SPHERICAL HARMONICS: ROTATION ABOUT THE X AXIS

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.5.14.

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

Here's another example of using spherical harmonics to study the behaviour of wave functions in 3-d. Under a rotation by θ_x about the x axis, the coordinates transform using the rotation matrix

$$R(\theta_x\hat{\mathbf{x}}) = \left[\begin{array}{ccc} 1 & 0 & 0 \\ 0 & \cos\theta_x & -\sin\theta_x \\ 0 & \sin\theta_x & \cos\theta_x \end{array}\right] \tag{1}$$

This results in the coordinate transformations

$$x \rightarrow x \tag{2}$$
$$y \rightarrow y\cos\theta_x - z\sin\theta_x \tag{3}$$
$$z \rightarrow z\cos\theta_x + y\sin\theta_x \tag{4}$$

Using similar techniques to those for translations, it is found that the wave function $\psi(x,y,z)$ transforms into the wave function at the position obtained by rotating by $-\theta_x$ (that is, by rotating by θ_x in the opposite direction):

$$\psi(x,y,z) \rightarrow \psi_R = \psi(x, y\cos\theta_x + z\sin\theta_x, z\cos\theta_x - y\sin\theta_x) \tag{5}$$

Suppose we have a wave function given by

$$\psi = Aze^{-r^2/a^2} \tag{6}$$

for some constants a and A. Under this rotation, using 5 it transforms to

$$\psi_R = A(z\cos\theta_x - y\sin\theta_x)e^{-r^2/a^2} \tag{7}$$

[Note that r^2 remains invariant under rotations about the origin, since the distance of a point from the origin is not affected by a rotation. You can verify this directly if you like by working out $r^2 = x^2 + y^2 + z^2$ after the rotation.]

Equatioin 7 differs from the equation given in Shankar, which is

$$\psi_R = A\left(z\cos\theta_x + y\sin\theta_x\right)e^{-r^2/a^2} \tag{8}$$

Curiously, in the errata for Shankar's book (2006 edition) 7 is listed as the incorrect version, which is 'corrected' to 8. In my copy of the book (which doesn't have a date on the title page), 8 is printed, but I don't think this is right. In any case, we'll proceed with the problem.

First, we write 6 in terms of spherical harmonics, using

$$x = \frac{1}{2}\sqrt{\frac{8\pi}{3}}r\left(Y_1^{-1} - Y_1^1\right) \tag{9}$$

$$y = -\frac{1}{2i}\sqrt{\frac{8\pi}{3}}r\left(Y_1^{-1} + Y_1^1\right) \tag{10}$$

$$z = \sqrt{\frac{4\pi}{3}}rY_1^0 \tag{11}$$

We have

$$\psi = A\sqrt{\frac{4\pi}{3}}rY_1^0 e^{-r^2/a^2} \tag{12}$$

With the three spherical harmonics Y_1^1, Y_1^0 and Y_1^{-1} as the basis, we can write this in vector notation as

$$\psi = A\sqrt{\frac{4\pi}{3}}re^{-r^2/a^2}\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \tag{13}$$

A rotation in 3-d for $\ell = 1$ is given by

$$D^{(1)}[R] = I^{(1)} + \frac{\left(\hat{\theta}\cdot\mathbf{J}^{(1)}\right)^2}{\hbar^2}\left(\cos\theta - 1\right) - \frac{i\hat{\theta}\cdot\mathbf{J}^{(1)}}{\hbar}\sin\theta \tag{14}$$

For $\hat{\theta} = \theta_x\hat{\mathbf{x}}$, this works out to

$$D^{(1)}[R(\theta_x\hat{\mathbf{x}})] = \frac{1}{2}\begin{bmatrix} 1+\cos\theta_x & -\sqrt{2}i\sin\theta_x & \cos\theta_x - 1 \\ -\sqrt{2}i\sin\theta_x & 2\cos\theta_x & -\sqrt{2}i\sin\theta_x \\ \cos\theta_x - 1 & -\sqrt{2}i\sin\theta_x & 1+\cos\theta_x \end{bmatrix} \tag{15}$$

We can use this to transform 13 to get

$$\psi_R = D^{(1)}\left[R\left(\theta_x\hat{\mathbf{x}}\right)\right]\psi \tag{16}$$

$$= A\sqrt{\frac{4\pi}{3}}re^{-r^2/a^2}\frac{1}{2}\begin{bmatrix} 1+\cos\theta_x & -\sqrt{2}i\sin\theta_x & \cos\theta_x-1 \\ -\sqrt{2}i\sin\theta_x & 2\cos\theta_x & -\sqrt{2}i\sin\theta_x \\ \cos\theta_x-1 & -\sqrt{2}i\sin\theta_x & 1+\cos\theta_x \end{bmatrix}\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \tag{17}$$

$$= A\sqrt{\frac{\pi}{3}}re^{-r^2/a^2}\begin{bmatrix} -\sqrt{2}i\sin\theta_x \\ 2\cos\theta_x \\ -\sqrt{2}i\sin\theta_x \end{bmatrix} \tag{18}$$

$$= Ae^{-r^2/a^2}\left\{\sqrt{\frac{4\pi}{3}}r\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}\cos\theta_x - \sqrt{\frac{2\pi}{3}}ri\sin\theta_x\left(\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}+\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}\right)\right\} \tag{19}$$

$$= Ae^{-r^2/a^2}\left\{\sqrt{\frac{4\pi}{3}}rY_1^0\cos\theta_x + \frac{1}{2i}\sqrt{\frac{8\pi}{3}}r\left(Y_1^1+Y_1^{-1}\right)\sin\theta_x\right\} \tag{20}$$

$$= Ae^{-r^2/a^2}\left(z\cos\theta_x - y\sin\theta_x\right) \tag{21}$$

where we used 10 to get the last line. This result agrees with 7 and not with the equation 8 given in Shankar, so (provided I got the signs right) it looks like Shankar's equation is wrong.