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

Maple 12

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

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]]);
```

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

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
```

$$\lambda^3 - 3\lambda^2 + 2\lambda$$

$$\lambda\,(\lambda - 1)\,(\lambda - 2)$$

$$[[\lambda = 0], [\lambda = 1], [\lambda = 2]] \quad \textbf{(2)}$$

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]);
```

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

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

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

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

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

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

Calculating the Expectation Value

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

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

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

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

$$\mathbf{v}_2 = \mathbf{y}, \quad \mathbf{v}_1 = \frac{\mathbf{x}+\mathbf{z}}{\sqrt{2}}, \quad \mathbf{v}_3 = \frac{-\mathbf{x}+\mathbf{z}}{\sqrt{2}};$$

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

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

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

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

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

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

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

The transpose of matrix

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

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

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

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

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

$$||r1|| = 1$$
$$||r2|| = 1$$
$$||r3|| = 1 \tag{12}$$

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 $\{u_1, u_2, u_3\}$

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

$$\mathbb{Y} := \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2}\sqrt{2} \\ \frac{1}{2} \end{bmatrix} \tag{13}$$

Changing from one basis to another

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

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

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

$$\mathbb{Y} := \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2}\sqrt{2} \\ \frac{1}{2} \end{bmatrix} \tag{14}$$

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

$$Y := \begin{bmatrix} 0 \\ \frac{1}{2}\sqrt{2} \\ \frac{1}{2}\sqrt{2} \end{bmatrix} \tag{15}$$

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

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

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

$$\mathbb{K} := \begin{bmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{16}$$

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($\mathbb{Y}$), Multiply($\mathbb{K}$, $\mathbb{Y}$));

$$E\ \ Value = 1 \tag{17}$$

Define the basis vectors:

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

basis set 2 { u1, u2, u3 }

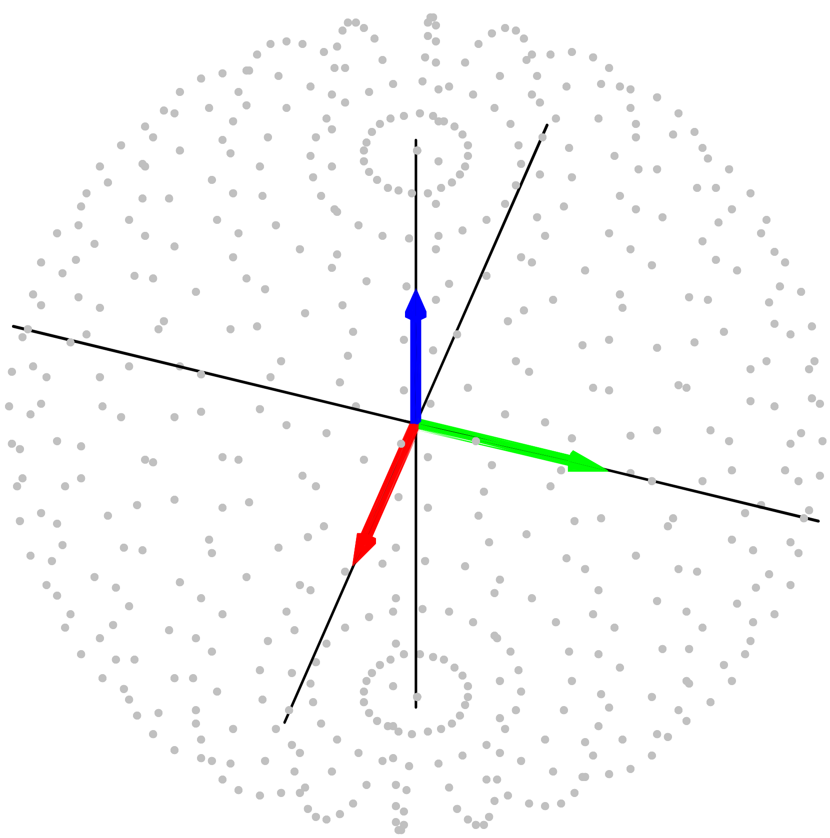
Notice that these are orthogonal bases: x • y = x · z = y · z = 0

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

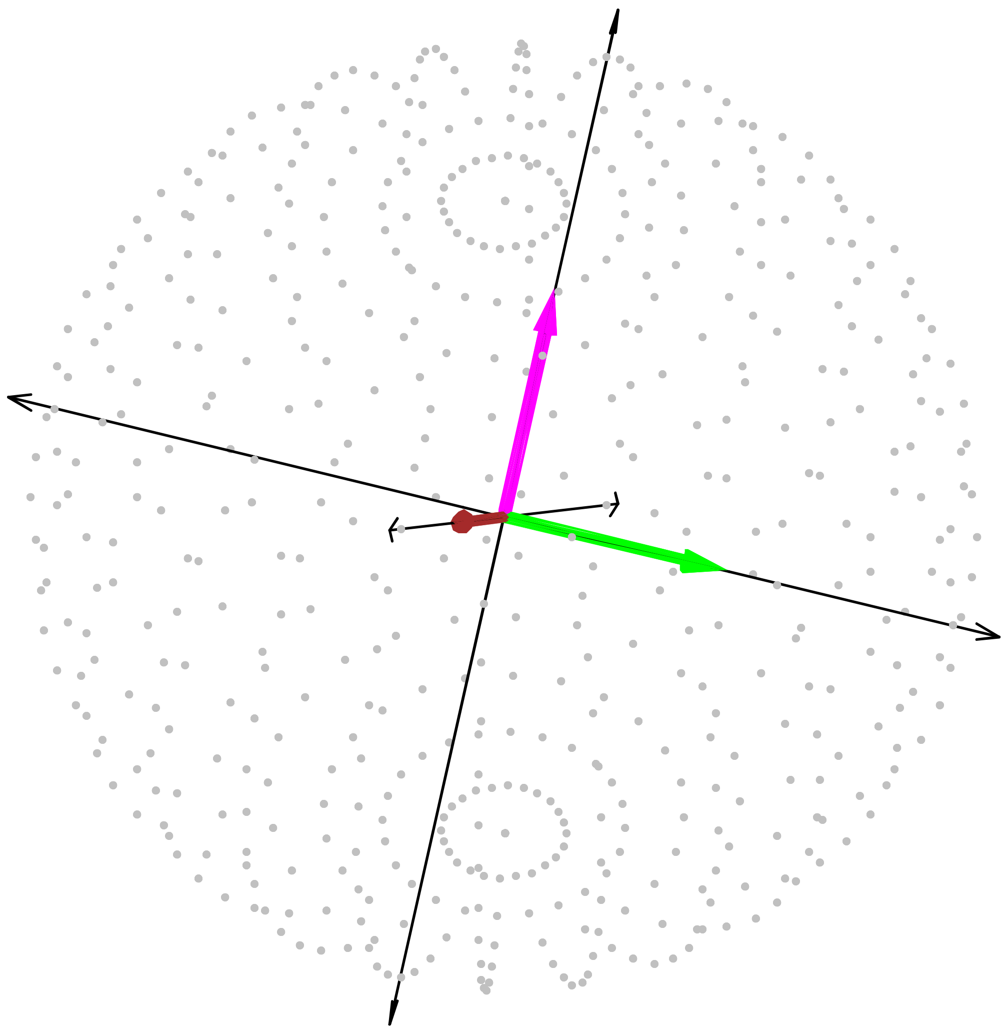
Plotting the standard basis { x, y, z }

> *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]);



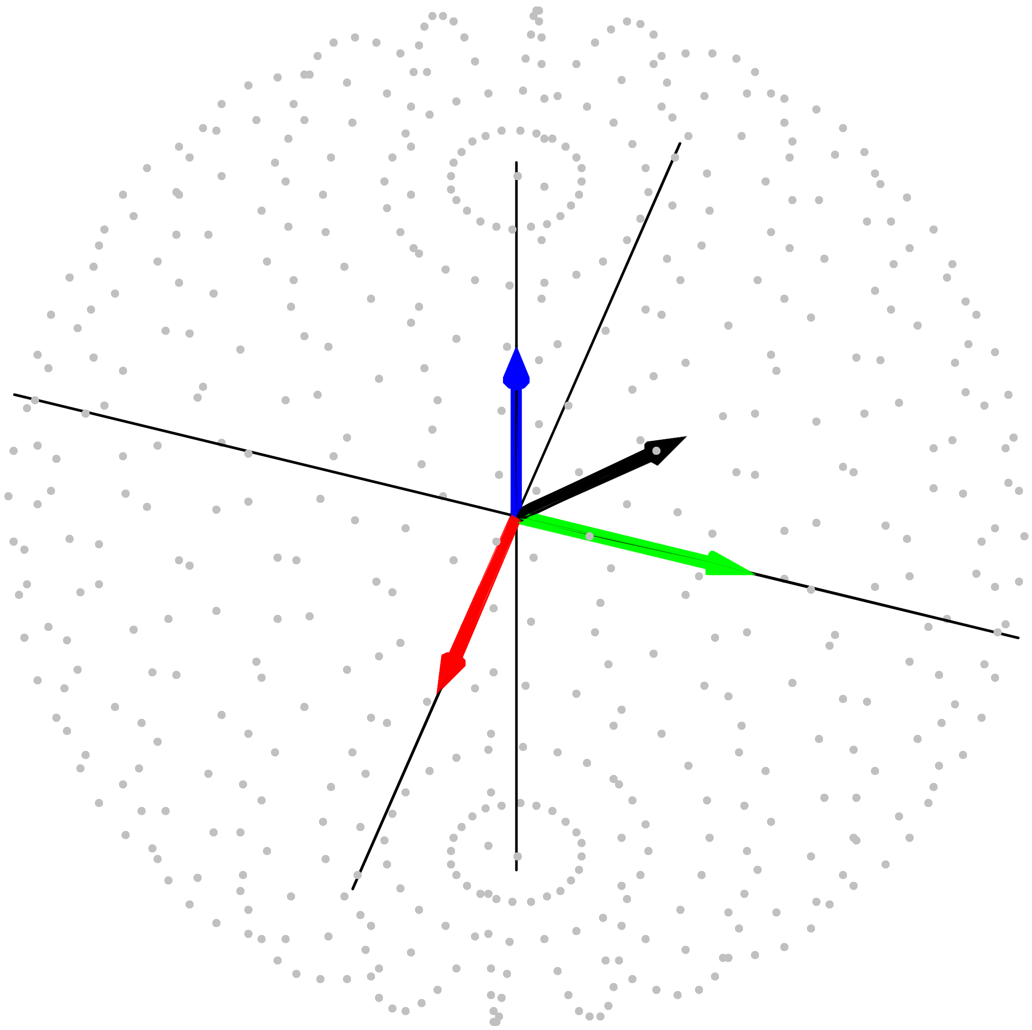
Plotting basis { v1, v2, v3 }

