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

Maple 12

This is Problem 5 from Chapter 3

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

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

$$K := \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \tag{1}$$

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

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

$$\lambda^3 - 3\lambda^2 + 2\lambda$$
$$\lambda(\lambda - 1)(\lambda - 2)$$
$$[[\lambda = 0], [\lambda = 1], [\lambda = 2]] \tag{2}$$

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

```
> L := Eigenvectors(K) :       # 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]);
```

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

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

$$eigenvalue = 1, eigenvector = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \tag{3}$$

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

> $Y := \frac{1}{\sqrt{2}} \cdot Vector([0, 1, 1]);$

$$Y := \begin{bmatrix} 0 \\ \frac{1}{2}\sqrt{2} \\ \frac{1}{2}\sqrt{2} \end{bmatrix} \tag{4}$$

Calculating the Expectation Value: $\langle K\rangle = \langle\psi|K|\psi\rangle$

> $'E\ \ Value' = Multiply(Transpose(Y), Multiply(K, Y));$

$$E\ \ Value = 1 \tag{5}$$

Defining the matrix S^{-1} as the transformation matrix from basis $\{u_1, u_2, u_3\}$ to basis {x, y, z}.
The columns of the matrix are the vectors u_1, u_2, u_3

> $u1 := \left(\frac{1}{Norm(L[2][1..3, 1], Euclidean)}\right) \cdot (L[2][1..3, 1]);$
> $u2 := \left(\frac{1}{Norm(L[2][1..3, 2], Euclidean)}\right) \cdot (L[2][1..3, 2]);$
> $u3 := \left(\frac{1}{Norm(L[2][1..3, 3], Euclidean)}\right) \cdot (L[2][1..3, 3]); \mathbb{S} := Matrix([u1, u2, u3]);$

$$u1 := \begin{bmatrix} -\frac{1}{2}\sqrt{2} \\ 0 \\ \frac{1}{2}\sqrt{2} \end{bmatrix}$$

$$u2 := \begin{bmatrix} \frac{1}{2}\sqrt{2} \\ 0 \\ \frac{1}{2}\sqrt{2} \end{bmatrix}$$

$$u3 := \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

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

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

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

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

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

$$\mathbb{S}\, S = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{8}$$

The transpose of matrix

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

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

Matrix S is an orthogonal matrix

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

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

$$\langle c\ 1 | c\ 2 \rangle = 0$$
$$\langle c\ 1 | c\ 3 \rangle = 0$$
$$\langle c\ 2 | c\ 3 \rangle = 0 \tag{10}$$

The row inner product of matrix S is also zero.

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

$$\langle r\ 1 | r\ 2 \rangle = 0$$
$$\langle r\ 1 | r\ 3 \rangle = 0$$
$$\langle r\ 2 | r\ 3 \rangle = 0 \tag{11}$$

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

```
> print(`||c1||`=Norm(S[1..3, 1], Euclidean));
  print(`||c2||`=Norm(S[1..3, 2], Euclidean));
  print(`||c3||`=Norm(S[1..3, 3], Euclidean));print( );
  print(`||r1||`=Norm(S[1, 1..3], Euclidean));
  print(`||r2||`=Norm(S[2, 1..3], Euclidean));
  print(`||r3||`=Norm(S[3, 1..3], Euclidean));
```

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

$$||r1|| = 1$$
$$||r2|| = 1$$
$$||r3|| = 1 \qquad \textbf{(12)}$$

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

Defining the state vector $|\psi'\rangle \equiv \mathbb{Y}$ in the new basis $\{u_1, u_2, u_3\}$

```
> 𝕐 := Multiply(S, Y);
```

$$\mathbb{Y} := \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2}\sqrt{2} \end{bmatrix} \qquad \textbf{(13)}$$

Changing from one basis to another

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

```
> 𝕐 := Multiply(S, Y);
```

$$\mathbb{Y} := \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2}\sqrt{2} \end{bmatrix} \qquad \textbf{(14)}$$

```
> Y := Multiply(𝕊, 𝕐);
```

$$Y := \begin{bmatrix} 0 \\ \frac{1}{2}\sqrt{2} \\ \frac{1}{2}\sqrt{2} \end{bmatrix} \qquad \textbf{(15)}$$

Determining the operator $\mathbb{K}$ in the $\{u_1, u_2, u_3\}$ basis:

$$\mathbb{K} = \mathbf{S} \cdot \mathbf{K} \cdot \mathbf{S}^{-1}$$

```
> 𝕂 := Multiply(S, Multiply(K, 𝕊));
```

$$\mathbb{K} := \begin{bmatrix} 0 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad \textbf{(16)}$$

