

[Link to Mathematica .nb file](#)

Definitions

Normalization constants

$$\text{In[1]:= } A[l_ , m_] := \sqrt{\frac{(2 - \text{KroneckerDelta}[m, 0]) (2 l + 1) (l - m)!}{4 \pi (l + m)!}};$$

$$B[l_ , m_ , j_ , k_] := \frac{2^l m! \left(\frac{l+m+k-1}{2}\right)!}{j! k! (m-j)! (l-m-k)! \left(\frac{-l+m+k-1}{2}\right)!};$$

Spherical harmonics in $x^i y^j z^k$ form

$$\text{In[3]:= } Y_{xyz}[l_ , m_ , x_ , y_ , z_] := \begin{cases} \text{Sum}[\text{Sum}[(-1)^{\frac{j}{2}} A[l, m] B[l, m, j, k] x^{m-j} y^j z^k, \{k, 0, l-m\}], \{ \\ \text{Sum}[\text{Sum}[(-1)^{\frac{j-1}{2}} A[l, \text{Abs}[m]] B[l, \text{Abs}[m], j, k] x^{\text{Abs}[m]-j} y^j z^k, \\ \{j, 1, \text{Abs}[m], 2\}] \end{cases}$$

Spherical harmonics in contracted form

$$\text{In[4]:= } Y[l_ , m_ , x_ , y_] := \text{Expand}[\text{FullSimplify}[Y_{xyz}[l, m, x, y, \sqrt{1-x^2-y^2}]]] /. \sqrt{1-x^2-y^2} \rightarrow z;$$

As a check, compute them from Mathematica's complex SphericalHarmonicY function

$$\text{In[5]:= } Y\theta\phi[l_ , m_ , \theta_ , \phi_] := \text{If}[m == 0, \\ \text{SphericalHarmonicY}[l, 0, \theta, \phi], \\ \text{If}[m < 0, \\ \frac{i}{\sqrt{2}} (\text{SphericalHarmonicY}[l, m, \theta, \phi] + (-1)^{m+1} \text{SphericalHarmonicY}[l, -m, \theta, \phi]), \\ \frac{1}{\sqrt{2}} (\text{SphericalHarmonicY}[l, -m, \theta, \phi] + (-1)^m \text{SphericalHarmonicY}[l, m, \theta, \phi])];$$

Benchmarks

Compare to the Mathematica version up to $l_{\max} = 10$

$$\text{In[6]:= } \text{With}[\{l_{\max} = 10\}, \text{AllTrue}[\text{Assuming}[\theta \in \text{Reals} \ \&\& \ \text{Cos}[\theta] \geq 0, \text{Flatten}[\text{Table}[\text{FullSimplify}[Y[l, m, \text{Sin}[\theta] \text{Cos}[\phi], \text{Sin}[\theta] \text{Sin}[\phi]] == Y\theta\phi[l, m, \theta, \phi]], \{l, 0, 3\}, \{m, -l, l\}]]], \text{TrueQ}]]$$

