hbar\omega^3}\right)^{1/2} \left(\sqrt{n+1}\,|n+1\rangle - \sqrt{n}\,|n-1\rangle\right)$$

* but since we are in the ground state $n=0$, and $|-1\rangle = 0$

$$= -\left(\frac{\alpha^2}{2m\hbar\omega^3}\right)^{1/2} |1\rangle$$

* Our full state is now $|\psi\rangle = |0\rangle - \left(\frac{\alpha^2}{2m\hbar\omega^3}\right)^{1/2} |1\rangle$

$$\Rightarrow \langle x\rangle = \langle\psi|x|\psi\rangle \; ; \quad x = \sqrt{\frac{\hbar}{2m\omega}}\,(a^\dagger + a)$$

$$= \overbrace{\langle 0|x|0\rangle}^{0} - \left(\frac{\alpha^2}{2m\hbar\omega^3}\right)^{1/2}\langle 0|x|1\rangle - \left(\frac{\alpha^2}{2m\hbar\omega}\right)^{1/2}\langle 1|x|0\rangle + \frac{\alpha^2}{2m\hbar\omega^3}\overbrace{\langle 1|x|1\rangle}^{0}$$

$$= -\left(\frac{\alpha^2}{2m\hbar\omega^3}\right)^{1/2}\left[\langle 0|\sqrt{\frac{\hbar}{2m\omega}}\,(a^\dagger + a)|1\rangle + \langle 1|\sqrt{\frac{\hbar}{2m\omega}}\,(a^\dagger + a)|0\rangle\right]$$

$$= -\left(\frac{\alpha^2}{4m^2\omega^4}\right)^{1/2}\left[\overbrace{\langle 0|a^\dagger|1\rangle}^{0} + \langle 0|a|1\rangle + \langle 1|a^\dagger|0\rangle + \overbrace{\langle 1|a|0\rangle}^{0}\right]$$

$$= \frac{-\alpha}{2m\omega^2}\left[\langle 0|0\rangle + \langle 1|1\rangle\right]$$

$$= \frac{-\alpha}{m\omega^2}$$

* The expectation value being negative implies that the potential is deeper on the negative side than the unperturbed potential

#3 (cont.)

c) The transition probability is: (assumes a two state problem of i, f as states

$$c_n^{(1)} = \frac{-i}{\hbar}\int_{t_0}^{t} e^{-i\omega_{ni}t'} V_{ni}(t')\,dt', \quad \omega_{ni} = \omega_n - \omega_f, \quad E = \hbar\omega$$

$$V = -e|\vec{E}|x e^{-t^2/\tau^2}$$

*Simplifing the equation, we see:

$$\begin{aligned} V_{ni} &= \langle f|V|i\rangle \\ &= \langle f|-e|\vec{E}|x e^{-t^2/\tau^2}|i\rangle \\ &= -e|\vec{E}|e^{-t^2/\tau^2}\langle f|\sqrt{\tfrac{\hbar}{2m\omega}}(a^\dagger + a)|i\rangle \\ &= -eEe^{-t^2/\tau^2}\sqrt{\tfrac{\hbar}{2m\omega}}\left[\langle f|a^\dagger|i\rangle + \langle f|a|i\rangle\right] \end{aligned}$$

d) $P = |c_n^{(1)}|^2$, now specifying $|f\rangle = |1\rangle$, $|i\rangle = |0\rangle$

$$\begin{aligned} V_{ni} &= -eEe^{-t^2/\tau^2}\sqrt{\tfrac{\hbar}{2m\omega}}\left[\langle 1|a^\dagger|0\rangle + \cancel{\langle 1|a|0\rangle}^{\,0}\right] \\ &= -eEe^{-t^2\tau^2}\sqrt{\tfrac{\hbar}{2m\omega}} \end{aligned}$$

$$\hookrightarrow c_{10}^{(1)} = \frac{-i}{\hbar}\int_{-\infty}^{\infty} e^{-i\omega_{10}t'}\left(-eEe^{-t^2/\tau^2}\right)dt' \cdot \sqrt{\tfrac{\hbar}{2m\omega}}$$

$$= \frac{ieE}{\hbar}\sqrt{\frac{\hbar}{2m\omega}}\int_{-\infty}^{\infty} e^{-i\omega_{10}t'} e^{-t'^2/\tau^2}\,dt'$$

$$= \frac{ieE}{\hbar}\sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{\pi}\tau \exp[-\omega_{10}^2\tau^2/4]\right)$$

$$\underline{P} = \frac{e^2E^2}{\hbar^2}\left(\frac{\hbar}{2m\omega}\right)\pi\tau \exp[-\omega_{10}^2\tau^2/2], \quad \omega_{10} = \frac{E_1^{(0)} - E_0^{(1)}}{\hbar}$$

PROBLEM 4: Two Particles in a 1D Box

Consider two noninteracting particles of mass m inside a 1D box,

$$V(x) = \begin{cases} 0 & , 0 < |x| < a \\ \infty & , \text{otherwise} \end{cases} .$$

Make sure to consider the spin part of the wavefunction in this problem.

a) Let n_1 and n_2 be the quantum numbers of particle 1 and 2 respectively. What are the wavefunctions of the single particle states for the each particle in the box? What are the single particle energies? (2 Points)

b) If the particles are distinguishable what is the two-particle wavefunction that describes the state? What is the energy? Write out explicitly the state (or states) and energies for the ground state and first excited states of the system. (2 Points)

c) If the two particles are identical spin 0 bosons what are the ground state and first excited state wavefunctions and energies? (2 Points)

d) If the two particles are identical spin 1/2 fermions what are the ground state and first excited state wavefunctions and energies? (2 Points)

e) Write down the Hamiltonian for the two particles in the box and show that when the particles are identical H commutes with the exchange operator. (2 Points)

#4 (cont.)

a) * Similarly, if $n=$ odd: $A=0$, $B=\sqrt{\frac{1}{a}}$

$\Rightarrow$ For any single particle: $\boxed{\psi(x) = \begin{cases} \sqrt{\frac{1}{a}} \sin\left(\frac{n\pi x}{2a}\right) & n = \text{even} \\ \sqrt{\frac{1}{a}} \cos\left(\frac{n\pi x}{2a}\right) & n = \text{odd} \end{cases}}$

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

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

b) Assuming distinguishable particles, our two particle wave functions will be the product of the two single particle states, plus a spin function

$$\psi_{sys} = \psi_{n_1}\psi_{n_2}\psi_{spin}, \qquad E_{sys} = \frac{(n_1^2+n_2^2)\pi^2\hbar^2}{2ma^2}$$

The ground state occurs when $n_1 = n_2 = 1$

$$\psi_{sys} = \frac{1}{a}\cos\left(\frac{\pi x_1}{2a}\right)\cos\left(\frac{\pi x_2}{2a}\right)$$

$$E = \frac{\pi^2\hbar^2}{ma^2}$$

The first excited state occurs when $(n_1 = 2, n_2 = 1)$ or $(n_1 = 1, n_2 = 2)$

$$\psi_{sys} = \frac{1}{a}\sin\left(\frac{\pi x_1}{a}\right)\cos\left(\frac{\pi x_2}{2a}\right) \qquad E = \frac{5\pi^2\hbar^2}{2ma^2}$$

or

$$\psi_{sys} = \frac{1}{a}\cos\left(\frac{\pi x_1}{2a}\right)\sin\left(\frac{\pi x_2}{a}\right) \qquad E = \frac{5\pi^2\hbar^2}{2ma^2}$$

c) Our spin function now becomes important. Bosons must have symmetric spin functions which we will denote ψ_{spin}^{sym}. Since our bosons are identical, and thus indistinguishable, it will be a superposition of the two possible single particle states

$\Rightarrow$ In the ground state, $E_{sys} = \frac{\pi^2\hbar^2}{ma^2}$

$$\psi_{sys} = A\left[\frac{1}{a}\cos\left(\frac{\pi x_1}{2a}\right)\cos\left(\frac{\pi x_2}{2a}\right) + \frac{1}{a}\cos\left(\frac{\pi x_1}{2a}\right)\cos\left(\frac{\pi x_2}{2a}\right)\right]$$

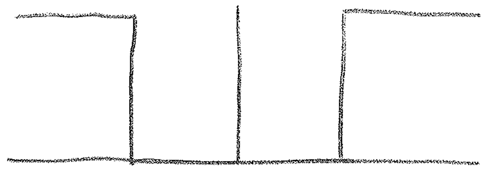
$$= \frac{2A}{a}\cos\left(\frac{\pi x_1}{2a}\right)\cos\left(\frac{\pi x_2}{2a}\right),$$ A is normalization constant

Aug 2014

Quantum #4

a) For two non-interacting particles in a box, where

$$V(x) = \begin{cases} 0 & 0 < |x| < a \\ \infty & \text{otherwise} \end{cases}$$



$-a$ $\qquad$ a

$$H\psi = E\psi$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

$$\frac{d^2\psi}{dx^2} = \frac{-\sqrt{2mE}}{\hbar}\psi$$

$$= -k^2\psi$$

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

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

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

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

$\hookrightarrow$ Our trig functions will be 0 when $ka = \frac{n\pi}{2} \Leftrightarrow k = \frac{n\pi}{2a}$

$\sin\left(\frac{n\pi}{2}\right) = 0$ if $n =$ even $(0, 2, 4, \text{etc})$

$\cos\left(\frac{n\pi}{2}\right) = 0$ if $n =$ odd $(1, 3, 5, \text{etc})$

*if $n =$ even,

$$\psi = A(0) + B\cos\left(\frac{n\pi}{2}\right) \Rightarrow B = 0$$

$$1 = A^2\int_{-a}^{a}\sin^2\left(\frac{n\pi x}{2}\right)dx$$

$$1 = \frac{A^2}{2}\int_{-a}^{a}\left[1 - \cos\left(\frac{n\pi x}{2a}\right)\right]dx$$

$$1 = \frac{A^2}{2}\left[x - \sin\left(\frac{n\pi x}{a}\right)\right]\Big|_{-a}^{a}$$

$$1 = \frac{A^2}{2}\left[\left(a - \frac{1}{n\pi}\overset{0}{\cancel{\sin\left(\frac{n\pi a}{a}\right)}}\right) - \left(-a - \frac{1}{n\pi}\overset{0}{\cancel{\sin\left(\frac{-n\pi a}{a}\right)}}\right)\right]$$

$$1 = \frac{A^2}{2}[2a] \Rightarrow A = \sqrt{\frac{1}{a}}$$

#4 (cont)

c) $\Rightarrow$ In the first excited state, $E_{sys} = \frac{5\pi^2\hbar^2}{2ma^2}$

$$\psi_{sys} = A\left[\frac{1}{a}\sin\left(\frac{\pi x_1}{2a}\right)\cos\left(\frac{\pi x_2}{a}\right) + \frac{1}{a}\cos\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{2a}\right)\right]$$

d) With two identical spin 1/2 fermions, we need an antisymmetric spin function, denoted ψ^{asym}_{spin}, and an antisymmetric wave function

$\Rightarrow$ In the ground state, $E_{sys} = \frac{\pi^2\hbar^2}{2ma^2}$ (1 particle spin up, 1 spin down will violate exclusion principle)

$$\psi_{sys} = A\left[\frac{1}{a}\sin\left(\frac{\pi x_1}{2a}\right)\sin\left(\frac{\pi x_2}{2a}\right) - \frac{1}{a}\sin\left(\frac{\pi x_1}{2a}\right)\sin\left(\frac{\pi x_2}{2a}\right)\right]$$

$$= 0$$

Therefore, our ground state becomes $E_{sys} = \frac{5\pi^2\hbar^2}{2ma^2}$

$$\psi_{sys} = A\left[\frac{1}{a}\sin\left(\frac{\pi x_1}{2a}\right)\cos\left(\frac{\pi x_2}{a}\right) - \frac{1}{a}\cos\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{2a}\right)\right]$$

$\Rightarrow$ Now the first excited state occurs when $(n_1 = 1, n_2 = 3)$ or $(n_1 = 3, n_2 = 1)$. with $E_{sys} = \frac{5\pi^2\hbar^2}{ma^2}$

$$\psi_{sys} = A\left[\frac{1}{a}\sin\left(\frac{\pi x_1}{2a}\right)\sin\left(\frac{3\pi x_2}{2a}\right) - \frac{1}{a}\sin\left(\frac{3\pi x_1}{2a}\right)\sin\left(\frac{\pi x_2}{2a}\right)\right]$$

e) The Hamiltonian for the system is:

$$H = \frac{-\hbar^2}{2m}\left[\frac{d^2}{dx_1^2} + \frac{d^2}{dx_2^2}\right]$$

PROBLEM 5: Addition of angular momenta

Consider an electron. We know its orbital angular momentum $\ell = 1$ and the z component $m = 1/2$ of its total angular momentum j.

a) What are the possible values of j? (2 Points).

b) Write down the kets $|\ell = 1, \frac{1}{2}; j, m = \frac{1}{2}\rangle$ in terms of products of spin and orbital angular momentum states (3 Points)

c) Calculate the expectation value of the spin operator $\mathbf{S}$ in the state $|\ell = 1, \frac{1}{2}; j, m = \frac{1}{2}\rangle$. Consider all possible values of j. (3 Points).

d) The magnetic dipole moment of the electron is

$$\boldsymbol{\mu} = \frac{e}{2m_e c}(\mathbf{L} + 2\mathbf{S}),$$

with $\mathbf{L}$ the orbital angular momentum operator, e the electron charge, m_e the mass and c the speed of light. Calculate the expectation value of $\boldsymbol{\mu}$ in the states $|\ell = 1, \frac{1}{2}; j, m = \frac{1}{2}\rangle$. (2 Points)

Raising and lowering angular momentum operators:

$$J_\pm |j, m\rangle = \hbar\sqrt{(j \mp m)(j \pm m + 1)}|j, m \pm 1\rangle$$

Aug 2014

Quantum #5

a) Given an electron w/ $\ell = 1$, $m = 1/2$, we know that

$$|\ell - m| \le j \le |\ell + s|$$

$$|1 - 1/2| \le j \le |1 + 1/2|$$

$$1/2 \le j \le 3/2$$

$$\hookrightarrow j = \{1/2, 3/2\}$$

b) We must use Clebsh-Gordon coefficients, we start in the highest state and use the lowering operator

$$|\ell=1, m=1/2; 3/2, 3/2\rangle = |\ell=1, m_\ell=1\rangle \otimes |s=1/2, m_s=1/2\rangle$$

$$J_-|\ell=1, m=1/2; 3/2, 3/2\rangle = \hbar\sqrt{(\tfrac{3}{2}+\tfrac{3}{2})(3/2-3/2+1)}\ |1, 1/2; 3/2, 1/2\rangle$$

$$= \hbar\sqrt{3}$$

$$J_-|1,1\rangle \otimes |1/2, 1/2\rangle = J_-^L|1,1\rangle \otimes |1/2, 1/2\rangle + |1,1\rangle \otimes J_-^S|1/2, 1/2\rangle$$

$$= \sqrt{2}\hbar|1,0\rangle \otimes |1/2, 1/2\rangle + \hbar|1,1\rangle \otimes |1/2, -1/2\rangle$$

$$|1, 1/2; 3/2, 1/2\rangle = \frac{\sqrt{2}}{\sqrt{3}}\left[|1,0\rangle \otimes |1/2, 1/2\rangle\right] + \frac{1}{\sqrt{3}}\left[|1,1\rangle \otimes |1/2, -1/2\rangle\right]$$

To determine the $|1, 1/2; 1/2, 1/2\rangle$ state, we use the orthogonality condition

$$\langle 1, 1/2; 3/2, 1/2 | 1, 1/2; 1/2, 1/2\rangle = 0$$

letting $|1, 1/2; 1/2, 1/2\rangle = A\left[|1,0\rangle \otimes |1/2, 1/2\rangle\right] + B\left[|1,1\rangle \otimes |1/2, -1/2\rangle\right]$

where $A^2 + B^2 = 1$

$$\hookrightarrow 0 = A \cdot \sqrt{\tfrac{2}{3}} + B\sqrt{\tfrac{1}{3}}$$

$$-B\sqrt{\tfrac{1}{3}} = A\sqrt{\tfrac{2}{3}} \Rightarrow A = \frac{-B}{\sqrt{2}}$$

$$1 = \frac{B^2}{2} + B^2 \Rightarrow B = \sqrt{\tfrac{2}{3}},\ A = \frac{-1}{\sqrt{3}}$$

$$\hookrightarrow |1, 1/2; 1/2, 1/2\rangle = \frac{-1}{\sqrt{3}}|1,0\rangle \otimes |1/2, 1/2\rangle + \sqrt{\tfrac{2}{3}}|1,1\rangle \otimes |1/2, -1/2\rangle$$

#5 (cont.)

c)

PROBLEM 6: Variational approach

A particle with mass, m, moving in one dimension finds itself in a potential given by,

$$V = \infty \quad \text{for} \quad x < 0$$

and

$$V = \beta x^3 \quad \text{for} \quad x > 0$$

where β is a positive constant.

a) Find an approximation to the ground state energy, using the trial wavefunction

$$\Psi = 0 \quad \text{for} \quad x < 0$$

and

$$\Psi = Cxe^{-\alpha x} \quad \text{for} \quad x > 0.$$

where C and α are positive constants. (5 Points)

b) Would you expect the exact ground state energy to be less than your answer to part (a), or greater than it? Justify. (3 Points)

c) How would you go about finding an excited state in this system using the same approach? (2 Points)

Hint: $\int_0^\infty x^2 \mathrm{e}^{-ax} = 2a^{-3}$, for $a > 0$.

Aug 2014

Quantum #6

a) The Variational principle states that $E_{gs} \le \langle \psi | H | \psi \rangle = \langle H \rangle$ where $|\psi\rangle$ is a normalized trial wave function

$$\hookrightarrow H = \frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \beta x^3 = E\psi$$

$$V = \begin{cases} 0 & x < 0 \\ \beta x^3 & x \ge 0 \end{cases}$$

$$\psi = \begin{cases} Cx e^{-\alpha x} & x \ge 0 \\ 0 & x < 0 \end{cases}$$

* We first normalize our trial wave function, domain of interest is $[0, \infty)$

$$1 = C^2 \int_0^\infty x^2 e^{-2\alpha x}\, dx$$

* we know $\int_0^\infty x^2 e^{-ax} = 2a^{-3}$, $a > 0$

$$\hookrightarrow a = 2\alpha$$

$$1 = C^2 \cdot 2(2\alpha)^{-3}$$

$$1 = C^2 \cdot \frac{1}{4\alpha^3}$$

$$\hookrightarrow C = 2\alpha^{3/2}$$

$$\Rightarrow \psi(x) = \begin{cases} 2\alpha^{3/2} x e^{-\alpha x} & x \ge 0 \\ 0 & x < 0 \end{cases}$$

$$\langle H \rangle = \langle \psi | H | \psi \rangle$$

$$= \int_0^\infty 2\alpha^{3/2} x e^{-\alpha x}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \beta x^3\right) 2\alpha^{3/2} x e^{-\alpha x}\, dx$$

$$= \int_0^\infty 2\alpha^{3/2} x e^{-\alpha x}\left[-\frac{\hbar^2 \alpha^{3/2}}{m}\frac{d^2(xe^{-\alpha x})}{dx^2} + 2\alpha^{3/2}\beta x^4 e^{-\alpha x}\right] dx$$

$$= \int_0^\infty 2\alpha^{3/2} x e^{-\alpha x}\left[-\frac{\hbar^2 \alpha^{3/2}}{m}(\alpha^2 x - 2\alpha) e^{-\alpha x} + 2\alpha^{3/2}\beta x^4 e^{-\alpha x}\right] dx$$

$$= \int_0^\infty -\frac{2\alpha^3 x \hbar^2}{m}(\alpha^2 x - 2\alpha) e^{-2\alpha x} + 4\alpha^3 \beta x^5 e^{-2\alpha x}\, dx$$

#6 (cont.)

a) $\langle H \rangle = \frac{-2\alpha^5\hbar^2}{m}\int_0^\infty x^2 e^{-2\alpha x}dx + \frac{4\alpha^4\hbar^2}{m}\int_0^\infty x e^{-2\alpha x}dx + 4\alpha^3\beta\int_0^\infty x^5 e^{-2\alpha x}dx$

* in general, $\int_0^\infty x^n e^{-bx} = \frac{n!}{b^{n+1}}$

$$= -\frac{2\alpha^5\hbar^2}{m}\left[\frac{2!}{(2\alpha)^3}\right] + \frac{4\alpha^4\hbar^2}{m}\left[\frac{1!}{(2\alpha)^2}\right] + 4\alpha^3\beta\left[\frac{5!}{(2\alpha)^6}\right]$$

$$= \frac{-4\alpha^5\hbar^2}{8\alpha^3 m} + \frac{4\alpha^4\hbar^2}{4\alpha^2 m} + \frac{4\alpha^3\beta\cdot 120}{64\alpha^6}$$

$$= \frac{-\alpha^2\hbar^2}{2m} + \frac{\alpha^2\hbar^2}{m} + \frac{30\beta}{4\alpha^3}$$

$$= \frac{\alpha^2\hbar^2}{2m} + \frac{15\beta}{2\alpha^3}$$

b) By definition, our $E_{gs} \leq \langle H \rangle$. To prove this, we write our trial function as an expansion in eigenfunctions of H

$$|\psi\rangle = \sum_n c_n |\psi_n\rangle \quad \text{where } H|\psi_n\rangle = E_n|\psi_n\rangle$$
$$|c_n|^2 = 1$$

$$\Rightarrow \langle H \rangle = \langle \psi | H | \psi \rangle$$
$$= \sum_{nm} \langle \psi_m | c_m^* H c_n | \psi_n \rangle$$
$$= \sum_{nm} c_m^* c_n \langle \psi_m | H | \psi_n \rangle$$
$$= \sum_{nm} c_m^* c_n E_n \langle \psi_m | \psi_n \rangle$$
$$= \sum_{nm} c_m^* c_n E_n \delta_{mn}$$
$$= \sum_n |c_n|^2 E_n$$

$\Rightarrow E_{gs} = \sum_n |c_n|^2 E_n$ if n is ground state, otherwise

$E_{gs} < \sum_n |c_n|^2 E_n$

#6 (cont.)

c) To get an upper bound on the first excited state, we need a wavefunction that is orthogonal to the ground state wave function ψ_{gs}. However, since this is difficult to know, an equivalent option is to use a trial wave function with a parity opposite to that of the potential. Then we proceed as before.

Quantum Mechanics
Qualifying Exam - January 2015

Notes and Instructions

- There are 6 problems. Attempt them all as partial credit will be given.
- 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

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

In spherical coordinates,

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

Problem 1: Solving the Harmonic Oscillator

Solving the differential equation form of the time-independent Schrödinger equation for the eigenstates of the harmonic oscillator Hamiltonian in 1D requires solving a second order differential equation. By using operator algebra, it is possible to simplify the solution to this problem.

The 1D harmonic oscillator is described by the Hamiltonian

$$H = \frac{P^2}{2m} + \frac{m}{2}\omega^2 X^2. \tag{1}$$

Define the unitless variables

$$x = \frac{X}{\lambda}, \quad p = \frac{\lambda}{\hbar}P, \quad \lambda = \sqrt{\frac{\hbar}{m\omega}}. \tag{2}$$

such that the Hamiltonian has the form

$$H = \frac{\hbar\omega}{2}\left(p^2 + x^2\right). \tag{3}$$

Note that x and p are conjugate observables, $[x,p] = i$

(a) [2 pt] Using the harmonic oscillator operators

$$\hat{a} = \frac{1}{\sqrt{2}}(x + ip), \quad \hat{a}^\dagger = \frac{1}{\sqrt{2}}(x - ip), \quad \hat{n} = \hat{a}^\dagger\hat{a}, \tag{4}$$

and their commutation relations, show that the Hamiltonian can be written as

$$H = \hbar\omega(\hat{n} + \frac{1}{2}). \tag{5}$$

(b) [2 pts] Define the eigenstates of the operator $\hat{n}$:

$$\hat{n}|n\rangle = n|n\rangle, \tag{6}$$

with n some (unitless) numbers. Use the operator commutation relations to show that

$$\begin{aligned} \hat{a}|n\rangle &= c(n)|n-1\rangle \\ \hat{a}^\dagger|n\rangle &= d(n)|n+1\rangle. \end{aligned} \tag{7}$$

Derive expressions for $c(n)$ and $d(n)$. Show your work.

