Phys 3810, Spring 2012 Exam #2

- 1. Give short definitions of the terms
- a) A complete set of eigenfunctions.

This means that any (legal) wave function can be expressed as a linear combination of the eigenfunctions of a certain operator.

b) The *spectrum* of an operator.

This is the set of all eigenvalues of the operator. It can have discrete and continuum parts.

c) Degenerate eigenvalues.

These are eigenvalues for which there are two or more independent eigenfunctions (eigenstates).

2. What did we show about the possibility of (energy) degenerate bound states for a one-dimensional potential?

We showed that there can't be degenerate eigenstates of the energy for bound states in a onedimensional potential. (Two wave functions with the same energy eigenvalue are not independent.)

3. An operator \hat{A} (representing observable A) has two normalized eigenstates ψ_1 and ψ_2 , with eigenvalues a_1 and a_2 , respectively. Operator \hat{B} has two normalized eigenstates ϕ_1 and ϕ_2 with eigenvalues b_1 and b_2 respectively. The eigenstates are related by

$$\psi_1 = (5\phi_1 + 4\phi_2)/\sqrt{41} \qquad \qquad \psi_2 = (-4\phi_1 + 5\phi_2)/\sqrt{41}$$
 (1)

a) Observable A is measured and the value a_2 obtained. What is the state of the system (immediately) after this measurement? (Easy.)

The state of the system is immediately set to be ψ_2 .

b) If B is now measured, what are the possible results and what are their probabilities? (Also not too hard.)

Reading off the coefficients of ϕ_1 and ϕ_2 in ψ_2 (and squaring them) we have

Probability of
$$\frac{16}{41}$$
 to be in ϕ_1 Probability of $\frac{25}{41}$ to be in ϕ_2

c) If the measurement in (b) had given b_1 what are the probabilities now that a measurement of A will give a_1 ?

With this measurement we now know that the system is in state ψ_1 . To answer the questions, write ϕ_1 in terms of ψ_1 and ψ_2 . Note that we can get the ϕ_2 's in 1 by taking $5\psi_1 - 4\psi_2$. This gives:

$$5\psi_1 - 4\psi_2 = \frac{1}{\sqrt{41}}(25\phi_1 + 16\phi_2) = \frac{41}{\sqrt{41}}\phi_1 = \sqrt{41}\phi_1$$

so this gives

$$\phi_1 = \frac{1}{\sqrt{41}} (5\psi_1 - 4\psi_2)$$

and from this we read off that the probability to give the measurement a_1 (which goes with state ψ_1) is

 $P_1 = \frac{25}{41}$

4. a) Give the definition of a hermitian operator.

Using the bra-ket notation if the operator \hat{Q} is Hermitian then for any legal states $|f\rangle$ and $|g\rangle$ we have

$$\langle f|Qg\rangle\rangle = \langle (Qf)|g\rangle$$

b) Say something about the importance or relevance of the Hermiticity property of an operator to quantum mechanics.

Any operator which corresponds to an observable quantity must be Hermitian.

c) How do you know that the coordinate operator x is Hermitian?

For our x-space wave functions the operator x is simply a multiplicative factor so it can be $applied\ to$ the bra- or ket- wave function. But it also real so that it can be written as x^* with no change and thus moved to the ket in $\langle (xf) ||$.

d) Show that our raising and lowering operators for the Harmonic oscillator are related by $a_{+}^{\dagger} = a_{-}$. So they are not Hermitian. Why is this not a problem for quantum mechanics?

Since $x^\dagger = x$ and $p^\dagger = p$, we have

$$a_{+}^{\dagger} = \frac{1}{\sqrt{2\hbar m\omega}} (-ip + m\omega x)^{\dagger} = \frac{1}{\sqrt{2\hbar m\omega}} (+ip^{\dagger} + m\omega x^{\dagger})$$
$$= \frac{1}{\sqrt{2\hbar m\omega}} (ip + m\omega x) = a_{-}$$

It is not a problem that $a_+^\dagger \neq a_+$ because the raising operator is not an observable.

5. Give a brief but *correct* summary of the meaning (i.e. the proper usage) of the energy-time uncertainty relation $\Delta t \Delta E \geq \frac{\hbar}{2}$.

If we choose some observable Q by which we will measure significant changes in a quantum system and take Δt to be the time it takes for the expectation value of Q to change substantially (one standard deviation) and if the uncertainty in the evergy is ΔE then

$$\Delta E \Delta t \ge \frac{\hbar}{2}$$

This is what the time--energy uncertainty relation really says.

