5. [15] It is often important to find expectations values of operators like \( R_i \), which when acting on a wave function \( \psi \) yields one of the quantities \( \{x, y, z\} \).

(a) [3] Write each of the quantities \( \{x, y, z\} \) in spherical coordinates, and then show how each of them can be written as \( r \) times some linear combination of spherical harmonics. I recommend against trying to “derive” them, just try looking for expressions similar to what you want.

Cartesian coordinates are related to spherical by
\[
x = r \sin \theta \cos \phi, \quad y = r \sin \theta \sin \phi, \quad z = r \cos \theta
\]

Now, glancing at the spherical harmonics, we see that reasonable functions to try would be the \( Y_l^m \)'s for which we have
\[
Y_l^0 (\theta, \phi) = r^{1/2} \sqrt{\frac{3}{2\pi}} \cos \theta = \frac{1}{2} \sqrt{2\pi} z
\]
\[
Y_{l-1}^1 (\theta, \phi) = \mp r^{1/2} \sqrt{\frac{3}{2\pi}} \sin \theta e^{\pm i\phi} = \mp r^{1/2} \sqrt{\frac{3}{2\pi}} \sin \theta (\cos \phi \pm i \sin \phi) = \frac{1}{2} \sqrt{3} \pi (\mp x - iy)
\]
It is pretty easy to see how to write \( z \) in terms of \( Y_l^0 \). For the other two, we note
\[
rY_l^1 (\theta, \phi) + rY_{l-1}^1 (\theta, \phi) = \frac{1}{2} \sqrt{\frac{3}{2\pi}} (-x - iy + x - iy) = -i \sqrt{\frac{3}{2\pi}} y
\]
\[
rY_{l-1}^1 (\theta, \phi) - rY_l^1 (\theta, \phi) = \frac{1}{2} \sqrt{\frac{3}{2\pi}} (x - iy + x + iy) = \frac{3}{2\pi} x
\]
So in summary, we have
\[
x = \sqrt{\frac{2\pi}{3}} r \left[ Y_{l-1}^1 (\theta, \phi) - Y_l^1 (\theta, \phi) \right]
\]
\[
y = \sqrt{\frac{2\pi}{3}} ir \left[ Y_l^1 (\theta, \phi) + Y_{l-1}^1 (\theta, \phi) \right]
\]
\[
z = 2 \sqrt{\frac{\pi}{3}} rY_l^0 (\theta, \phi)
\]

(b) [12] Show that the six quantities \( \{x^2, y^2, z^2, xy, xz, yz\} \) can similarly be written as \( r^2 \) times various combinations of spherical harmonics. There should not be any products or powers of spherical harmonics, so you can’t derive them from part (a).

Inspired by our previous successes, this time we try using the \( Y_{l-1}^m \)'s times \( r^2 \). Writing them out, we have
\[ r^2 Y_0^0 (\theta, \phi) = r^2 \frac{1}{4} \sqrt{\frac{5}{\pi}} \left( 3 \cos^2 \theta - 1 \right) = \frac{1}{4} \sqrt{\frac{5}{\pi}} (2 z^2 - r^2) = \frac{1}{4} \sqrt{\frac{5}{\pi}} \left( 2 z^2 - x^2 - y^2 \right) \]

\[ r^2 Y_2^{\pm 1} (\theta, \phi) = \mp r^2 \frac{1}{2} \sqrt{\frac{15}{2\pi}} \sin \theta \cos \theta e^{\pm i \phi} = \mp \frac{1}{2} \sqrt{\frac{15}{2\pi}} r \sin \theta (\cos \phi \pm i \sin \phi) = \frac{1}{2} \sqrt{\frac{15}{2\pi}} \sin \theta (z \pm i y) \]

\[ r^2 Y_2^{\pm 2} (\theta, \phi) = r^2 \frac{1}{4} \sqrt{\frac{15}{2\pi}} \sin^2 \theta e^{\pm 2i \phi} = \frac{1}{4} \sqrt{\frac{15}{2\pi}} \left[ r \sin \theta (\cos \phi \pm i \sin \phi) \right]^2 = \frac{1}{4} \sqrt{\frac{15}{2\pi}} \left( x \pm iy \right)^2 \]