(c) [3 pts] The potential, $V(x) = \frac{\hbar\omega}{2}x^2 \geq 0$ for all x. Explain why this implies that:

1. The eigenenergies of the Harmonic Oscillator must be positive
2. The eigenvalues of $\hat{n}$ must be non-negative integers
3. There is a lowest eigenstate of $\hat{n}$, $|0\rangle$ defined by $\hat{a}|0\rangle = 0$.

(d) [2 pts] Show that results above define a first order differential equation in X that can be solved for the ground state harmonic oscillator wavefunction $\psi_0(X)$. Determine this equation and solve for this wavefunction.

(e) [1 pt] Use the result from (e) and the operators to determine the first excited state wavefunction for the harmonic oscillator, $\psi_1(X)$.

Quantum #1

a) Given: $H = \frac{\hbar\omega}{2}(p^2 + x^2)$, $[x,p] = i$

$a = \frac{1}{\sqrt{2}}(x + ip) \quad a^+ = \frac{1}{\sqrt{2}}(x - ip) \quad n = a^+ a$

* Rewrite H in terms a, a^+ then n

$$\Rightarrow \begin{aligned} \sqrt{2}\,a &= (x + ip) \\ \sqrt{2}\,a^+ &= (x - ip) \end{aligned} \iff \begin{aligned} x &= \frac{1}{\sqrt{2}}(a + a^+) \\ p &= \frac{-i}{\sqrt{2}}(a - a^+) \end{aligned}$$

$$\begin{aligned}
\Rightarrow H &= \frac{\hbar\omega}{2}\left(\left[\frac{-i}{\sqrt{2}}(a-a^+)\right]^2 + \left[\frac{1}{\sqrt{2}}(a+a^+)\right]^2\right) \\
&= \frac{\hbar\omega}{2}\left(\frac{-1}{2}(\cancel{aa} - a^+a - aa^+ + \cancel{a^+a^+}) + \frac{1}{2}(\cancel{aa} + aa^+ + a^+a + \cancel{a^+a^+})\right) \\
&= \frac{\hbar\omega}{2}(aa^+ + a^+a) \\
&= \frac{\hbar\omega}{2}(a^+a + 1 + a^+a) \quad (\text{from } [a, a^+] = 1) \\
&= \hbar\omega(n + 1/2) \checkmark
\end{aligned}$$

b) * Remember that $[n, a] = -a$, $[n, a^+] = a^+$

$\Rightarrow$ Solve by using the above commutator relations

$$\begin{aligned}
n(a|n\rangle) &= (an - a)|n\rangle \\
&= a(n-1)|n\rangle \\
&= (n-1)(a|n\rangle) \quad \Rightarrow a|n\rangle = c_n|n-1\rangle
\end{aligned}$$

$$\begin{aligned}
n(a^+|n\rangle) &= (a^+n + a^+)|n\rangle \\
&= a^+(n+1)|n\rangle \\
&= (n+1)(a^+|n\rangle) \quad \Rightarrow a^+|n\rangle = d_n|n+1\rangle
\end{aligned}$$

$\Rightarrow$ Determine c_n and d_n through normalization

$$\begin{aligned}
\langle n|a^+a|n\rangle &= |c_n|^2\langle n-1|n-1\rangle \\
n\langle n|n\rangle &= |c_n|^2 \\
n &= |c_n|^2 \quad \Rightarrow \boxed{c_n = \sqrt{n}}
\end{aligned}$$

#1 (cont.)

b) $\langle n|aa^\dagger|n\rangle = |d_n|^2\langle n+1|n+1\rangle$

$\langle n|a^\dagger a+1|n\rangle = |d_n|^2$

$(n+1)\langle n|n\rangle = |d_n|^2$

$n+1 = |d_n|^2 \Rightarrow d_n = \sqrt{n+1}$

c) ① Given a potential $V(x) = \frac{1}{2}\hbar\omega x^2 \geq 0$ for all x and combined with the fact that $T \geq 0$ (since kinetic energy can never be negative), then $(H = T+V) \geq 0$ at all times, thus its eigenenergies must also be positive

② We can rewrite our potential as: $V = \frac{1}{2}\hbar\omega\left(\frac{a+a^\dagger}{\sqrt{2}}\right)^2$

$\Rightarrow V = \frac{\hbar\omega}{4}(aa + aa^\dagger + a^\dagger a + a^\dagger a^\dagger)$

$V|n\rangle = \frac{\hbar\omega}{4}(aa + aa^\dagger + a^\dagger a + a^\dagger a^\dagger)|n\rangle$

$= \frac{\hbar\omega}{4}\left[\sqrt{n(n-1)}\,|n-2\rangle + \sqrt{n+1}\sqrt{n+1}\,|n\rangle + \sqrt{n}\sqrt{n}\,|n\rangle + \sqrt{(n+1)(n+2)}\,|n+2\rangle\right]$

$= \frac{\hbar\omega}{4}\left[\sqrt{n(n-1)}\,|n-2\rangle + (2n+1)|n\rangle + \sqrt{(n+1)(n+2)}\,|n+2\rangle\right]$

* For the above equation to be greater than or equal to 0, n must also be greater than or equal to 0

③ In order for the above to be true $a|0\rangle = 0$ because $n \geq 0$. Following our work from part b

$n(a|0\rangle) = (an - a)|0\rangle$

$= a(0-1)|0\rangle$

$= -a|0\rangle = c_n|-1\rangle$

$\langle 0|-a^\dagger - a|0\rangle = |c_n|^2\langle -1|-1\rangle$

$0\,\cancel{\langle 0|0\rangle}^{1} = |c_n|^2\langle -1|-1\rangle$

$0 = |c_n|^2\langle -1|-1\rangle$

$\hookrightarrow \langle -1|-1\rangle = 0$

#1 (cont.)

d) If we let $|0\rangle = \psi_0$

$$a\psi_0 = 0$$

$$\frac{1}{\sqrt{2}}(x + ip)\psi_0 = 0$$

$$\frac{1}{\sqrt{2}}\left(\frac{1}{\lambda}x + i\frac{\lambda}{\hbar}p\right)\psi_0 = 0$$

$$\frac{1}{\sqrt{2}}\left(\frac{1}{\lambda}x + i\frac{\lambda}{\hbar}\left(\frac{-i\hbar\partial}{\partial x}\right)\right)\psi_0 = 0$$

$$\frac{1}{\sqrt{2}}\left(\frac{1}{\lambda}x + \lambda\frac{\partial}{\partial x}\right)\psi_0 = 0$$

$$\frac{1}{\lambda}x\psi_0 = -\lambda\frac{\partial\psi_0}{\partial x}$$

$$\int x\,\partial x = \int -\lambda^2\frac{\partial\psi_0}{\psi_0}$$

$$\frac{-1}{2\lambda^2}x^2 + C = \ln(\psi_0)$$

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

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

* Normalizing our wavefunction

$$1 = \int |\psi_0|^2 dx$$

$$1 = c^2\int \left|\exp\left[\frac{-m\omega}{2\hbar}x^2\right]\right|^2 dx$$

$$1 = c^2\int \exp\left[\frac{-m\omega}{\hbar}x^2\right]dx$$

$$1 = c^2\sqrt{\frac{\hbar\pi}{m\omega}}$$

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

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

#1 (cont.)

e) * Following a similiar progression to part d

$$|1\rangle = \psi_1 = a^\dagger|0\rangle$$

$$\psi_1 = \frac{1}{\sqrt{2}}(x - ip)\psi_0$$

$$= \frac{1}{\sqrt{2}}\left(\frac{x}{\lambda} - i\frac{\lambda}{\hbar}\left(-i\hbar\frac{\partial}{\partial x}\right)\right)\psi_0$$

$$= \frac{1}{\sqrt{2}}\left(\frac{x}{\lambda} - \lambda\frac{\partial}{\partial x}\right)\psi_0$$

$$= \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x - \sqrt{\frac{\hbar}{m\omega}}\frac{\partial}{\partial x}\right)\left[\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left[\frac{-m\omega}{2\hbar}x^2\right]\right]$$

$$= \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x\psi_0 - \sqrt{\frac{\hbar}{m\omega}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left(-x\frac{m\omega}{\hbar}\right)\exp\left[\frac{-m\omega}{2\hbar}x^2\right]\right.$$

$$= \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x\psi_0 + \sqrt{\frac{m\omega}{\hbar}}x\psi_0\right)$$

$$= \sqrt{\frac{2m\omega}{\hbar}}x\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left[\frac{-m\omega}{2\hbar}x^2\right]$$

Problem 2: Angular Momentum States

Consider the electron in a hydrogen atom in the presence of a homogeneous magnetic field $\mathbf{B} = B\hat{\mathbf{z}}$. In this problem, ignore the electron spin and only consider the orbital angular momentum. The Hamiltonian of the system is

$$\mathcal{H} = \mathcal{H}_0 - \omega L_z, \tag{1}$$

where $\mathcal{H}_0$ is the Hamiltonian for the hydrogen atom, $\omega \equiv |e|B/2m_e c$, and L_z is the angular momentum operator along the z direction. The eigenstates $|n, \ell, m\rangle$ and eigenvalues $E_n^{(0)}$ of the unperturbed hydrogen atom are to be considered as known. Assume that initially (at $t = 0$) the system is in the state

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}} \left(|2, 1, -1\rangle - |2, 1, 1\rangle\right). \tag{2}$$

(a) [1 pt] Write down the time-dependent state for this atom, $|\psi(t)\rangle$, given the initial state and the full Hamiltonian.

(b) [2 pts] Calculate the probability of finding the atom at some later time $t > 0$ in the state

$$|2p_y\rangle = \frac{1}{\sqrt{2}} \left(|2, 1, -1\rangle + |2, 1, 1\rangle\right). \tag{3}$$

When is the probability equal to 1?

(c) [3 pts] Define the state $|\mathbf{e}_\phi\rangle$ defined by

$$(\mathbf{e}_\phi \cdot \mathbf{L})\, |\mathbf{e}_\phi\rangle = \hbar |\mathbf{e}_\phi\rangle, \qquad \mathbf{L}^2 |\mathbf{e}_\phi\rangle = 2\hbar^2 |\mathbf{e}_\phi\rangle. \tag{4}$$

$\mathbf{e}_\phi$ is a unit vector in the $x - y$ plane, $\mathbf{e}_\phi = \cos(\phi)\mathbf{e_x} + \sin(\phi)\mathbf{e_y}$.

This state has quantum number $\ell = 1$ and angular momentum projection along the direction $\mathbf{e}_\phi$ equal to $+\hbar$. Solve for the state $|\mathbf{e}_\phi\rangle$ in the basis of states $|2, 1, m\rangle$, with $m = \pm 1, 0$.

(d) [2 pts] Calculate the time-dependent probability of finding the system in the state $|\mathbf{e}_\phi\rangle$, if it starts in the state $|\psi(0)\rangle$ above, and show that this is a periodic function of time. Calculate the times when the probability is maximum and minimum.

(e) [2 pts] If the electron starts in the state $|\psi(0)\rangle$, calculate the expectation value of the magnetic dipole

$$\langle \vec{\mu} \rangle(t) = \frac{e}{2m_e c} \langle \mathbf{L} \rangle(t), \quad \mathbf{L} = L_x \mathbf{e_x} + L_y \mathbf{e_y} + L_z \mathbf{e_z} \tag{5}$$

as a function of time.

Hint: It will be useful to use:

$$\begin{aligned} J_\pm &= J_x \pm i J_y \\ J_\pm |j, m\rangle &= \hbar \sqrt{j(j+1) - m(m \pm 1)}\; |j, m \pm 1\rangle \end{aligned} \tag{6}$$

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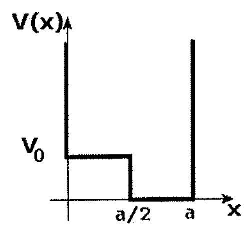
Quantum #2

Problem 3: Double Step Potential

Consider a single particle of mass m in a one dimensional well of width a and a potential, $V(x)$, given by:

$$V(x) = \begin{cases} \infty, & x < 0 \\ V_0, & 0 < x < \frac{a}{2} \\ 0, & \frac{a}{2} < x < a \\ \infty, & x > a \end{cases} \tag{1}$$



In this question, you will consider the special cases where this potential well has a bound state at the energy $E = V_0$. There are only certain values of V_0 and a where this will happen.

In this problem, use the constant

$$k = \sqrt{\frac{2mV_0}{\hbar^2}} \tag{2}$$

(a) [2 pts] For the energy $E = V_0$ in this potential, determine the general eigenfunction solutions to the time-independent Schrödinger equation in all regions of x. Show your work.

(b) [3 pts] Apply boundary conditions to determine relationships between the constants you introduced in writing the wave functions in part (a).

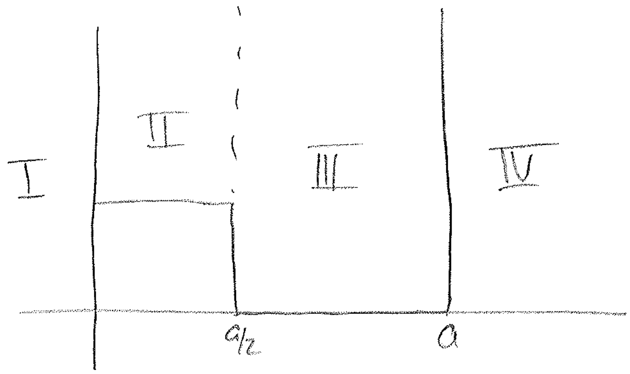
(c) [2 pts] From your results above, derive a transcendental equation that gives the values of V_0 where there is an energy eigenstate with $E = V_0$, for a fixed well width a. This equation will have the form $z = f(z)$ with $z = k\frac{a}{2}$. Plot this function and determine a relationship between the first energy V_0 that satisfies this equation and the bound state energies of a square well of width a.

(d) [2 pts] Qualitatively sketch the wave function that corresponds to the smallest value of V_0 that satisfies the transcendental equation from part (c), for a fixed value of a.

(e) [1 pt] Finally, consider the case where the width of the well is fixed but the potential step, V_0, can be changed. There are an infinite number of possible values of V_0 where the well contains an energy eigenstate with $E = V_0$. Describe, qualitatively, the changes in the wavefunctions of these eigenstates as V_0 gets larger.

Jan 2015

Quantum #3



a) $H\psi_i = E\psi_i$

* In regions I + IV: $\psi_I = 0 = \psi_{IV}$ (due to infinite potential)

* In region III:

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

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

* if $k = \sqrt{\frac{2mV_0}{\hbar}}$ ($E = V_0$ as stated in problem)

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

$\hookrightarrow \psi_{III}(x) = Ae^{-ikx} + Be^{ikx}$

* In region II:

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

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

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

$\hookrightarrow$ let $k = \sqrt{\frac{2m(E-V)}{\hbar^2}}$, $E = V_0$ as stated in problem

$$\frac{\partial^2\psi}{\partial x^2} = 0$$

$\hookrightarrow \psi_{II} = Cx + D$

#3(cont.)

b) * Remember, our two boundary conditions are that: ψ is continuous

$\frac{d\psi}{dx}$ is continuous where $V \neq \infty$

$0 = C(0) + D$

$\hookrightarrow \boxed{D = 0}$

$0 = Ae^{-ika} + Be^{ika}$

$= A + Be^{2ika}$

$\hookrightarrow \boxed{A = -Be^{2ika}}$

$C(\frac{a}{2}) = -Be^{3ika/2} + Be^{ika/2}$

$C = \frac{2B}{a}(e^{ika/2} - e^{3ika/2})$

$C = ikA(e^{ika/2} + e^{3ika/2})$

Problem 4: Finite Quantum System

Consider a quantum system that can be described by three basis states, $|n\rangle$, $n = 1, 2, 3$, and the Hamiltonian in this basis:

$$H = \frac{\hbar\omega}{2}\begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & i \\ 0 & -i & 1 \end{pmatrix} \tag{1}$$

(a) [3 pts] Solve for the energy eigenvalues and eigenstates of this system.

(b) [2 pts] If the system starts in the state

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

determine the time-dependence of the state $|\psi(t)\rangle$. You may write your answer in terms of either the states $|n\rangle$ or the eigenstates you found in part (a).

(c) [3 pts] Calculate the time dependent probabilities for measuring the system to be in each of the states $|1\rangle$, $|2\rangle$, and $|3\rangle$, if the system starts in the state given in part (b). Explain why the different states can or cannot be measured and the frequency of the oscillations you found.

(d) [2 pts] Finally, assume that the states $|n\rangle$ are the eigenstates of some observable O where

$$O|n\rangle = (-1)^n n|n\rangle \tag{3}$$

If, again, the system starts in the state given in part (b), what is the time dependent expectation value of O, $\langle O\rangle(t)$?

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Quantum #4

a) $H = \frac{\hbar\omega}{2}\begin{bmatrix} 2 & 0 & 0 \\ 0 & 1 & i \\ 0 & -i & 1 \end{bmatrix}$

* Solving eigenvalue equation $\det(H - \lambda \mathbb{I}) = 0$

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

$$\Rightarrow \quad 0 = (2-\lambda)\left[(1-\lambda^2) - 1\right]$$
$$= (2-\lambda)\left[(1-\lambda)-1\right]\left[(1-\lambda)+1\right]$$

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

* Solving eigenvector equation: $H\vec{x} = \lambda\vec{x}$

Case $\lambda = 0$:

$2x_1 = 0$

$x_2 + ix_3 = 0 \rightarrow x_2 = -ix_3$

$-ix_2 + x_3 = 0 \rightarrow x_3 = ix_2$

$\rightarrow \vec{x} = \begin{bmatrix} 0 \\ -i \\ 1 \end{bmatrix} \cdot \frac{1}{\sqrt{2}}$

Case $\lambda = 2$

$2x_1 = 2x_1$

$x_2 + ix_3 = 2x_2 \rightarrow ix_3 = x_2$

$-ix_2 + x_3 = 2x_3 \qquad -ix_2 = x_3$

$\vec{x} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$ or $\begin{bmatrix} 0 \\ i \\ 1 \end{bmatrix} \cdot \frac{1}{\sqrt{2}}$

b) $\boxed{\begin{aligned} &\text{* Proceed according to: } |1\rangle = \langle 1,0,0\rangle,\ \lambda_1 = 2 \\ &|2\rangle = \tfrac{1}{\sqrt{2}}\langle 0,i,1\rangle,\ \lambda_2 = 2 \\ &|3\rangle = \tfrac{1}{\sqrt{2}}\langle 0,-i,1\rangle,\ \lambda_3 = 0 \end{aligned}}$ * for rest of problem

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

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

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

$= \frac{1}{\sqrt{2}} e^{-i2t/\hbar}\left(|1\rangle + |2\rangle\right)$

#4 (cont.)

c) We want to calculate $|\langle n|\Psi(t)\rangle|^2$ where $n\in\{1,2,3\}$

$$|\langle 1|\tfrac{1}{\sqrt{2}}e^{-i2t/\hbar}(|1\rangle+|2\rangle)|^2$$
$$=\tfrac{1}{2}|\langle 1|1\rangle+\langle 1|2\rangle|^2$$
$$=\tfrac{1}{2}$$

$$|\langle 3|\tfrac{1}{\sqrt{2}}e^{-i2t/\hbar}(|1\rangle+|2\rangle)|^2$$
$$=\tfrac{1}{2}|\langle 3|1\rangle+\langle 3|2\rangle|^2$$
$$=0$$

$$|\langle 2|\tfrac{1}{\sqrt{2}}e^{-i2t/\hbar}(|1\rangle+|2\rangle)|^2$$
$$=\tfrac{1}{2}|\langle 2|1\rangle+\langle 2|2\rangle|^2$$
$$=\tfrac{1}{2}$$

$\Rightarrow$ Oscillations will only occur if $|2\rangle$ has $\lambda=0$ as this will prevent $e^{-i2t/\hbar}e^{i2t/\hbar}=1$ term from forming. In an abstract notation, you would find oscillations with frequency $\frac{1}{\hbar}(\lambda_i-\lambda_j)$ where $i,j\in\{1,2,3\}$ and $i\neq j$

d) * Expectation values are by definition time-independent

$$\Rightarrow |\Psi(0)\rangle=\tfrac{1}{\sqrt{2}}(|1\rangle+|2\rangle)$$

$$\langle O(t)\rangle = \langle\Psi(0)|U^\dagger O U|\Psi(0)\rangle$$
$$=\tfrac{1}{2}\left[(\langle 1|+\langle 2|)U^\dagger O U(|1\rangle+|2\rangle)\right]$$
$$=\tfrac{1}{2}\left[\langle 1|U^\dagger OU|1\rangle+\langle 1|U^\dagger OU|2\rangle+\langle 2|U^\dagger OU|1\rangle+\langle 2|U^\dagger OU|2\rangle\right)$$
$$=\tfrac{1}{2}\left[\langle 1|O|1\rangle+\langle 1|O|2\rangle+\langle 2|O|1\rangle+\langle 2|O|2\rangle\right]$$
$$=\tfrac{1}{2}\left[(-1)^1 1+(-1)^2(2)+(-1)^1 1+(-1)^2(2)\right]$$
$$=\tfrac{1}{2}\left[-1+2-1+2\right]$$
$$=1$$

* See note from part c about oscillatory term if states $|2\rangle$ and $|3\rangle$ are mislabled. In the context of this problem, $e^{-i2t/\hbar}$ term introduced in cross terms

$$\hookrightarrow \langle O(t)\rangle=\tfrac{1}{2}\left[1+e^{-i2t/\hbar}\right]$$

Problem 5: Interaction Picture of Quantum Mechanics

The "Interaction Picture" of quantum mechanics is in some ways in-between the Schrödinger formulation and the Heisenberg formulation.

Consider a system with the Hamiltonian $H = H_0 + V(t)$ where H_0 is independent of time and $V(t)$ may or may not be time dependent. The Interaction Picture is defined by the transformation of the Schrödinger states:

$$\begin{aligned} |\psi\rangle_I &= {U_0}^{-1}|\psi\rangle_S \\ U_0 &= e^{-\frac{i}{\hbar}(t-t_0)H_0}. \end{aligned} \tag{1}$$

The subscripts I and S refer to the Interaction Picture and Schrödinger Picture respectively. t_0 is a time when the pictures coincide, and we will set $t_0 = 0$ for this problem.

(a) [1 pt] Show that U_0 is a unitary operator. Why is it important for the transformation between pictures be unitary?

(b) [3 pts] The transformation between $|\psi\rangle_S$ and $|\psi\rangle_I$ implies that there is also a transformation of the observables between the pictures. If A_S and A_I are operators for an observable in the Schrödinger and Interaction pictures respectively, derive the relation between A_S and A_I. Show that this implies that H_0 is the same in the two pictures.

(c) [3 pts] Derive the differential equation that determines the time dependence of the Interaction Picture states, $|\psi(t)\rangle_I$. Be sure to show and explain your work. Explain why the Interaction Picture may be particularly useful when $V(t)$ is "small".

(d) [1 pt] Define the eigenstates of H_0 to be

$$H_0|\lambda\rangle_S = E_\lambda|\lambda\rangle_S \tag{2}$$

Show that if $V(t) = 0$, the Interaction Picture energy eigenstates $|\lambda\rangle_I$ are equal to $|\lambda(t=0)\rangle_S$ and independent of time.

(e) [2 pts] Consider a potential of the form

$$V(t) = 0, \quad t \leq 0 \quad V(t) \neq 0, \quad t > 0 \tag{3}$$

The system is in a state $|\psi_0\rangle_I$ for $t < 0$. For $t > 0$ the Interaction Picture state will depend on time. It can be expanded as:

$$|\psi(t)\rangle_I = \sum_\lambda c_\lambda(t)|\lambda(0)\rangle_I \tag{4}$$

In this expression, $c_\lambda(t)$ are time-dependent expansion coefficients for the state and $|\lambda(0)\rangle_I$ is the complete set of time-independent eigenstates of H_0 in the interaction picture.

Use the time dependence found in part (c) to derive a set of coupled equations relating $c_\lambda(t)$ and $\partial_t c_\lambda(t)$.

