Link to Mathematica .nb file

Definitions

Define the spherical harmonics

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

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

$$\texttt{Yxyz[l\_, m\_, x\_, y\_, z\_]} := \begin{cases} \texttt{Sum}\left[\texttt{Sum}\left[(-1)^{\frac{j}{2}}\ \texttt{A[l, m] B[l, m, j, k]}\ x^{m-j}\ y^{j}\ z^{k},\ \{k, 0, l - m\}\right], \{ \right. \\ \texttt{Sum}\left[\texttt{Sum}\left[(-1)^{\frac{j-1}{2}}\ \texttt{A[l, Abs[m]] B[l, Abs[m], j, k]}\ x^{\texttt{Abs[m]}-j}\ y^{j}\ z^{k}, \right.\right. \\ \left. \{j, 1, \texttt{Abs[m]}, 2\}\right] \end{cases}$$

$$\texttt{Y[l\_, m\_, x\_, y\_, z\_]} :=$$
$$\texttt{Expand}\left[\texttt{FullSimplify}\left[\texttt{Yxyz}\left[l, m, x, y, \sqrt{1 - x^2 - y^2}\right]\right]\right]\ /.\ \sqrt{1 - x^2 - y^2} \to z;$$

Bases

Compute our spherical harmonic basis **by**

```
by[n_, x_, y_, z_] := Module[{l, m},
    l = Floor[√n];
    m = n - l² - l;
    Y[l, m, x, y, z]];
```

```
Table[by[n, x, y, z], {n, 0, 8}] // TableForm
```

$$\frac{1}{2\sqrt{\pi}}$$

$$\frac{1}{2}\sqrt{\frac{3}{\pi}}\ y$$

$$\frac{1}{2}\sqrt{\frac{3}{\pi}}\ z$$

$$\frac{1}{2}\sqrt{\frac{3}{\pi}}\ x$$

$$\frac{1}{2}\sqrt{\frac{15}{\pi}}\ x\ y$$

$$\frac{1}{2}\sqrt{\frac{15}{\pi}}\ y\ z$$

$$\frac{\sqrt{\frac{5}{\pi}}}{2} - \frac{3}{4}\sqrt{\frac{5}{\pi}}\ x^2 - \frac{3}{4}\sqrt{\frac{5}{\pi}}\ y^2$$

$$\frac{1}{2}\sqrt{\frac{15}{\pi}}\ x\ z$$

$$\frac{1}{4}\sqrt{\frac{15}{\pi}}\ x^2 - \frac{1}{4}\sqrt{\frac{15}{\pi}}\ y^2$$

Compute our polynomial basis **bp**

```
bp[n_, x_, y_, z_] := Module[{l, m, μ, ν},
   l = Floor[√n];
   m = n - l^2 - l;
   μ = l - m;
   ν = l + m;
   If[EvenQ[ν], x^(μ/2) y^(ν/2), x^((μ-1)/2) y^((ν-1)/2) z]];
```

```
Table[bp[n, x, y, z], {n, 0, 8}] // TableForm
```

1
x
z
y
x^2
x z
x y
y z
y^2

Compute the spherical harmonic vectors in the polynomial basis, **p**

```
p[l_, m_, lmax_] := Module[{Ylm},
   Ylm = Y[l, m, x, y, z];
   Table[If[n == 0, Ylm, Coefficient[Ylm, bp[n, x, y, z]]] /. {x → 0, y → 0, z → 0},
    {n, 0, (lmax + 1)^2 - 1}]];
```

The columns of the change of basis matrix $\boldsymbol{A_1}$ are just **p**

```
A1[lmax_] := Transpose[Flatten[Table[p[l, m, lmax], {l, 0, lmax}, {m, -l, l}], 1]];
```

```
A1[2] // MatrixForm
```

$$
\begin{pmatrix}
\frac{1}{2\sqrt{\pi}} & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{\frac{5}{\pi}}}{2} & 0 & 0 \\
0 & 0 & 0 & \frac{\sqrt{\frac{3}{\pi}}}{2} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \frac{\sqrt{\frac{3}{\pi}}}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{\sqrt{\frac{3}{\pi}}}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -\frac{3\sqrt{\frac{5}{\pi}}}{4} & 0 & \frac{\sqrt{\frac{15}{\pi}}}{4} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{\frac{15}{\pi}}}{2} & 0 \\
0 & 0 & 0 & 0 & \frac{\sqrt{\frac{15}{\pi}}}{2} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{\sqrt{\frac{15}{\pi}}}{2} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -\frac{3\sqrt{\frac{5}{\pi}}}{4} & 0 & -\frac{\sqrt{\frac{15}{\pi}}}{4}
\end{pmatrix}
$$

LaTeXify

Make $\boldsymbol{A}_{\mathbf{l}}$ LaTeX-friendly

$$\texttt{A1TeX[lmax\_] := TeXForm}\left[\frac{1}{2\sqrt{\pi}}\right]\ \texttt{TeXForm}\left[\texttt{FullSimplify}\left[2\sqrt{\pi}\ \texttt{A1[lmax]}\right]\right];$$

Print $\boldsymbol{A}_{\mathbf{l}}$ for $l_{max} = 2$

```
A1TeX[2]
```

```
\frac{1}{2 \sqrt{\pi }} \left(
\begin{array}{ccccccccc}
 1 & 0 & 0 & 0 & 0 & 0 & \sqrt{5} & 0 & 0 \\
 0 & 0 & 0 & \sqrt{3} & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & \sqrt{3} & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & \sqrt{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & -\frac{3 \sqrt{5}}{2} & 0 & \frac{\sqrt{15}}{2} \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sqrt{15} & 0 \\
 0 & 0 & 0 & 0 & \sqrt{15} & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & \sqrt{15} & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & -\frac{3 \sqrt{5}}{2} & 0 & -\frac{\sqrt{15}}{2} \\
\end{array}
\right)
```