6. Evaluate

$$[x,p^2]$$

(Recall $[x, p] = i\hbar$.)

Use $xp = i\hbar + px$ (operator relation), then

$$[x, p^{2}] = xp^{2} - p^{2}x = (xp)p - p^{2}x = (i\hbar + px)p - p^{2}x$$

$$= i\hbar p + p(xp) - p^{2}x = i\hbar p + p(i\hbar + px) - p^{2}x$$

$$= 2i\hbar p + p^{2}x - p^{2}x = 2i\hbar p = 2i\hbar \frac{\hbar}{i} \frac{d}{dx} = 2\hbar^{2} \frac{d}{dx}$$

7. The Hamiltonian for a certain two-level system is given by (in the basis of these states, $|1\rangle$ and $|2\rangle$),

$$H = \left(\begin{array}{cc} 2a & 2a \\ 2a & -a \end{array}\right)$$

If the system starts out in state

$$|\mathcal{S}(0)\rangle = \begin{pmatrix} 0\\1 \end{pmatrix}$$

what is $|\mathcal{S}(t)\rangle$?

Find the eigenvalues and eigenvectors for the H matrix (omit the overall factor of a for simplicity; eigenvalues are then a times the ones we find below). Solve:

$$\begin{vmatrix} 2 - \lambda & 2 \\ 2 & -1 - \lambda \end{vmatrix} = (2 - \lambda)(-1 - \lambda) - 4 = \lambda^2 - \lambda - 6 = (\lambda - 3)(\lambda + 2) = 0$$

so that the eigenvalues are -2 and 3 (or rather for H they are -2a and 3a).

For the eigenvalue -2 (i.e. -2a) solve for the eigenvector:

$$\begin{pmatrix} 2 & 2 \\ 2 & -1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = -2 \begin{pmatrix} a \\ b \end{pmatrix} \implies 2a + 2b = -2a \implies b = -2a$$

giving the normalized eigenvector

$$\begin{pmatrix} 1 \\ -2 \end{pmatrix} \implies \chi_1 = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ -2 \end{pmatrix}$$

For the eigenvalue 3 (i.e. 3a) solve for the eigenvector:

$$\begin{pmatrix} 2 & 2 \\ 2 & -1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = 3 \begin{pmatrix} a \\ b \end{pmatrix} \implies 2a + 2b = 3a \implies 2b = a$$

giving the normalized eigenvector

$$\begin{pmatrix} 2 \\ 1 \end{pmatrix} \implies \chi_2 = \frac{1}{\sqrt{5}} \begin{pmatrix} 2 \\ 1 \end{pmatrix}$$

Now if the initial value of $\chi(t)$ can be written in terms of χ_1 and χ_2 as:

$$(\chi_2 - 2\chi_1) = \frac{1}{\sqrt{5}} \begin{pmatrix} 0 \\ 5 \end{pmatrix} = \frac{5}{\sqrt{5}} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \sqrt{5} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Then

$$\chi(0) = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{2}{\sqrt{5}}\chi_1 + \frac{1}{\sqrt{5}}\chi_2$$

We can now restore the time dependence by multiplying each stationary-sate x-part byt the wiggly $\Phi(t)$ factor:

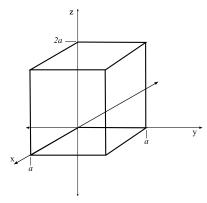
$$\chi(t) = -\frac{2}{\sqrt{5}} \chi_1 e^{\frac{-iE_1t}{\hbar}} + \frac{1}{\sqrt{5}} \chi_2 e^{\frac{-iE_2t}{\hbar}}$$

where $E_1 = -2a$ and $E_2 = 3a$.

- **8.** A particle of mass m is confined to move in three dimensions. It is confined to move inside a box of sides a a, and 2a (see figure).
- a) What are the energy eigenvalues for the particle?

The Schrödinger separates in the three cartesian coordinates to give equations of the form

$$\frac{d^2X}{dx^2} + k^2X = 0 \qquad \text{etc}$$



which has solutions

$$\psi(\mathbf{r}) = X(x)Y(y)Z(z) = \sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}}\sqrt{\frac{2}{2a}}\sin\left(\frac{n_x\pi^2\hbar^2}{2m(a)^2}\right)\sin\left(\frac{n_y\pi^2\hbar^2}{2m(a)^2}\right)\sin\left(\frac{n_z\pi^2\hbar^2}{2m(2a)^2}\right)$$

with eigenvalues

$$E_{n_x,n_y,n_z} = E_{n_x} + E_{n_y} + E_{n_z} = \frac{n_x^2 \pi^2 \hbar^2}{2ma^2} + \frac{n_y^2 \pi^2 \hbar^2}{2ma^2} + \frac{n_z^2 \pi^2 \hbar^2}{2m(2a)^2}$$
$$= \frac{\pi^2 \hbar^2}{2ma^2} \left(n_x^2 + n_y^2 + \frac{n_z^2}{4} \right)$$

b) Give the values and degeneracies of the first four energy levels of this system.