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Quantum #5

a) An operator is unitary if: $U^{+}U = \mathbb{I}$

$$\hookrightarrow U = \exp\left[\frac{-i(t-t_0)H_0}{\hbar}\right]$$

$$U^{+} = \exp\left[\frac{i(t-t_0)H_0}{\hbar}\right]$$

$$U^{+}U = \exp\left[\frac{i(t-t_0)H_0}{\hbar}\right]\exp\left[\frac{-i(t-t_0)H_0}{\hbar}\right]$$

$$= 1 \checkmark$$

Our transformation must be a unitary operator b/c it preserves lengths of vectors, as well as the angles b/w them

b) This transformation is best seen in terms of an expectation value. In the Schrödinger picture:

$$\langle A \rangle = {}_S\langle\psi| A_S |\psi\rangle_S$$

Since we can only multiply by 1 and we want $|\psi\rangle_I = U_0^{-1}|\psi\rangle_S$

$$= {}_S\langle\psi| U_0 U_0^{-1} A_S U_0 U_0^{-1} |\psi\rangle_S$$

$$= {}_I\langle\psi| U_0^{-1} A_S U_0 |\psi\rangle_I$$

$$\hookrightarrow U_0^{-1} A_S U_0 = A_I$$

*Not sure I've fully answered this part

c) $|\psi\rangle_I = \exp\left[\frac{i(t-t_0)H_0}{\hbar}\right]|\psi\rangle_S$

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle_I = i\hbar\frac{\partial}{\partial t}\left(\exp\left[\frac{i(t-t_0)H_0}{\hbar}\right]|\psi\rangle_S\right)$$

$$= i\hbar\left(\frac{H_0}{-i\hbar}\exp\left[\frac{i(t-t_0)H_0}{\hbar}\right]|\psi\rangle_S + \left[\frac{i(t-t_0)H_0}{\hbar}\right]\frac{\partial}{\partial t}|\psi\rangle_S\right)$$

$$= -H_0\exp\left[\frac{i(t-t_0)H_0}{\hbar}\right]|\psi\rangle_S + (H_0+V)|\psi_S\rangle\exp\left[\frac{i(t-t_0)H_0}{\hbar}\right]$$

$$= V\exp\left[\frac{i(t-t_0)H_0}{\hbar}\right]|\psi\rangle_S$$

$$= V|\psi\rangle_I$$

5 (cont.)

c) $i\hbar \frac{\partial}{\partial t} \langle n | \psi \rangle_I = \langle n | V | \psi \rangle_I$

$$i\hbar \frac{\partial}{\partial t} c_n(t) = \sum_m \langle n | V | m \rangle \langle m | \psi \rangle_I$$

$$= \sum_m c_m V_{nm}$$

expanding $c_n(t)$ as $c_n^{(0)}(t) + \lambda c_n^{(1)}(t) + \ldots$

$$i\hbar \frac{\partial}{\partial t} \left(c_n^{(0)}(t) + \lambda c_n^{(1)}(t) + \ldots \right) = \sum_m \left[c_m^{(0)}(t) + \lambda c_n^{(1)}(t) \right.$$

Problem 6: Perturbations in a 2D well

Consider a spinless particle of mass m and charge q confined to a hard-walled square well (in two dimensions) with sides of length L. The potential can be written:

$$\begin{aligned} V(x,y) &= 0, \quad -\frac{L}{2} \leq x \leq \frac{L}{2}, \quad -\frac{L}{2} \leq y \leq \frac{L}{2} \\ V(x,y) &= \infty \quad otherwise \end{aligned}$$

(a) [2 pts] Write down the eigenenergies, eigenstates, and degeneracies of the first three energy levels for this well. You do not have to solve for these explicitly, but you must explain and justify how you obtained these results.

(b) [2 pts] Consider applying a constant electric field in the x-direction to this system,

$$\vec{E} = E_0 \hat{e}_x \tag{1}$$

Assuming that E_0 is small, determine the first order shift in the energies for the ground state and first excited states. Be sure to show your work.

(c) [3 pts] The second-order, in E_0, energy shift of the ground state can be written in terms of a sum. Write down an expression for this sum using the general form for the eigentstates you determined in part (a). Calculate an approximate value for this energy shift by solving for the largest term in the sum. Your answer should be in terms of the parameters given in the problem, and fundamental constants.

(d) [1 pt] Considering the sum you wrote down in part (c), what is the next largest term that will contribute a non-zero value to the sum? Explain your answer, but you do not need to compute this term.

(e) [2 pts] Finally, instead of an electric field, consider the effect of a localized perturbation:

$$V(x,y) = V_0 L^2 \delta(x - x_0)\delta(y - y_0) \tag{2}$$

where (x_0, y_0) is some point in the well. Write down an expression for the first order energy shift for the ground state, showing how the energy shift depends on the position of the perturbation (x_0, y_0).

Determine a position for the perturbation where the ground state energy changes, but the first excited state does not.

Determine a position for the perturbation that splits the degeneracy of the first excited state.

Jan 2015

Quantum #6

a) For a square well with walls at $[-L/2, L/2]$, our general wavefunctions and energies are:

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

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

Thus for a 2-D well, our wavefunctions/energies become:

$$\psi_{n_x n_y}(x,y) = \psi_{n_x}(x)\,\psi_{n_y}(y) \quad \text{where } \psi_{n_i}(i) \text{ is as above}$$

$$E_{n_x n_y} = \frac{(n_x^2 + n_y^2)\pi^2\hbar^2}{2mL^2}$$

Our first three energy levels will be:

$$g$$

① $n_x = 1,\ n_y = 1 \Rightarrow E_{11} = \frac{2\pi^2\hbar^2}{2mL^2}$

$$\psi_{11} = \frac{2}{L}\cos\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi y}{L}\right) \qquad 1$$

② $n_x = 1,\ n_y = 2$ or $n_x = 2,\ n_y = 1 \Rightarrow E_{12} = E_{21} = \frac{5\pi^2\hbar^2}{2mL^2}$

$$\psi_{12} = \frac{2}{L}\cos\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi y}{L}\right) \qquad 2$$

$$\psi_{21} = \frac{2}{L}\sin\left(\frac{2\pi x}{L}\right)\cos\left(\frac{\pi y}{L}\right)$$

③ $n_x = 2,\ n_y = 2 \Rightarrow E_{22} = \frac{8\pi^2\hbar^2}{2mL^2}$

$$\psi_{22} = \frac{2}{L}\sin\left(\frac{2\pi x}{L}\right)\sin\left(\frac{2\pi y}{L}\right) \qquad 1$$

#6 (cont.)

b) Applying a constant E field $\vec{E} = E_0 \hat{x}$, yields a potential $V(x,y) = qE_0 x$

The equation that determines the first order energy correction is:

$$\Delta E^{(1)}_{n_x n_y} = \langle n_x n_y | V | n_x n_y \rangle$$

$$\Rightarrow \Delta E^{(1)}_{11} = \langle 1,1 | qE_0 x | 1,1 \rangle$$

$$= \int_{-L/2}^{L/2} dy \int_{-L/2}^{L/2} dx \left(\frac{2}{L}\right)^2 \cos^2\left(\frac{\pi x}{L}\right) \cos^2\left(\frac{\pi y}{L}\right) qE_0 x$$

$$= \int_{-L/2}^{L/2} qE_0 \cos^2\left(\frac{\pi y}{L}\right) dy \int_{-L/2}^{L/2} x \cos^2\left(\frac{\pi x}{L}\right) dx \cdot \left(\frac{2}{L}\right)^2$$

$$= \frac{4qE_0}{L^2} \int_{-L/2}^{L/2} \cos^2\left(\frac{\pi y}{L}\right) dy \left[\frac{x^2}{4} + \frac{x \sin\left(\frac{2\pi x}{L}\right)}{4(\pi/L)} + \frac{\cos\left(\frac{2\pi x}{L}\right)}{8(\pi/L)^2}\right] \Bigg|_{-L/2}^{L/2}$$

$$= \frac{4qE_0}{L^2} \int_{-L/2}^{L/2} \cos^2\left(\frac{\pi y}{L}\right) dy \left[\frac{(L/2)^2}{4} + \frac{L/2 \sin(\pi)}{4(\pi/L)} + \frac{\cos(\pi)}{8\pi^2/L^2} - \left(\frac{(-L/2)^2}{4} + \frac{-L/2 \sin(-\pi)}{4(\pi/L)} + \frac{\cos(-\pi)}{8\pi^2/L^2}\right)\right]$$

$$= \frac{4qE_0}{L^2} \int_{-L/2}^{L/2} \cos^2\left(\frac{\pi y}{L}\right) dy \left(\frac{L^2}{16} - \frac{L^2}{8\pi^2} - \left(\frac{L^2}{16} - \frac{L^2}{8\pi^2}\right)\right)$$

$$= 0$$

$$\Rightarrow \Delta E^{(1)}_{21} = \Delta E^{(1)}_{12}$$

$$= \langle 1,2 | V | 1,2 \rangle$$

$$= qE_0 \int_{-L/2}^{L/2} dy \int_{-L/2}^{L/2} \left(\frac{2}{L}\right)^2 \cos^2\left(\frac{\pi x}{L}\right) \sin^2\left(\frac{2\pi y}{L}\right) x \, dx$$

$$= qE_0 \int_{-L/2}^{L/2} \sin^2\left(\frac{2\pi y}{L}\right) dy \underbrace{\int_{-L/2}^{L/2} x \cos^2\left(\frac{\pi x}{L}\right) dx}_{\text{same as above, equals } 0} \cdot \frac{4}{L^2}$$

$$= 0$$

#6 (cont.)

c) We know that the second order energy correction is given by:

$$\Delta E^{(2)} = \sum_{k \neq n}' \frac{|\langle k|V|n\rangle|^2}{E_n^{(0)} - E_k^{(0)}}$$

$$= \sum_{k \neq n}' \frac{\left| \int_{-L/2}^{L/2} dy \int_{-L/2}^{L/2} dx \; qE_0 \, \psi^*_{k_x k_y} \psi_{n_x n_y} \right|^2}{(n_x^2 + n_y^2) - (k_x^2 + k_y)^2 \cdot \frac{\pi^2 \hbar^2}{2mL^2}}$$

* Note that $\psi^*_{k_x k_y}$ and $\psi_{n_x n_y}$ will vary based on the values of the x-y states.

* Parity says that only odd functions will be non-zero over symmetric bounds, therefore since $n = (n_x = 1, n_y = 1)$ always yields an even function, our second order correction will always be 0 as even · odd = even

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

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

Angular Momentum Operators,

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

In spherical coordinates,

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

In cylindrical coordinates,

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

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

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

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

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:

$$j(x,t) = \frac{1}{m} Re\left(\Psi^*(x,t) P \Psi(x,t)\right) \tag{1}$$

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

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

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

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

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

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,

$$\frac{j_T}{j_I}, \tag{4}$$

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

(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,

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

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

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

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

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

(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:

$$E_a = \frac{\pi^2\hbar^2}{2ma^2} \tag{2}$$

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 $\mathcal{P}_\gamma$ 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 $\mathcal{P}_\gamma$. Solve for this probability.

Aug 2015

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 $A^\dagger A = AA^\dagger = \mathbb{I}$

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

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

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

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

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

$$\hookrightarrow \lambda = \alpha, \alpha, -\alpha$$

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: $\lambda = -\alpha$

$$\begin{aligned} -i\alpha \overset{-ix_1}{x_3} &= -\alpha x_1 \\ \alpha x_2 &= -\alpha x_2 \\ i\alpha x_1 &= -\alpha x_3 \end{aligned} \quad \Rightarrow \begin{bmatrix} 1 \\ 0 \\ i \end{bmatrix} \cdot \frac{1}{\sqrt{2}}$$

Case: $\lambda = \alpha$

$$\begin{aligned} -i\alpha x_3 &= \alpha x_1 \\ \alpha x_2 &= \alpha x_2 \\ i\alpha x_1 &= \alpha x_3 \end{aligned} \quad \Rightarrow \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \text{ or } \begin{bmatrix} -i \\ 0 \\ 1 \end{bmatrix} \cdot \frac{1}{\sqrt{2}}$$

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

$$\Rightarrow P_\gamma = |2\rangle\langle 2|$$

$$= \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

e) $|\psi\rangle = \frac{2}{3}|1\rangle + \frac{2}{3}|2\rangle - \frac{5}{3}|3\rangle$

$$P(\lambda = \gamma) = |\langle\gamma|A|\psi\rangle|^2$$

$$= \langle\psi|A^\dagger|\gamma\rangle\langle\gamma|A|\psi\rangle$$

$$= \Big[\left(\frac{2}{3}\langle 1| + \frac{2}{3}\langle 2| - \frac{5}{3}\langle 3|\right)$$

Problem 4: Square Well Expansion

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

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

(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

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

(d) [3 pts] Calculate the limiting functional form for $P_{11}(a/L)$ from part (c) for $L >> a$, $\frac{a}{L} \to 0$. (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 $\frac{a}{L} \to 1$. 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.

Aug 2015

Quantum #4

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

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

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

b) For our expanded well with $L > a$, our solutions above are valid with $a \to L$. 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)
$$P_{n',n} = |\langle n'|n\rangle|^2$$

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

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

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

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

$$= \frac{4}{La}\left|\left(\frac{\sin\left(\left[\frac{\pi}{L}-\frac{\pi}{a}\right]\frac{a}{2}\right)}{2\left(\frac{\pi}{L}-\frac{\pi}{a}\right)} + \frac{\sin\left(\left[\frac{\pi}{L}+\frac{\pi}{a}\right]\frac{a}{2}\right)}{2\left(\frac{\pi}{L}+\frac{\pi}{a}\right)}\right) - \left(\frac{\sin\left(\left(\frac{\pi}{L}-\frac{\pi}{a}\right)\frac{-a}{2}\right)}{2\left(\frac{\pi}{L}-\frac{\pi}{a}\right)} + \frac{\sin\left(\left[\frac{\pi}{L}-\frac{\pi}{a}\right]?\right.}{2\left(\frac{\pi}{L}+\frac{\pi}{a}\right)}\right.$$

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

#4 (cont.)

c) $$P_{1,1} = \frac{4}{La}\left| \frac{1}{\left(\frac{\pi^2}{L^2}-\frac{\pi^2}{a^2}\right)}\left[\left(\frac{\pi}{L}+\frac{\pi}{a}\right)\sin\left(\frac{\pi a}{2L}-\frac{\pi}{2}\right)+\left(\frac{\pi}{L}-\frac{\pi}{a}\right)\sin\left(\frac{\pi a}{2L}+\frac{\pi}{2}\right)\right]\right|^2$$

$$= \frac{4}{La}\left| \frac{1}{\frac{\pi^2}{L^2}-\frac{\pi^2}{a^2}}\left[\left(\frac{\pi}{L}+\frac{\pi}{a}\right)\sin\left(\frac{\pi a}{2L}-\frac{\pi}{2}\right)-\left(\frac{\pi}{L}-\frac{\pi}{a}\right)\sin\left(\frac{\pi a}{2L}-\frac{\pi}{2}\right)\right]\right|^2$$

$$= \frac{4}{La}\left| \frac{1}{\frac{\pi^2}{L^2}-\frac{\pi}{a^2}} \cdot \frac{2\pi}{a}\sin\left(\frac{\pi a}{2L}-\frac{\pi}{2}\right)\right|^2$$

$$= \frac{16\pi^2}{La^2}\sin^2\left(\frac{\pi a}{2L}-\frac{\pi}{2}\right)\cdot\frac{1}{\left(\frac{\pi^2}{L^2}-\frac{\pi^2}{a^2}\right)^2}$$

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

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

$$= \frac{16\cos^2\left(\frac{\pi a}{2L}\right)}{\pi^2 L\left(1-\left(\frac{a}{L}\right)^2\right)^2 a^6}$$ off by factor a^7??

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

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

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

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

(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)?

Aug 2015

Quantum #5

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

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

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

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

$$\hookrightarrow H_0 + V_1 = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{m\omega^2}{2}\left(y - \frac{\gamma_1}{m\omega^2}\right)^2 + \gamma_1\left(y - \frac{\gamma'}{m\omega^2}\right)$$

$$= \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{m\omega^2}{2}\left(y^2 - \frac{2\gamma_1 y}{m\omega^2} + \frac{\gamma_1^2}{m^2\omega^4}\right) + \gamma_1 y - \frac{\gamma_1^2}{m\omega^2}$$

$$= \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{m\omega^2 y^2}{2} - \cancel{\gamma_1 y} + \frac{\gamma_1^2}{2m\omega^2} + \cancel{\gamma_1 y} - \frac{\gamma_1^2}{m\omega}$$

$$= \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{m\omega^2 y^2}{2} - \frac{\gamma_1^2}{2m\omega}$$

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

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

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

b) Our first order energy corrections are determined by:

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

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

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

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

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

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

#5 (cont.)

b) Our second order energy corrections are determined by:

$$\Delta E^{(2)} = \sum_{k \neq n}' \frac{|\langle k|V_1|n\rangle|^2}{E_n^{(0)} - E_k^{(0)}}$$

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

$$= \frac{\gamma_1^2 \hbar}{2m\omega} \cdot \frac{1}{\hbar\omega} \sum_{k \neq n}' |\langle k|a^\dagger|n\rangle + \langle k|a|n\rangle|^2/(n-k)$$

$$= \frac{\gamma_1^2}{2m\omega^2} \sum_{k \neq n}' |\sqrt{n+1}\langle k|n+1\rangle + \sqrt{n}\langle k|n-1\rangle|^2/n-k$$

$$= \frac{\gamma_1^2}{2m\omega^2}\left[\frac{n+1}{n-(n+1)} + \frac{n}{n-(n-1)}\right]$$

$$= \frac{\gamma_1^2}{2m\omega^2}\left[-(n+1) + n\right]$$

$$= \frac{-\gamma_1^2}{2m\omega^2}$$

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

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

$$H_0 + V_2 = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{m}{2}x^2 \underbrace{\left(\omega^2 + \frac{2\gamma_2}{m}\right)}_{\omega_1^2}$$

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

$$\hookrightarrow E_n'' = \hbar\omega_1(n + 1/2)$$

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

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

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

#5 (cont.)

d) Again, our first order energy corrections are:

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

$$= \langle n | \gamma_2 x^2 | n^{(0)} \rangle$$

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

$$= \frac{\gamma_2 \hbar}{2m\omega}\left[\langle n | \cancel{a^\dagger a^\dagger} | n \rangle^{0} + \langle n | a^\dagger a | n \rangle + \langle n | a a^\dagger | n \rangle + \langle n | \cancel{aa} | n \rangle^{0}\right]$$

$$= \frac{\gamma_2 \hbar}{2m\omega}\left[n + n+1\right]$$

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

* 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 $|2,1,1\rangle$,

$$\frac{\langle z^2\rangle_{2,1,0}}{\langle z^2\rangle_{2,1,1}} \tag{1}$$

Hydrogen Atom States:

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

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

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

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}}, \quad Y_{1,0} = \sqrt{\frac{3}{4\pi}}cos\theta, \quad Y_{1,\pm1} = \mp\sqrt{\frac{3}{8\pi}}sin\theta\; e^{\pm i\phi}$$

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

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.

Aug 2015

Quantum #6

a) $\langle r \rangle = \langle 1,0,0 | r | 1,0,0 \rangle$

$$= \int_0^\infty r^2 dr \int_0^{2\pi} \sin\theta\, d\theta \int_0^{\pi} d\varphi \cdot r \left(\frac{1}{\sqrt{4\pi}}\right)^2 \left(\frac{2}{a_0^{3/2}}\right)^2 e^{-2r/a_0}$$

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

$$= \frac{4}{a_0^3}\left(\frac{3!}{(2/a_0)^4}\right)$$

$$= \frac{a_0 \cdot 3 \cdot 2}{2^4}$$

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

b) We must determine what the forbidden region is

$$E < V(r)$$

$$\frac{-e^2/2a_0}{n^2} < \frac{-e^2}{r}$$

$$r > 2a_0 n^2$$

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

$\hookrightarrow$ $$P = \int_{2a_0}^\infty \frac{4}{a_0^3} r^2 e^{-2r/a_0} dr$$

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

$$= \frac{4}{a_0^3}\left(\frac{2!}{(2/a_0)^3} e^{-2/a_0 \cdot 2a_0} \sum_{k=0}^{2} \frac{((2/a_0)\cdot 2a_0)^k}{k!}\right)$$

$$= e^{-4}\left[\frac{1}{0!} + \frac{4}{1!} + \frac{16}{2!}\right]$$

$$1 + 4 + 8$$

$$= 13e^{-4}$$

#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:

$$\langle z\rangle = \int_0^\infty r^2 dr \int_0^{2\pi} d\varphi \int_0^\pi \sin\theta\, d\theta \cdot r\cos\theta \cdot \frac{1}{(2a_0)^3} \frac{r^2}{\cancel{3}a_0^2} e^{-r/a_0} \frac{\cancel{3}}{4\pi} \cos^2\theta$$

$$= \int_0^\infty \frac{1}{32\pi a_0^5} r^4 e^{-r/a_0} \int_0^{2\pi} d\varphi \int_0 \cos^3\theta \sin\theta\, d\theta$$

$$= \int_0^\infty dr \frac{1}{16 a_0^5} r^4 e^{-r/a_0} \int_0^\pi -\cos^3\theta\, d(\cos\theta)$$

$$= \int_0^\infty dr \frac{1}{16a_0^5} r^4 e^{-r/a_0} \left[-\frac{1}{4}\cos^4\theta \Big|_0^\pi \right]$$

$$= \int_0^\infty \frac{1}{16a_0^5} r^4 e^{-r/a_0} dr \left[\underbrace{-\frac{1}{4} - -\frac{1}{4}}_{0} \right]$$

$$= 0$$

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

$$\langle z\rangle = \int_0^\infty r^2 dr \int_0^{2\pi} d\varphi \int_0^\pi \sin\theta\, d\theta \cdot r\cos\theta \cdot \left(\frac{-1}{(2a_0)^3}\right) \frac{r^2}{\cancel{3}a_0^2} e^{-r/a_0} \frac{\cancel{3}}{8\pi} \sin^2\theta\, e^{i\varphi}$$

$$= \int_0^\infty \frac{-1}{64\pi a_0^5} r^4 e^{-r/a_0} dr \int_0^{2\pi} e^{i\varphi} d\varphi \int_0^\pi \sin^3\theta \cos\theta\, d\theta$$

$$= \qquad\qquad \cdot\, 0$$

$$= 0$$

* 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

$$\langle z^2 \rangle = \int_0^\infty \frac{1}{16 a_0^5} r^5 e^{-r/a_0} dr \int_0^\pi \cos^4(\theta) \sin\theta \, d\theta$$

$$= \int_0^\infty \frac{1}{16a_0^5} r^5 e^{-r/a_0} dr \left[\frac{-1}{5}\cos^5(\theta) \Big|_0^\pi \right]$$

$$= \int_0^\infty \frac{1}{16a_0^5} r^5 e^{-r/a_0} dr \cdot \left(\frac{-1}{5}(-1)^5 - \frac{-1}{5}(1)^5 \right)$$

$$= \frac{2}{80 a_0^5} \int_0^\infty r^5 e^{-r/a_0} dr$$

$$= \frac{1}{40a_0^5} \left[\frac{5!}{(2/a_0)^6} \right]$$

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

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

$$\langle z^2 \rangle = \int_0^\infty \frac{-1}{64 \pi a_0^5} r^5 e^{-r/a_0} dr \int_0^{2\pi} \overset{1}{\cancel{e^{-i\varphi} e^{i\varphi}}} d\varphi \int_0^\pi \sin^3\theta \cos^2\theta \, d\theta$$

$$= \frac{-1}{32 a_0^5} \left[\frac{5!}{(2/a_0)^6} \right] \int_0^\pi \sin^3\theta - \sin^5\theta \, d\theta$$

$$= \frac{1}{32 a_0^5} \left(\frac{120 a_0^6}{2^6} \right) \cdot \frac{4}{15} \text{ (from mathematica)}$$

$$= \frac{a_0}{64}$$

Quantum Mechanics

Qualifying Exam - January 2016

Notes and Instructions

- There are 6 problems. Attempt them all as partial credit will be given.
- 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

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

In spherical coordinates,

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

Harmonic oscillator wave functions

$u_0(x) = (\frac{m\omega}{\pi\hbar})^{1/4}e^{-\frac{m\omega x^2}{2\hbar}}$

$u_1(x) = (\frac{m\omega}{\pi\hbar})^{1/4}\sqrt{\frac{2m\omega}{\hbar}}xe^{-\frac{m\omega x^2}{2\hbar}}$

