Phys 3810, Spring 2010
Exam #2

1. Give short definitions of the terms (as used by Griffiths)

a) A *complete* set of eigenfunctions.

A set of functions with which one can form a linear combination to express any $other$ possible stats of the system.

b) Determinate state.

State for which the measurement of a particular observable always returns the same value.

c) Compatible observables.

Compatible observables allow us to find eigenfunctions which are $simultaneously$ eigenfunctions of the operators for both observables. This is possible when those operators commute.

d) The *spectrum* of an operator.

The spectrum of an operator is the full set of eigenvalues of that operator.

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

The equation $\Delta E \Delta t =\geq \hbar/2$ has the meaning that if we pick some observable Q then for a state which is not a stationary state, if Δt represents the time required for $\langle Q \rangle$ to change by a significant fraction then ΔE for that state satisfies the given equation.

It does not mean all the erroneous things that people say it means.

3. (Not too hard...) 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

$$\psi_1 = (-3\phi_1 + 4\phi_2)/5 \qquad\qquad \psi_2 = (4\phi_1 + 3\phi_2)/5$$

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

After the measurement, the state of the system must be ψ_2.

b) If B is now measured, what are the possible results and what are their probabilities?

Since $\psi_2 = (4\phi_1 + 3\phi_2)/5$, we have a probability of

$$(4/5)^2 = \frac{16}{25} \qquad \text{to be measured as} \qquad b_1$$

and a probability of

$$(3/5)^2 = \frac{9}{25} \qquad \text{to be measured as} \qquad b_2$$

4. Evaluate the commutator of the momentum operator and square of the coordinate operator,

$$\left[p, x^2\right] \ .$$

Evaluate and explain all the steps.

Consider some "test function" $f(x)$, then

$$\begin{aligned}
[p, x^2]f(x) &= \frac{\hbar}{i}[d/dx, x^2]f(x) = \frac{\hbar}{i}\left[\frac{d}{dx}(x^2 f(x)) - x^2\frac{d}{dx}f(x)\right] \\
&= \frac{\hbar}{i}\left[2xf(x) + x^2\frac{df}{dx} - x^2\frac{df}{dx}\right] = \frac{\hbar}{i}2xf(x) = \frac{2\hbar x}{i}f(x)
\end{aligned}$$

which tells us that the commutator is

$$[p, x^2] = \frac{2\hbar x}{i}$$

5. In the space of states consisting of $|1\rangle$, $|2\rangle$, express as a matrix the operator

$$H = a|1\rangle\langle 1| + b|2\rangle\langle 2| + \epsilon|1\rangle\langle 2| + \epsilon|2\rangle\langle 1|$$

$$\text{where} \qquad |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

Find the eigenvalues and eigenvectors of H.

The matrix which represents H is

$$H = \begin{pmatrix} a & \epsilon \\ \epsilon & b \end{pmatrix}$$

Solve for values of E such that $|H - EI| = 0$:

$$\begin{vmatrix} a - E & \epsilon \\ \epsilon & b - E \end{vmatrix} = (a-E)(b-E) - \epsilon^2 = E^2 - (a+b)E + (ab - \epsilon^2) = 0$$

So that

$$E = \frac{(a+b) \pm \sqrt{(a+b)^2 - 4(ab-\epsilon^2)}}{2} = \tfrac{1}{2}\left[(a+b) \pm \sqrt{(a-b)^2 - 4\epsilon^2}\right]$$

The algebra is getting a little messy at this so I'll go a little further and then we'll punt. Define $\alpha = \frac{1}{2}(a+b)$ and $\beta = \frac{1}{2}\sqrt{(a-b)^2 - 4\epsilon^2}$ so that the eigenvalues are $E = \alpha \pm \beta$. To get the eigenvector of $E = \alpha + \beta$, solve for x and y in

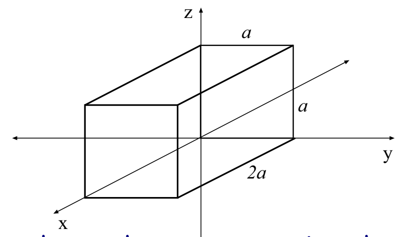
$$H\begin{pmatrix} x \\ y \end{pmatrix} = (\alpha+\beta)\begin{pmatrix} x \\ y \end{pmatrix} \qquad \Longrightarrow \qquad \begin{pmatrix} a & \epsilon \\ \epsilon & b \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = (\alpha+\beta)\begin{pmatrix} x \\ y \end{pmatrix}$$

We find

$$ax + \epsilon y = (\alpha + \beta)x \qquad \Longrightarrow \qquad y = \frac{(\alpha + \beta - a)}{\epsilon}x$$

which gives the eigenvector, which one should then normalize. The other case, $E = \alpha - \beta$ is similar.

6. A particle of mass m is confined to a 3-dimensional box which has sides $2a$, a and a which are oriented along the x, y and z axes,respectively.



a) Write down the wave function(s) and energy eigenvalue for the ground state.