The main diagonal lists the eigenvalues

Calculating the Expectation Value in the new basis $\{u_1, u_2, u_3\}$: $\langle \mathbb{K} \rangle = \langle \psi' | \mathbb{K} | \psi' \rangle$

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

$$E\ \ Value = 1 \qquad \textbf{(17)}$$

Define the basis vectors:

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

basis set 2 { u1, u2, u3 }

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

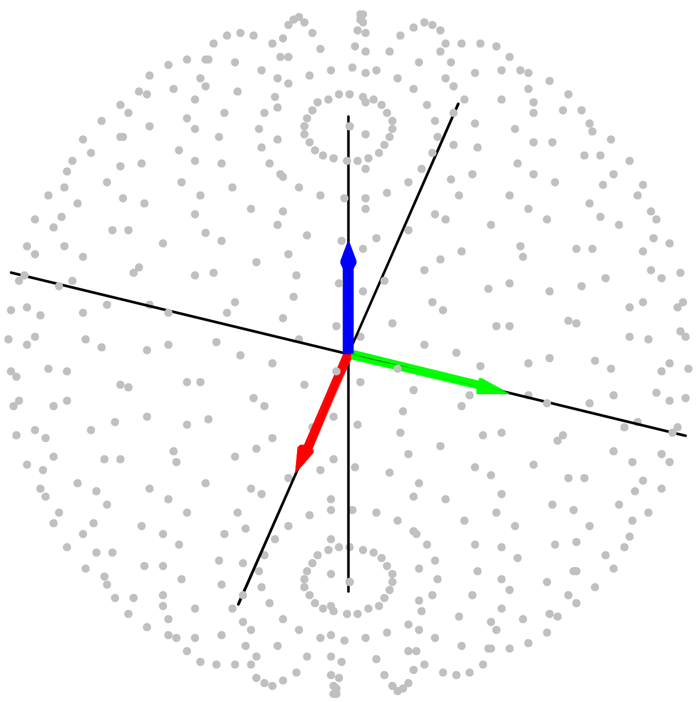
u1 · u2 = u1 · u3 = u2 · u3 =0

```
> e1 := Vector([1, 0, 0]) : e2 := Vector([0, 1, 0]) :
  e3 := Vector([0, 0, 1]) : u2 := Vector([0, 1, 0]) :
```

$$u1 := \frac{1}{\sqrt{2}} \cdot \text{Vector}([1, 0, 1]) : u3 := \frac{1}{\sqrt{2}} \cdot \text{Vector}([-1, 0, 1]) :$$

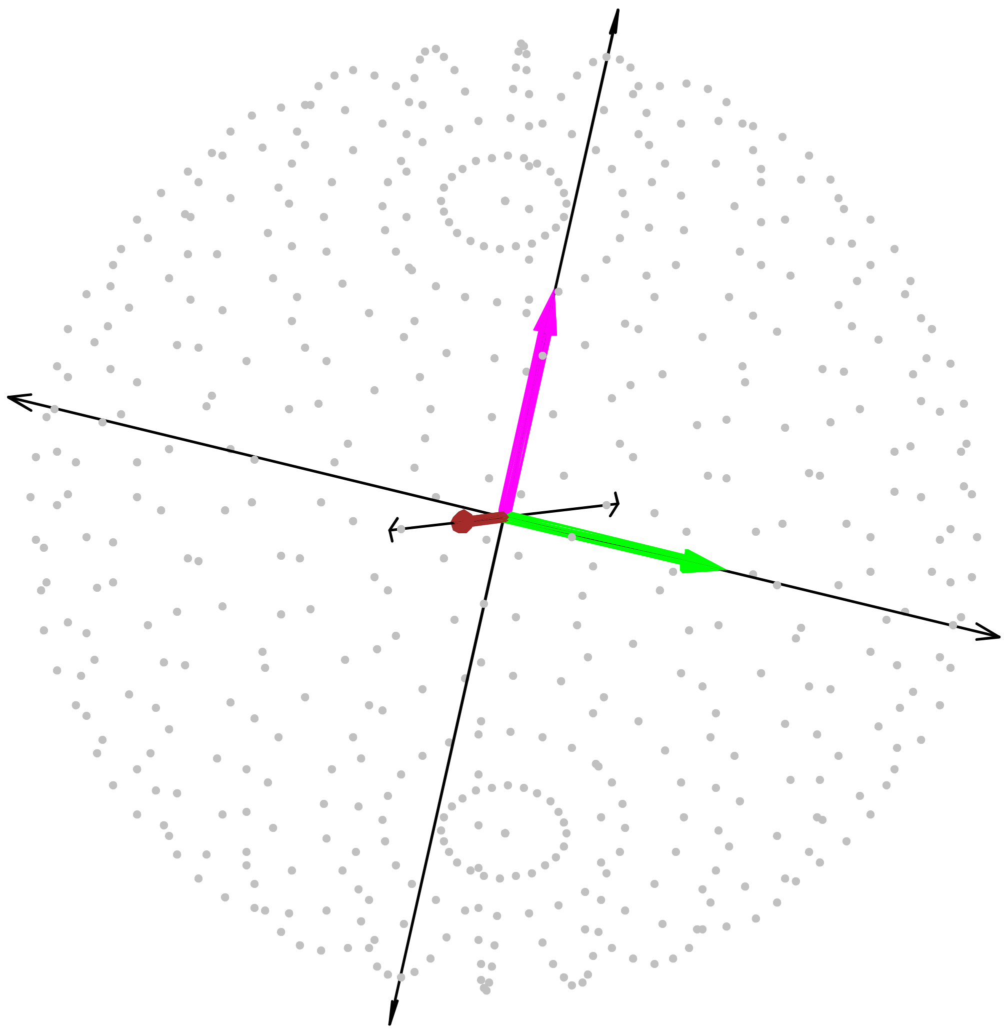
Plotting the standard basis { x, y, z }

```
> 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 = [18, 42]);
```