Problem 1: Clebsh-Gordon coefficients (10 pts)

A system of two particles with spins $s_1 = \frac{3}{2}$ and $s_2 = \frac{1}{2}$ is described by the Hamiltonian

$$\mathcal{H} = \alpha \mathbf{S}_1 \cdot \mathbf{S}_2$$

with α a constant and $\mathbf{S}_i$ $(i = 1, 2)$ is the spin operator of the i-th particle.

a) What are the allowed values for the quantum numbers of the total spin $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$? (2 Points)

b) Calculate the energy levels of the Hamiltonian. (2 Points)

c) Let us define the basis of eigenstates of the $\mathbf{S}_1^2$, $\mathbf{S}_2^2$, S_{1z}, S_{2z} operators, $|s_1 s_2; m_1 m_2\rangle$, where m_1 and m_2 are the quantum numbers of the projection operators S_{1z} and S_{2z} respectively. The system at time $t = 0$ is initially in the state

$$\left| s_1 s_2; \frac{1}{2}, \frac{1}{2} \right\rangle .$$

Find the state of the system at times $t > 0$. (4 Points)

d) Assuming the initial state above, what is the probability of finding the system in the state

$$\left| s_1 s_2; \frac{3}{2}, -\frac{1}{2} \right\rangle$$

at $t > 0$? (2 Points)

Jan 2016

Quantum #1

a) The allowed S values are:

$$|S_1 - S_2| < S < S_1 + S_2$$
$$\left|\tfrac{3}{2} - \tfrac{1}{2}\right| < S < \tfrac{3}{2} + \tfrac{1}{2}$$
$$\hookrightarrow S = 1, 2$$

b) $H = \alpha S_1 \cdot S_2$

$\times$ Remember $S^2 = S_1^2 + S_2^2 + 2 S_1 \cdot S_2$

$$\hookrightarrow S_1 \cdot S_2 = \tfrac{1}{2}(S^2 - S_1^2 - S_2^2)$$

$$H|S_1, S_2; S, S_z\rangle = \frac{\alpha}{2}(S^2 - S_1^2 - S_2^2)|3/2, 1/2; 2, S_z\rangle = \frac{\alpha\hbar^2}{2}\left(2(2+1) - \tfrac{3}{2}(\tfrac{3}{2}+1) - \tfrac{1}{2}(\tfrac{1}{2}+1)\right)|\rangle$$

or

$$\frac{\alpha}{2}(S^2 - S_1^2 - S_2^2)|3/2, 1/2; 1, S_z\rangle = \frac{\alpha\hbar^2}{2}\left(1(1+1) - \tfrac{3}{2}(\tfrac{3}{2}+1) - \tfrac{1}{2}(\tfrac{1}{2}+1)\right)|\rangle$$

$\Rightarrow$ Our energy states are $E = \frac{\alpha\hbar^2}{2}\left(6 - \frac{15}{4} - \frac{3}{4}\right) = \frac{3\alpha\hbar^2}{2}$ $\quad S=2$

$E = \frac{\alpha\hbar^2}{2}\left(2 - \frac{15}{4} - \frac{3}{4}\right) = -\frac{\alpha\hbar^2}{2}$ $\quad S=1$

c) $S_1 \cdot S_2 = S_{1x}S_{2x} + S_{1y}S_{2y} + S_{1z}S_{2z}$

$$= \tfrac{1}{2}(S_{1+}S_{2-} + S_{1-}S_{2+}) + S_{1z}S_{2z}$$

To determine $|S_1, S_2; \tfrac{1}{2}, \tfrac{1}{2}\rangle$ in basis of H_1 we must start in max S state $|S_1, S_2; S, S_z\rangle$ and lower to appropriate state

$$|2,2\rangle = |3/2, 1/2\rangle$$

$$S_-|2,2\rangle = \sqrt{(2+2)(2-2+1)}\,|2,1\rangle$$
$$= 2|2,1\rangle$$

$$S_-|3/2, 1/2\rangle = S_{1-}|3/2, 1/2\rangle + S_{2-}|3/2, 1/2\rangle$$
$$= \sqrt{(\tfrac{3}{2}+\tfrac{3}{2})(\tfrac{3}{2}-\tfrac{3}{2}+1)}\,|1/2, 1/2\rangle + \sqrt{(\tfrac{1}{2}+\tfrac{1}{2})(\tfrac{1}{2}-\tfrac{1}{2}+1)}\,|3/2, -1/2\rangle$$
$$= \sqrt{3}\,|1/2, 1/2\rangle + |3/2, -1/2\rangle$$

#1(cont.)

c) $\Rightarrow |2,1\rangle = \sqrt{3/4}\,|1/2, 1/2\rangle + \frac{1}{\sqrt{4}}|3/2,-1/2\rangle$

*Note: The $|1,1\rangle$ state is also a linear combination of $|1/2, 1/2\rangle$ and $|3/2,-1/2\rangle$

$$|1,1\rangle = \frac{-1}{\sqrt{4}}|1/2,1/2\rangle + \sqrt{\frac{3}{4}}\,|3/2,-1/2\rangle$$

$$-\sqrt{3}\,|2,1\rangle + |1,1\rangle = -|1/2, 1/2\rangle$$

$$\Downarrow$$

$$|1/2, 1/2\rangle = \sqrt{\tfrac{3}{4}}\,|2,1\rangle - \sqrt{\tfrac{1}{4}}\,|1,1\rangle$$

$$|\Psi(t)\rangle = U(t,t_0)\,|\Psi(0)\rangle, \quad U(t,t_0) = \exp\left[\frac{-iHt}{\hbar}\right]$$

$$\hookrightarrow |1/2, 1/2\,(t)\rangle = \sqrt{\tfrac{3}{4}}\exp\left[\frac{-i3\alpha\hbar t}{2}\right]|2,1\rangle - \sqrt{\tfrac{1}{4}}\exp\left[\frac{i\alpha\hbar t}{2}\right]|1,1\rangle$$

d) $|\langle 3/2,-1/2\,|\,1/2,1/2\,(t)\rangle|^2$

$$|3/2,-1/2\rangle = \sqrt{\tfrac{1}{4}}\,|2,1\rangle + \sqrt{\tfrac{3}{4}}\,|1,1\rangle$$

$$\left|\left[\sqrt{\tfrac{3}{4}}\langle 1,1| + \sqrt{\tfrac{1}{4}}\langle 2,1|\right]\left[\sqrt{\tfrac{3}{4}}\exp\left[\frac{-i3\alpha\hbar t}{2}\right]|2,1\rangle - \sqrt{\tfrac{1}{4}}\exp\left[\frac{i\alpha\hbar t}{2}\right]|1,1\rangle\right]\right|^2$$

$$\left|\frac{\sqrt{3}}{4}\exp\left[\frac{i\alpha\hbar t}{2}\right] + \frac{\sqrt{3}}{4}\exp\left[\frac{-i3\alpha\hbar t}{2}\right]\right|^2$$

$$\frac{3}{16}\left(\exp\left[\frac{-i\alpha\hbar t}{2}\right] - \exp\left[\frac{i3\alpha\hbar t}{2}\right]\right)\left(\exp\left[\frac{i\alpha\hbar t}{2}\right] - \exp\left[\frac{-i3\alpha\hbar t}{2}\right]\right)$$

$$\frac{3}{16}\left(2 - \exp[2i\alpha\hbar t] - \exp[-2i\alpha\hbar t]\right)$$

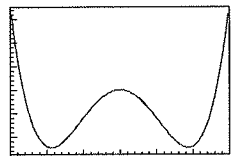


Figure 1: U(x)

Problem 2: Perturbation to a Harmonic Oscillator (10 pts)

Consider a particle of mass, m, moving in a 1-dimensional potential (see Figure 1)

$$U(x) = \lambda x^4 - kx^2.$$

λ and k are positive, and $\lambda \ll \frac{(k^{3/2} m^{1/2})}{4\hbar}$. Approximate the potential near the minima by a simple harmonic oscillator. Here are some useful integrals:

$$\int_{-\infty}^{\infty} x^4 e^{-A(x-a)^2} dx = \frac{1}{4A^{5/2}}(3 + 4a^2 A(3 + a^2 A))\sqrt{\pi}, \text{ for A} > 0$$

$$\int_{-\infty}^{\infty} x^4 e^{-A(x-a)^2} e^{-A(x+a)^2} dx = \frac{3}{16A^{5/2}} e^{-2a^2 A} \sqrt{\frac{\pi}{2}}, \text{ for A} > 0$$

a. Sketch the wavefunctions of the state $|\psi_R\rangle$ which is defined as the state when the particle is found at $x > 0$ and the state $|\psi_L\rangle$ which is the state when the particle is found at $x < 0$. Only consider the lowest energy states near the minima. **(2 Points)**

b. Since the potential is invariant under reflection about the origin, the stationary states must be eigenstates of the parity operator. Express the ground-state and first excited state wavefunctions in terms of $|\psi_R\rangle$ and $|\psi_L\rangle$. **(2 Points)**

c. Estimate the energies of the 2 lowest states using the approximations already described. Hint: use the space representation of the harmonic oscillator wavefunctions and carry out the integrals to find the perturbed energies. **(6 Points)**

Problem 3: Identical particles (10 pts)

Two non-interacting particles of mass m are trapped in a 1-dimensional infinite box of length L situated between $x = 0$ and $x = L$. (In the cases you are considering fermions, assume them to all be spin up.)

(a) [1 points] Write down the single particle energy eigenvalues and wavefunctions.

(b) [1 points] Write down the energy eigenvalues and wavefunctions for two distinguishable particles. Label the states by n_1 for particle 1 and n_2 for particle 2.

(c) [2 points] An energy measurement of the *two identical particle* system yields $E = \hbar^2\pi^2/mL^2$. Write down the state vector/wave function of the system.

(d) [2 points] Suppose instead the energy of the two identical particle system is measured to be $E = 5\hbar^2\pi^2/mL^2$. What is the wave function? *Hint: there are two possibilities.*

(e) [2 points] Show that the fermion state you found in part (d) is an eigenfunction of the Hamiltonian, with the appropriate eigenvalue.

(f) [1 points] Write down the wavefunction for two identical spin-up fermions in the $n_1 = 2$ and $n_2 = 2$ state.

(g) [1 points] If instead you had three particles in the orthonormal states Ψ_1, Ψ_2, and Ψ_3, construct the three particle state for identical fermions.

Jan 2016

Quantum #3

a) For an infinite well b/w 0 and L, our solution is:

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

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

for any single particle

b) Assuming the particles are distinguishable, we simply use the above equations

$$\psi_{n_1} = \sqrt{\tfrac{2}{L}} \sin\left(\tfrac{n_1\pi x}{L}\right) \qquad E_{n_1} = \frac{n_1^2\pi^2\hbar^2}{2mL^2}$$

$$\psi_{n_2} = \sqrt{\tfrac{2}{L}} \sin\left(\tfrac{n_2\pi x}{L}\right) \qquad E_{n_2} = \frac{n_2^2\pi^2\hbar^2}{2mL^2}$$

c) Considering two identical spin-up fermions, the exclusion principle prevents both particles from being in the same state. Since the only combination that yields $E_{n_1 n_2} = \frac{(n_1^2+n_2^2)\pi^2\hbar^2}{2mL^2} = \frac{\pi^2\hbar^2}{mL^2}$ is $n_1 = n_2 = 1$, this state is disallowed by the exclusion principle, therefore

$$\psi_{1,1} = 0$$

d) If $E_{n_1,n_2} = \frac{5\pi^2\hbar^2}{mL^2}$, our possible configurations are $n_1 = 1, n_2 = 3$; $n_1 = 3, n_2 = 1$

Our general wavefunction for identical fermions is:

$$\psi_{n_1 n_2} = \frac{1}{\sqrt{2}}\left(\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)\right)$$

This yields the following potential wave functions:

$$\psi_{13} = \frac{1}{\sqrt{2}}\left(\psi_1(x_1)\psi_2(x_2) - \psi_1(x_2)\psi_2(x_1)\right)$$

$$= \frac{\sqrt{2}}{L}\left(\sin\left(\tfrac{\pi x_1}{L}\right)\sin\left(\tfrac{3\pi x_2}{L}\right) - \sin\left(\tfrac{\pi x_2}{L}\right)\sin\left(\tfrac{3\pi x_1}{L}\right)\right)$$

$$\psi_{31} = \frac{\sqrt{2}}{L}\left(\sin\left(\tfrac{3\pi x_1}{L}\right)\sin\left(\tfrac{\pi x_2}{L}\right) - \sin\left(\tfrac{3\pi x_2}{L}\right)\sin\left(\tfrac{\pi x_1}{L}\right)\right)$$

#3 (cont.)

e) We know that $H\psi_n = E_n \psi_n$ where $H = \frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}\right)$

$\Rightarrow$ For the ψ_{13} state;

$$\frac{\partial^2}{\partial x_1^2}\psi_{13} = \frac{\sqrt{2}}{L}\left(\frac{-\pi^2}{L^2}\sin\left(\frac{\pi x_1}{L}\right)\sin\left(\frac{3\pi x_2}{L}\right) + \left(\frac{3\pi}{L}\right)^2 \sin\left(\frac{\pi x_2}{L}\right)\sin\left(\frac{3\pi x_1}{L}\right)\right)$$

$$\frac{\partial^2}{\partial x_2^2}\psi_{13} = \frac{\sqrt{2}}{L}\left(-\left(\frac{3\pi}{L}\right)^2 \sin\left(\frac{\pi x_1}{L}\right)\sin\left(\frac{3\pi x_2}{L}\right) + \left(\frac{\pi}{L}\right)^2 \sin\left(\frac{\pi x_2}{L}\right)\sin\left(\frac{3\pi x_1}{L}\right)\right)$$

$$\hookrightarrow H\psi_{13} = \frac{-\hbar^2}{2m}\left(\frac{\sqrt{2}}{L}\left[\frac{-\pi^2}{L^2}\sin\left(\frac{\pi x_1}{L}\right)\sin\left(\frac{3\pi x_2}{L}\right) + \frac{9\pi^2}{L^2}\sin\left(\frac{\pi x_2}{L}\right)\sin\left(\frac{3\pi x_1}{L}\right)\right.\right.$$

$$\left.\left. + \frac{\sqrt{2}}{L}\left[-\frac{9\pi^2}{L^2}\sin\left(\frac{\pi x_1}{L}\right)\sin\left(\frac{3\pi x_2}{L}\right) + \frac{\pi^2}{L^2}\sin\left(\frac{\pi x_2}{L}\right)\sin\left(\frac{3\pi x_1}{L}\right)\right)\right)$$

$$= \frac{\hbar^2 10\pi^2}{2mL^2}\left(\frac{\sqrt{2}}{L}\left[\sin\left(\frac{\pi x_1}{L}\right)\sin\left(\frac{3\pi x_2}{L}\right) + \sin\left(\frac{\pi x_2}{L}\right)\sin\left(\frac{3\pi x_1}{L}\right)\right]\right)$$

$$= \frac{10\hbar^2\pi^2}{2mL^2}\psi_{13} \checkmark$$

* A similar process will reach the same conclusion for the ψ_{31} state

f) The $n_1 = n_2 = 2$ state is disallowed by the exclusion principle

$\hookrightarrow \psi_{22} = 0$

g) My guess is this follows something like a cyclic permutation

$$\Rightarrow \psi_{n_1 n_2 n_3} = \frac{1}{\sqrt{6}}\left[\psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3) - \psi_{n_1}(x_2)\psi_{n_2}(x_3)\psi_{n_3}(x_1)\right.$$

$$- \psi_{n_1}(x_3)\psi_{n_2}(x_1)\psi_{n_3}(x_2) + \psi_{n_1}(x_3)\psi_{n_2}(x_2)\psi_{n_3}(x_1)$$

$$\left. + \psi_{n_1}(x_2)\psi_{n_2}(x_1)\psi_{n_3}(x_3) + \psi_{n_1}(x_1)\psi_{n_2}(x_3)\psi_{n_3}(x_2)\right]$$

Problem 4: Matrix Mechanics (10 pts)

Consider a system governed by a Hamiltonian H, with an observable C. The Hamiltonian is represented in the $|e_i\rangle$ basis as:

$$H = \hbar\omega \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

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

The eigenvalues and eigenvectors of H are

$$|E_1 = -\hbar\omega\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}, |E_2 = \hbar\omega, 1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, |E_2 = \hbar\omega, 2\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}.$$

Let C be represented in the $|e_i\rangle$ basis as

$$C = \begin{bmatrix} 0 & 0 & 2 \\ 0 & 1 & 0 \\ 2 & 0 & 0 \end{bmatrix}$$

At t=0, the system is in the state: $|\Psi(t=0)\rangle = \frac{1}{\sqrt{2}}|e_1\rangle + \frac{1}{\sqrt{2}}|e_2\rangle$

a) At time t=0, the observable C is measured. What results are possible and with what probabilities? (2 pts)

b) Determine the representation of the time evolution operator $U(t, t_0 = 0)$ in the $|e_i\rangle$ representation. (2 pts)

c) Determine $|\Psi(t)\rangle$ in the $|e_i\rangle$ basis. (2 pts)

d) If C is measured at some later time t, what results are possible and with what probabilities? (2 pts)

e) Are your probabilities time dependent or time independent? Explain (2 pts)

Jan 2016

Quantum #4

a) * Read question as: Starting in $|\Psi(t=0)\rangle$, what is the probability of obtaining each eigenvalue of C

* Determine eigenvalues

$$|C-\lambda \mathbb{I}| = 0$$

$$\Rightarrow \quad 0 = \begin{vmatrix} -\lambda & 0 & 2 \\ 0 & 1-\lambda & 0 \\ 2 & 0 & -\lambda \end{vmatrix}$$

$$0 = -\lambda\left[(1-\lambda)(-\lambda)-0\right] - 0\left[0(-\lambda)-0(2)\right] + 2\left[0(0)-(1-\lambda)(2)\right]$$

$$= (-\lambda)^2(1-\lambda) - 4(1-\lambda)$$

$$= (1-\lambda)\left[\lambda^2-4\right]$$

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

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

* Determine eigenvectors

$$C\vec{v} = \lambda\vec{v}$$

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

$$\hookrightarrow \quad 2x_3 = \lambda x_1$$

$$x_2 = \lambda x_2$$

$$2x_1 = \lambda x_3$$

* for $\lambda = 1$

$$2x_3 = x_1$$

$$x_2 = x_2$$

$$2x_1 = x_3$$

$$\Rightarrow \vec{v} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

* for $\lambda = 2$

$$2x_3 = 2x_1$$

$$x_2 = 2x_2$$

$$2x_1 = 2x_3$$

$$\Rightarrow \vec{v} = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}\frac{1}{\sqrt{2}}$$

* for $\lambda = -2$

$$2x_3 = -2x_1$$

$$x_2 = -2x_2$$

$$2x_1 = -2x_3$$

$$\Rightarrow \vec{v} = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}\frac{1}{\sqrt{2}}$$

#4 (cont.)

a) * Rewriting $|\Psi(t=0)\rangle = \frac{1}{\sqrt{2}}(|e_1\rangle + |e_2\rangle)$

$$= \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\\0\end{bmatrix}$$

$$= \frac{1}{\sqrt{2}}\left(|\lambda=1\rangle + \frac{1}{2}[\,|\lambda=2\rangle + |\lambda=-2\rangle]\right)$$

* Probabilities of form

$$|\langle i|\,C\,|\Psi(t=0)\rangle|^2$$

$$C|\Psi(t=0)\rangle = \frac{1}{\sqrt{2}}\left(|\lambda=1\rangle + \frac{1}{2}(2|\lambda=2\rangle - 2|\lambda=-2\rangle)\right)$$

$$= \frac{1}{\sqrt{2}}|\lambda=1\rangle + \frac{1}{\sqrt{2}}|\lambda=-2\rangle - \frac{1}{\sqrt{2}}|\lambda=-2\rangle$$

$$\Rightarrow |\langle\lambda=1|\,C\,|\Psi(t=0)\rangle|^2 = \frac{1}{2}$$

$$|\langle\lambda=+2|\,C\,|\Psi(t=0)\rangle|^2 = \frac{1}{4}$$

$$|\langle\lambda=-2|\,C\,|\Psi(t=0)\rangle|^2 = \frac{1}{4}$$

b) $U(t, t_0=0) = e^{-iHt/\hbar}$

$$= e^{-i\omega t}(|e_1\rangle\langle e_1| + |e_2\rangle\langle e_3| + |e_3\rangle\langle e_2|)$$

c) $|\Psi(t)\rangle = U(t,t_0=0)\,|\Psi(t=0)\rangle$

$$= \frac{1}{\sqrt{2}}\left[e^{-i\omega t}|e_1\rangle + e^{-i\omega t}|e_3\rangle\right]$$

d) * Rewriting $|\Psi(t)\rangle = \frac{1}{\sqrt{2}}e^{-i\omega t}(|e_1\rangle + e_3\rangle)$

$$= \frac{1}{\sqrt{2}}e^{-i\omega t}\begin{bmatrix}1\\0\\1\end{bmatrix}$$

$$= e^{-i\omega t}|\lambda=2\rangle$$

Problem 5: Magnetic Moments and Spin (10 pts)

Consider a spin 1/2 particle with a magnetic moment. We can write the interaction between the spin and an external magnetic field using the Hamiltonian:

$$H = -\gamma \vec{B} \cdot \vec{S} \tag{1}$$

where $\vec{B}$ is the external field, $\vec{S}$ is the spin operator for the particle, and γ is a real positive constant. In this problem, use the usual basis states that are eigenstates of S_z

$$S_z \chi_{\pm} = \pm \frac{\hbar}{2} \chi_{\pm}, \quad \chi_{+} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi_{-} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{2}$$

For this problem, assume the magnetic field lies in the x-z plane:

$$\vec{B} = B_x \hat{e}_x + B_z \hat{e}_z \tag{3}$$

(a) [1 pt] Solve for the eigenenergies for the Hamiltonian, showing your work. Explain the physics of your results.

(b) [2 pts] Any state of the spin can be written in the $\chi_{\pm}$ basis as:

$$\Psi(t) = \begin{pmatrix} \alpha(t) \\ \beta(t) \end{pmatrix} \tag{4}$$

Using the Hamiltonian, derive the first-order coupled differential equations that give the time dependence for $\alpha(t)$ and $\beta(t)$. In other words, derive the equations for $\dot{\alpha}(t)$ and $\dot{\beta}(t)$.

(c) [2 pts] Show that you can re-write your results from part (b) as two uncoupled second-order differential equations:

$$\begin{aligned} \ddot{\alpha}(t) &= -\frac{\gamma^2 B_T^2}{4} \alpha(t) \\ \ddot{\beta}(t) &= -\frac{\gamma^2 B_T^2}{4} \beta(t) \end{aligned} \tag{5}$$

where $B_T = \sqrt{B_x^2 + B_z^2}$ is the magnitude of the total magnetic field. How is this result related to what you found in part (a)?

Of course, the solutions to these equations are:

$$\begin{aligned} \alpha(t) &= C_1 \cos(\omega t) + C_2 \sin(\omega t) \\ \beta(t) &= C_3 \cos(\omega t) + C_4 \sin(\omega t) \end{aligned} \tag{6}$$

with $\omega = \frac{\gamma B_T}{2}$.

(d) [3 pts] Consider the situation where the spin is in the spin-up S_z state χ_{+} at time $t = 0$. Using the boundary conditions at time $t = 0$, determine the values for the constants C_1, C_2, C_3, C_4 that will solve for the time-dependence of the state. Remember that the equations in part (c) are second-order, so you need two boundary conditions at $t = 0$ for each.

(e) [2 pt] Write down the time-dependent probabilities, $P_{\pm}$ of the spin being in the spin-up and spin-down S_z states. Show that your results are correct in the two cases where $B_x = 0$ and $B_z = 0$.

