```
> restart;
> interface(warnlevel = 0) :        #
```

Maple 12

```
> with(LinearAlgebra) :
> with(plots) :
```

This is Problem 4 from Chapter 3

Defining the H operator/matrix in the standard basis {x, y, z}

```
> H := Matrix([[1, 0, 0], [0, 0, 2], [0, 2, 0]]);
```

$$H := \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 2 \\ 0 & 2 & 0 \end{bmatrix} \quad \textbf{(1)}$$

Finding the roots of the characteristic polynomial (CP) to obtain the eigenvalues of matrix H

```
> CharacteristicPolynomial(H, λ);   # the polynomial in terms of λ
  factor(%);                        # factor the polynomial
  solve( %= 0, [λ]);                # the root of the polynomial by solving CP = 0
```

$$4 + \lambda^3 - \lambda^2 - 4\,\lambda$$
$$(\lambda - 1)\ (\lambda - 2)\ (\lambda + 2)$$
$$[[\lambda = 1], [\lambda = 2], [\lambda = -2]] \quad \textbf{(2)}$$

Determining the eigenvalues and eigenvectors of matrix H using Maple's Eigenvectors() function

```
> L := Eigenvectors(H) :     # a list of the eigenvalues with their corresponding eigenvectors
  print(eigenvalue = L[1][1], eigenvector =L[2][1 ..3, 1]);
  print(eigenvalue = L[1][2], eigenvector = L[2][1 ..3, 2] );
  print(eigenvalue = L[1][3],  eigenvector = L[2][1 ..3, 3]);
```

$$eigenvalue = 2, eigenvector = \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix}$$

$$eigenvalue = 1, eigenvector = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

$$eigenvalue = -2, eigenvector = \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix} \quad \textbf{(3)}$$

Defining the state vector $|\psi\rangle \equiv$ Y in the standard basis {x, y, z}

> Y := $\frac{1}{3} \cdot Vector([2, 2, 1]);$

$$Y := \begin{bmatrix} \frac{2}{3} \\ \frac{2}{3} \\ \frac{1}{3} \end{bmatrix} \qquad (4)$$

Calculating the Expectation Value

$$\langle \mathbf{H} \rangle = \langle \psi | \mathbf{H} | \psi \rangle$$

> 'E Value'= Multiply(Transpose(Y), Multiply(H, Y));

$$E\ \ Value = \frac{4}{3} \qquad (5)$$

Defining the matrix S^{-1} as the transformation matrix from basis $\{v_1, v_2, v_3\}$ to basis {x, y, z}.
The columns of the matrix are the vectors v_1, v_2, v_3

$$\mathbf{v_1 = x,} \quad \mathbf{v_2} = \frac{-\mathbf{y}+\mathbf{z}}{\sqrt{2}}, \quad \mathbf{v_3} = \frac{\mathbf{y}+\mathbf{z}}{\sqrt{2}};$$

> $\mathbb{S}$:=Matrix$\left(\left[[1, 0, 0], \left[0, -\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right], \left[0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right]\right]\right);$

$$\mathbb{S} := \begin{bmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{2}\sqrt{2} & \frac{1}{2}\sqrt{2} \\ 0 & \frac{1}{2}\sqrt{2} & \frac{1}{2}\sqrt{2} \end{bmatrix} \qquad (6)$$

Defining the transformation matrix S from basis {x, y, z} to basis $\{v_1, v_2, v_3\}$

> S := MatrixInverse($\mathbb{S}$);

$$S := \begin{bmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{2}\sqrt{2} & \frac{1}{2}\sqrt{2} \\ 0 & \frac{1}{2}\sqrt{2} & \frac{1}{2}\sqrt{2} \end{bmatrix} \qquad (7)$$

Notice that these two matrices are equal

> '$\mathbb{S}\cdot S$'= Multiply($\mathbb{S}$, S);

$$\mathbb{S}\ S = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (8)$$

Matrix S is a symmetric matrix: S = S^T

> ST := Transpose(S);

$$ST := \begin{bmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{2}\sqrt{2} & \frac{1}{2}\sqrt{2} \\ 0 & \frac{1}{2}\sqrt{2} & \frac{1}{2}\sqrt{2} \end{bmatrix} \quad (9)$$

