

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

$$R(\theta_x \hat{\mathbf{x}}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos \theta_x & -\sin \theta_x \\ 0 & \sin \theta_x & \cos \theta_x \end{bmatrix} \quad (1)$$

This results in the coordinate transformations

$$x \rightarrow x \quad (2)$$

$$y \rightarrow y \cos \theta_x - z \sin \theta_x \quad (3)$$

$$z \rightarrow z \cos \theta_x + y \sin \theta_x \quad (4)$$

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):

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

Suppose we have a wave function given by

$$\psi = A z e^{-r^2/a^2} \quad (6)$$

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

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

[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.]

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

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

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

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

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

$$z = \sqrt{\frac{4\pi}{3}} r Y_1^0 \quad (11)$$

We have

$$\psi = A \sqrt{\frac{4\pi}{3}} r Y_1^0 e^{-r^2/a^2} \quad (12)$$

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

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

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

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

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

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

We can use this to transform 13 to get

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

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

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

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

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

$$= A e^{-r^2/a^2} (z \cos \theta_x - y \sin \theta_x) \quad (21)$$

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.