Jan 2016

Quantum #5

a) Given $H = -\gamma \vec{B} \cdot \vec{S}$

$$= -\gamma (B_x S_x + B_z S_z)$$

$$= -\gamma \left(B_x \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + B_z \hbar/2 \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \right)$$

$$= -\gamma \frac{\hbar}{2} \begin{bmatrix} B_z & B_x \\ B_x & -B_z \end{bmatrix}$$

We can determine the energy eigenvalues by $\det(H - \lambda \mathbb{I}) = 0$

$$\begin{vmatrix} -\frac{\gamma\hbar B_z}{2} - \lambda & -\frac{\gamma\hbar B_x}{2} \\ -\frac{\gamma\hbar B_x}{2} & \frac{\gamma\hbar B_z}{2} - \lambda \end{vmatrix} = \left(-\frac{\gamma\hbar B_z}{2} - \lambda\right)\left(\frac{\gamma\hbar B_z}{2} - \lambda\right) - \frac{\gamma^2\hbar^2 B_x^2}{4}$$

$$= -\frac{\gamma^2\hbar^2 B_z^2}{4} \cancel{- \frac{\lambda\gamma\hbar B_z}{2} + \frac{\lambda\gamma\hbar B_z}{2}} + \lambda^2 - \frac{\gamma^2\hbar^2 B_x^2}{4}$$

$$0 = \lambda^2 - \frac{\gamma^2\hbar^2(B_z^2 + B_x^2)}{4}$$

$$\lambda^2 = \frac{\gamma^2\hbar^2}{4}(B_z^2 + B_x^2)$$

$$\lambda = \pm \frac{\gamma\hbar}{2}(B_z^2 + B_x^2)^{1/2}$$

b) The time-dependent Schrödinger eqn states:

$$i\hbar \frac{\partial}{\partial t} \Psi = H\Psi$$

$$i\hbar \frac{\partial}{\partial t} \begin{bmatrix} \alpha(t) \\ \beta(t) \end{bmatrix} = -\frac{\gamma\hbar}{2} \begin{bmatrix} B_z & B_x \\ B_x & -B_z \end{bmatrix} \begin{bmatrix} \alpha(t) \\ \beta(t) \end{bmatrix}$$

$$i \frac{\partial\alpha}{\partial t} = -\frac{\gamma}{2}(B_z \alpha(t) + B_x \beta(t))$$

$$i \frac{\partial\beta}{\partial t} = -\frac{\gamma}{2}(B_x \alpha(t) - B_z \beta(t))$$

or

$$\dot{\alpha}(t) = \frac{i\gamma}{2}(B_z \alpha(t) + B_x \beta(t))$$

$$\dot{\beta}(t) = \frac{i\gamma}{2}(B_x \alpha(t) - B_z \beta(t))$$

#5 (cont.)

c) To get 2^{nd} order differential equations, we take another set of time derivatives

$$\ddot{\alpha}(t) = \frac{i\gamma}{2}\left(B_z\,\dot{\alpha}(t) + B_x\,\dot{\beta}(t)\right)$$

$$\ddot{\beta}(t) = \frac{i\gamma}{2}\left(B_x\,\dot{\alpha}(t) - B_z\,\dot{\beta}(t)\right)$$

Substituting our first order differential equations into the above equations yield:

$$\ddot{\alpha}(t) = \frac{-\gamma^2}{4}\left(B_z[B_z\alpha(t) + B_x\beta(t)] + B_x[B_x\alpha(t) - B_z\beta(t)]\right)$$

$$\ddot{\beta}(t) = \frac{-\gamma^2}{4}\left(B_x[B_z\alpha(t) + B_x\beta(t)] - B_z[B_x\alpha(t) - B_z\beta(t)]\right)$$

Simplifying and letting $B_T^2 = B_x^2 + B_z^2$

$$\ddot{\alpha}(t) = \frac{-\gamma^2 B_T^2}{4}\alpha(t)$$

$$\ddot{\beta}(t) = \frac{-\gamma^2 B_T^2}{4}\beta(t)$$

d) If we are in the spin-up state at $t=0$

$$1 = C_1\cos(\omega t) + C_2\sin(\omega t) = \alpha(t)$$

$$0 = C_3\cos(\omega t) + C_4\sin(\omega t) = \beta(t)$$

$\Rightarrow$ From this, we immediately determine $C_1 = 1$, $C_3 = 0$ b/c $\cos(\omega t) = 1$ at $t=0$

Our other condition comes from the first order differential equations

$\hookrightarrow$ $\dot{\alpha}(0) = \frac{i\gamma}{2}B_z \qquad \dot{\beta}(0) = \frac{i\gamma}{2}B_x$

$$\dot{\alpha}(t) = -\omega C_1\sin(\omega t) + \omega C_2\cos(\omega t) \rightarrow \dot{\alpha}(0) = \omega C_2$$

$$\dot{\beta}(t) = -\omega C_3\sin(\omega t) + \omega C_4\cos(\omega t) \rightarrow \dot{\beta}(0) = \omega C_4$$

$$\Rightarrow C_2 = \frac{i\gamma}{2\omega}B_z = \frac{iB_z}{B_T}$$

$$C_4 = \frac{i\gamma}{2\omega}B_x = \frac{iB_x}{B_T}$$

#5 (cont.)

e) We now know our time-dependent initial state

$$|\psi\rangle = \begin{bmatrix} \cos(\omega t) + \frac{iB_z}{B_T}\sin(\omega t) \\ \frac{iB_x}{B_T}\sin(\omega t) \end{bmatrix}$$

$$P_\pm = |\langle \chi_\pm | \psi(t) \rangle|^2$$

$$P_+ = |\langle \chi_+ | \psi(t) \rangle|^2$$

$$= \left| [1 \;\; 0] \begin{bmatrix} \cos(\omega t) + \frac{iB_z}{B_T}\sin(\omega t) \\ \frac{iB_x}{B_T}\sin(\omega t) \end{bmatrix} \right|^2$$

$$= \left| \cos(\omega t) + \frac{iB_z}{B_z}\sin(\omega t) \right|$$

$$= \cos^2(\omega t) + \cancel{\frac{iB_z}{B_T}\sin(\omega t)\cos(\omega t)} - \cancel{\frac{iB_z}{B_T}\sin(\omega t)\cos(\omega t)} + \frac{B_z^2}{B_T^2}\sin^2(\omega t)$$

$$= \cos^2(\omega t) + \frac{B_z^2}{B_T^2}\sin^2(\omega t)$$

$$P_- = |\langle \chi_- | \psi(t) \rangle|^2$$

$$= \left| [0 \;\; 1] \begin{bmatrix} \cos(\omega t) + \frac{iB_z}{B_T}\sin(\omega t) \\ \frac{iB_x}{B_T}\sin(\omega t) \end{bmatrix} \right|^2$$

$$= \frac{B_x^2}{B_T^2}\sin^2(\omega t)$$

$$P_+ + P_- = \cos(\omega t) + \frac{B_z^2}{B_T^2}\sin^2(\omega t) + \frac{B_x^2}{B_T^2}\sin^2(\omega t)$$

$$= \cos^2(\omega t) + \underbrace{\frac{B_z^2 + \cancel{B_x^2}}{\cancel{B_x^2} + B_z^2}}_{1}\sin^2(\omega t)$$

$$= \cos^2(\omega t) + \sin^2(\omega t)$$

$$= 1 \quad \Rightarrow \text{ Valid at all times}$$

* if $B_x = 0$

$P_+ = 1, \quad P_- = 0$

* if $B_z = 0$

$P_+ = \cos^2(\omega t)$

$P_- = \sin^2(\omega t)$

Problem 6: Electron in a Finite Square Well (10 pts)

Consider an electron of energy E incident from x=$-\infty$ on a symmetric one-dimensional square well of depth V_0 and width L.

$$V(x) = \begin{cases} 0, & \text{x < -L/2} \\ -V_0, & \text{-L/2 < x < L/2} \\ 0, & \text{x > L/2} \end{cases}$$

a) Write down the solutions to the time-independent Schrodinger Equation for this situation. There should be five integration constants (2 points)

b) Apply boundary conditions to find the probability that the electron is transmitted past the finite well (4 points)

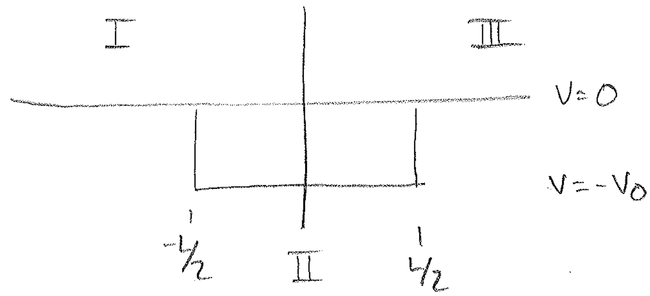
c) For what values of E is there a 100% probability for transmission past the well? (2 points)

d) Consider a potential well with V_0 large enough for there to be two bound states. For this well, what is the smallest electron energy (E > 0) for which there is a 100% probability for transmission? Your answer will depend on V_0 and other parameters in the problem. (2 points)

Jan 2016

Quantum #6

a)



The time-independent Schrödinger equation states:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi + V\psi = E\psi$$

Regions I and III:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

$$\frac{d^2\psi}{dx^2} = \frac{-2mE}{\hbar^2}\psi$$

$$\text{let } \kappa = \frac{\sqrt{-2mE}}{\hbar}$$

$$\frac{d^2\psi}{dx^2} = \kappa^2\psi$$

$$\hookrightarrow \psi_I = Ae^{\kappa x} + Be^{-\kappa x}$$

$$\psi_{III} = Fe^{\kappa x} + Ge^{-\kappa x}$$

Region II:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - V_0\psi = E\psi$$

$$\frac{d^2\psi}{dx^2} = \frac{-2m(E+V_0)}{\hbar^2}\psi$$

$$\text{let } k = \frac{\sqrt{2m(E+V_0)}}{\hbar}$$

$$\frac{d^2\psi}{dx^2} = -k^2\psi \Rightarrow \psi_{II} = Ce^{ikx} + De^{-ikx}$$

#6 (cont.)

a) * Note: The above derivation assumes we have a bound state ($-V_0 < E < 0$)

If $E > 0$, then our wave functions become

$$\psi_{I} = Ae^{ikx} + Be^{-ikx} \qquad k_I = k_{III} = \frac{\sqrt{2mE}}{\hbar} = k$$

$$\psi_{II} = Ce^{ikx} + De^{ikx} \qquad k_{II} = \frac{\sqrt{2m(E+V_0)}}{\hbar}$$

$$\psi_{III} = Fe^{ikx}$$ (Assume no incoming wave from left)

b) Our boundary conditions are that ψ and $\frac{d\psi}{dx}$ are continuous

↳ at $-L/2$:

$$Ae^{-ikL/2} + Be^{ikL/2} = C\sin\left(-k_{II}\tfrac{L}{2}\right) + D\cos\left(-\tfrac{k_{II}L}{2}\right)$$

$$ik_I\left(Ae^{-ik\cdot L/2} - Be^{ik\cdot L/2}\right) = k_{II}\left[C\cos\left(-k_{II}\tfrac{L}{2}\right) - D\sin\left(-\tfrac{k_{II}L}{2}\right)\right]$$

↳ at $L/2$:

$$C\sin\left(k_{II}\tfrac{L}{2}\right) + D\cos\left(k_{II}\tfrac{L}{2}\right) = Fe^{ikL/2}$$

$$k_{II}\left[C\cos\left(k_{II}\tfrac{L}{2}\right) - D\sin\left(k_{II}\tfrac{L}{2}\right)\right] = ikFe^{ikL/2}$$

* In the end, the transmission probability $T = \frac{|F|^2}{|A|^2}$

⇒ After using $\frac{L}{2}$ B.C's to eliminate C and D and substituting them into our $-\frac{L}{2}$ B.C, with <u>waste of time algebra</u> we find:

$$F = \frac{\exp[-ikL]}{\cos(k_{II}L) - i\frac{k^2 + k_{II}^2}{2kk_{II}}\sin(k_{II}L)} A$$

$(-i)(i) = 1$

$$\Rightarrow T = \frac{1}{\left|\cos(k_{II}L) - i\frac{k^2+k_{II}^2}{2kk_{II}}\sin(k_{II}L)\right|^2}$$

$$= \frac{1}{\cos^2(k_{II}L) + \left(\frac{k^2+k_{II}^2}{2kk_{II}}\right)^2\sin^2(k_{II}L)}$$

#6 (cont.)

c) Perfect transmission will occur when $F = A$

$$\hookrightarrow E_n = \frac{n^2 \pi^2 \hbar^2}{2m L^2} - V_0 \qquad \text{(from Griffiths)}$$

d) $$E = \frac{2\pi^2\hbar^2}{mL^2} - V_0$$ for 2 bound states

Quantum Mechanics
Qualifying Exam - August 2016

Notes and Instructions

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Spin Operator

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

In spherical coordinates,

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

Harmonic oscillator wave functions

$u_0(x) = (\frac{m\omega}{\pi\hbar})^{1/4}e^{-\frac{m\omega x^2}{2\hbar}}$

$u_1(x) = (\frac{m\omega}{\pi\hbar})^{1/4}\sqrt{\frac{2m\omega}{\hbar}}xe^{-\frac{m\omega x^2}{2\hbar}}$

Problem 1: Time dependent solutions to Schrodinger's Equation (10 pts)

Consider a particle of mass m in an infinite square well.

$$V(x) = \begin{cases} 0, & -\frac{a}{2} \leq x \leq -\frac{a}{2} \\ \infty, & x < -\frac{a}{2} \text{ or } x > +\frac{a}{2} \end{cases}$$

The solutions to the time independent Schrodinger Equation are: $H|\Psi_n\rangle = E_n|\Psi_n\rangle$ for n=1,2,3, ... where $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$ and

$$\langle x|\Psi_n\rangle = \Psi_n(x) = \sqrt{\frac{2}{a}}\cos(\frac{n\pi x}{a})\ n = 1, 3, 5, ... \quad \sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a})\ n = 2, 4, 6, ...$$

Assume at t_o, the particle is in the state:

$$|\Psi(t_o = 0)\rangle = \sqrt{3/10}\,|\Psi_1\rangle - i\sqrt{7/10}\,|\Psi_3\rangle$$

Answer the following questions:

a) Using Dirac notation, write down the expression for the time evolution operator, $U(t, t_o = 0)$ in terms of energy eigenvalues and eigenstates. (1 pt)

b) Find $|\Psi(t)\rangle = U(t, t_o = 0)|\Psi(t_o = 0)\rangle$ (1 pt)

c) Does your $|\Psi(t)\rangle$ in part b) satisfy the time independent Schrodinger Equation? Demonstrate explicitly. (1 pt)

d) Does your $|\Psi(t)\rangle$ in part b) satisfy the time dependent Schrodinger Equation? Demonstrate explicitly. (1 pt)

e) Is the uncertainty in the energy $\Delta E > 0$, < 0 or $= 0$ for $|\Psi(t)\rangle$? Discuss. (1 pt)

f) State whether the following properties are time dependent or time independent for a system in the state $|\Psi(t)\rangle$. (4 pts)

i) ΔE

ii) $\langle x^2\rangle$

iii) $\langle p\rangle$

iv) $\langle P\rangle$, where P is the parity operator

g) How do your answers to part f) change after the energy is measured at time t and the result is $E = \frac{9\pi^2\hbar^2}{2ma^2}$? (1 pt)

Problem 2: Hydrogen Atom (10 pts)

In this problem you will calculate the relativistic correction to the energies of the hydrogen atom. The hydrogen atom Hamiltonian is in terms of its electron in the field of the positively charged nucleus

$$H_0 = \frac{p^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0 r}$$

where p is the electrons momentum, r its position, m_e its mass, and e the charge. This Hamiltonian is nonrelativistic ($p/(mc) \ll 1$). The correct relativistic expression to use for the kinetic energy is

$$T = \sqrt{p^2c^2 + m_e^2c^4} - m_ec^2$$

recall that

$$\langle r \rangle_{nl} = n^2 a_0 \{1 + \frac{1}{2}[1 - \frac{l(l+1)}{n^2}]\}$$

$$\langle r^2 \rangle_{nl} = n^4 a_0^2 \{1 + \frac{3}{2}[1 - \frac{l(l+1) - 1/3}{n^2}]\}$$

$$\langle \frac{1}{r} \rangle_{nl} = \frac{1}{a_0 n^2}$$

$$\langle \frac{1}{r^2} \rangle_{nl} = \frac{1}{a_0^2 n^3} \frac{1}{l + 1/2}$$

$$\langle \frac{1}{r^3} \rangle_{nl} = \frac{1}{a_0^3 n^3} \frac{1}{l(l+1/2)(l+1)}$$

a. Use this information to find the first non-zero order correction to the Hamiltonian due to the relativistic motion of the electron. **(2 Points)**

b. Show that this correction is diagonal in the $|nlm\rangle$ basis by proving that it commutes with the angular momentum operator $\vec{L}$. Why is it sufficient to prove that the perturbation commutes with $\vec{L}$ to show that the perturbation is diagonal in the $|nlm\rangle$ basis? **(4 Points)**

c. Using the fact that

$$\frac{p^2}{2m_e} = H_0 + \frac{e^2}{4\pi\epsilon_0 r}$$

find the relativistic energy correction to the energy levels of the Hydrogen atom. **(4 Points)**

Problem 3: Angular momentum (10 pts)

One particle has spin j_1 and another particle has spin j_2.

(a) [1 point] What are the good quantum numbers for the two-particle system with $\vec{J} = \vec{J}_1 + \vec{J}_2$ in the direct product basis? Write down the basis vectors labelled according to their eigenvalues.

(b) [1 points] Write down the basis vectors in the total j basis. What are the good quantum numbers in this case?

(c) [2 points] Write down the completeness relation for the direct product basis states.

(d) [2 points] Use the completeness relation to relate the total -j basis to the direct product basis. Identify the Clebsch-Gordon coefficient.

(e) [2 points] Write down the relation between total-j and direct product bases for $j_1 = 1/2$ and $j_2 = 1/2$. Recall

$$J_{\pm}|j, m> = \hbar\sqrt{(j \mp m)(j \pm m + 1)}|j, m \pm 1>$$

(f) [2 points] Suppose you have an interaction of the form $H_I = A\vec{J}_1 \cdot \vec{J}_2$ where $\vec{J} = \vec{J}_1 + \vec{J}_2$. Which basis vectors are best to use and why?

Problem 4: 3D Attractive Potential (10 pts)

Consider a particle that moves subjected to a three dimensional attractive potential

$$V(x,y,z) = -\frac{\hbar^2}{2m}[\lambda_1\delta(x) + \lambda_2\delta(y) + \lambda_3\delta(z)],$$

where $\lambda_1, \lambda_2, \lambda_3 > 0$.

a) Find the energy and the wavefunction of the particle in this potential. (4 points)

b) Interpret the meaning of this state. Calculate the probability of finding the particle inside a rectangular volume centered at the origin, with size $\ell_i = 1/\lambda_i$, with $i = 1, 2, 3$ for the x, y, z directions respectively. (2 points)

c) Compute the spatial and momentum uncertainties $(\Delta \mathbf{x})^2$ and $(\Delta \mathbf{p})^2$ for the state of item a) and explicitly check Heisenberg's inequality. (4 points)

Hint:

$$\frac{d|x|}{dx} = \frac{x}{|x|} \equiv \text{sign}(x) \qquad \frac{d}{dx}\text{sign}(x) = 2\delta(x)$$

Problem 5: Expanding Harmonic Oscillator (10 pts)

Consider a particle of mass m confined in a 1D harmonic oscillator potential with frequency ω_0

$$H_a = \frac{P^2}{2m} + \frac{m}{2}\omega_0^2 \, X^2 \tag{1}$$

The raising and lowering operators are useful for harmonic oscillator problems:

$$a^\dagger = \frac{1}{\sqrt{2}}\left(\frac{X}{\lambda} - i\frac{\lambda}{\hbar}P\right) \qquad a = \frac{1}{\sqrt{2}}\left(\frac{X}{\lambda} + i\frac{\lambda}{\hbar}P\right) \tag{2}$$

where $\lambda = \sqrt{\frac{\hbar}{m\omega_0}}$ is the length scale for the harmonic oscillator:

(a) [2 pts] Use the raising and lowering operators to derive the ground state wavefuction, $\psi_0(x)$, and the first excited state wavefuction, $\psi_1(x)$, for the Hamiltonian H_a. Be sure to show your work.

(b) [1 pt] Consider a sudden change in the potential, modeled by a change in the original frequency of the oscillator by some multiplicative value f, to the new Hamiltonian:

$$H_b = \frac{P^2}{2m} + \frac{m}{2}\omega_1^2 \, X^2, \quad \omega_1 = f\omega_0, \quad 0 < f < 1 \tag{3}$$

"Sudden" in this case means that one can ignore the time it takes to change the potential.

If $\phi_0(x)$ and $\phi_1(x)$ are the ground and first excited state wavefunctions of H_b, what are the functional forms for these wavefunctions? Explain your answer.

(c) [3 pts] The oscillator is in the ground state $\psi_0(x)$ when the potential suddenly changes. What is the expectation value of the energy of the oscillator after the potential changes? Show your work.

(d) [2 pts] If the oscillator is in the state $\psi_0(x)$ when the potential suddenly changes, what is the probability of the oscillator being in the ground state of H_b after the potential changes? Show your work.

(e) [1 pt] If the oscillator is in the state $\psi_0(x)$ when the potential suddenly changes, what is the probability of the oscillator being in the first excited state of H_b after the potential changes? Explain your answer.

(f) [1 pt] Finally, assume the oscillator is in the first excited state of H_a, $\psi_1(x)$, when the potential suddenly changes. What is the expectation value of the energy of the oscillator after the potential changes? Is the change in the expectation value of the energy, from H_a to H_b, for ψ_1 larger than, smaller than, or the same as ψ_0? Explain.