From our experience in separating the Schrödinger equations, we know that we can write the wave function as a product of the appropriate "box" wave functions for x, y and z and the energy eigenvalue is the sum of the values for each term in the product. For the ground state, we have:

$$\begin{aligned}
\psi_{(000)}(x, y, z) &= \sqrt{\frac{2}{2a}} \left(\sqrt{\frac{2}{a}} \right)^2 \sin(\frac{\pi x}{2a}) \sin(\frac{\pi y}{a}) \sin(\frac{\pi z}{a}) \\
&= \frac{2}{a^{3/2}} \sin\left(\frac{\pi x}{2a}\right) \sin\left(\frac{\pi y}{a}\right) \sin\left(\frac{\pi z}{a}\right)
\end{aligned}$$

Energy eigenvalues are

$$E_{n_x,n_y,n_z} = \frac{n_x^2 \pi^2 \hbar^2}{8ma^2} + \frac{n_x^2 \pi^2 \hbar^2}{2ma^2} + \frac{n_x^2 \pi^2 \hbar^2}{2ma^2} = \frac{\pi^2 \hbar^2}{2ma^2}(\tfrac{1}{4}n_x^2 + n_y^2 + n_z^2)$$

so the ground state with $\mathbf{n} = (1, 1, 1)$ has energy

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

where E_0 is just the common factor in all the energies.

b) Find the energy eigenvalues of the next-lowest three states. Note any degeneracies which are present.

The next lowest state has

$$(n_x, n_y, n_z) = (2, 1, 1) \qquad \Longrightarrow \qquad E = 3E_0$$

The next lowest has

$$(n_x, n_y, n_z) = (3, 1, 1) \qquad \Longrightarrow \qquad E = \frac{17}{4} E_0$$

For the next energy level, there are two possible combinations,

$$(n_x, n_y, n_z) = (1, 2, 1), \quad (1, 1, 2) \qquad \Longrightarrow \qquad E = \frac{21}{4} E_0$$

7. Suppose an electron is trapped inside a spherical box of radius 2.0×10^{-10} m. (Inside the "box", $V = 0$.)

Find the energy of the ground state.

The ground state radial wave function for this problem was $R_0(r) = Aj_0(kr)$ and it had to satisfy the condition

$$j_0(ka) = 0 \qquad \Longrightarrow \qquad \sin(ka) = 0 \qquad \Longrightarrow \qquad ka = \pi$$

Since as usual we had $k \equiv \sqrt{2mE}/\hbar$, this gives

$$\frac{\sqrt{2mE}}{\hbar} = \frac{\pi}{a} \qquad \Longrightarrow \qquad 2mE = \frac{\pi^2\hbar^2}{a^2} \qquad \Longrightarrow \qquad E = \frac{\pi^2\hbar^2}{2ma^2}$$

Plugging in some numbers,

$$E = \frac{\pi^2(1.0546 \times 10^{-34}\ \mathsf{J}\cdot\mathrm{s})^2}{8(9.11 \times 10^{-31}\ \mathsf{kg})(2.0 \times 10^{-10}\ \mathsf{m})^2} = 1.5 \times 10^{-18}\ \mathsf{J} = 9.4\ \mathsf{eV}$$

8. Find $\langle z^2 \rangle$ for ground state of the H atom.

This is

$$\int_0^\infty (r^2 \cos^2\theta)|\psi_{000}|^2\, d^3\mathbf{r}$$

The angular integral for this is

$$\int \cos^2\theta |Y_0^0|^2 d\Omega = \frac{2\pi}{4\pi}\int_0^\pi \cos^2\theta \sin\theta d\theta = \tfrac{1}{2}\int_{-1}^{1} x^2\, dx = \frac{1}{3}$$

The radial part is

$$\int_0^\infty |R_{00}(r)|^2 r^4\, dr = \frac{2}{a^3}\int_0^\infty r^4 e^{-2r/a} = \frac{2}{a^3}(4!)\left(\frac{a}{2}\right)^5 = \frac{48a^2}{32} = \frac{3a^2}{2}$$

The product of the two gives

$$\langle z^2 \rangle = \frac{1}{3}\frac{3a^2}{2} = \frac{a^2}{2}$$

9. Show that the wave functions for the $(n = 1, l = 0, m = 0)$ and $(n = 2, l = 0, m = 0)$ are orthogonal.

Since

$$\psi_{100}(\mathbf{r}) = R_{10}(r)Y_0^0(\theta,\phi) \qquad \text{and} \qquad \psi_{200}(\mathbf{r}) = R_{20}(r)Y_0^0(\theta,\phi)$$

we really need to show that the radial functions are orthogonal. Using

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

the radial part of the "dot product" of the two wave functions is

$$\Longrightarrow \qquad = \frac{2}{\sqrt{2}} a^3 \int_0^\infty e^{-r/a} \left(1 - \frac{1}{2}\frac{r}{a}\right) e^{-r/2a} r^2 dr$$

Do some algebra:

$$\Longrightarrow \qquad = \sqrt{2} a^3 \int_0^\infty \left(r^2 - \frac{r^3}{2a}\right) e^{-3r/2a} dr$$

Use the exponential integral formulae. This gives:

$$\Longrightarrow \qquad = \sqrt{2} a^3 \left[2\left(\frac{2a}{3}\right)^3 - \frac{1}{2a} 6 \left(\frac{2a}{3}\right)^4\right] = \sqrt{2} a^3 \left[\frac{16a^3}{27} - \frac{16a^3}{27}\right] = 0$$

so the wave functions are orthogonal.

