```
> 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]]);
```

$$H := \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 2 \\ 0 & 2 & 0 \end{bmatrix} \tag{1}$$

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
```

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

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]);
```

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

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

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

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

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

$$Y := \begin{bmatrix} \frac{2}{3} \\ \frac{2}{3} \\ \frac{1}{3} \end{bmatrix} \tag{4}$$

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

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

$$E\ \ Value = \frac{4}{3} \tag{5}$$

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

$> \; v1 := \left(\frac{1}{Norm(L[2][1..3, 1], Euclidean)}\right) \cdot (L[2][1..3, 1]);$

$v2 := \left(\frac{1}{Norm(L[2][1..3, 2], Euclidean)}\right) \cdot (L[2][1..3, 2]);$

$v3 := \left(\frac{1}{Norm(L[2][1..3, 3], Euclidean)}\right) \cdot (L[2][1..3, 3]); \mathbb{S} := Matrix([v1, v2, v3]);$

$$v1 := \begin{bmatrix} 0 \\ \frac{1}{2}\sqrt{2} \\ \frac{1}{2}\sqrt{2} \end{bmatrix}$$

$$v2 := \begin{bmatrix} 0 \\ -\frac{1}{2}\sqrt{2} \\ \frac{1}{2}\sqrt{2} \end{bmatrix}$$

$$v3 := \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

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

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

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

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

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

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

The transpose of matrix S. Notice that if S is a symmetric matrix then $S = S^T$

> $ST := Transpose(S);$

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

Matrix S is an orthogonal matrix

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

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

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

The row inner product of matrix S is also zero.

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

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

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));
```

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

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

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 $\{v_1, v_2, v_3\}$

```
> 𝕐 := Multiply(S, Y);
```

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

Changing from one basis to another

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

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