```
> 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]);
```



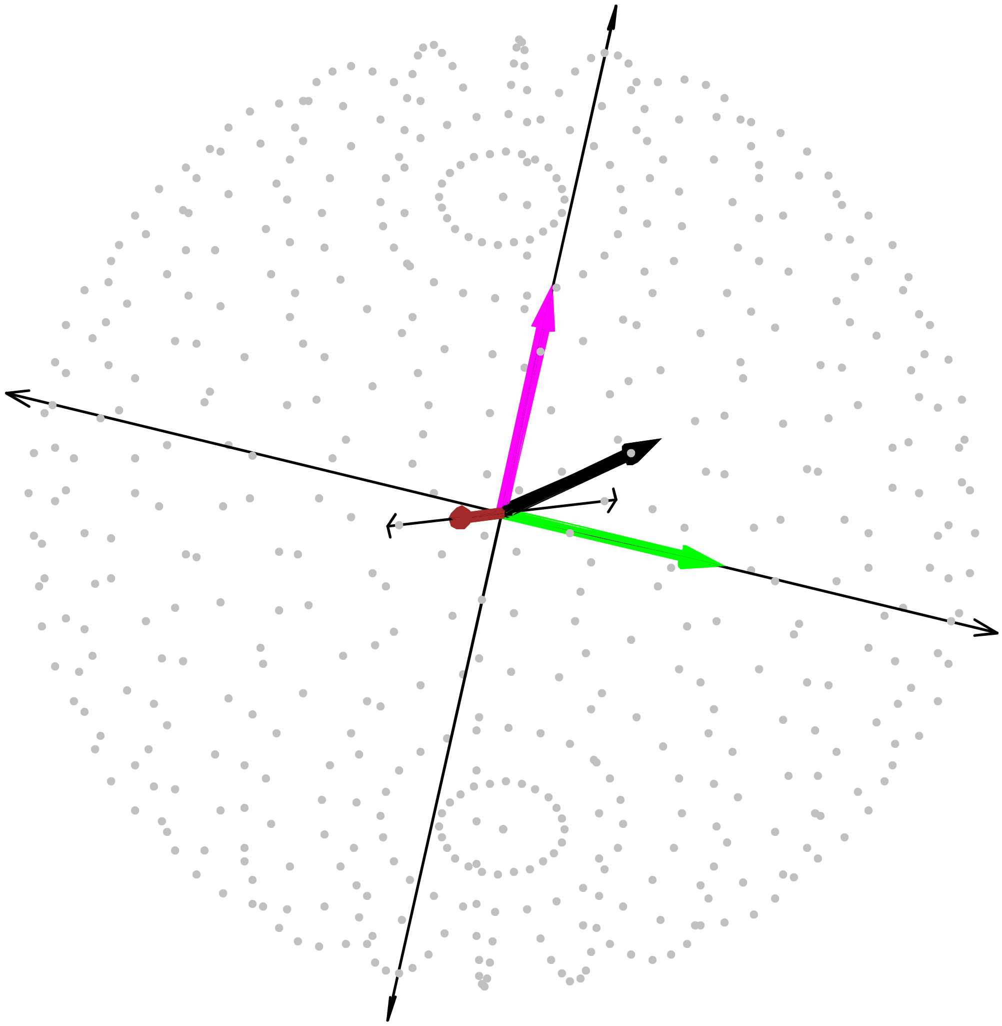
Plotting the state vector Y and the standard basis