10. Find the probability that the electron in the ground state of the H atom will be "found" at a distance $r < a$ from the proton.

This is given by

$$\int_0^a |\psi_{000}(r)|^2 \, d^3\mathbf{r} = \frac{4}{a^3} \int_0^a e^{-2r/a} r^2 \, dr$$

where we can just do that radial integral because the angular part is separately normalized. This gives:

$$P_{r<a} = \frac{4}{a^3} \left[-\frac{a}{2} e^{-2r/a} \left(r^2 + ar + \frac{a^2}{2}\right)\right] \Big|_0^a$$

Factoring out some things,

$$\Longrightarrow \qquad 2(-e^{-2} \cdot \frac{5}{2} + \frac{1}{2}) = 1 - 5e^{-2} \approx 0.323$$

Possibly surprising in that it is a bit less than $\frac{1}{2}$.

11. For the one-electron H-like atom with a central (very massive) charge Ze, find the value of Z at which we would probably need relativity for the electron in the ground state.

The criterion for this is would be the value of Z where the expectation value of the for the kinetic or potential energy is comparable to the mass energy $m_e c^2$. For this you may want to note the results from a problem we didn't do; for state n of the H atom,

$$\langle T \rangle = -E_n \qquad \langle V \rangle = 2E_n$$

Get a number! Does this correspond to the nucleus of any known element?

We found that the (total) energy of the ground state is proportional to Z^2, that is, it is $(-13.6 \text{ eV})Z^2$ so that if, say, the magnitude of this energy is *half* of the rest energy then

$$(13.6 \text{ eV})Z^2 = 511 \times 10^3 \text{ eV} \qquad \Longrightarrow \qquad Z = 193$$

which is significantly bigger than the nucleus of any element. But such a big nucleus might be made in the temporary smash-ups of two large nuclei!

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

It is non-relativistic so that its form for the kinetic energy, $p^2/2m$, is in some way erroneous. It does not include any way in which the electron spin can enter the Hamiltonian, for example as from an interaction with the proton spin.

Useful Equations

Math

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

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

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

Numbers

$$\hbar = 1.05457\times 10^{-34}\ \mathrm{J\cdot s} \qquad m_{\mathrm{e}} = 9.10938\times 10^{-31}\ \mathrm{kg} \qquad m_{\mathrm{p}} = 1.67262\times 10^{-27}\ \mathrm{kg}$$

$$e = 1.60218\times 10^{-19}\ \mathrm{C} \qquad c = 2.99792\times 10^{8}\ \tfrac{\mathrm{m}}{\mathrm{s}}$$

Physics

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

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

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

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

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

$$\int \psi_m(x)^*\psi_n(x)\,dx = \delta_{mn} \qquad c_n = \int \psi_n(x)^*\,f(x)\,dx \qquad \sum_{n=1}^{\infty}|c_n|^2 = 1 \qquad \langle H\rangle = \sum_{n=1}^{\infty}|c_n|^2E_n$$

Harmonic Oscillator: $$V(x) = \tfrac{1}{2}m\omega^2x^2 \qquad \frac{1}{2m}[p^2 + (m\omega x)^2]\psi = E\psi$$

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

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

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} \qquad \psi_1(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\sqrt{\frac{2m\omega}{\hbar}}\,xe^{-\frac{m\omega}{2\hbar}x^2}$$

Free particle: $$\Psi_k(x) = Ae^{i(kx - \frac{\hbar k^2}{2m})t} \qquad v_{\mathrm{phase}} = \frac{\omega}{k} \qquad v_{\mathrm{group}} = \frac{d\omega}{dk}$$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx - \frac{\hbar k^2}{2m} t)}\, dk \qquad \phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-ikx}\, dx$$

$$\text{Delta Fn Potl:} \qquad \psi(x) = \frac{\sqrt{m\alpha}}{\hbar} e^{-m\alpha|x|/\hbar^2} \qquad E = -\frac{m\alpha^2}{2\hbar^2}$$

$$f_p(x) = \frac{1}{\sqrt{2\pi\hbar}} \exp(ipx/\hbar) \qquad [\hat{A},\hat{B}] \equiv \hat{A}\hat{B} = \hat{B}\hat{A} \qquad \Phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \Psi(x,t)\, dx$$

$$\sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2i} \langle [\hat{A},\hat{B}] \rangle \right)^2 \qquad \sigma_x \sigma_p \geq \frac{\hbar}{2} \qquad \Delta E \Delta t \geq \frac{\hbar}{2}$$

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

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

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

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

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

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

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

where $E_1 = -13.6$ eV.

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

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