Remember that the Gaussian integrals have the form:

$$\begin{aligned} \int_{-\infty}^{\infty} e^{-ax^2} dx &= \sqrt{\frac{\pi}{a}} \\ \int_{-\infty}^{\infty} x^{2n} e^{-ax^n} dx &= \frac{1 \cdot 3 \cdot 5 \ldots (2n-1)}{2^n a^2} \sqrt{\frac{\pi}{a}} \end{aligned} \tag{4}$$

Problem 6: Delta function in a 1-D well(10 pts)

A particle of mass m is placed in an attractive 1-D delta function potential

$$V(x) = -\hbar^2 \lambda \delta(x)/m$$

with positive λ. The particle and the potential are located in an infinite box with walls at x=$\pm\, a/2$ (i.e $V(a/2) = V(-a/2) = \infty$)

a) Determine the condition on the parameters for which the system will have exactly one bound state with negative energy eigenvalue E and give its wave function (4 pts).

b) For the same system, determine the energy eigenvalues and eigenvectors for states with positive E. (3 pts)

c) If the coefficient $\lambda < 0$, explain in detail how your results change for parts a) and b) (3 pts)

Quantum Mechanics
Qualifying Exam - January 2017

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In spherical coordinates,

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

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$$u_1(x) = (\tfrac{m\omega}{\pi\hbar})^{1/4} \sqrt{\tfrac{2m\omega}{\hbar}}\, x e^{-\frac{m\omega x^2}{2\hbar}}$$

Spherical Harmonics:

$$Y_{0,0}(\theta,\phi) = \tfrac{1}{\sqrt{4\pi}} \qquad Y_{2,0}(\theta,\phi) = \sqrt{\tfrac{5}{16\pi}}(3\cos^2\theta - 1)$$

$$Y_{1,0}(\theta,\phi) = \sqrt{\tfrac{3}{4\pi}}\cos\theta \qquad Y_{2,\pm1}(\theta,\phi) = \mp\sqrt{\tfrac{15}{8\pi}} e^{\pm i\phi}\cos\theta\sin\theta$$

$$Y_{1,\pm1}(\theta,\phi) = \mp\sqrt{\tfrac{3}{8\pi}} e^{\pm i\phi}\sin\theta \qquad Y_{2,\pm2}(\theta,\phi) = \sqrt{\tfrac{15}{32\pi}} e^{\pm 2i\phi}\sin^2\theta$$

Problem 1: Harmonic Oscillator (10 Points)

Consider the quantum mechanical simple harmonic oscillator.

a. Using the raising and lower operators, $\hat{a}$ and $\hat{a}^\dagger$ find the average value of X and P for the state $|n>$. **(1 Points)**

b. Using the raising and lower operators, $\hat{a}$ and $\hat{a}^\dagger$, find the average value of X^2 and P^2 for the state $|n>$. **(2 Points)**

c. Using the raising and lower operators, $\hat{a}$ and $\hat{a}^\dagger$ find the root mean square deviations of X and P for the state $|n>$. **(2 Points)**

d. Find the uncertainty product for the state $|n>$ **(2 Points)**

e. Fine the average potential energy and average kinetic energy for the oscillator when it is in state $|n>$ **(3 Points)**

Jan 2017

Quantum #1

a) * Remember that: $a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{i}{m\omega}p\right)$

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

$$\Rightarrow \quad x = \frac{1}{\sqrt{2}}\sqrt{\frac{2\hbar}{m\omega}}(a + a^{+}) = \sqrt{\frac{\hbar}{2m\omega}}\,(a + a^{+}) \qquad p = \frac{m\omega}{2i}\sqrt{\frac{2\hbar}{m\omega}}(a - a^{+}) = -i\sqrt{\frac{m\omega\hbar}{2}}\,(a - a^{+})$$

$$\Rightarrow \langle x \rangle = \langle n| \sqrt{\tfrac{\hbar}{2m\omega}}(a + a^{+})|n\rangle$$
$$= \sqrt{\tfrac{\hbar}{2m\omega}}\left[\langle n|a|n\rangle + \langle n|a^{+}|n\rangle\right]$$
$$= \sqrt{\tfrac{\hbar}{2m\omega}}\left[\sqrt{n}\,\langle n|n-1\rangle + \sqrt{n+1}\,\langle n|n+1\rangle\right]$$
$$= 0$$

$$\langle p \rangle = -i\sqrt{\tfrac{m\omega\hbar}{2}}\left[\langle n|\, a - a^{+}|n\rangle\right]$$
$$= -i\sqrt{\tfrac{m\omega\hbar}{2}}\left[\langle n|a|n\rangle - \langle n|a^{+}|n\rangle\right]$$
$$= -i\sqrt{\tfrac{m\omega\hbar}{2}}\left[\sqrt{n}\,\langle n|n-1\rangle - \sqrt{n+1}\,\langle n|n+1\rangle\right]$$
$$= 0$$

b) $$\langle x^2 \rangle = \frac{\hbar}{2m\omega}\left[\langle n|\, aa + a^{+}a + aa^{+} + a^{+}a^{+}|n\rangle\right]$$
$$= \frac{\hbar}{2m\omega}\left[\sqrt{n(n-1)}\,\langle n|n-2\rangle + \sqrt{(n+1)^2}\,\langle n|n\rangle + \sqrt{n^2}\,\langle n|n\rangle + \sqrt{(n+1)(n+2)}\,\langle n|n+2\rangle\right]$$
$$= \frac{\hbar}{2m\omega}(2n+1)$$

$$\langle p^2 \rangle = -\frac{m\omega\hbar}{2}\left[\langle n|\, aa - aa^{+} - a^{+}a + a^{+}a^{+}|n\rangle\right]$$
$$= -\frac{m\omega\hbar}{2}\left[\sqrt{n(n-1)}\,\langle n|n-2\rangle - (n+1)\langle n|n\rangle - \sqrt{n^2}\,\langle n|n\rangle + \sqrt{(n+1)(n+2)}\,\langle n|n+2\rangle\right]$$
$$= \frac{m\omega\hbar}{2}(2n+1)$$

c) * In general, the RMS value of an operator is defined by $\langle(\Delta A)^2\rangle = \langle A^2\rangle - \langle A\rangle^2$

$$\Rightarrow \langle(\Delta x)^2\rangle = \langle x^2\rangle - \langle x\rangle^2 = \frac{\hbar}{2m\omega}(2n+1) \qquad \langle(\Delta p)^2\rangle = \langle p^2\rangle - \langle p\rangle^2 = \frac{m\omega\hbar}{2}(2n+1)$$

#1 (cont.)

d) $\sqrt{\langle(\Delta x^2)\rangle\langle(\Delta p)^2\rangle} = \sqrt{\frac{\hbar}{2m\omega}(2n+1)\frac{m\omega\hbar}{2}(2n+1)}$

$= \frac{\hbar}{2}(2n+1)$

e) $T = \frac{p^2}{2m}$

$\langle T\rangle = \langle \frac{p^2}{2m}\rangle$

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

$= \frac{\hbar\omega}{4}(2n+1)$

$V = \frac{1}{2}m\omega^2x^2$

$\langle V\rangle = \langle \frac{1}{2}m\omega^2x^2\rangle$

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

$= \frac{\hbar\omega}{4}(2n+1)$

4?

Problem 2: Variational Method (10 Points)

The Hamiltonian of a one-dimensional harmonic oscillator is

$$H = \frac{P^2}{2m} + \frac{m\omega^2 X^2}{2} .$$

The ground state energy is $E_0 = \hbar\omega/2$.

Let us employ the variational method with the following trial function as the ground-state wave function

$$\langle x|\psi\rangle = \psi(x) = Ne^{-\beta|x|} .$$

a. Determine the constant N by applying the normalization condition. (2 points)

b. Find the value of β that minimizes $\langle\psi|H|\psi\rangle$. (2 points)

c. What is the ground-state energy calculated with the variational method? (5 points)
N.B. *The derivative of the trial function has a discontinuity.*

d. How close do you get to the true ground-state energy? (1 points)

Jan 2017

Quantum #2

a) The normalization condition is: $1 = \int_{-\infty}^{\infty} |\psi|^2 dx$

$$\Rightarrow 1 = N^2 \int_{-\infty}^{\infty} e^{-2\beta|x|}$$

$$1 = N^2 \left[\int_{-\infty}^{0} e^{2\beta x} dx + \int_{0}^{\infty} e^{-2\beta x} dx \right]$$

$$1 = N^2 \left[\frac{1}{2\beta} e^{2\beta x} \Big|_{-\infty}^{0} + \frac{-1}{2\beta} e^{-2\beta x} \Big|_{0}^{+\infty} \right]$$

$$1 = N^2 \left[\frac{1}{2\beta} \left(\cancel{e^{2\beta(0)}}^{1} - \cancel{e^{2\beta(-\infty)}}^{0} - \cancel{e^{-2\beta(\infty)}}^{0} + \cancel{e^{-2\beta(0)}}^{1} \right) \right]$$

$$1 = N^2 \frac{1}{2\beta} (2)$$

$$1 = \frac{N^2}{\beta} \Rightarrow N = \sqrt{\beta}$$

b) $\langle \psi | H | \psi \rangle = \langle \psi | x' \rangle \langle x' | H | x \rangle \langle x | \psi \rangle$

$$= \int dx' \int dx \; \psi^*(x') H \psi(x)$$

$$= \int dx' \int dx \; \psi^*(x') \left[\frac{p^2}{2m} + \frac{m\omega^2 x^2}{2} \right] \psi(x)$$

$$= \int dx' \int dx \; \psi^*(x') \left[\frac{1}{2m} \left(-i\hbar \frac{\partial}{\partial x} \delta(x-x')\right)^2 + \frac{m\omega^2}{2} x^2 \delta(x-x') \right] \psi(x)$$

$$= \int_{-\infty}^{\infty} dx \; \psi^*(x) \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{m\omega^2}{2} x^2 \right] \psi(x)$$

* minimum occurs when $\frac{d}{d\beta} \langle \psi | H | \psi \rangle = 0$

$$0 = \frac{d}{d\beta} \int_{-\infty}^{\infty} \frac{1}{\sqrt{\beta}} e^{-\beta|x|} \left[\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{m\omega^2}{2} x^2 \right] \frac{1}{\sqrt{\beta}} e^{-\beta|x|} dx$$

$$= \frac{d}{d\beta} \int_{-\infty}^{\infty} \frac{1}{\beta} e^{\beta x} \left[\frac{-\hbar^2 \beta^2}{2m} e^{\beta x} + \frac{m\omega^2}{2} x^2 \right] e^{\beta x} dx + \int_{0}^{\infty} \frac{1}{\beta} e^{-\beta x} \left[\frac{-\hbar^2 \beta^2}{2m} e^{-\beta x} + \frac{m\omega^2}{2} x^2 e^{-\beta x} \right] dx$$

$$= \frac{d}{d\beta} \int_{-\infty}^{0} \frac{-\hbar^2 \beta}{2m} e^{2\beta x} + \frac{m\omega^2 x^2}{2\beta} e^{2\beta x} dx + \int_{0}^{\infty} \frac{-\hbar^2 \beta}{2m} e^{-2\beta x} + \frac{m\omega^2 x^2}{2\beta} e^{-2\beta x} dx$$

$$= \frac{d}{d\beta} \left[\frac{-\hbar^2}{4m} e^{2\beta x} \Big|_{-\infty}^{0} + \frac{m\omega^2}{2} \frac{1}{4\beta^4} + \frac{\hbar^2}{2m} \cdot \frac{1}{2} e^{-2\beta x} \Big|_{0}^{\infty} + \frac{m\omega^2}{2} \frac{1}{4\beta^4} \right.$$

$$= \frac{d}{d\beta} \left[\frac{-\hbar^2}{4m} + \frac{m\omega^2}{8\beta^4} - \frac{\hbar^2}{4m} + \frac{m\omega^2}{8\beta} \right]$$

$$= \frac{d}{d\beta} \left[\frac{-\hbar^2}{2m} + \frac{m\omega^2}{4\beta^4} \right]$$

#2 (cont.)

b) $0 = \frac{-m\omega^2}{\beta^5}$

Problem 3: Angular Momentum Hamiltonian (10 points)

Consider the following Hamiltonian for a spinless particle with orbital angular momentum ℓ=2.

$$\hat{H} = \frac{3a}{2\hbar}\hat{L}_z - \frac{a}{\hbar^2}(\hat{L}_x^2 + \hat{L}_y^2)$$

where a is a constant greater than 0 and $\hat{L}_i$ denotes the i^{th} component of the angular momentum operator.

✓ a) Calculate the energy spectrum of this Hamiltonian (2 pts)

b) Suppose a particle with this Hamiltonian has the wavefunction

$$\Psi(\theta, \phi) = A(\sin\theta\cos\theta\cos\phi + \sin^2\theta\sin\phi\cos\phi)$$

where θ is the polar angle, ϕ is the azimuthal angle, and A is a normalization constant. What is the average energy obtained in energy measurements on an ensemble of particles described by the wavefunction above? (3 pts)

c) Assume the particle is in the lowest energy state (with ℓ=2) for $t < 0$. Starting at t=0, an external magnetic field is applied with

$$\hat{V}(t) = \frac{\lambda}{\hbar}\hat{L}_x e^{-t/\tau}$$

where τ is the decay constant and λ is a constant. Calculate the transition probabilities to possible excited states after a very long time ($\tau \ll t \to \infty$) using first order time-dependent perturbation theory. (5 pts)

Jan 2017

Quantum #3

a) We know that we can write simultaneous eigenkets of L^2, L_z as $|l,m\rangle$ in systems where angular momentum is under investigation

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

$$L_\pm = L_x \pm iL_y$$

$$\Rightarrow H = \frac{3a}{2\hbar} L_z - \frac{a}{\hbar^2}(L_x^2 + L_y^2)$$
$$= \frac{3a}{2\hbar} L_z - \frac{a}{\hbar^2}(L^2 - L_z^2)$$

* We know that $H|l,m\rangle = E|l,m\rangle$

$$\hookrightarrow \frac{3a}{2\hbar} L_z - \frac{a}{\hbar^2}(L^2 - L_z^2)|l,m\rangle = \frac{3a}{2\hbar} m - \frac{a}{\hbar^2}\left(l(l+1) - m^2\right)|l,m\rangle$$

$$\Rightarrow E = \frac{3am}{2\hbar} - \frac{a^2}{\hbar^2}\left(l(l+1) - m^2\right)$$

b) $\Psi(\theta,\varphi) = A(\sin\theta\cos\theta\cos\varphi + \sin^2\theta\sin\varphi\cos\varphi)$

$$\hookrightarrow Y_{2,\pm1}(\theta,\varphi) = \mp\sqrt{\tfrac{15}{8\pi}}\, e^{\pm i\varphi}\cos\theta\sin\theta = \mp\sqrt{\tfrac{15}{8\pi}}(\cos\varphi \pm i\sin\varphi)\cos\theta\sin\theta$$

$$Y_{2,\pm2}(\theta,\varphi) = \sqrt{\tfrac{15}{32\pi}}\, e^{\pm 2i\varphi}\sin^2\theta = \sqrt{\tfrac{15}{32\pi}}(\cos 2\varphi \pm i\sin 2\varphi)\sin^2\theta$$

* From wolfram, $\int d\theta d\varphi\, |\Psi|^2 = \frac{7\pi^2 A^2}{32} = 1 \Rightarrow A = \sqrt{\frac{32}{7\pi^2}}$

* Notice that: $Y_{2,-1} - Y_{2,+1} = 2\sqrt{\tfrac{15}{8\pi}}\cos\theta\sin\theta\cos\varphi$

$$Y_{2,+2} - Y_{2,-2} = 2i\sqrt{\tfrac{15}{8\pi}}\sin^2\theta\sin\varphi\cos\varphi$$

$$\Rightarrow \Psi,\theta,\varphi) = \langle r,\theta,\varphi| \left(\tfrac{1}{2}\sqrt{\tfrac{8\pi}{15}}\left[|2,-1\rangle - |2,1\rangle\right] + \tfrac{1}{2i}\sqrt{\tfrac{8\pi}{15}}\left[|2,+2\rangle - |2,-2\rangle\right]\right)$$

$$\hookrightarrow \langle\Psi|H|\Psi\rangle = \left(\tfrac{1}{2}\sqrt{\tfrac{8\pi}{15}}\right)^2\left[\langle 2,-1| - \langle 2,1| + i\langle 2,2| - i\langle 2,-2|\right] H \left[|2,-1\rangle - |2,1\rangle - i|2,2\rangle + i|2,-2\rangle\right]$$

$$= \left(\tfrac{1}{2}\sqrt{\tfrac{8\pi}{15}}\right)^2\left[\langle 2,-1|H|2,-1\rangle - \langle 2,1|H|2,1\rangle + \langle 2,2|H|2,2\rangle + \langle 2,-2|H|2,-2\rangle\right]$$

* All other terms 0 by orthogonality of spherical harmonics as kets are unaltered by Hamiltonian

3 (cont.)

b) $$\langle \Phi | H | \Phi \rangle = \left(\frac{1}{2}\sqrt{\frac{8\pi}{15}}\right)^2 \left[\left(\cancel{\frac{3a}{2\hbar}} - \cancel{\frac{a}{\hbar^2}[6+1]} \right) - \left(\cancel{\frac{3a}{2\hbar}} - \cancel{\frac{a}{\hbar^2}[6+1]} \right) + \left(\cancel{\frac{6a}{2\hbar}} - \frac{a}{\hbar^2}[6+4] \right) + \frac{6a}{2\hbar} - \frac{a}{\hbar^2}[6+4] \right]$$

$$= \left(\frac{1}{2}\sqrt{\frac{8\pi}{15}}\right)^2 \left[\frac{6a}{2\hbar} - \frac{20a}{\hbar^2} \right]$$

$$= \frac{8\pi}{60}\left(\frac{6a}{2\hbar} - \frac{20a}{\hbar^2} \right)$$

c) First order time dependant perturbation theory (for two states) says:

Problem 4: Hydrogen Atom (10 points)

Schrodinger's equation in spherical coordinates where the potential is only a function of r can be solved by using separation of variables: $\Psi(r,\theta,\phi)=R(r)Y(\theta,\phi)$.

✓ a) In units $2m = 1$ and $\hbar=1$, show that using the change of variables $u(r) \equiv rR(r)$, one can obtain the radial Schrodinger's equation for the hydrogen atom. (1 pt)

$$[-\frac{d^2}{dr^2} - \frac{g^2}{r} + \frac{\ell(\ell+1)}{r^2}]u(r) = \epsilon u(r)$$

where g^2 is the Coulomb strength and ϵ is the energy.

b) The lowest eigenstate of a given ℓ is known to have the form

$$u_\ell^0 = C_\ell r^{\ell+1} exp(-r/a_\ell)$$

For a given ℓ, determine the eigenvalue ϵ_ℓ^0 and the size parameter a_ℓ, in terms of g^2 (2 pts).

Consider that the initial 3-dimensional wave function at time t=0 is a superposition of the above states

$$\Psi(r,0) = D(e^{-g^2\frac{r}{2}} + g^2 r e^{-g^2\frac{r}{4}}\cos\theta)$$

c) Determine $\Psi(r,t)$ (1 pt)

d) Determine $\langle\cos\theta\rangle$ as a function of time (3 pts).

e) Consider the hydrogen atom. Determine the most probable value of r for the ground state. (1 pt)

f) Consider a hydrogen atom placed in a weak constant uniform external electric field. Determine how the energy levels shift for the n=2 state of hydrogen due to the electric field. (2 pts)

Jan 2017

Quantum #4

a)

Problem 5: 1/x potential (10 points)

An electron moves in one dimension and is confined to the right half space (x > 0) where it has potential energy

$$V(x) = -\frac{e^2}{4x}$$

where e is the charge on an electron.

a) What is the solution of Schrodinger's equation at large x? (2 pts)

b) What are the necessary boundary conditions (1 pt)

c) Using the results of part a) and b), determine the ground state solution of the equation. (3 pts)

d) Determine the ground state energy (2 pts)

e) Find the expectation value $\langle x \rangle$ in the ground state (2 pts)

Problem 6: Measurements and Probability (10 points)

A three-level quantum system has a non-degenerate ground state and a two-fold degenerate excited state, defined by:

$$H|0\rangle = 0\ , \qquad H|a\rangle = \epsilon|a\rangle\ , \qquad H|b\rangle = \epsilon|b\rangle$$

where ϵ is a positive constant energy.

(a) (1 pt) Write down the matrix representation of H in the basis $|0\rangle$, $|a\rangle$, $|b\rangle$.

(b) (2 pts.) Define the observable C by its operation on the eigenstates of H.

$$C|0\rangle = \gamma|a\rangle\ , \quad C|a\rangle = \gamma|0\rangle\ , \quad C|b\rangle = -\gamma|b\rangle \tag{3}$$

$\gamma > 0$. What are all the possible outcomes of a measurement of C?

(c) (2 pts.) For each of the eigenstates of H, calculate the probability of measuring the different possible values for C if the system is in that eigenstate.

(d) (1 pts.) Do H and C have common eigenstates? Are H and C compatible observables? Explain.

(e) (2 pts.) At time $t = 0$, the system is in the eigenstate of C with the largest eigenvalue. Calculate the probabilities, as functions of time, of obtaining the different possible results of a measurement of C.

(f) (2 pt.) At time $t = 0$, the system is in the state $|\psi\rangle = \frac{1}{\sqrt{2}}\left(|a\rangle + |b\rangle\right)$. Calculate the probabilities, as functions of time, of obtaining the different possible results of a measurement of C. Explain the differences in this result and what was found in part (e).

Jan 2017

Quantum #6

a) $$H \doteq \begin{array}{c|ccc} & |0\rangle & |a\rangle & |b\rangle \\ \hline \langle 0| & 0 & 0 & 0 \\ \langle a| & 0 & \epsilon & 0 \\ \langle b| & 0 & 0 & \epsilon \end{array}$$

b) $$C \doteq \begin{bmatrix} 0 & \gamma & 0 \\ \gamma & 0 & 0 \\ 0 & 0 & -\gamma \end{bmatrix} \qquad C - \lambda \mathbb{I} = \begin{bmatrix} -\lambda & \gamma & 0 \\ \gamma & -\lambda & 0 \\ 0 & 0 & -\gamma-\lambda \end{bmatrix}$$

* Reading the question as asking us to determine the eigenvalues of C

$$|C - \lambda \mathbb{I}| = 0 = -\lambda(-\lambda(-\lambda-\gamma)-0) - \gamma(\gamma(-\gamma-\lambda)-0)$$

$$= -\lambda^2(\lambda+\gamma) + \gamma^2(\lambda+\gamma)$$

$$\doteq (\lambda+\gamma)(\gamma^2-\lambda^2)$$

$$\hookrightarrow \boxed{\lambda = -\gamma, -\gamma, +\gamma}$$

c) * To do this, we must rewrite eigenstates of H in the eigenbasis of C

$$C\vec{x} = \lambda\vec{x}$$

$$\begin{bmatrix} 0 & \gamma & 0 \\ \gamma & 0 & 0 \\ 0 & 0 & -\gamma \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \lambda\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad \begin{aligned} \gamma x_2 &= \lambda x_1 \\ \gamma x_1 &= \lambda x_2 \\ -\gamma x_3 &= \lambda x_3 \end{aligned}$$

* for $\lambda = \gamma$

$$\gamma x_2 = \gamma x_1$$
$$\gamma x_1 = \gamma x_2$$
$$-\gamma x_3 = \gamma x_3$$

$$\Rightarrow \vec{x} = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} \cdot \frac{1}{\sqrt{2}}$$

$$= |\lambda_c = \gamma\rangle$$

* for $\lambda = -\gamma$

$$\gamma x_2 = -\gamma x_1$$
$$\gamma x_1 = -\gamma x_2$$
$$-\gamma x_3 = -\gamma x_3$$

$$\vec{x} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \text{ or } \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix} \frac{1}{\sqrt{2}}$$

$$= |\lambda_c = -\gamma, 1\rangle \text{ or } |\lambda_c = -\gamma, 2\rangle$$

#6 (cont.)

c) $\Rightarrow$ $|0\rangle = \frac{1}{\sqrt{2}}\left[|\lambda_c = \gamma\rangle + |\lambda_c = -\gamma, 2\rangle\right]$ $P(\gamma) = \frac{1}{2}$ $P(-\gamma) = \frac{1}{2}$

$|a\rangle = \frac{1}{\sqrt{2}}\left[|\lambda_c = \gamma\rangle - |\lambda_c = -\gamma, 2\rangle\right]$ $P(\gamma) = \frac{1}{2}$ $P(-\gamma) = \frac{1}{2}$

$|b\rangle = |\lambda_c = -\gamma, 1\rangle$ $P(\gamma) = 0$ $P(-\gamma) = 1$

d) No, H and C are not compatible b/c they do not share an eigenbasis

e) $|\psi(t=0)\rangle = |\lambda_c = \gamma\rangle$

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

$\hookrightarrow$ $|\psi(t)\rangle = \exp\left[-\frac{i}{\hbar}Ht\right]|\lambda_c = \gamma\rangle$

$= \exp\left[-\frac{i}{\hbar}Ht\right]\left(\frac{1}{\sqrt{2}}\left[|0\rangle + |a\rangle\right]\right)$

$= \frac{1}{\sqrt{2}}\left[|0\rangle + e^{-i\epsilon t/\hbar}|a\rangle\right]$

$= \frac{1}{2}\left[|\lambda_c = \gamma\rangle + |\lambda_c = -\gamma, 2\rangle + e^{-i\epsilon t/\hbar}\left(|\lambda_c = \gamma\rangle - |\lambda_c = -\gamma, 2\rangle\right)\right]$

$= \frac{1}{2}\left[\left(1 + e^{-i\epsilon t/\hbar}\right)|\lambda_c = \gamma\rangle + \left(1 - e^{-i\epsilon t/\hbar}\right)|\lambda_c = -\gamma, 2\rangle\right]$

$P(\gamma) = \frac{1}{4}\left|1 + e^{-i\epsilon t/\hbar}\right|^2$

$= \frac{1}{4}\left(1 + e^{-i\epsilon t/\hbar} + e^{i\epsilon t/\hbar} + 1\right)$

$= \frac{1}{4}\left(2 + 2\cos\left(\frac{\epsilon t}{\hbar}\right)\right)$

$= \frac{1}{2} + \frac{1}{2}\cos\left(\frac{\epsilon t}{\hbar}\right)$

$P(-\gamma) = \frac{1}{4}\left|1 - e^{-i\epsilon t/\hbar}\right|^2$

$= \frac{1}{4}\left(1 - e^{-i\epsilon t/\hbar} - e^{i\epsilon t/\hbar} + 1\right)$

$= \frac{1}{4}\left(2 - 2\cos\left(\frac{\epsilon t}{\hbar}\right)\right)$

$= \frac{1}{2} - \frac{1}{2}\cos\left(\frac{\epsilon t}{\hbar}\right)$

f) $|\psi(t=0)\rangle = \frac{1}{\sqrt{2}}\left(|a\rangle + |b\rangle\right)$

$|\psi(t)\rangle = \frac{1}{\sqrt{2}}e^{-iHt/\hbar}\left(|a\rangle + |b\rangle\right)$

$= \frac{1}{\sqrt{2}}e^{-i\epsilon t/\hbar}\left(|a\rangle + |b\rangle\right)$

$= \frac{1}{\sqrt{2}}e^{-i\epsilon t/\hbar}\left(\frac{1}{\sqrt{2}}\left[|\lambda_c = \gamma\rangle - |\lambda_c = -\gamma, 2\rangle\right]\right) + \frac{1}{\sqrt{2}}e^{-i\epsilon t/\hbar}|\lambda_c = -\gamma, 1\rangle$

#6 (cont)

f) $P(\gamma) = \left|\frac{1}{2}e^{-i\epsilon t/\hbar}\right|^2$

$= \frac{1}{4}$

$P(-\gamma) = \left|\frac{1}{2}e^{-i\epsilon t/\hbar}\right|^2 + \left|\frac{1}{\sqrt{2}}e^{-i\epsilon t/\hbar}\right|^2$

$= \frac{1}{4} + \frac{1}{2}$

$= 3/4$

$\Rightarrow$ In this case, we have probabilities that are not time dependent.

