your name(s)____

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Physics 852 Exercise #4b - Friday, Feb. 4th

The radial hydrogen-atom wave functions are

$$\psi_{n,\ell}(r,\theta,\phi) = \left\{ \left(\frac{2}{na_0}\right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]^3} \right\}^{1/2} e^{-r/(na_0)} \left(\frac{2r}{na_0}\right)^\ell L_{n+\ell}^{2\ell+1}\left(\frac{2r}{na_0}\right) Y_{\ell,m}(\theta,\phi).$$

Here, $L_n^k(x)$ are Laguerre polynomials.
Consider the operator

$$A \equiv e^{-R^2/R_0^2} X^2,$$

where R_0 is some arbitrary constant. The operators X, Y, Z are the position operators and $R^2 = X^2 + Y^2 + Z^2$.

1. Write the operator X^2 in terms of a sum over irreducible tensor operators, T_q^k, where you define the operators. (You can find this in the lecture notes or peak at the FYI below).

2. You need to calculate the matrix elements

   $$\langle n,\ell,m|A|0\rangle.$$

   For which values of n,ℓ,m might the matrix element be non-zero? Use the orthogonality properties of spherical harmonics.

3. Repeat (2) but replace A with the operator

   $$B \equiv e^{-R^2/R_0^2} P_x^2,$$

   where P_x, P_y, P_z are the momentum operators. You may wish to use the expression for P_x^2 in spherical coordinates given in the FYI.

4. After completing 1-3, go home and think about how you would go about answering the same questions but with the ket being $|n',\ell',m'\rangle$. Don't do it!

FYI: Some spherical harmonics are:

$$
\begin{aligned}
Y_{0,0} &= \frac{1}{\sqrt{4\pi}}, \\
Y_{1,0} &= \sqrt{\frac{3}{4\pi}} \cos\theta, \\
Y_{1,\pm 1} &= \mp\sqrt{\frac{3}{8\pi}} \sin\theta e^{\pm i\phi}, \\
Y_{2,0} &= \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1), \\
Y_{2,\pm 1} &= \mp\sqrt{\frac{15}{8\pi}} \sin\theta\cos\theta e^{\pm i\phi}, \\
Y_{2,\pm 2} &= \sqrt{\frac{15}{32\pi}} \sin^2\theta e^{\pm 2i\phi}, \\
Y_{\ell -m}(\theta,\phi) &= (-1)^m Y^*_{\ell m}(\theta,\phi).
\end{aligned}
$$

Using the following definition of some irreducible tensor operators,

$$
\begin{aligned}
T^0_0 &= 1, \\
T^1_1 &= -\frac{1}{\sqrt{2}}(x+iy), \\
T^1_0 &= z, \\
T^1_{-1} &= \frac{1}{\sqrt{2}}(x-iy), \\
T^2_2 &= \sqrt{\frac{3}{8}}(x^2+2ixy-y^2), \\
T^2_1 &= -\frac{\sqrt{3}}{2}z(x+iy), \\
T^2_0 &= \frac{1}{2}(3z^2-r^2), \\
T^2_{-1} &= \frac{\sqrt{3}}{2}z(x-iy), \\
T^2_{-2} &= \sqrt{\frac{3}{8}}(x^2-2ixy-y^2),
\end{aligned}
$$

one can express various powers of x, y and z.

$$
\begin{aligned}
1 &= T_0^0, \\
x &= \frac{1}{\sqrt{2}}(T_{-1}^1 - T_1^1), \\
y &= \frac{i}{\sqrt{2}}(T_{-1}^1 + T_1^1), \\
z &= T_0^1, \\
x^2 &= \frac{1}{2}\sqrt{\frac{2}{3}}(T_2^2 + T_{-2}^2) - \frac{1}{3}T_0^2 + \frac{1}{3}T_0^0 r^2, \\
y^2 &= -\frac{1}{2}\sqrt{\frac{2}{3}}(T_2^2 + T_{-2}^2) - \frac{1}{3}T_0^2 + \frac{1}{3}T_0^0 r^2, \\
z^2 &= \frac{2}{3}T_0^2 + \frac{1}{3}T_0^0 r^2, \\
xy &= i\frac{1}{\sqrt{6}}(T_{-2}^2 - T_2^2), \\
xz &= \frac{1}{\sqrt{3}}(T_{-1}^2 - T_1^2), \\
yz &= \frac{i}{\sqrt{3}}(T_{-1}^2 + T_1^2).
\end{aligned}
$$

Some algebra,

$$
\begin{aligned}
\partial_x f(r,\theta,\phi) &= \frac{\partial r}{\partial x}\partial_r f + \frac{\partial \theta}{\partial x}\partial_\theta f + \frac{\partial \phi}{\partial x}\partial_\phi f \\
&= \frac{\sin\theta\cos\phi}{r}\partial_r f + \frac{\cos\theta\cos\phi}{r}\partial_\theta f - \frac{\sin\phi}{r\sin\theta}\partial_\phi f
\end{aligned}
$$

If $f(r,\theta,\phi)$ depends only on r,

$$
\begin{aligned}
\partial_x^2 f(r) &= \left(\frac{\sin\theta\cos\phi}{r}\partial_r + \frac{\cos\theta\cos\phi}{r}\partial_\theta - \frac{\sin\phi}{r\sin\theta}\partial_\phi\right)\frac{\sin\theta\cos\phi}{r}\partial_r f \\
&= \frac{\sin^2\theta\cos^2\phi}{r^2}\partial_r^2 f + (\cos^2\theta\cos^2\phi + \sin^2\phi)\frac{1}{r}\partial_r f \\
&= \frac{\sin^2\theta\cos^2\phi}{r^2}\partial_r^2 f + (1 - \sin^2\theta\cos^2\phi)\frac{1}{r}\partial_r f
\end{aligned}
$$

Solution:
1. Read them off the FYI.

2. Because $x^2\psi_0(r)$ looks like something along the lines of

$$[a + bY_{\ell=2,m=-2}(\theta,\phi) + cY_{\ell=2,m=0}(\theta,\phi) + dY_{\ell=2,m=2}(\theta,\phi)]\psi_0(r),$$

only states with $\ell = 0, m = 0$ or $\ell = 2, m = -2, 0, 2$ can have non-zero overlaps. Any n is possible.

3. By inspection of $\partial_x^2\psi_0(r)$, one can see that the

$$\partial_x^2\psi \sim \alpha(r) + \beta(r)x^2,$$

so the answer is exactly the same as for (2).

4. First, you would have to include all the terms for P_x^2, i.e. include the ones that have derivatives w.r.t. θ or ϕ. Second, the angular integral would involve three powers of spherical harmonics. Yuk!