Matrix S is an orthogonal matrix

The column inner product of matrix S is zero; columns are orthogonal

> '$\langle c_1|c_2\rangle$'= DotProduct(S[1 ..3, 1], S[1 ..3, 2]);
> '$\langle c_1|c_3\rangle$' = DotProduct(S[1 ..3, 1], S[1 ..3, 3]);
> '$\langle c_2|c_3\rangle$' = DotProduct(S[1 ..3, 2], S[1 ..3, 3]);

$$\langle c\ \ 1|c\ \ 2\rangle = 0$$
$$\langle c\ \ 1|c\ \ 3\rangle = 0$$
$$\langle c\ \ 2|c\ \ 3\rangle = 0 \quad (10)$$

The row inner product of matrix S is also zero.

> '$\langle r_1|r_2\rangle$'= DotProduct(S[1, 1 ..3], S[2, 1 ..3]);
> '$\langle r_1|r_3\rangle$' = DotProduct(S[1, 1 ..3], S[3, 1 ..3]);
> '$\langle r_2|r_3\rangle$' = DotProduct(S[2, 1 ..3], S[3, 1 ..3]);

$$\langle r\ \ 1|r\ \ 2\rangle = 0$$
$$\langle r\ \ 1|r\ \ 3\rangle = 0$$
$$\langle r\ \ 2|r\ \ 3\rangle = 0 \quad (11)$$

The length of the columns and rows of matrix S is 1

> print(`$\|c_1\|$` = Norm(S[1 ..3, 1], Euclidean));
> print(`$\|c_2\|$` = Norm(S[1 ..3, 2], Euclidean));
> print(`$\|c_3\|$` = Norm(S[1 ..3, 3], Euclidean)); print( );
> print(`$\|r_1\|$` = Norm(S[1, 1 ..3], Euclidean));
> print(`$\|r_2\|$` = Norm(S[2, 1 ..3], Euclidean));
> print(`$\|r_3\|$` = Norm(S[3, 1 ..3], Euclidean));

$$||c1|| = 1$$
$$||c2|| = 1$$
$$||c3|| = 1$$

$$||r1|| = 1$$
$$||r2|| = 1$$
$$||r3|| = 1 \quad (12)$$

The inverse of an orthogonal matrix is its own transpose. Thus $S^{-1} = S^T = S$

Defining the state vector $|\psi'\rangle \equiv \mathbb{Y}$ in the new basis $\{v_1, v_2, v_3\}$

> $\mathbb{Y} := Multiply(S, Y);$

$$\mathbb{Y} := \begin{bmatrix} \frac{2}{3} \\ -\frac{1}{6}\sqrt{2} \\ \frac{1}{2}\sqrt{2} \end{bmatrix} \quad \textbf{(13)}$$

Changing from one basis to another

$|\psi'\rangle = S\,|\psi\rangle$

$|\psi\rangle = S^{-1}\,|\psi'\rangle = S\,|\psi'\rangle$

> $\mathbb{Y} := Multiply(S, Y);$

$$\mathbb{Y} := \begin{bmatrix} \frac{2}{3} \\ -\frac{1}{6}\sqrt{2} \\ \frac{1}{2}\sqrt{2} \end{bmatrix} \quad \textbf{(14)}$$

> $Y := Multiply(\mathbb{S}, \mathbb{Y});$

$$Y := \begin{bmatrix} \frac{2}{3} \\ \frac{2}{3} \\ \frac{1}{3} \end{bmatrix} \quad \textbf{(15)}$$

Determining the operator $\mathbb{H}$ in the $\{v_1, v_2, v_3\}$ basis

$\mathbb{H} = S \cdot H \cdot S^{-1}$

> $\mathbb{H} := Multiply(S, Multiply(H, \mathbb{S}));$

$$\mathbb{H} := \begin{bmatrix} 1 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 2 \end{bmatrix} \quad \textbf{(16)}$$