The ground state has

$$E_{\rm gs} = \frac{\pi^2 \hbar^2}{2ma^2} (1 + 1 + \frac{1}{4}) \equiv E_0(\frac{9}{4}) = \frac{9}{4} E_0$$

The next state, with $n_z=2$ has

$$E_2 = E_0(1+1+1) = \frac{12}{4}E_0$$

and with $n_z = 3$ we get

$$E_3 = E_0(1 + 1 + \frac{9}{4}) = \frac{17}{4}E_0$$

and with $n_z = 4$ we get

$$E = E_0(1 + 1 + \frac{16}{4}) = \frac{24}{4}E_0$$

But note that with the quantum numbers (2,1,1) or (1,2,1) the energy is

$$E = E_0(4 + 1 + \frac{1}{4}) = \frac{21}{4}E_0$$

so in fact the fourth state is the doubly degenerate one with

$$E_4 = \frac{21}{4} E_0$$

9. Big, Really Easy Problem!! Show how to separate the Schrödinger equation in two dimensions in polar coordinates (s, ϕ) when the potential depends only on s.

For cylindrical coordinates s and ϕ , the laplacian is

$$\nabla^2 = \frac{1}{s} \frac{\partial}{\partial s} \left(s \frac{\partial}{\partial s} \right) + \frac{1}{s^2} \frac{\partial^2}{\partial \phi^2}$$

a) Find the separated (differential) equations for the s and ϕ coordinates that come from the trial solution

$$\psi(\mathbf{r}) = S(s)\Phi(\phi)$$

Put this trial solution into

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(s) = E\psi(\mathbf{r})$$

then get

$$-\frac{\hbar^2}{2m} \left[\Phi(\phi) \frac{1}{s} \frac{d}{ds} \left(s \frac{dS}{ds} \right) + S(s) \frac{1}{s^2} \frac{d^2 \Phi}{d\phi^2} \right] + V(s) S(s) \Phi(\phi) = ES(s) \Phi(\phi)$$

Multiply by s^2 and divide by $S(s)\Phi(\phi)$. Get:

$$-\frac{\hbar^2}{2m} \left[\frac{s}{S} \frac{d}{ds} \left(s \frac{dS}{ds} \right) + \frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} \right] + s^2 V(s) = s^2 E$$

This is a some of terms of the $f(s) + g(\phi) = C$ with $s \phi$ independent and we can conclude in the usual way that these functions are constants. This leads to the equations:

$$-\frac{\hbar^2}{2m}\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = C \qquad \Longrightarrow \qquad \frac{d^2\Phi}{d\phi^2} = C_1\Phi$$

and

$$-\frac{\hbar^2}{2m}\frac{s}{S}\frac{d}{ds}\left(s\frac{dS}{ds}\right) + s^2V(s) - s^2E = C \qquad \Longrightarrow \qquad \frac{s}{S}\frac{d}{ds}\left(s\frac{dS}{ds}\right) + \frac{2m}{\hbar^2}s^2(E - V(s)) = C_2$$

b) Solve the equation for ϕ ; it has easy solutions, and the values of the separation constant are restricted by the fact that the solution must be periodic in ϕ with period 2π .

For the angular function this gives

$$\frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} = C \qquad \Longrightarrow \qquad \frac{d^2 \Phi}{d\phi^2} = C \Phi$$

which has the solution

$$\Phi(\phi) = e^{\pm i\alpha\phi} \qquad \text{with} \quad -\alpha^2 = C$$

But for the wave function to be single--valued, α must be an integer, say $\alpha=m$ with $m=0,\pm 1,\pm 2\dots$ which will absorb the \pm sign; also to normalize the Φ part separately, the integral over all ϕ of $|\Phi|^2$ must give 1 and this gives

$$\Phi(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi} \quad \text{for} \quad m = 0, \pm 1, \pm 2 \dots$$

c) Now suppose we want to consider a particle of mass m trapped in a 2D circular box of radius R with V=0 on the inside. With with result of part (b) put the s (differential) equation in a simple form that someone might solve. Give the boundary condition it must satisfy for the trapped particle problem. You don't need to say what the solution is.