The cross terms aren't too hard to work out, for example

\[ r^2 \left[ Y_2^1 (\theta, \phi) + Y_2^{-1} (\theta, \phi) \right] = \frac{1}{4} \sqrt{\frac{15}{2\pi}} z (-x - iy + x - iy) = -i \sqrt{\frac{15}{2\pi}} y z \]

\[ r^2 \left[ Y_2^{-1} (\theta, \phi) - Y_2^1 (\theta, \phi) \right] = \frac{1}{2} \sqrt{\frac{15}{2\pi}} z (x + iy + x - iy) = \frac{1}{2} \sqrt{\frac{15}{2\pi}} x z \]

\[ r^2 \left[ Y_2^2 (\theta, \phi) - Y_2^{-2} (\theta, \phi) \right] = \frac{1}{4} \sqrt{\frac{15}{2\pi}} \left[ (x + iy)^2 - (x - iy)^2 \right] = i \sqrt{\frac{15}{2\pi}} x y \]

From these we see that

\[ xy = i \sqrt{\frac{15}{2\pi}} r^2 \left[ Y_2^{-2} (\theta, \phi) - Y_2^2 (\theta, \phi) \right] \]

\[ xz = \frac{1}{2} \sqrt{\frac{15}{2\pi}} r^2 \left[ Y_2^{-1} (\theta, \phi) - Y_2^1 (\theta, \phi) \right] \]

\[ yz = i \sqrt{\frac{15}{2\pi}} r^2 \left[ Y_2^1 (\theta, \phi) + Y_2^{-1} (\theta, \phi) \right] \]

The problem is the other ones. We notice quickly that we can write

\[ 2z^2 - x^2 - y^2 = 4 \sqrt{\frac{\pi}{2}} r^2 Y_0^0 (\theta, \phi) \]

\[ x^2 - y^2 = 2 \sqrt{\frac{15}{2\pi}} r^2 \left[ Y_2^0 (\theta, \phi) + Y_2^{-2} (\theta, \phi) \right] \]

Unfortunately, we can find none of the desired quantities using only these. Hunting around through the other choices, we see that

\[ r^2 = x^2 + y^2 + z^2 = 2 \sqrt{\pi} r^2 Y_0^0 (\theta, \phi) \]

At this point it doesn’t take a genius to see that we can get any combination we want by taking combinations of these three expressions. We have

\[ x^2 = \frac{1}{4} \left( x^2 + y^2 + z^2 \right) - \frac{1}{6} \left( 2z^2 - x^2 - y^2 \right) + \frac{1}{2} \left( x^2 - y^2 \right) \]

\[ = \frac{2}{3} \sqrt{\pi} r^2 Y_0^0 (\theta, \phi) - \frac{2}{3} \sqrt{\frac{15}{2\pi}} r^2 \left[ Y_2^0 (\theta, \phi) + Y_2^{-2} (\theta, \phi) \right] \]

\[ y^2 = \frac{1}{3} \left( x^2 + y^2 + z^2 \right) - \frac{1}{6} \left( 2z^2 - x^2 - y^2 \right) - \frac{1}{2} \left( x^2 - y^2 \right) \]

\[ = \frac{2}{3} \sqrt{\pi} r^2 Y_0^0 (\theta, \phi) - \frac{2}{3} \sqrt{\frac{15}{2\pi}} r^2 \left[ Y_2^0 (\theta, \phi) + Y_2^{-2} (\theta, \phi) \right] \]

\[ z^2 = \frac{1}{4} \left( x^2 + y^2 + z^2 \right) + \frac{1}{3} \left( 2z^2 - x^2 - y^2 \right) = \frac{2}{3} \sqrt{\pi} r^2 Y_0^0 (\theta, \phi) + \frac{1}{3} \sqrt{\frac{15}{2\pi}} r^2 Y_2^0 (\theta, \phi) \]