The main diagonal lists the eigenvalues

Calculating the Expectation Value in the new basis $\{v_1, v_2, v_3\}$

$$\langle \mathbb{H} \rangle = \langle \psi' | \mathbb{H} | \psi' \rangle$$

```
> 'E Value'= Multiply(Transpose(𝕐), Multiply(ℍ, 𝕐));
```

$$E\ \ Value = \frac{4}{3} \quad (17)$$

Define the basis vectors:

basis set 1 { x, y, z }; the standard basis

basis set 2 { v1, v2, v3 }

Notice that these are orthogonal bases: x • y = x · z = y · z = 0

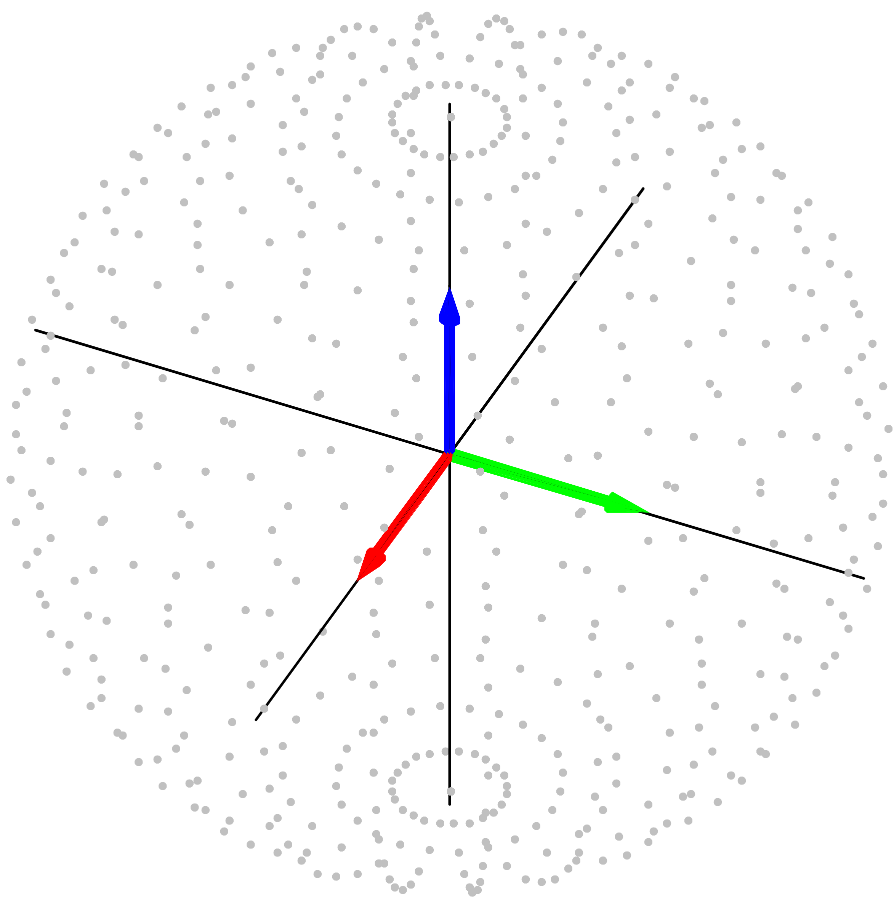
v1 · v2 = v1 · v3 = v2 · v3 =0

```
> e1 := Vector([1, 0, 0]) : e2 := Vector([0, 1, 0]) :
  e3 := Vector([0, 0, 1]) : v1 := Vector([1, 0, 0]) :
```

$$v2 := \frac{1}{\sqrt{2}} \cdot \text{Vector}([0, -1, 1]) : v3 := \frac{1}{\sqrt{2}} \cdot \text{Vector}([0, 1, 1]) :$$