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



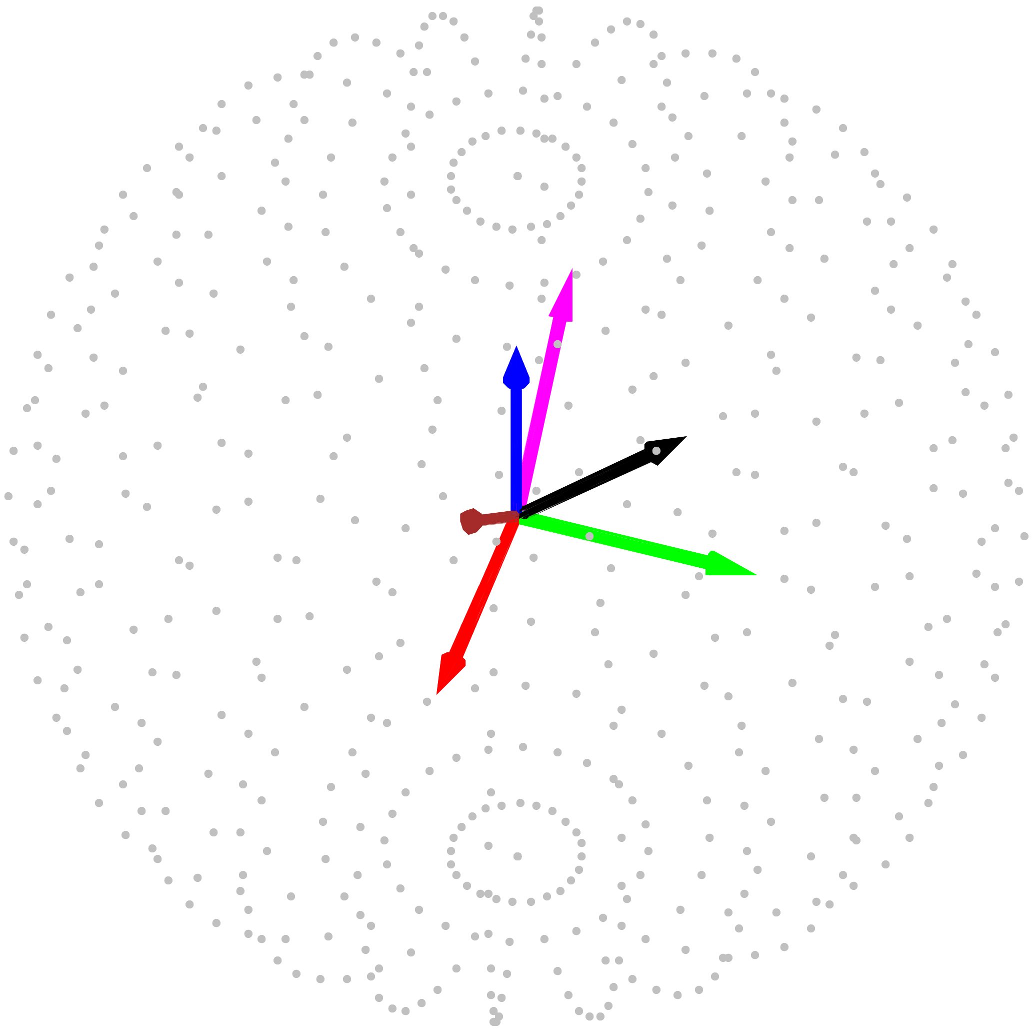
Plotting the state vector Y and basis { u1, u2, u3 }

```
> 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]);
```