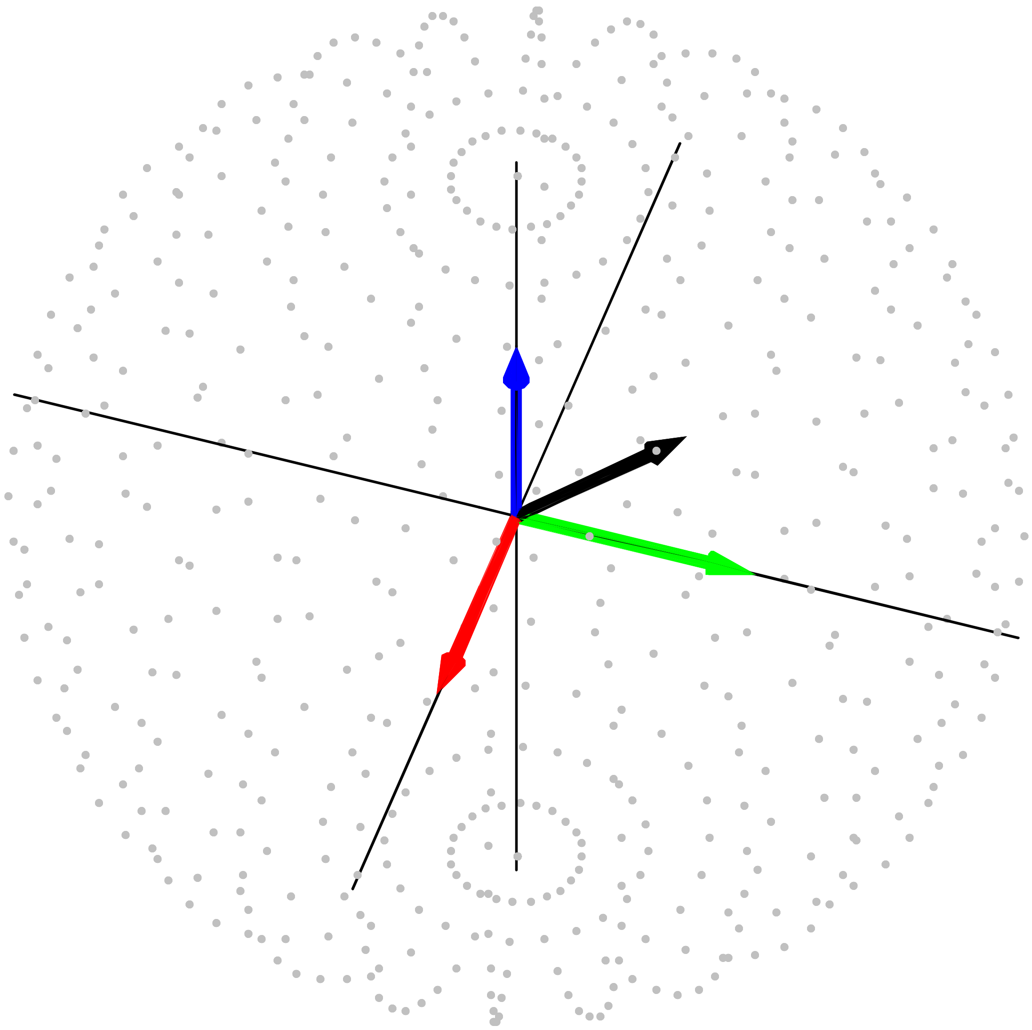
Plotting basis { v1, v2, v3 }

```
> q1 := arrow(u1, color = brown, width = 0.05) :
  q2 := arrow(u2, color = green, width = 0.05) :
  q3 := arrow(u3, color = magenta, width = 0.05) :
  a := arrow(2.2· u1, color = black, width = 0.05, shape = arrow, head_length = 0.1, head_width = 0.1) :
  b := arrow(2.2· u2, color = black, width = 0.05, shape = arrow, head_length = 0.1, head_width = 0.1) :
  c := arrow(2.2 · u3, color = black, width = 0.05, shape = arrow, head_length = 0.1, head_width = 0.1) :
  d := arrow( − 2.2· u1, color = black, width = 0.05, shape = arrow, head_length = 0.1, head_width = 0.1) :
  e := arrow( − 2.2· u2, color = black, width = 0.05, shape = arrow, head_length = 0.1, head_width = 0.1) :
  f := arrow( − 2.2· u3, color = black, width = 0.05, shape = arrow, head_length = 0.1, head_width = 0.1) :
  display([q1, q2, q3, a, b, c, d, e, f, sp], axes = none, scaling = constrained, orientation = [18, 42]);
```