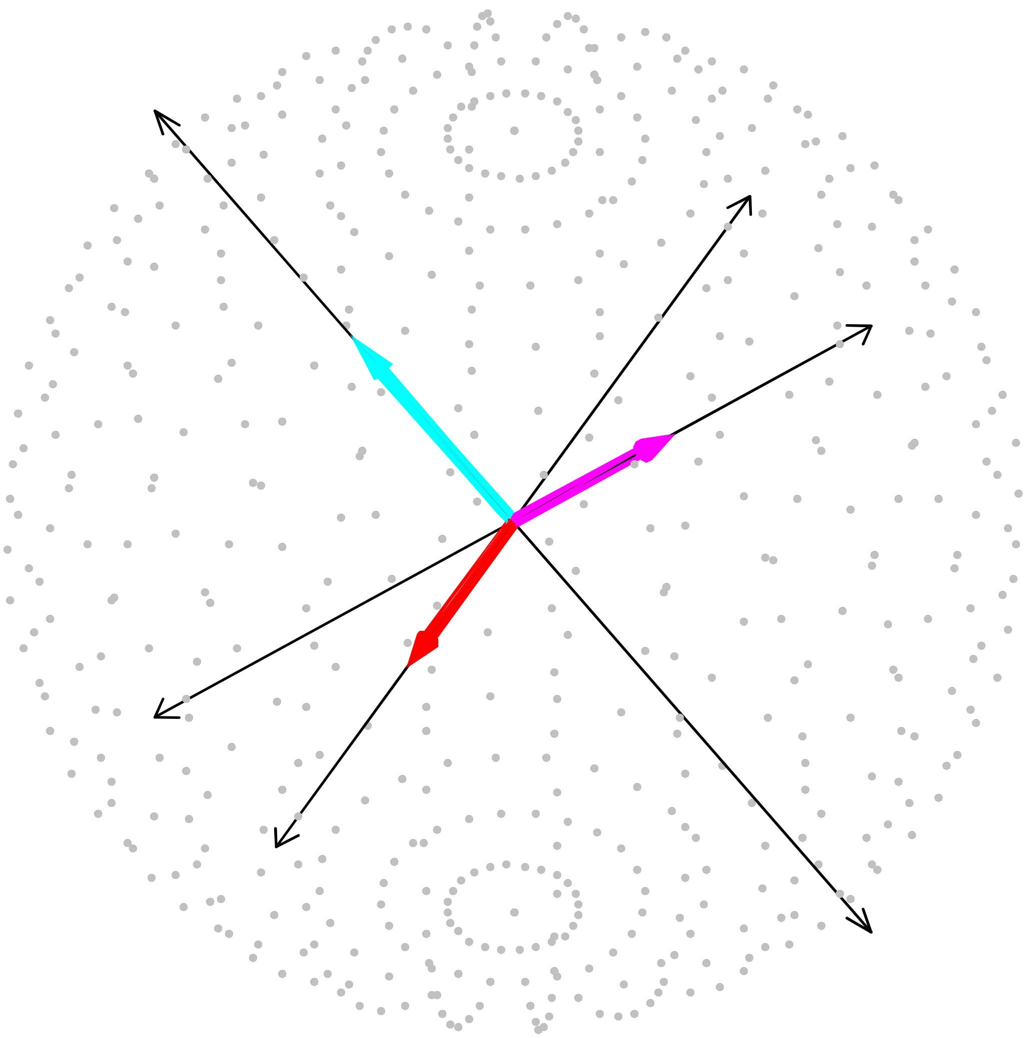
Plotting the standard basis { x, y, z }

```
> sp := plottools[sphere]([0, 0, 0], 2, style = point, color = gray) :
  x := arrow(e1, color = red, width = 0.05) : y := arrow(e2, color = green, width = 0.05) :
  z := arrow(e3, color = blue, width = 0.05) :
  display([x, y, z, sp], axes = normal, scaling = constrained, tickmarks = [2, 2, 2], orientation = [25, 50]);
```