Go back to the s equation, and with $C=-\alpha^2$ so that

$$\frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} = -m^2$$

and specializing to ${\cal V}=0$ we now have

$$s\frac{d}{ds}\left(s\frac{dS}{ds}\right) - m^2S + s^2\frac{2mE}{\hbar^2}S = 0$$

As usual define

$$k^2 \equiv \frac{2mE}{\hbar^2}$$

and then get

$$s^{2}\frac{d^{2}S}{ds^{2}} + s\frac{dS}{ds} + (k^{2}s^{2} - m^{2})S = 0$$

Replacing x by the unitless x = ks gives (for S now considered as a function of x):

$$x^{2}\frac{d^{2}S}{dx^{2}} + x\frac{dS}{dx} + (x^{2} - m^{2})S = 0$$

which is known as Bessel's differential equation.

The condition that

$$S(x) = 0$$
 for $s = R$

gives the discrete values for the energy E.

10. Find the energy difference between the n = 1 and n = 4 levels in the H atom. (Express the answer in eV and as a wavelength for the corresponding photon.)

Using the formula $E_n = (-13.6 \text{ eV})/n^2$ we get

$$|\Delta E| = (13.6 \text{ eV})(\frac{1}{1} - \frac{1}{16}) = 12.8 \text{ eV} = 2.04 \times 10^{-18} \text{ J}$$

The wavelength this corresponds to (using $\Delta E = h \nu$ is

$$\lambda = \frac{c}{\nu} = \frac{hc}{E} = \frac{(6.626 \times 10^{-34} \text{ J} \cdot \text{s}(2.998 \times 10^8 \frac{\text{m}}{\text{s}})}{(2.04 \times 10^{-18} \text{ J})} = 9.74 \times 10^{-8} \text{ m} = 97.4 \text{ nm}$$

11. Our solution for the H atom is a first-order answer, good to at least 1%, but some "physics" has been left out. Identify two ways in which our simple H-atom Hamiltonian is deficient.

Our treatment with the Schrödinger equation neglects the effects of relativity and any dependence of the Hamiltonian on the spin of the electron and the proton. There are also corrections from QED (not included in the "basic" relativity treatment).

Useful Equations

Math

$$\int_0^\infty x^n e^{-x/a} = n! \, a^{n+1}$$

$$\int_0^\infty x^{2n} e^{-x^2/a^2} \, dx = \sqrt{\pi} \frac{(2n)!}{n!} \left(\frac{a}{2}\right)^{2n+1} \qquad \int_0^\infty x^{2n+1} e^{-x^2/a^2} \, dx = \frac{n!}{2} a^{2n+2}$$

$$\int_a^b f \, \frac{dg}{dx} \, dx = -\int_a^b \frac{df}{dx} \, g \, dx + fg \bigg|_a^b \qquad \delta(x) = \frac{1}{2\pi} \int_{-\infty}^\infty e^{ikx} \, dk$$

Numbers

$$\hbar = 1.05457 \times 10^{-34} \text{ J} \cdot \text{s}$$
 $m_{\rm e} = 9.10938 \times 10^{-31} \text{ kg}$ $m_{\rm p} = 1.67262 \times 10^{-27} \text{ kg}$ $e = 1.60218 \times 10^{-19} \text{ C}$ $c = 2.99792 \times 10^8 \frac{\text{m}}{\text{s}}$

Physics

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi \qquad P_{ab} = \int_a^b |\Psi(x,t)|^2 dx \qquad p \to \frac{\hbar}{i}\frac{d}{dx}$$

$$\int_{-\infty}^\infty |\Psi(x,t)|^2 dx = 1 \qquad \langle x \rangle = \int_{-\infty}^\infty x |\Psi(x,t)|^2 dx \qquad \langle p \rangle = \int_{-\infty}^\infty \Psi^* \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) \Psi dx$$

$$\sigma = \sqrt{\langle j^2 \rangle - \langle j \rangle^2} \qquad \sigma_x \sigma_p \ge \frac{\hbar}{2}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + V\Psi = E\Psi \qquad \phi(t) = e^{-iEt/\hbar} \qquad \Psi(x,t) = \sum_{n=1}^\infty c_n \psi_n(x) e^{-iE_nt/\hbar} = \sum_{n=1}^\infty \Psi_n(x,t)$$