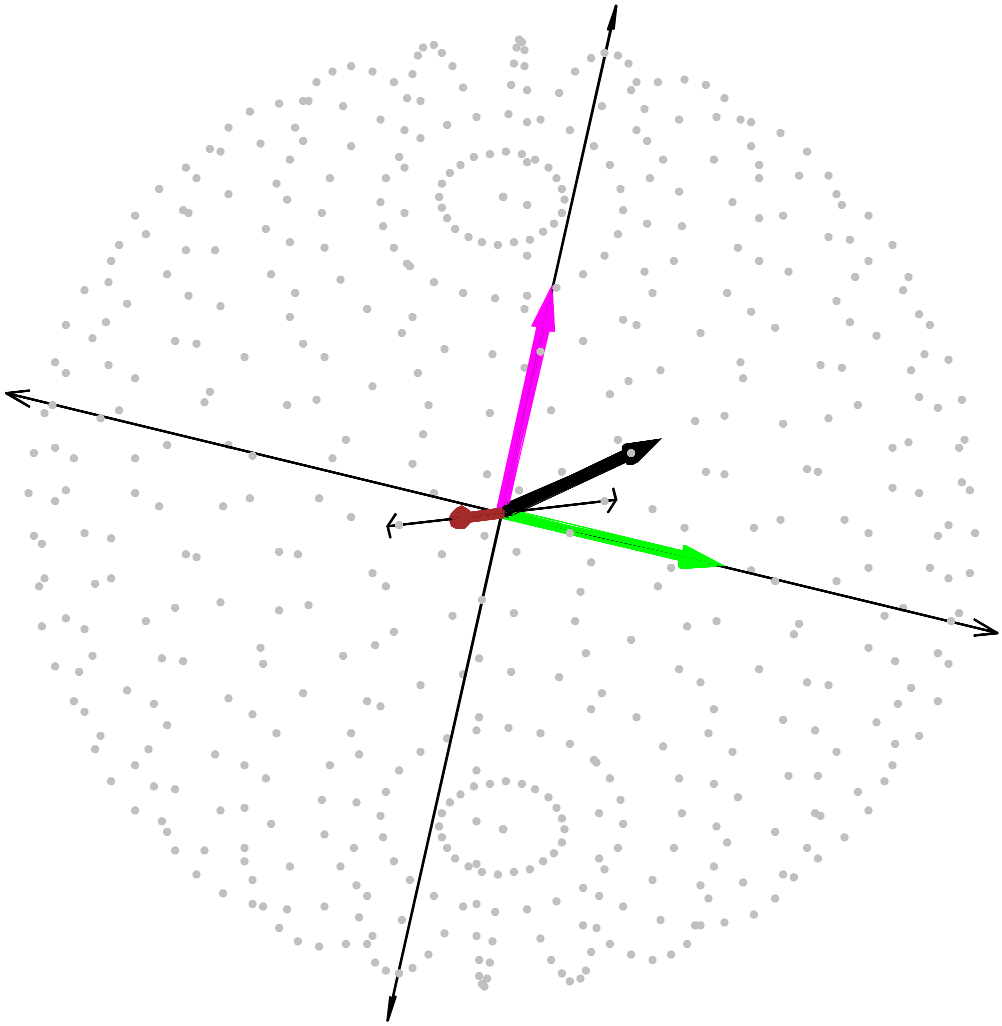
Plotting the state vector Y and the standard basis