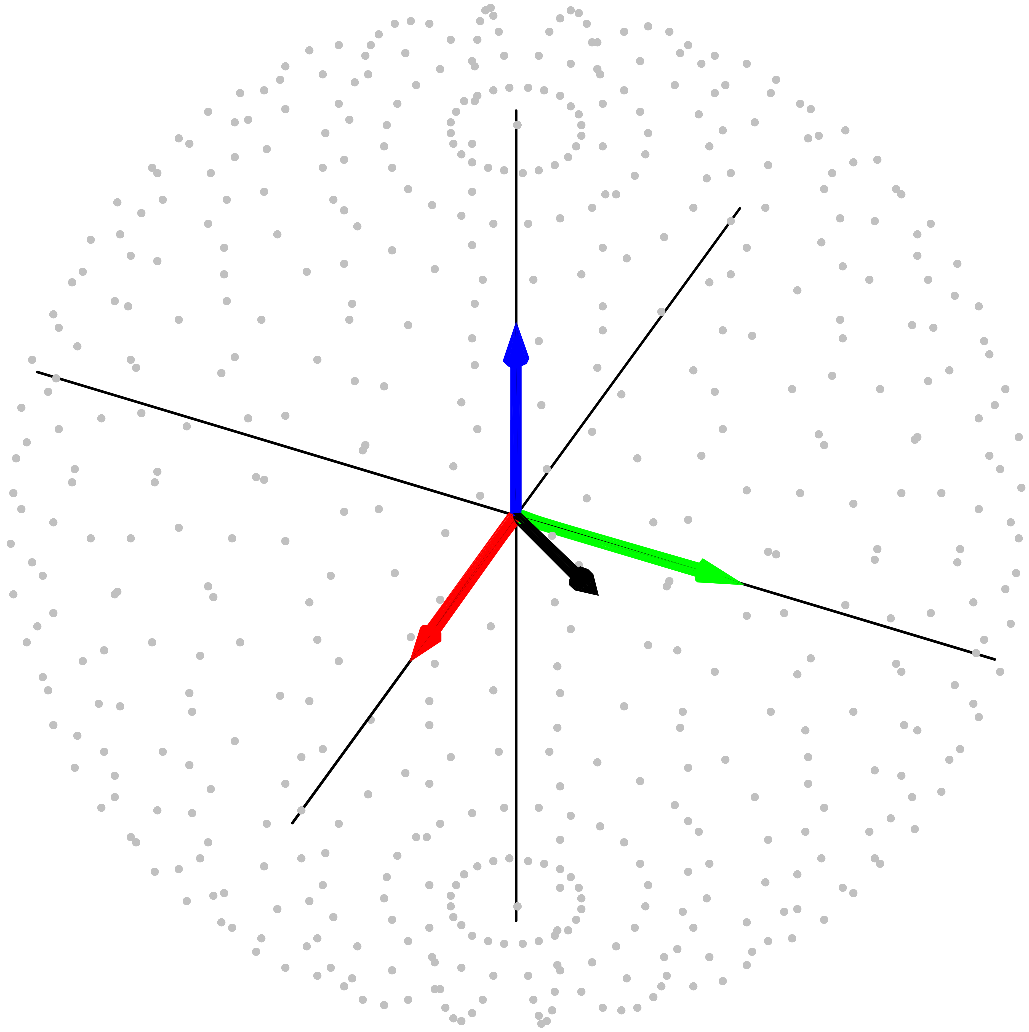
Plotting basis { v1, v2, v3 }

```
> u1 := arrow(v1, color = red, width = 0.05) :
  u2 := arrow(v2, color = cyan, width = 0.05) :
  u3 := arrow(v3, color = magenta, width = 0.05) :
  a := arrow(2.2· v1, color = black, width = 0.05, shape = arrow, head_length = 0.1, head_width = 0.1) :
  b := arrow(2.2· v2, color = black, width = 0.05, shape = arrow, head_length = 0.1, head_width = 0.1) :
  c := arrow(2.2 · v3, color = black, width = 0.05, shape = arrow, head_length = 0.1, head_width = 0.1) :
  d := arrow(− 2.2· v1, color = black, width = 0.05, shape = arrow, head_length = 0.1, head_width = 0.1) :
  e := arrow( − 2.2· v2, color = black, width = 0.05, shape = arrow, head_length = 0.1, head_width = 0.1) :
  f := arrow(− 2.2· v3, color = black, width = 0.05, shape = arrow, head_length = 0.1, head_width = 0.1) :
  display([u1, u2, u3, a, b, c, d, e, f, sp], axes = none, scaling = constrained, orientation = [25, 50]);
```