Out[6]= True

Examples

Show the spherical harmonics up to $l_{\max} = 4$

```
In[7]:= With[{lmax = 4},
  Grid[Table[CenterArray[Table[Text[Style[Y[l, m, x, y], FontSize → 7]], {m, -l, l}],
    2 lmax + 1, ""], {l, 0, lmax}], Frame → All]]
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Out[7]=

				$\frac{1}{2\sqrt{\pi}}$				
			$\frac{1}{2}\sqrt{\frac{3}{\pi}}y$	$\frac{1}{2}\sqrt{\frac{3}{\pi}}z$	$\frac{1}{2}\sqrt{\frac{3}{\pi}}x$			
		$\frac{1}{2}\sqrt{\frac{15}{\pi}}xy$	$\frac{1}{2}\sqrt{\frac{15}{\pi}}yz$	$\frac{\sqrt{5}}{2} - \frac{3}{4}\sqrt{\frac{5}{\pi}}x^2 - \frac{3}{4}\sqrt{\frac{5}{\pi}}y^2$	$\frac{1}{2}\sqrt{\frac{15}{\pi}}xz$	$\frac{1}{4}\sqrt{\left(\frac{15}{\pi}\right)}x^2 - \frac{1}{4}\sqrt{\left(\frac{15}{\pi}\right)}y^2$		
	$\frac{3}{4}\sqrt{\left(\frac{35}{2\pi}\right)}x^2y - \frac{1}{4}\sqrt{\left(\frac{35}{2\pi}\right)}y^3$	$\frac{1}{2}\sqrt{\frac{105}{\pi}}xyz$	$\sqrt{\frac{21}{2\pi}}y - \frac{5}{4}\sqrt{\left(\frac{21}{2\pi}\right)}x^2y - \frac{5}{4}\sqrt{\left(\frac{21}{2\pi}\right)}y^3$	$\frac{1}{2}\sqrt{\frac{7}{\pi}}z - \frac{5}{4}\sqrt{\frac{7}{\pi}}x^2z - \frac{5}{4}\sqrt{\frac{7}{\pi}}y^2z$	$\sqrt{\frac{21}{2\pi}}x - \frac{5}{4}\sqrt{\left(\frac{21}{2\pi}\right)}x^3 - \frac{5}{4}\sqrt{\left(\frac{21}{2\pi}\right)}xy^2$	$\frac{1}{4}\sqrt{\left(\frac{105}{\pi}\right)}x^2z - \frac{1}{4}\sqrt{\left(\frac{105}{\pi}\right)}y^2z$	$\frac{1}{4}\sqrt{\left(\frac{35}{2\pi}\right)}x^3 - \frac{3}{4}\sqrt{\left(\frac{35}{2\pi}\right)}xy^2$	
$\frac{3}{4}\sqrt{\left(\frac{35}{\pi}\right)}x^3y - \frac{3}{4}\sqrt{\left(\frac{35}{\pi}\right)}xy^3$	$\frac{9}{4}\sqrt{\left(\frac{35}{2\pi}\right)}x^2yz - \frac{3}{4}\sqrt{\left(\frac{35}{2\pi}\right)}y^3z$	$\frac{9}{2}\sqrt{\frac{5}{\pi}}xy - \frac{21}{4}\sqrt{\frac{5}{\pi}}x^3y - \frac{21}{4}\sqrt{\frac{5}{\pi}}xy^3$	$3\sqrt{\left(\frac{5}{2\pi}\right)}yz - \frac{21}{4}\sqrt{\left(\frac{5}{2\pi}\right)}x^2yz - \frac{21}{4}\sqrt{\left(\frac{5}{2\pi}\right)}y^3z$	$\frac{3}{2\sqrt{\pi}} - \frac{15x^2}{2\sqrt{\pi}} + \frac{(105x^4)}{(16\sqrt{\pi})} - \frac{15y^2}{2\sqrt{\pi}} + \frac{(105x^2y^2)}{(8\sqrt{\pi})} + \frac{(105y^4)}{(16\sqrt{\pi})}$	$3\sqrt{\left(\frac{5}{2\pi}\right)}xz - \frac{21}{4}\sqrt{\left(\frac{5}{2\pi}\right)}x^3z - \frac{21}{4}\sqrt{\left(\frac{5}{2\pi}\right)}xy^2z$	$\frac{9}{4}\sqrt{\frac{5}{\pi}}x^2 - \frac{21}{8}\sqrt{\frac{5}{\pi}}x^4 - \frac{9}{4}\sqrt{\frac{5}{\pi}}y^2 + \frac{21}{8}\sqrt{\frac{5}{\pi}}y^4$	$\frac{3}{4}\sqrt{\left(\frac{35}{2\pi}\right)}x^3z - \frac{9}{4}\sqrt{\left(\frac{35}{2\pi}\right)}xy^2z$	$\frac{3}{16}\sqrt{\left(\frac{35}{\pi}\right)}x^4 - \frac{9}{8}\sqrt{\left(\frac{35}{\pi}\right)}x^2y^2 + \frac{3}{16}\sqrt{\left(\frac{35}{\pi}\right)}y^4$