

## E462: Wave function rotation

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### The problem:

A particle is described by the wave function:

$$\psi(\vec{r}) = f(r)(\sqrt{2} \sin \theta \cos \phi + \cos \theta)$$

We rotate the wave function 90 degrees around the Y axis, and then 90 degrees around the Z axis. what is the new wave function?

(1) The simpler way is to switch to cartesian coordinates, and use euclidean (spatial) rotation matrix.

(2) Another way, more complex, is to present the wave function as a superposition of  $Y^{lm}(\theta, \phi)$  and to use the standard rotation matrix over the coefficients vector.

### The solution:

(1) In cartesian coordinates  $\hat{r}$  is represented as  $\hat{r} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$  therefore:

$$\psi(\vec{r}) = f(r)(\sqrt{2}\hat{x} + \hat{z})$$

Lucky for us  $f(r)$  is invariant to rotation. Vector presentation of  $\psi(\vec{r})$  in the euclidean basis:

$$\psi(\vec{r}) \rightarrow f(r) \begin{pmatrix} \sqrt{2} \\ 0 \\ 1 \end{pmatrix}$$

The euclidean 90 degrees rotation matrix around Y and Z:

$$R_y(90^0) = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \quad ; \quad R_z(90^0) = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Now all is left to do is multiply the rotation matrix with the wave function:

$$\tilde{\psi}(\vec{r}) = R_z(90^0)R_y(90^0)\psi(\vec{r}) = f(r) \begin{pmatrix} 1 \\ 0 \\ \sqrt{2} \end{pmatrix} = f(r)(\sin \theta \cos \phi - \sqrt{2} \cos \theta)$$

(2) Using the following  $Y^{lm}$

$$Y^{10} = \sqrt{\frac{3}{4\pi}} \cos \theta \quad ; \quad Y^{1-1} = \sqrt{\frac{3}{8\pi}} \sin \theta e^{-i\phi} \quad ; \quad Y^{11} = -\sqrt{\frac{3}{8\pi}} \sin \theta e^{i\phi}$$

We obtain:

$$\psi(\vec{r}) = f(r)(\sqrt{2}\frac{1}{2}\sqrt{\frac{8\pi}{3}}(Y^{1-1} - Y^{11}) + \sqrt{\frac{4\pi}{3}}Y^{10}) = f(r)\sqrt{\frac{4\pi}{3}}(Y^{1-1} + Y^{10} - Y^{11})$$

Presented as Vector in the standard basis:

$$\psi(\vec{r}) \rightarrow f(r)\sqrt{\frac{4\pi}{3}} \begin{pmatrix} -1 \\ 1 \\ 1 \end{pmatrix}$$

The standard rotation matrix of 90 degrees is derived from the generators of rotations  $S_n$  in the standard basis:

$$U(\bar{\Phi}) = e^{-i\bar{\Phi} \cdot \bar{S}_n} = 1 - (1 - \cos \Phi) S_n^2 - i \sin \Phi S_n$$

$$U_y(90^\circ) = \begin{pmatrix} \frac{1}{2} & -\frac{1}{\sqrt{2}} & \frac{1}{2} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \end{pmatrix} ; \quad U_z(90^\circ) = \begin{pmatrix} -i & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & i \end{pmatrix}$$

Multiplication of those rotations with the wave function gives the following:

$$\tilde{\psi}(\bar{r}) = U_z(90^\circ) U_y(90^\circ) \psi(\bar{r}) = f(r) \sqrt{\frac{4\pi}{3}} \begin{pmatrix} \frac{i}{2} \\ -\sqrt{2} \\ \frac{i}{2} \end{pmatrix}$$

Switching back to spherical coordinates:

$$\tilde{\psi}(\bar{r}) = f(r) \sqrt{\frac{4\pi}{3}} \left( \frac{i}{2} Y^{1-1} - \sqrt{2} Y^{10} + \frac{i}{2} Y^{11} \right) = f(r) (\sin \theta \cos \phi - \sqrt{2} \cos \theta)$$

To verify - we get the same result as (1).