Physics 346: QM EXAM 2 23 October 2008

Complete no more than 5 of the following problems

1. Chemists typically talk about different angular functions than do physicists. I dug out my old Physical Chemistry book and found reference to the following angular functions. Note that all of these functions just depend on the angles θ and ϕ, as in:

$$p_x(\theta,\phi) = N_x\ (-Y_{11}(\theta,\phi) + Y_{1-1}(\theta,\phi))$$

but I've not bothered below to repeat "(θ,ϕ)" as each function's arguments. The Ns are positive constants that normalize each function; "p" is referring to $\ell = 1$ not momentum.

$$\begin{aligned}
p_x &= N_x\,(-Y_{11} + Y_{1-1}) \\
p_y &= iN_y\,(Y_{11} + Y_{1-1}) \\
p_z &= Y_{10} \\
\text{hybridized } sp^3 &= N\,(\sqrt{2}Y_{00} + (1+i)Y_{11} + \sqrt{2}Y_{10} - (1-i)Y_{1-1}) \\
d_{x^2-y^2} &= N_{x^2-y^2}\,(Y_{22} + Y_{2-2}) \\
d_{yz} &= iN_{yz}\,(Y_{21} + Y_{2-1}) \\
d_{y^2-z^2} &= -N_{y^2-z^2}\,(Y_{22} + \sqrt{6}Y_{20} + Y_{2-2}) \\
d_{xy} &= iN_{xy}\,(-Y_{22} + Y_{2-2}) \\
d_{zx} &= N_{zx}\,(-Y_{21} + Y_{2-1})
\end{aligned}$$

(a) Using the raising and lowering operators, show p_x is an eigenfunction of L_x with eigenvalue 0, i.e., $L_x p_x = 0 \cdot p_x$.

(b) Show:

$$L_z\, d_{xy} = \lambda\, d_{x^2-y^2}$$

and report the value of λ.

(c) Consider the hybridized sp^3 wavefunction. Find N. If you measured L^2 and L_z of this wavefunction, what values would be found and with what probability?

(d) The $Y_{\ell m}(\theta,\phi)$ angular functions are eigenfunctions of L_z. Are any of the chemist's wavefunctions eigenfunctions of L_z? (If so list them.) In performing the separation of variables to produce the radial Schrödinger's equation, we needed eigenfunctions of L^2. Are any of the chemist's wavefunctions not eigenfunctions of L^2? (If so list them.)

2. The following state is a normalized eigenfunction of $\vec{J}^2$, J_z, $\vec{L}^2$, and $\vec{S}^2$, where $\vec{J} = \vec{L} + \vec{S}$.

$$\sqrt{\tfrac{3}{5}}Y_{21}\chi_- - \sqrt{\tfrac{2}{5}}Y_{20}\chi_+$$

Show directly that this is an eigenfunction of $\vec{J}^2$ and find the eigenvalue. What are the eigenvalues of J_z, $\vec{L}^2$, and $\vec{S}^2$?

3. In the H-atom a state (wavefunction) is typically denoted: $|n\ell m\rangle$. What do the integers n, ℓ, and m represent? (That is, connect these integers with Newtonian quantities discussed in PHYS 339/191.) What is the range of possible values for these integers? List (in approximate order of energy from ground state up) the (n,ℓ,m) values that represent the ten lowest energy states. Many of these states have the same energy in the simple Bohr picture. In your list, circle those groups of states that Bohr would call degenerate. The Bohr states are typically labeled with a number and a letter, e.g., $3p$ as in problem 6. Properly so label each circled set of sets in your list.

4. Show $[L_x, p_y] = i\hbar p_z$.

5. Consider the following wave function for two (free, noninteracting, identical, mass m) particles in one dimension (x_1 refers to particle 1 and x_2 refers to 2).

$$\psi(x_1, x_2) = \exp(i5(x_1 + x_2)) \sin(3(x_1 - x_2))$$

By direct calculation, show that this is a solution to the time independent Schrödinger's equation: $H\psi = E\psi$, where H is the free particle Hamiltonian:

$$H = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x_1^2} + \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x_2^2}$$

Is this a possible state if the particles are electrons in the same spin state (e.g., $\uparrow\uparrow$)? WHY?

6. The normalized wavefunction for a H-atom electron in a $3p$ state is:

$$\psi = \frac{\left(4 - \frac{2}{3}\, r'\right) r' e^{-r'/3} \cos\theta}{27\sqrt{2\pi}\; a_0^{3/2}}$$

where $r' = r/a_0$ and a_0 is the Bohr radius. Write down the integral that would be required to find the expectation value of z^2 (i.e., $\langle\psi|z^2|\psi\rangle$) for this $3p$ H-atom state. (Include full details—like range of integration—but do not bother to actually evaluate the integral.)

7. Consider the spin $\frac{1}{2}$ operators:

Operator	Eigen vector	Eigen value	Eigen vector	Eigen value
$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 \\ 1 \end{pmatrix}$			
$S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$	$\begin{pmatrix} 1 \\ i \end{pmatrix}$		$\begin{pmatrix} i \\ 1 \end{pmatrix}$	
$S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$	$+\frac{\hbar}{2}$	$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$	$-\frac{\hbar}{2}$

(a) Fill in the five missing entries in the above table: one new eigenvector and four eigenvalues.

(b) Consider the state given by the column vector: $\begin{pmatrix} 5i+1 \\ 3i-1 \end{pmatrix}$.

i. Normalize this state; normalize the S_y eigenvectors.

ii. If S_z is measured, what results will occur? What is the probability of each result?

iii. If S_y is measured, what results will occur? What is the probability of each result?

(c) In class, three different schemes have been use to denote the S_z eigenvectors, with notations like $|sm\rangle$, χ_+, and $\uparrow$. Report the three notations that apply to the eigenvector $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ shown above.