Physics 741 – Graduate Quantum Mechanics 1

Solutions to Chapter 7

5. [15] It is often important to find expectations values of operators like R_i, which when acting on a wave function ψ 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 the spherical harmonics Y_1^m. 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_1^m's for which we have

$$rY_1^0(\theta,\phi) = r\tfrac{1}{2}\sqrt{\tfrac{3}{\pi}}\cos\theta = \tfrac{1}{2}\sqrt{\tfrac{3}{\pi}}z$$

$$rY_1^{\pm1}(\theta,\phi) = \mp r\tfrac{1}{2}\sqrt{\tfrac{3}{2\pi}}\sin\theta e^{\pm i\phi} = \mp r\tfrac{1}{2}\sqrt{\tfrac{3}{2\pi}}\sin\theta(\cos\phi \pm i\sin\phi) = \tfrac{1}{2}\sqrt{\tfrac{3}{2\pi}}(\mp x - iy)$$

It is pretty easy to see how to write *z* in terms of Y_1^0. For the other two, we note

$$rY_1^1(\theta,\phi) + rY_1^{-1}(\theta,\phi) = \tfrac{1}{2}\sqrt{\tfrac{3}{2\pi}}(-x-iy+x-iy) = -i\sqrt{\tfrac{3}{2\pi}}y$$

$$rY_1^{-1}(\theta,\phi) - rY_1^1(\theta,\phi) = \tfrac{1}{2}\sqrt{\tfrac{3}{2\pi}}(x-iy+x+iy) = \sqrt{\tfrac{3}{2\pi}}x$$

So in summary, we have

$$x = \sqrt{\tfrac{2\pi}{3}}r\left[Y_1^{-1}(\theta,\phi) - Y_1^1(\theta,\phi)\right],\quad y = \sqrt{\tfrac{2\pi}{3}}ir\left[Y_1^1(\theta,\phi) + Y_1^{-1}(\theta,\phi)\right],\quad z = 2\sqrt{\tfrac{\pi}{3}}rY_1^0(\theta,\phi).$$

(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 Y_2^m and Y_0^0. 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_2^m's times r^2. Writing them out, we have

$$r^2Y_2^0(\theta,\phi) = r^2\tfrac{1}{4}\sqrt{\tfrac{5}{\pi}}(3\cos^2\theta - 1) = \tfrac{1}{4}\sqrt{\tfrac{5}{\pi}}(3z^2 - r^2) = \tfrac{1}{4}\sqrt{\tfrac{5}{\pi}}(2z^2 - x^2 - y^2)$$

$$r^2Y_2^{\pm1}(\theta,\phi) = \mp r^2\tfrac{1}{2}\sqrt{\tfrac{15}{2\pi}}\sin\theta\cos\theta e^{\pm i\phi} = \mp\tfrac{1}{2}\sqrt{\tfrac{15}{2\pi}}zr\sin\theta(\cos\phi \pm i\sin\phi) = \tfrac{1}{2}\sqrt{\tfrac{15}{2\pi}}z(\mp x - iy)$$

$$r^2Y_2^{\pm2}(\theta,\phi) = r^2\tfrac{1}{4}\sqrt{\tfrac{15}{2\pi}}\sin^2\theta e^{\pm 2i\phi} = \tfrac{1}{4}\sqrt{\tfrac{15}{2\pi}}\left[r\sin\theta(\cos\phi \pm i\sin\phi)\right]^2 = \tfrac{1}{4}\sqrt{\tfrac{15}{2\pi}}(x \pm iy)^2$$

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

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

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

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

From these we see that

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

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

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

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

$$2z^2-x^2-y^2=4\sqrt{\tfrac{\pi}{5}}r^2Y_2^0(\theta,\phi)$$

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

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

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

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

$$\begin{aligned}
x^2&=\tfrac{1}{3}\left(x^2+y^2+z^2\right)-\tfrac{1}{6}\left(2z^2-x^2-y^2\right)+\tfrac{1}{2}\left(x^2-y^2\right)\\
&=\tfrac{2}{3}\sqrt{\pi}r^2Y_0^0(\theta,\phi)-\tfrac{2}{3}\sqrt{\tfrac{\pi}{5}}r^2Y_2^0(\theta,\phi)+\sqrt{\tfrac{2\pi}{15}}r^2\left[Y_2^2(\theta,\phi)+Y_2^{-2}(\theta,\phi)\right],\\
y^2&=\tfrac{1}{3}\left(x^2+y^2+z^2\right)-\tfrac{1}{6}\left(2z^2-x^2-y^2\right)-\tfrac{1}{2}\left(x^2-y^2\right)\\
&=\tfrac{2}{3}\sqrt{\pi}r^2Y_0^0(\theta,\phi)-\tfrac{2}{3}\sqrt{\tfrac{\pi}{5}}r^2Y_2^0(\theta,\phi)-\sqrt{\tfrac{2\pi}{15}}r^2\left[Y_2^2(\theta,\phi)+Y_2^{-2}(\theta,\phi)\right],\\
z^2&=\tfrac{1}{3}\left(x^2+y^2+z^2\right)+\tfrac{1}{3}\left(2z^2-x^2-y^2\right)=\tfrac{2}{3}\sqrt{\pi}r^2Y_0^0(\theta,\phi)+\tfrac{4}{3}\sqrt{\tfrac{\pi}{5}}r^2Y_2^0(\theta,\phi)
\end{aligned}$$