> $ay := arrow(Y, color = black)$: $display([\mathrm{x}, \mathrm{y}, \mathrm{z}, ay, sp], \mathrm{axes} = \mathrm{normal}, \mathrm{scaling} = \mathrm{constrained}, \mathrm{tickmarks} = [2, 2, 2], orientation = [18, 42])$;



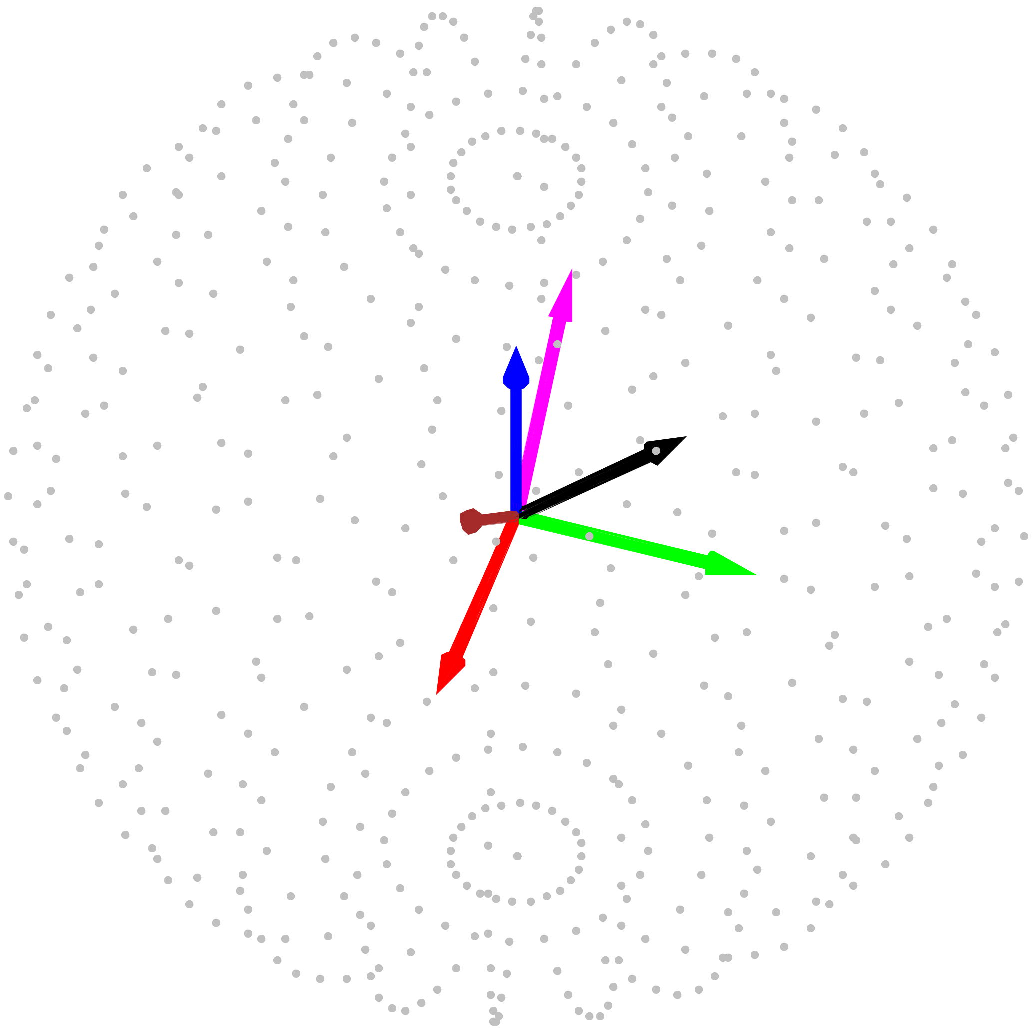
Plotting the state vector Y and basis { u1, u2, u3 }

> display([q1, q2, q3, *a*, *b*, *c*, *d*, *e*, *f*, *ay*, *sp*], axes = *none*, scaling = constrained, *orientation* = [18, 42]);



Plotting the state vector Y and both bases

```
> display([x, y, z, q1, q2, q3, ay, sp], axes = none, scaling = constrained, orientation = [18, 42]);
```



> display([x, y, z, q1, q2, q3, *a*, *b*, *c*, *d*, *e*, *f*, *ay*, *sp*], axes = *normal*, *tickmarks* = [0, 0, 0], scaling = constrained, *orientation* = [18, 42]);