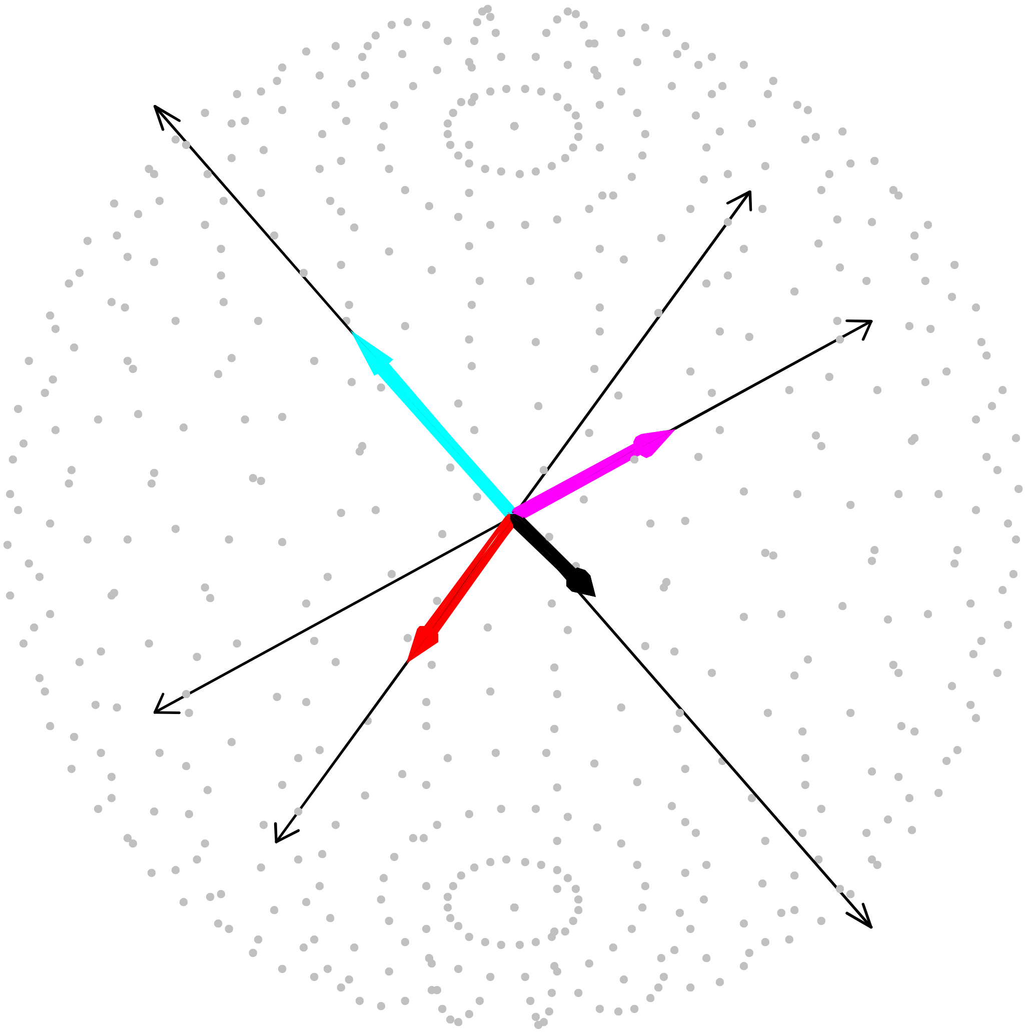
Plotting the state vector Y and the standard basis

> $ay := arrow(Y, color = black) : display([\mathrm{x}, \mathrm{y}, \mathrm{z}, ay, sp], \mathrm{axes} = \mathrm{normal}, \mathrm{scaling} = \mathrm{constrained}, \ \mathrm{tickmarks} = [2, 2, 2], orientation = [25, 50]);$