Quantum Mechanics
Qualifying Exam - August 2017

Notes and Instructions

- There are 6 problems. Attempt them all as partial credit will be given.
- 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

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

In spherical coordinates,

$$\frac{1}{r^2}\left(\frac{\partial}{\partial r} r^2 \frac{\partial \psi}{\partial r}\right)$$

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

Harmonic oscillator wave functions

$$u_0(x) = (\tfrac{m\omega}{\pi\hbar})^{1/4} e^{-\frac{m\omega x^2}{2\hbar}}$$

$$u_1(x) = (\tfrac{m\omega}{\pi\hbar})^{1/4}\sqrt{\tfrac{2m\omega}{\hbar}}\, x e^{-\frac{m\omega x^2}{2\hbar}}$$

Spherical Harmonics:

$$Y_{0,0}(\theta,\phi) = \tfrac{1}{\sqrt{4\pi}}$$

$$Y_{1,0}(\theta,\phi) = \sqrt{\tfrac{3}{4\pi}}\cos\theta$$

$$Y_{1,\pm1}(\theta,\phi) = \mp\sqrt{\tfrac{3}{8\pi}} e^{\pm i\phi}\sin\theta$$

$$Y_{2,0}(\theta,\phi) = \sqrt{\tfrac{5}{16\pi}}(3\cos^2\theta - 1)$$

$$Y_{2,\pm1}(\theta,\phi) = \mp\sqrt{\tfrac{15}{8\pi}} e^{\pm i\phi}\cos\theta\sin\theta$$

$$Y_{2,\pm2}(\theta,\phi) = \sqrt{\tfrac{15}{32\pi}} e^{\pm 2i\phi}\sin^2\theta$$

Problem 1: Periodic Perturbation (10 Points):

Consider a two-level system under a periodic perturbation, $V(t) = V_0 e^{i\omega t}$, where V_0 is real. Take the time dependent amplitude for the lower state $|a\rangle$ to be $a(t)$ and the upper state $|b\rangle$ to be $b(t)$. Take the energy of the upper level to be at $\hbar\omega_0$ and the lower level to be at 0.

a. Find differential equations for the time-dependent probability amplitudes to be in the upper state $b(t)$ and the amplitude to be in the lower state $a(t)$. **(3 Points)**

b. Solve the equations you obtained in (a.) for the initial conditions $a(0) = 1$ and $b(0) = 0$. These initial conditions correspond to the system starting in the ground state. Take $\Delta = \omega - \omega_0 = 0$. Use the following unitary transformation to simplify the Hamiltonian you used in (a.) to solve for the time dependent wavefunction:

$$U = \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\omega t} \end{pmatrix}$$

(3 Points)

c. Using your result in (b.) find the probability for the system to be in $|b\rangle$. **(2 Points)**

d. Sketch the probability as a function of time that you found in (c.) and interpret the result. **(2 Points)**

Problem 2: WKB approximation (10 Points):

The one-dimensional Schrodinger equation,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

can be rewritten as

$$\frac{d^2\psi}{dx^2} = -\frac{p^2}{\cancel{2m}\ \hbar^2}\psi\,,$$

where

$$p(x) \equiv \sqrt{2m[E - V(x)]}\,.$$

The wave function $\psi(x)$ is often expressed as $\psi(x) = A(x)e^{i\phi(x)}$ where $A(x)$ is the amplitude and $\phi(x)$ is the phase. Both $A(x)$ and $\phi(x)$ can be real.

(a) Show that the amplitude is $A = \frac{C}{\sqrt{\phi'}}$ where C is a constant and prime is the derivative with respect to x. (2 points)

(b) (3 points) Let us assume that $A''/A \ll (\phi')^2$ and $A''/A \ll p^2/\hbar^2$. Show that the wave function in the WKB approximation is

$$\psi(x) \simeq \frac{C}{\sqrt{p(x)}} e^{\pm\frac{i}{\hbar}\int p(x)dx}\,.$$

In parts (c)–(e), the potential energy of the one-dimensional harmonic oscillator is

$$V(x) = \frac{1}{2}m\omega^2x^2\,.$$

(c) Find the classical turning points $x_1 < x_2$ for an energy E. (1 points)

(d) Evaluate the phase ϕ in terms of E and ω with the WKB method. (3 points)

(e) Apply the eigenvalue condition $\phi = \left(n + \frac{1}{2}\right)\pi\hbar$ and find energy eigenvalues E_n. (1 points)

Aug 2017

Quantum #2

a) To show $A = \frac{c}{\sqrt{\varphi'}}$, assuming $\psi(x) = A(x)e^{i\varphi(x)}$, we substitute ψ into the rewritten Schrödinger eqn: $\frac{d^2\psi}{dx^2} = \frac{-p^2}{\hbar^2}\psi$, $p = \sqrt{2m(E-V(x))}$

$$\hookrightarrow \frac{d\psi}{dx} = A'e^{i\varphi(x)} + Ai\varphi' e^{i\varphi(x)}$$

$$\frac{d^2\psi}{dx^2} = A''e^{i\varphi(x)} + iA'\varphi' e^{i\varphi(x)} + iA'\varphi' e^{i\varphi(x)} + iA\varphi'' e^{i\varphi(x)} - A(\varphi')^2 e^{i\varphi(x)}$$

$$e^{i\varphi(x)} \cdot \left[A'' - A(\varphi')^2 + i\left[2A'\varphi' + A\varphi''\right]\right] = \frac{-p^2}{\hbar^2}A(x)e^{i\varphi(x)}$$

Real: $\frac{-p^2}{\hbar^2}A = A'' - A(\varphi')^2$

Imaginary: $0 = 2A'\varphi' + A\varphi''$

$$0 = \frac{d}{dx}(A^2\varphi')$$

$$\boxed{\begin{array}{l} \frac{d}{dx}(A^2\varphi') = 2AA'\varphi' + A^2\varphi'' = 0 \\ \text{*divide by } A \\ 2A'\varphi' + A\varphi'' = 0 \end{array}}$$

$$\hookrightarrow c^2 = A^2\varphi'$$

$$\hookrightarrow A = \frac{c}{\sqrt{\varphi'}} \checkmark$$

b) Assuming $A''/A \ll (\varphi')^2$ and $A''/A \ll p^2/\hbar^2$, we can now use the real equation from part A to show $\psi(x) \approx \frac{C}{\sqrt{p(x)}} e^{\pm\frac{i}{\hbar}\int p(x)dx}$

$$\frac{-p^2}{\hbar^2}A = A'' - A(\varphi')^2$$

$$\frac{p^2}{\hbar^2}\frac{\cancel{c}}{\cancel{\sqrt{\varphi'}}} = \frac{\cancel{c}}{\cancel{\sqrt{\varphi'}}}(\varphi')^2$$

$$\varphi' = \pm\frac{p}{\hbar} \Rightarrow \varphi = \pm\frac{1}{\hbar}\int_0^x p(x)dx$$

$$\hookrightarrow \psi(x) = Ae^{i\varphi(x)}$$

$$= \frac{C}{\sqrt{\varphi'}}\exp\left[\frac{\pm i}{\hbar}\int p(x)dx\right]$$

#2 (cont.)

c) The classical turning points occur when $E = V(x)$

$\hookrightarrow E = \frac{1}{2} m \omega^2 x^2$

$\hookrightarrow x = \pm \sqrt{\frac{2E}{m}}\,\omega$

d) Note: In the region where $E < V$, $p(x)$ is imaginary
$E > V$, $p(x)$ is real
$E = V$ $p(x)$ is 0

* If $p(x) = 0$, $\varphi(x) = 0$

* If $p(x)$ is real $(E < V)$

$$\varphi(x) = \int_{x_1}^{x_2} p(x)\,dx$$

$$= \int_{x_1}^{x_2} \left[2m \left(E - \tfrac{1}{2} m\omega^2 x^2\right)\right]^{1/2} dx$$

$$= \int_{x_1}^{x_2} \left(2mE - m^2\omega^2 x^2\right)^{1/2} dx$$

*let $a = \sqrt{2mE}$, $u = m\omega x$

$$= \int_{x_1}^{0} \sqrt{a^2 - u^2}\, \frac{du}{m\omega} + \int_{0}^{x_2} \sqrt{a^2 - u^2}\, du/m\omega$$

$$= \int_{0}^{x_2} \frac{1}{m\omega} \sqrt{a^2 - u^2}\, du - \int_{0}^{x_1} \frac{1}{m\omega} \sqrt{a^2 - u^2}\, du$$

$$= \frac{1}{m\omega}\left[\frac{\pi x_2^2}{4} - \frac{\pi x_1^2}{4} \right]$$

$$= \frac{\pi}{4m\omega}\left[x_2^2 - x_1^2 \right]$$

$$= \frac{\pi}{4m\omega^2}$$

See Griffiths QM
ex. 8.4

$\frac{1}{2}[1 \quad 1]\begin{bmatrix}1\\-1\end{bmatrix} = 0 \qquad \frac{1}{10}[1 \quad 3]\begin{bmatrix}1\\-3\end{bmatrix} = \frac{-8}{10} \neq 1$

$[-3 \quad 1]\begin{bmatrix}1\\3\end{bmatrix} = 0$

Problem 3: Two-State Problem (10 Points):

Consider a two-state quantum system. In the orthonormal and complete set of basis vectors $|1\rangle$ and $|2\rangle$, the Hamiltonian operator for the system is represented by ($\omega > 0$)

$$\hat{H} = 10\hbar\omega|1\rangle\langle 1| - 3\hbar\omega|1\rangle\langle 2| - 3\hbar\omega|2\rangle\langle 1| + 2\hbar\omega|2\rangle\langle 2|$$

7

Consider another complete and orthonormal basis $|\alpha\rangle$, $|\beta\rangle$, such that $\hat{H}|\alpha\rangle = E_1|\alpha\rangle$, and $\hat{H}|\beta\rangle = E_2|\beta\rangle$ (with $E_1 < E_2$). Let the action of operator $\hat{A}$ on the $|\alpha\rangle$, $|\beta\rangle$ basis vectors be given as

$$\hat{A}|\alpha\rangle = 2ia_0|\beta\rangle$$
$$\hat{A}|\beta\rangle = -2ia_0|\alpha\rangle - 3a_0|\beta\rangle$$

where $a_0 > 0$ is real.

✓a) Find the eigenvalues and eigenvectors of H in the $|1\rangle, |2\rangle$ basis (1 pt).

✓b) Find the eigenvalues and eigenvectors of $\hat{A}$ in the $|\alpha\rangle, |\beta\rangle$ basis (1 pt).

Suppose a measurement of $\hat{A}$ is carried out at t=0 on an arbitrary state and the largest possible value is obtained.

✓c) Calculate the probability P(t) that another measurement made at time t will yield the value as the one measured at t=0. (2 pts)

✓d) Calculate the time dependence of the expectation value $\langle\hat{A}\rangle$. What is the minimum value of $\langle\hat{A}\rangle$? At what time is the minimum value first achieved? (3 pts)

Now suppose that the average value obtained from a large number of measurements of $\hat{A}$ on identical quantum systems at a given time is -$a_0/4$.

e) (3 pts) Construct the most general normalized state vector (just before the measurement of $\hat{A}$) for your system consistent with this information in Dirac notation using the $|\alpha\rangle$, $|\beta\rangle$ basis. Express your answer as

$$|\Psi\rangle = C|\alpha\rangle + D|\beta\rangle$$

$[1 \quad \frac{-i}{2}]\begin{bmatrix}1\\-\frac{2}{i}\end{bmatrix}$

$1 \cdot 1 + \frac{-i}{2} \cdot \frac{-2}{i}$

$[1 \quad \frac{1}{2i}]\begin{bmatrix}1\\-\frac{2}{i}\end{bmatrix}$

$1 \cdot 1 + \frac{1}{2i} \cdot \frac{-2}{i} = \frac{-1}{i^2}$

$1 \cdot 1 + (2i)(-2i)$

$1 + 4(-i^2) =$

Aug 2017 <u>Quantum #3</u>

a) $H = 10\hbar\omega\,|1\rangle\langle 1| - 3\hbar\omega\,|1\rangle\langle 2| - 3\hbar\omega\,|2\rangle\langle 1| + 2\hbar\omega\,|2\rangle\langle 2|$

$$\doteq \begin{array}{c c} & \begin{array}{cc} |1\rangle & |2\rangle \end{array} \\ \begin{array}{c} \langle 1| \\ \langle 2| \end{array} & \begin{bmatrix} 10\hbar\omega & -3\hbar\omega \\ -3\hbar\omega & 2\hbar\omega \end{bmatrix} \end{array}$$

Using the eigenvalue equation $\det(H - \lambda \mathbb{I}) = 0$

$$\begin{vmatrix} 10\hbar\omega - \lambda & -3\hbar\omega \\ -3\hbar\omega & 2\hbar\omega - \lambda \end{vmatrix} = 0 = (10\hbar\omega - \lambda)(2\hbar\omega - \lambda) - (-3\hbar\omega)^2$$

$$= 20\hbar^2\omega^2 - 12\hbar\omega\lambda + \lambda^2 - 9\hbar^2\omega^2$$

$$= \lambda^2 - 12\hbar\omega\lambda + 11\hbar^2\omega^2$$

$$= (\lambda - \hbar\omega)(\lambda - 11\hbar\omega)$$

$\hookrightarrow \lambda_1 = \hbar\omega$

$\lambda_2 = 11\hbar\omega$

Using the eigenvector equation $H\vec{a} = \lambda\vec{a}$

$$\begin{bmatrix} 10\hbar\omega & -3\hbar\omega \\ -3\hbar\omega & 2\hbar\omega \end{bmatrix}\begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \lambda\begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \Rightarrow \begin{array}{l} 10\hbar\omega a_1 - 3\hbar\omega a_2 = \lambda a_1 \\ -3\hbar\omega a_1 + 2\hbar\omega a_2 = \lambda a_2 \end{array}$$

* if $\lambda = \hbar\omega$

$10a_1 - 3a_2 = a_1$

$-3a_1 + 2a_2 = a_2$

$\hookrightarrow a_1 = \frac{1}{3}a_2$

$|\lambda = \hbar\omega\rangle = \langle 1, 3\rangle \frac{1}{\sqrt{10}}$

* if $\lambda = 11\hbar\omega$

$10a_1 - 3a_2 = 11a_1$

$-3a_1 + 2a_2 = 11a_2$

$\hookrightarrow -3a_2 = a_1$

$|\lambda = 11\hbar\omega\rangle = \langle -3, 1\rangle \cdot \frac{1}{\sqrt{10}}$

* Dot product verifies orthogonality $\frac{1}{10}(1\cdot -3 + 3\cdot 1) = 0$

b) $A|\alpha\rangle = 2ia_0|\beta\rangle$

$A|\beta\rangle = -2ia_0|\alpha\rangle - 3a_0|\beta\rangle$

$$\Rightarrow A \doteq \begin{bmatrix} 0 & 2ia_0 \\ -2ia_0 & -3a_0 \end{bmatrix}$$

#3 (cont.)

b) Similarly to part a:

$$\begin{vmatrix} 0-\lambda & 2ia_0 \\ -2ia_0 & -3a_0-\lambda \end{vmatrix} = 0 = -\lambda(-3a_0-\lambda) - (2ia_0)(-2ia_0)$$

$$= \lambda^2 + 3a_0\lambda - 4a_0^2$$

$$= (\lambda+4a_0)(\lambda-a_0)$$

$$\Rightarrow \lambda = -4a_0, +a_0$$

Using the eigenvector equation:

$$\begin{bmatrix} 0 & 2ia_0 \\ -2ia_0 & -3a_0 \end{bmatrix}\begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \lambda\begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \Rightarrow \begin{matrix} 2ia_0a_2 = \lambda a_1 \\ -2ia_0a_1 - 3a_0a_2 = \lambda a_2 \end{matrix}$$

* if $\lambda = 4a_0$

$2ia_0a_2 = -4a_0a_1$

$-2ia_0a_1 - 3a_0a_2 = -4a_0a_2$

$\hookrightarrow \quad ia_2 = -2a_1$

$-2ia_1 = -a_2$

$\Rightarrow |\lambda = -4a_0\rangle = \langle -i, 2\rangle$

* if $\lambda = a_0$

$2ia_0a_2 = a_0a_1$

$-2ia_0a_1 - 3a_0a_2 = a_0a_2$

$\hookrightarrow \quad 2ia_2 = a_1$

$-ia_1 = 2a_2$

$\Rightarrow |\lambda = a_0\rangle = \langle 2i, 1\rangle$

c) To obtain the largest possible value of A at $t=0$, $|\psi\rangle = |\lambda = a_0\rangle$

But since $U(t,t_0) = \exp[-iHt/\hbar]$, we must convert $|\lambda = a_0\rangle$ to the basis of the Hamiltonian.

$|\lambda_A = a_0\rangle = \frac{1}{\sqrt{5}}\langle 2i, 1\rangle$

Hamiltonian basis vectors: $|\lambda_H = \hbar\omega\rangle = \frac{1}{\sqrt{10}}\langle 1, 3\rangle$

$|\lambda_H = 11\hbar\omega\rangle = \frac{1}{\sqrt{10}}\langle -3, 1\rangle$

$$\frac{2i}{\sqrt{5}} = a\frac{1}{\sqrt{10}} + b\frac{-3}{\sqrt{10}}$$

$$\frac{1}{\sqrt{5}} = a\frac{3}{\sqrt{10}} + b\frac{1}{\sqrt{10}}$$

$2\sqrt{2}\,i = a - 3b$

$\sqrt{2} = 3a + b \quad \Rightarrow b = \sqrt{2} - 3a$

$2\sqrt{2}\,i = a - 3(\sqrt{2} - 3a)$

$2\sqrt{2}\,i = 10a - 3\sqrt{2} \quad \Rightarrow \quad a = \frac{3\sqrt{2} - 2\sqrt{2}\,i}{10}$

$$b = \frac{-\sqrt{2} + 6\sqrt{2}\,i}{10}$$

#3 (cont.)

c) $\Rightarrow |\lambda_A = a_0\rangle = \frac{3\sqrt{2} - 2\sqrt{2}i}{10} |\lambda_H = \hbar\omega\rangle + \frac{\sqrt{2} + 6\sqrt{2}i}{10} |\lambda_H = 11\hbar\omega\rangle$

$$|\lambda_A = a_0 (t)\rangle = U(t,t_0) |\lambda_A = a_0\rangle$$
$$= \exp[-iHt/\hbar]\left[\frac{3\sqrt{2} - 2\sqrt{2}i}{10} |\lambda_H = \hbar\omega\rangle + \frac{\sqrt{2} + 6\sqrt{2}i}{10} |\lambda_H = 11\hbar\omega\rangle\right]$$
$$= \exp[-i\omega t]\left(\frac{3\sqrt{2} - 2\sqrt{2}i}{10}\right) |\lambda_H = \hbar\omega\rangle + \exp[-11i\omega t]\left(\frac{\sqrt{2} + 6\sqrt{2}i}{10}\right) |\lambda_H = 11\hbar\omega\rangle$$

$$P(t) = \langle \lambda_a = a_0 | A | \lambda_a = a_0 (t)\rangle$$
$$= \left[\frac{3\sqrt{2} + 2\sqrt{2}i}{10} \langle \lambda_H = \hbar\omega |\right.$$

Problem 4: Indistinguishable particles (10 Points):

Consider a system of two indistinguishable spin-1/2 particles.

?✓a) Which of the following two-particle spin states are eigenstates of the operator of the scalar product $\hat{S}_1 \cdot \hat{S}_2$ of the spin vectors? What are their eigenvalues? (1 point)

- $|\uparrow\uparrow\rangle \equiv |\uparrow\rangle \otimes |\uparrow\rangle$
- $|\uparrow\downarrow\rangle \equiv |\uparrow\rangle \otimes |\downarrow\rangle$
- $|\downarrow\uparrow\rangle \equiv |\downarrow\rangle \otimes |\uparrow\rangle$
- $|\downarrow\downarrow\rangle \equiv |\downarrow\rangle \otimes |\downarrow\rangle$

$\begin{bmatrix} \frac{1-i}{\sqrt{2}} & 1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{\sqrt{2}}{1+i} \end{bmatrix}$

$\frac{1-i}{\sqrt{2}} - \frac{\sqrt{2}}{1+i}\frac{(1-i)}{1-i} = 0$

?✓b) Show that the states:
$|s_+\rangle \equiv \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ and $|s_-\rangle \equiv \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ are eigenstates of $\hat{S}_1 \cdot \hat{S}_2$. What are their eigenvalues? (1 point)

These two particles, separated by a distance a, interact with one another via the field of their magnetic dipole moments. This interaction is described by the Hamiltonian

$$\hat{H} = \frac{\mu_0}{4\pi a^3}\left(\hat{m}_{x,1}\hat{m}_{x,2} + \hat{m}_{y,1}\hat{m}_{y,2} - 2\hat{m}_{z,1}\hat{m}_{z,2}\right),$$

where $\hat{m}_j = \gamma \hat{S}_j$ and γ is the gyromagnetic ratio of the particles.

?✓ c) Show that the anti-aligned states $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ are not eigenstates of the Hamiltonian. (1 point)

d) Derive the Hamiltonian in the basis of the anti-aligned states. (2 points)

e) What are the eigenvalues of this Hamiltonian? (1 point)

f) Find a unitary transformation matrix which diagonalizes the Hamiltonian. (2 points)

g) Use this transformation to diagonalize the Hamiltonian. (1 point)

h) What are the eigenstates of the Hamiltonian in this basis? (1 point)

Aug 2017

Quantum #4

a) Given two indistinguishable spin $1/2$ particles,

Problem 5: Angular Momentum (10 Points):

10

Suppose an electron is in a state described by the wave function

$$\psi = \frac{1}{\sqrt{4\pi}}(e^{i\phi}\sin\theta + \cos\theta)g(r)$$

where $\int_0^\infty |g(r)|^2 r^2 dr = 1$
and ϕ, θ are the azimuth and polar angles respectively.

✓(a) Express ψ in terms of spherical harmonics functions. (2 pts.)

✓(b) What are the possible results of a measurement of the z-component L_z of the angular momentum of the electron in this state? (2 pts.)

✓(c) Determine if $\int |\psi|^2 \; d^3\vec{r} = 1$. (2 pts.)

✓(d) Use the result in (c) to find the probability of obtaining each of the possible results in part (b). (2 pts.)

✓(e) What is the expectation value of L_z? (2 pts.)