$$\infty \text{ Square Well:} \qquad E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \qquad \psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$$

$$\int \psi_m(x)^*\psi_n(x) dx = \delta_{mn} \qquad c_n = \int \psi_n(x)^*f(x) dx \qquad \sum_{n=1}^\infty |c_n|^2 = 1 \qquad \langle H \rangle = \sum_{n=1}^\infty |c_n|^2 E_n$$
 Harmonic Oscillator:
$$V(x) = \frac{1}{2}m\omega^2 x^2 \qquad \frac{1}{2m}[p^2 + (m\omega x)^2]\psi = E\psi$$

$$a_{\pm} \equiv \frac{1}{\sqrt{2\hbar m\omega}}(\mp ip + m\omega x) \qquad [A,B] = AB - BA \qquad [x,p] = i\hbar$$

$$H(a_+\psi) = (E + \hbar\omega)(a_+\psi) \qquad H(a_-\psi) = (E - \hbar\omega)(a_+\psi) \qquad a_-\psi_0 = 0$$

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} \qquad \psi_1(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \sqrt{\frac{2m\omega}{\pi}} x e^{-\frac{m\omega}{2\hbar}x^2}$$
 Free particle:
$$\Psi_k(x) = Ae^{i(kx - \frac{\hbar k^2}{2m})t} \qquad v_{\text{phase}} = \frac{\omega}{t} \qquad v_{\text{group}} = \frac{d\omega}{dt}$$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx - \frac{\hbar k^2}{2m}t)} dk \qquad \phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-ikx} dx$$
Delta Fn Potl:
$$\psi(x) = \frac{\sqrt{m\alpha}}{\hbar} e^{-m\alpha|x|/\hbar^2} \qquad E = -\frac{m\alpha^2}{2\hbar^2}$$

$$f_p(x) = \frac{1}{\sqrt{2\pi\hbar}} \exp(ipx/\hbar) \qquad [\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} = \hat{B}\hat{A} \qquad \Phi(p, t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \Psi(x, t) \, dx$$
$$\sigma_A^2 \sigma_B^2 \ge \left(\frac{1}{2i} \langle [\hat{A}, \hat{B}] \rangle \right)^2 \qquad \sigma_x \sigma_p \ge \frac{\hbar}{2} \qquad \Delta E \Delta t \ge \frac{\hbar}{2}$$

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

$$\psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi) \qquad \frac{d^2\Phi}{d\phi^2} = -m^2\Phi \qquad \sin \theta \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + [\ell(\ell+1)\sin^2 \theta - m^2]\Theta = 0$$

$$Y_0^0 = \sqrt{\frac{1}{4\pi}} \qquad Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos \theta \qquad Y_1^{\pm 1} = \mp \sqrt{\frac{3}{8\pi}}\sin \theta e^{\pm i\phi}$$

$$Y_2^0 = \sqrt{\frac{5}{16\pi}} (3\cos^2 \theta - 1) \qquad Y_2^{\pm 1} = \mp \sqrt{\frac{15}{8\pi}}\sin \theta \cos \theta e^{\pm i\phi} \qquad \text{etc.}$$

$$R(r) = Aj_l(kr) \qquad k \equiv \sqrt{\frac{2mE}{\hbar}}$$

$$j_1(x) = \frac{\sin x}{x} \qquad j_1 = \frac{\sin x}{x^2} - \frac{\cos x}{x} \qquad j_2(x) = \left(\frac{3}{x^3} - \frac{1}{x}\right)\sin x - \frac{3}{x^2}\cos x$$

$$a = \frac{4\pi\epsilon_0\hbar^2}{me^2} = 0.529 \times 10^{-10} \text{ m}$$
 $E_n = -\left[\frac{m}{2\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right] \frac{1}{n^2} \equiv \frac{E_1}{n^2}$ for $n = 1, 2, 3, \dots$

where $E_1 = -13.6 \text{ eV}$.

$$R_{10}(r) = 2a^{-3/2}e^{-r/a} R_{20}(r) = \frac{1}{\sqrt{2}}a^{-3/2}\left(1 - \frac{1}{2}\frac{r}{a}\right)e^{-r/2a} R_{21}(r)\frac{1}{\sqrt{24}}a^{-3/2}\frac{r}{a}e^{-r/2a}$$

$$\lambda f = c$$
 $E_{\gamma} = hf$ $\frac{1}{\lambda} = R\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$ where $R = \frac{m}{4\pi c\hbar^3} \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 = 1.097 \times 10^7 \text{ m}^{-1}$