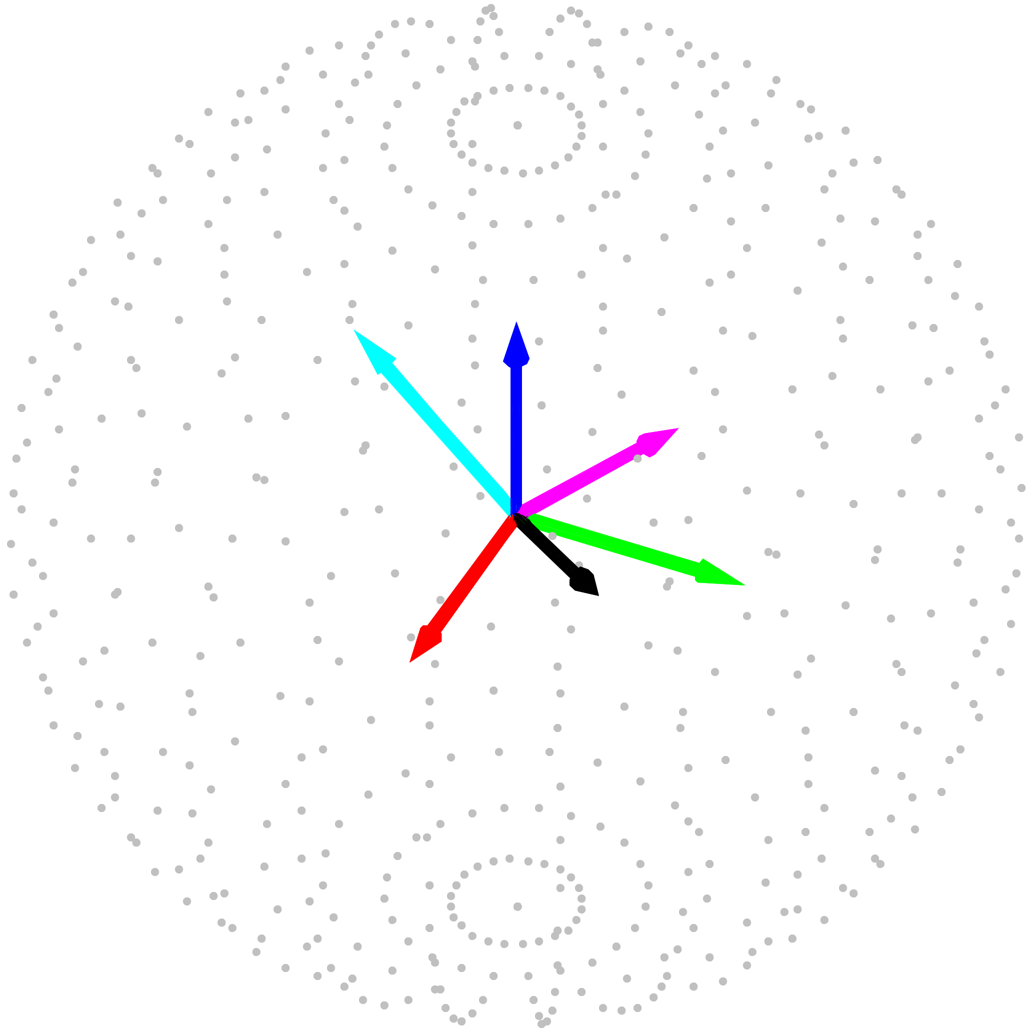
Plotting the state vector Y and basis { v1, v2, v3 }

> display([u1, u2, u3, *a*, *b*, *c*, *d*, *e*, *f*, *ay*, *sp*], axes = *none*, scaling = constrained, *orientation* = [25, 50]);



Plotting the state vector Y and both bases

```
> display([x, y, z, u1, u2, u3, ay, sp], axes = none, scaling = constrained, orientation = [25, 50]);
```



> display([x, y, z, u1, u2, u3, *a*, *b*, *c*, *d*, *e*, *f*, *ay*, *sp*], axes = *normal*, *tickmarks* = [0, 0, 0],
scaling = constrained, *orientation* = [25, 50]);