$\cos\varphi = \frac{1}{2} e^{i\varphi} + e^{-i\varphi}$

$\sin\varphi = \frac{1}{2i} e^{i\varphi} - e^{-i\varphi}$

$\cos\varphi - i\sin\varphi = e^{-i\varphi}$

$\cos 2\theta = 1 - 2\sin^2\theta$

$\sin^2\theta = \frac{1-\cos 2\theta}{2}$

Aug 2017

Quantum #5

a) $\psi = \frac{1}{\sqrt{4\pi}}\left(e^{i\varphi}\sin\theta + \cos\theta\right) g(r)$

* But we know $Y_{1,0} = \sqrt{\frac{3}{4\pi}}\cos\theta$

$$Y_{1,\pm 1} = \mp\sqrt{\frac{3}{8\pi}}\, e^{\pm i\varphi}\sin\theta$$

$$\hookrightarrow \psi = \frac{1}{\sqrt{4\pi}}\cdot\left(-\sqrt{\frac{8\pi}{3}}\, Y_{1,1} + \sqrt{\frac{4\pi}{3}}\, Y_{1,0}\right) g(r)$$

$$= \left(\frac{1}{\sqrt{3}} Y_{1,0} - \sqrt{\frac{2}{3}}\, Y_{1,1}\right) g(r)$$

* Check normalization

$$1 = \frac{1}{4\pi}A^2 \int_0^{\infty} r^2 dr \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta\, |g(r)|^2 \left(e^{-i\varphi}\sin\theta + \cos\theta\right)\left(e^{i\varphi}\sin\theta + \cos\theta\right)$$

$$1 = \frac{1}{4\pi}A^2 \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta\, d\theta \cdot \cancelto{1}{\sin^2\theta + \cos^2\theta} + e^{-i\varphi}\sin\theta\cos\theta + e^{i\varphi}\sin\theta\cos\theta$$

$$1 = \frac{1}{4\pi}A^2 \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta\, d\theta \cdot \left(1 + \sin\theta\cos\theta\left(e^{-i\varphi} + e^{i\varphi}\right)\right)$$

$$1 = \frac{1}{4\pi}A^2 \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta + 2\sin^2\theta\cos\theta\cos\varphi\, d\theta$$

$$1 = \frac{1}{4\pi}A^2 \int_0^{2\pi} d\varphi \left[-\cos\theta + \frac{2}{3}\sin^3\theta\cos\varphi\right]\Big|_0^{\pi}$$

$$1 = \frac{1}{4\pi}A^2 \int_0^{2\pi} d\varphi \left[(1 + 0) - (-1 + 0\right.$$

$$1 = \frac{1}{2\pi}A^2 \int_0^{2\pi} d\varphi$$

$$1 = A^2 \Rightarrow A = 1 \checkmark$$

b) Rewriting our function in bra-ket notation

$$\psi = \frac{1}{\sqrt{3}}|1,0\rangle - \sqrt{\frac{2}{3}}|1,1\rangle$$

$$\hookrightarrow L_z|\psi\rangle = L_z\cdot\frac{1}{\sqrt{3}}|1,0\rangle - \sqrt{\frac{2}{3}} L_z|1,1\rangle$$

* possible measurements are $L_z = 0, 1$

#5 (cont.)

c) See work from part a checking normalization

d) $\langle \psi | L_z | \psi \rangle = 0 \cdot \frac{1}{3} \overset{1}{\langle 1,0 | 1,0 \rangle} + \frac{2}{3} \overset{1}{\langle 1,1 | 1,1 \rangle} \cdot 1$ (Other terms ignored due to orthogonality)

↳ $L_z = 0$ $\frac{1}{3}$ of the time

$L_z = 1$ $\frac{2}{3}$ of the time

(Expectation value is weighted sum of possible measurements)

e) $\langle \psi | L_z | \psi \rangle = \frac{2}{3}$

Problem 6: 3D Square Well (10 Points):

Consider a particle of mass m moving in a 3D spherical well given by the potential

$$V(\vec{r}) = -V_0 \quad 0 \leq |\vec{r}| \leq a_0, \qquad V(\vec{r}) = 0 \quad |\vec{r}| > a_0$$

where $V_0 > 0$ and $a_0 > 0$.

5?

In this problem, only consider bound states in this well, so $-V_0 < E < 0$.

?✓(a) (1 pt.) Show that the energy eigenstates for this potential can be written in the form:

$$\Psi_{k,\ell,m}(\vec{r}) = f_{k,\ell}(r) Y_\ell^m(\theta, \phi)$$

r, θ, ϕ are the usual spherical coordinates. and Y_ℓ^m the spherical harmonics.

?✓(b) (1 pt.) Defining the function $u_{k,\ell}(r) = r f_{k,\ell}(r)$, write the radial Schrodinger equation for $u_{k,\ell}(r)$.

?✓(c) (2 pts.) Consider the zero angular momentum states, $\ell = 0$. Write down the functional form for the states $u_{k,0}(r)$ in the two regions, $0 \leq r \leq a_0$ and $r \geq a_0$. Define any constants that you use in these functions.

?✓(d) (1 pt.) What are the boundary conditions on the functions $u_{k,0}(r)$ as $r \to 0$, at $r = a_0$, and as $r \to \infty$? Hint: Consider the function $f_{k,\ell}(r)$ as $r \to 0$.

(e) (2 pts.) Using your boundary conditions, derive an equation that can be solved to give the bound state energies for the $\ell = 0$ states.

(f) (2 pt.) For a fixed value of the radius of the well, a_0, calculate the minimum depth, $V_0 = V_{min}$ for the potential well to have a bound state.

(g) (1 pt.) give a physical reason why there is always a bound state in a symmetric 1D quantum square well, but not in the 3D well studied in this problem.

In spherical coordinates, (L^2 is the usual angular momentum operator)

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r} \psi\right)$$

$$\nabla^2 \psi(\vec{r}) = \cancel{\frac{1}{r}\frac{\partial^2}{\partial r^2} r\psi(\vec{r})} + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial \psi(\vec{r})}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial \phi^2}\psi(\vec{r})$$

$$\nabla^2 \psi(\vec{r}) = \cancel{\frac{1}{r}\frac{\partial^2}{\partial r^2} r\psi(\vec{r})} - \frac{L^2}{\hbar^2 r^2}\psi(\vec{r})$$

Aug 2017

Quantum #6

a) $V(r) = \begin{cases} -V_0 & 0 \leq r \leq a_0 \\ 0 & r > a_0 \end{cases}$

* Note: We only consider the bound region

$$\frac{-\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

$$\hookrightarrow \frac{-\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2\psi}{\partial\varphi^2}\right)\right] + V(r)\psi = E\psi$$

* Assuming a solution of the form $\psi = f_{k,\ell}(r)\, Y_\ell^m(\theta,\varphi)$

$$\frac{-\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right)\cdot Y + \frac{f}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{f}{r^2\sin^2\theta}\left(\frac{\partial^2 Y}{\partial\varphi^2}\right) + VfY = EfY\right.$$

* multiplying by $\frac{-2mr^2}{fY\hbar^2}$ yields

$$\frac{1}{f}\left(\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) - \frac{2mr^2 f(V-E)}{\hbar^2}\right) + \frac{1}{Y}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2}\right) = 0$$

* Note: Our assumption of a seperable solution works where the angular equation can be solved to find that $Y_\ell^m(\theta,\varphi)$ is the solution we expect (ie spherical harmonics)

b) Defining $U_{k,\ell}(r) = r f_{k,\ell}(r) \Rightarrow f_{k,\ell} = \frac{U_{k,\ell}(r)}{r}$, the Schrödinger eqn becomes:

$$\frac{1}{f}\left(\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) - \frac{2mr^2 f(V-E)}{\hbar^2}\right) = \ell(\ell+1)$$

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) - \frac{2mr^2 f(V-E)}{\hbar^2} = \ell(\ell+1)f$$

$$\frac{\partial}{\partial r}\left(r^2\frac{d}{dr}\left(\frac{u}{r}\right)\right) - \frac{2mr\, U_{k,\ell}(r)(V-E)}{\hbar^2} = \ell(\ell+1)\frac{u(r)}{r}$$

$$\frac{\partial}{\partial r}\left(\cancel{r^2}\left[\frac{r\,du/dr - u}{\cancel{r^2}}\right]\right) - \frac{2mr\,u(V-E)}{\hbar^2} = \frac{\ell(\ell+1)u}{r}$$

$$\frac{\partial}{\partial r}\left(r\frac{du}{dr} - u\right) - \frac{2mr\,u(V-E)}{\hbar^2} = \frac{\ell(\ell+1)u}{r}$$

$$\left[\frac{du}{dr} + r\frac{d^2u}{dr^2} - \frac{du}{dr}\right] - \frac{2mru(V-E)}{\hbar^2} = \frac{\ell(\ell+1)u}{r}$$

$$\frac{-\hbar^2}{2m}\frac{d^2u}{dr^2} + \left(V + \frac{\hbar^2\ell(\ell+1)}{2m}\right)u = Eu$$

#6 (cont)

c) If we only consider $\ell = 0$, our equation becomes:

$$\frac{-\hbar^2}{2m}\frac{d^2u}{dr} + Vu = Eu$$

$$\hookrightarrow \frac{d^2u}{dr^2} = \frac{-2mE-V}{\hbar^2}u$$

let $k = \frac{\sqrt{2m(E+V_0)}}{\hbar}$ where $0 \le r \le a_0$

$$\frac{d^2u}{dr^2} = -k^2 u \Rightarrow u = Ae^{ikr} + Be^{-ikr} = C\sin(kr) + D\cos(kr)$$

let $\kappa = \frac{\sqrt{-2mE}}{\hbar}$ where $r > a_0$

$$\frac{d^2u}{dr^2} = \kappa^2 u \Rightarrow u = Ae^{\kappa r} + Be^{-\kappa r}$$

d) Our function must go to 0 at $r=0$ and $r=\infty$

$$\hookrightarrow f = \frac{u}{r} = C\frac{\sin(kr)}{r} + D\frac{\cos(kr)}{r}$$

(Inside well)

$\sin(0) = 0$

$\cos(0) = 1 \Rightarrow D = 0$

$$f = \frac{u}{r} = A\frac{1}{r}e^{\kappa r} + B\frac{1}{r}e^{-\kappa r}$$

$e^{\kappa\infty} = \infty \Rightarrow A = 0$

$e^{-\kappa\infty} = 0$

e) Therefore, inside the well (bound states), it must be true that

$$\sin(kr) = 0 \Rightarrow kr = n\pi$$

$$\frac{\sqrt{2m(E+V_0)}\,r}{\hbar} = n\pi$$

$$2m(E+V_0) = \frac{n^2\pi^2\hbar^2}{r^2}$$

$$E = \frac{n^2\pi^2\hbar^2}{2mr^2} - V_0$$

#6 (cont.)

f) Assuming a_0 is fixed, we need to find the minimum depth for a bound state

$$\hookrightarrow E > 0 \Rightarrow \frac{n^2\pi^2\hbar^2}{2mr^2} > V_{min}$$

* potential error in definitions of k and κ

$$\frac{n^2\pi^2\hbar^2}{2ma_0^2} = V_{min}$$

Quantum Mechanics
Qualifying Exam - January 2018

Notes and Instructions

- There are 6 problems. Attempt them all as partial credit will be given.
- 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

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

In spherical coordinates,

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

$$\nabla^2\psi(\vec{r}) = \frac{1}{r}\frac{\partial^2}{\partial r^2}r\psi(\vec{r}) - \frac{L^2}{\hbar^2 r^2}\psi(\vec{r})$$

where L^2 is the usual angular momentum operator.

Clebsch-Gordon coefficients

1/2 × 1/2	1 +1	1 0	0 0	1 −1
+1/2 +1/2	1			
+1/2 −1/2		1/2	1/2	
−1/2 +1/2		1/2	−1/2	
−1/2 −1/2				1

Spherical Harmonics:

$Y_{0,0}(\theta,\phi) = \frac{1}{\sqrt{4\pi}}$

$Y_{1,0}(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta$

$Y_{1,\pm1}(\theta,\phi) = \mp\sqrt{\frac{3}{8\pi}}e^{\pm i\phi}\sin\theta$

$Y_{2,0}(\theta,\phi) = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1)$

$Y_{2,\pm1}(\theta,\phi) = \mp\sqrt{\frac{15}{8\pi}}e^{\pm i\phi}\cos\theta\sin\theta$

$Y_{2,\pm2}(\theta,\phi) = \sqrt{\frac{15}{32\pi}}e^{\pm 2i\phi}\sin^2\theta$

8-10

Problem 1: Matrix Mechanics (10 points):

Consider a particle with mass m and one continuous degree of freedom (spatial coordinate z with associated momentum operator $\hat{p}_z = -\imath\hbar\frac{d}{dz}$) and two discrete internal (pseudo-) spin states described by the Hamiltonian operator $\hat{H}$:

$$\hat{H} = \frac{\hat{p}_z^2}{2m}\hat{I} + \frac{\hbar k_{so}}{m}\hat{\sigma}_z\hat{p}_z + \frac{\Omega}{2}\hat{\sigma}_x. \tag{1}$$

Here, $\hat{I}$ is the identity operator in spin space, k_{so} and Ω are constants, and $\hat{\sigma}_x$ and $\hat{\sigma}_z$ are the usual Pauli spin operators for a spin-1/2 particle. Different from what you might be used to, the Hamiltonian $\hat{H}$, Eq. (1), couples the spin and spatial degrees of freedom.

✓ a) (1 pt) What are the units of k_{so} and Ω? Explain your answer.

✓ b) (1 pt) Choose a convenient basis that spans the spin space and express the Hamiltonian operator $\hat{H}$ in this spin basis (you should obtain a 2×2 matrix). Explain your reasoning.

? c) (1 pt) Show that the operator $\hat{p}_z$ commutes with every element of the 2×2 matrix obtained in b).

✓ d) (3 pts) (Use your results from parts b) and c) to determine the eigen energies $E(p_z)$ of $\hat{H}$. Here, p_z is not an operator but a number.

✓ e) (1 pt) What happens to the eigen energies in the large p_z limit?

? f) (3 pts) Plot the eigen energies obtained in d) as a function of p_z for:
2? i) vanishing Ω
ii) large Ω
iii) small Ω

Explain what the terms "large" and "small" mean in this context, i.e., identify the quantity that Ω needs to be compared with in both cases.

$S^2 = S_1^2 + S_2^2 + 2 S_1 \cdot S_2$

5-7 ?

Problem 2: Perturbation with 2 spins (10 points):

Let $\vec{S_1}$ and $\vec{S_2}$ be the spin operators of two spin-1/2 particles. Then $\vec{S} = \vec{S_1} + \vec{S_2}$ is the spin operator for this two-particle system.

a) (2 pts) Consider the Hamiltonian

$$\hat{H}_0 = \alpha(\hat{S}_x^2 + \hat{S}_y^2 - \hat{S}_z^2)/\hbar^2 \quad \alpha: \text{ real constant greater than } 0$$

Determine the Energy eigenvalues and degeneracies for this Hamiltonian.

b) (4 pts) Consider a perturbation to the above Hamiltonian:

$$\hat{H}_1 = \lambda(\hat{S_{1x}} - \hat{S_{2x}}) \quad \lambda: \text{ real constant greater than } 0.$$

Calculate the new energies and degeneracies to first-order in perturbation theory.

? c) (3 pts) Now consider an unperturbed Hamiltonian

$$\hat{H}_0 = -A(\hat{S}_{1z} + \hat{S}_{2z}) \quad A: \text{ real constant greater than } 0$$

with a perturbing Hamiltonian of the form

$$\hat{H}_1 = B(\hat{S}_{1x}\hat{S}_{2x} - \hat{S}_{1y}\hat{S}_{2y}) \quad B: \text{ real constant greater than } 0$$

by means of perturbation theory, calculate the ground state energy of $\hat{H}_0$ and calculate the first and second order shifts of the ground state energy of $\hat{H}_0$ as a consequence of the perturbation $\hat{H}_1$.

? d) (1 pt) The exact ground state energy for $\hat{H}_0 + \hat{H}_1$ found in part c) is

$$E_{ground} = -\frac{\hbar}{2}\sqrt{4A^2 + B^2\hbar^2}$$

Compare your results from c) to the exact energy. What conditions on A and B are required so that your results from c) and d) agree?

$S_1^2 = S_{1x}^2 + S_{1y}^2 + S_{1z}^2$

$S_2^2 = S_{2x}^2 + S_{2y}^2 + S_{2z}^2$

$S^2 = S_x^2 + S_y^2 + S_z^2 - 2 S_1 \cdot S_2$

$S_x^2 + S_y^2 = S^2 - S_z^2 + 2S_1 \cdot S_2$

10

Problem 3: Infinite Well (10 points):

Assume that a particle is placed in a one dimensional infinitely deep square well potential of width $L = 1$, which has the analytic form

$$V(x) = \begin{cases} \infty & x < 0 \\ 0 & 0 \leq x \leq 1 \\ \infty & x > 1. \end{cases}$$

a) (2 pts) Calculate the eigenfunctions and eigenvalues for this potential.

b) (1 pt) Sketch the ground state wave function and the first 2 excited states

c) (2 pts) Assume that a particle is placed in the potential well in the state given by the following wavefunction at $t = 0$

$$\psi(x,0) = \sqrt{\frac{8}{13}}\sin(\pi x) + \sqrt{\frac{72}{13}}\sin(\pi x)\cos(\pi x).$$

Calculate the probability that the particle is in each of the following eigenstates: the ground state, the first excited state, in any state greater than the first excited state.

d) (1 pt) Calculate the expectation value of the energy.

e) (2 pts) Calculate the expectation value of the position operator for the initial state that is given in c).

f) (2 pts) The energy of the particle is measured and is found to be in the ground state. The wall located at $x = 1$ is quickly moved to $x = 2$. What is the probability that the energy is found equal to that of the ground state?

7

Problem 4: Coherent States and the Harmonic Oscillator (10 pts)

Consider a one dimensional harmonic oscillator with mass m and frequency ω

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

The raising and lowering operators are useful for harmonic oscillator problems:

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(x - i\frac{p}{m\omega} \right) \qquad a = \sqrt{\frac{m\omega}{2\hbar}} \left(x + i\frac{p}{m\omega} \right) \quad .$$

✓ (a) (1 pt) Verify that the Hamiltonian can be recast to the form $H = \hbar\omega(N + \frac{1}{2})$, where $N = a^\dagger a$. Be sure to show your work.

(b) (3 pts) Prove by induction that

$$[a, (a^\dagger)^n] = n(a^\dagger)^{n-1}$$

$a a^{\dagger n} - a^{\dagger n} a = n(a^\dagger)^{n-1}$

$a a^{\dagger n} - n (a^\dagger)^{n-1}$

where $n \geq 1$ denotes a positive integer.

✓ (c) (4 pts) Define a state

$$|f\rangle \quad = \quad e^{-|f|^2/2} \times e^{fa^\dagger} |0\rangle$$

where f is a complex number. This state is called a coherent state. Starting from your results in part (b) of this problem, show that

$$a|f\rangle \quad = \quad f|f\rangle \ .$$

✓ (d) (2 pts) Check that

$$\langle f|f\rangle \quad = \quad 1$$

If needed, you can use the fact that $(a^\dagger)^n|0\rangle \ = \ \sqrt{n!}|n\rangle$ for level n of the harmonic oscillator.

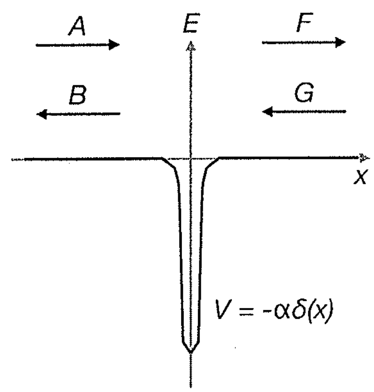
$\sqrt{(a+ib)(a-ib)} = a^2+b^2$

2

Problem 5: Transmission across delta functions(10 points):

a) (1 pt) Consider the potential $V(x) = -\alpha\delta(x)$. Show that the derivative of the wave function is discontinuous across the potential.
i.e $lim_{\epsilon\to 0}\left(\left(\frac{\partial\psi(x)}{\partial x}\right)_{x=\epsilon} - \left(\frac{\partial\psi(x)}{\partial x}\right)_{x=-\epsilon}\right) = -\frac{2m\alpha}{\hbar^2}\psi(0)$

b) (2 pts) A particle with $E > 0$ is incident on the delta function potential from $x < 0$. Determine the probability that the particle will be transmitted across the potential. Can the probability of transmission $= 1$?



c) (3 pts) One can define a transfer matrix M, which gives the amplitudes to the right of the potential in terms of those on the left.

$$\begin{pmatrix} F \\ G \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix}$$

Construct the M-matrix for scattering from a single delta-function potential at point a.

$$V(x) = -\alpha\delta(x-a)$$

d) (1 pt) Show that if you have a potential consisting of 2 isolated pieces, the M-matrix for the combination is the product of the two M-matrices for each section separately.

$$M = M_2 M_1$$

e) (3 pts) Now consider a double delta function potential

$$V(x) = -\alpha[\delta(x+a) + \delta(x-a)]$$

Determine the probability of transmission across the double delta function potential ($T = \frac{1}{|M_{22}|^2}$). Can the probability of transmission $= 1$?

Problem 6: Hydrogenic Systems (10 pts):

(Note this problem is 2 pages and has 5 parts)

Consider the quantum system consisting of two charged particles interacting due to the Coulomb Potential:

$$H = \frac{\vec{p}_1^2}{2m_1} + \frac{\vec{p}_2^2}{2m_2} - \frac{qe^2}{|\vec{r}_1 - \vec{r}_2|}$$

$\vec{p}_1$ and $\vec{r}_1$ are the position and momentum of particle 1 with mass m_1. $\vec{p}_2$ and $\vec{r}_2$ are the position and momentum of particle 2 with mass m_2.

The charge of particle 1 is $-e$ and the charge of particle 2 is $+qe$, where q is an integer greater than or equal to 1.

a) (2 pts.) To solve this problem, you first want to convert to the center-of-mass and relative coordinates:

$$\vec{R} = \frac{m_1}{m_1 + m_2}\vec{r}_1 + \frac{m_2}{m_1 + m_2}\vec{r}_2 \ , \quad \vec{r} = \vec{r}_1 - \vec{r}_2$$

Derive the conjugate momenta to these spatial coordinates, $\vec{P}$ and $\vec{p}$, defined by:

$$[r_i, p_j] = i\hbar\delta_{i,j}, \quad [R_i, P_j] = i\hbar\delta_{i,j}, \quad [r_i, P_j] = [R_i, p_j] = 0$$

In these expressions, the subscripts indicate the vector components $x,\ y,\ z,\ p_x,\ p_y, p_z$, etc. Show your work.

Using these coordinates, the 2-particle Hamiltonian can be written:

$$H = \frac{\vec{P}^2}{2(m_1 + m_2)} + \frac{\vec{p}^2}{2\mu} - \frac{qe^2}{|\vec{r}|} \quad \frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2} \tag{1}$$

For the rest of the problem, assume $\vec{P} = 0$ (the center-of-mass reference frame).

b) (2 pts.) Define the wavefunction for the system as:

$$\Psi_{n,\ell,m}(\vec{r}) = \frac{u_{n,\ell}(r)}{r} Y_\ell^m(\theta, \phi)$$

where $r,\ \theta,\ \phi$ are the usual spherical coordinates, and Y_ℓ^m the spherical harmonics.

Problem 6 continued

Show, in detail, that the Radial (Schrodinger) wave equation for the bound eigen-states, $u_{n,\ell}(r)$ can be written as:

$$\frac{\partial^2}{\partial r^2}u(r) - \frac{\ell(\ell+1)}{r^2}u(r) + \frac{2}{a_0}\frac{u(r)}{r} = \kappa_n^2 u(r)$$

What are a_0 and κ_n in terms of properties of the bound state system (μ, e, q, etc.)?

c) (3 pts.) Using the radial wave equation, determine the form of the function $u_{n,\ell}(r)$ in the limit as $r \to \infty$. How does $u_{n,\ell}(r)$ depend on the quantum number n for large values of r?

d) (2 pts.) In the limit that $r \to 0$, show that there are two possible solutions for $u_{n,\ell}(r)$, with the physical solution being $u_{n,\ell}(r) \propto r^{\ell+1}$. Do this for $\ell > 0$. (The $\ell = 0$ solution is a bit more complicated.)

e) (1 pt.) What are the ground-state energy and radius (Bohr radius) of the hydrogen-like system of a muon bound to an alpha particle?

Some potentially useful information:

- Fine structure constant - $\alpha = \frac{e^2}{\hbar c}$
- Bohr radius for a hydrogen atom - $a_B = \frac{\hbar}{\alpha m_e c}$
- Rydberg - $\frac{1}{2}\alpha^2 m_e c^2$
- Electron mass - $m_e c^2 = 0.51 MeV$
- Proton and Neutron mass - $m_N c^2 = 940 MeV$
- muon mass - $m_\mu c^2 = 106 MeV$.

$$a_0 = \frac{\hbar}{\frac{e^2}{\hbar c} m_e c} = \frac{\hbar^2}{e^2 m_e^2}$$