```
> 𝕐 := Multiply(S, Y);
```

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

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

$$Y := \begin{bmatrix} \frac{2}{3} \\ \frac{2}{3} \\ \frac{1}{3} \end{bmatrix} \tag{15}$$

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

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

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

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

The main diagonal lists the eigenvalues

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

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

> $'E\ Value' = Multiply(Transpose(\mathbb{Y}), Multiply(\mathbb{H}, \mathbb{Y}));$

$$E\ \ Value = \frac{4}{3} \tag{17}$$

Define the basis vectors:

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

basis set 2 { v1, v2, v3 }

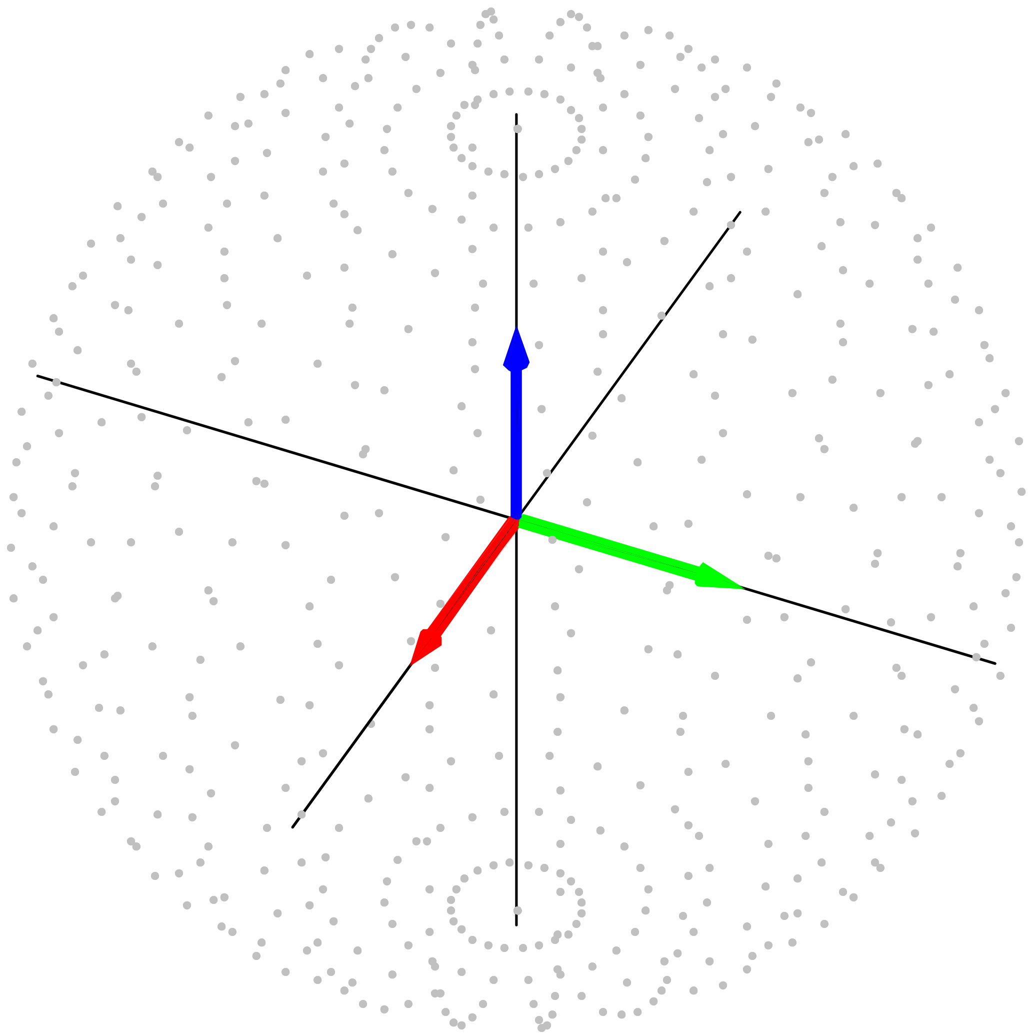
Notice that these are orthogonal bases: x • y = x · z = y · z = 0

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

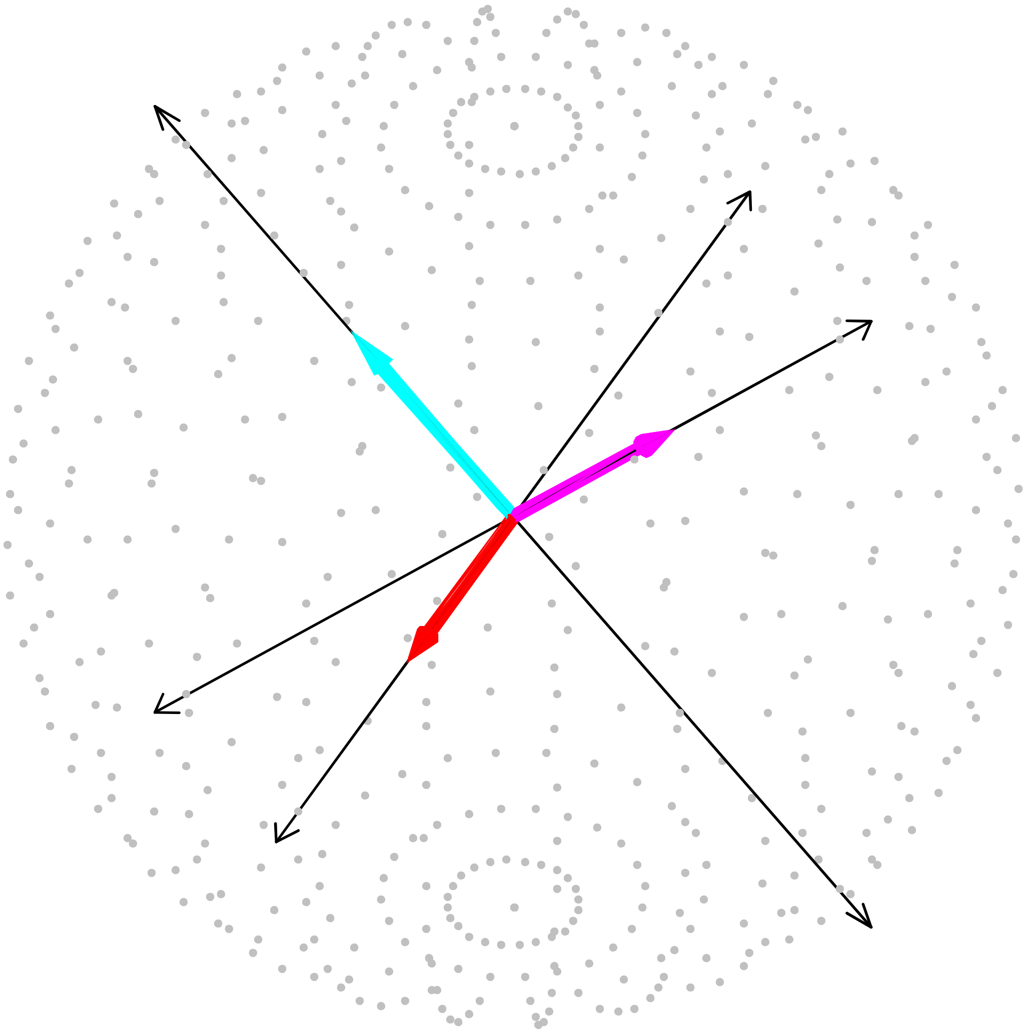
Plotting the standard basis { x, y, z }

> *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]);



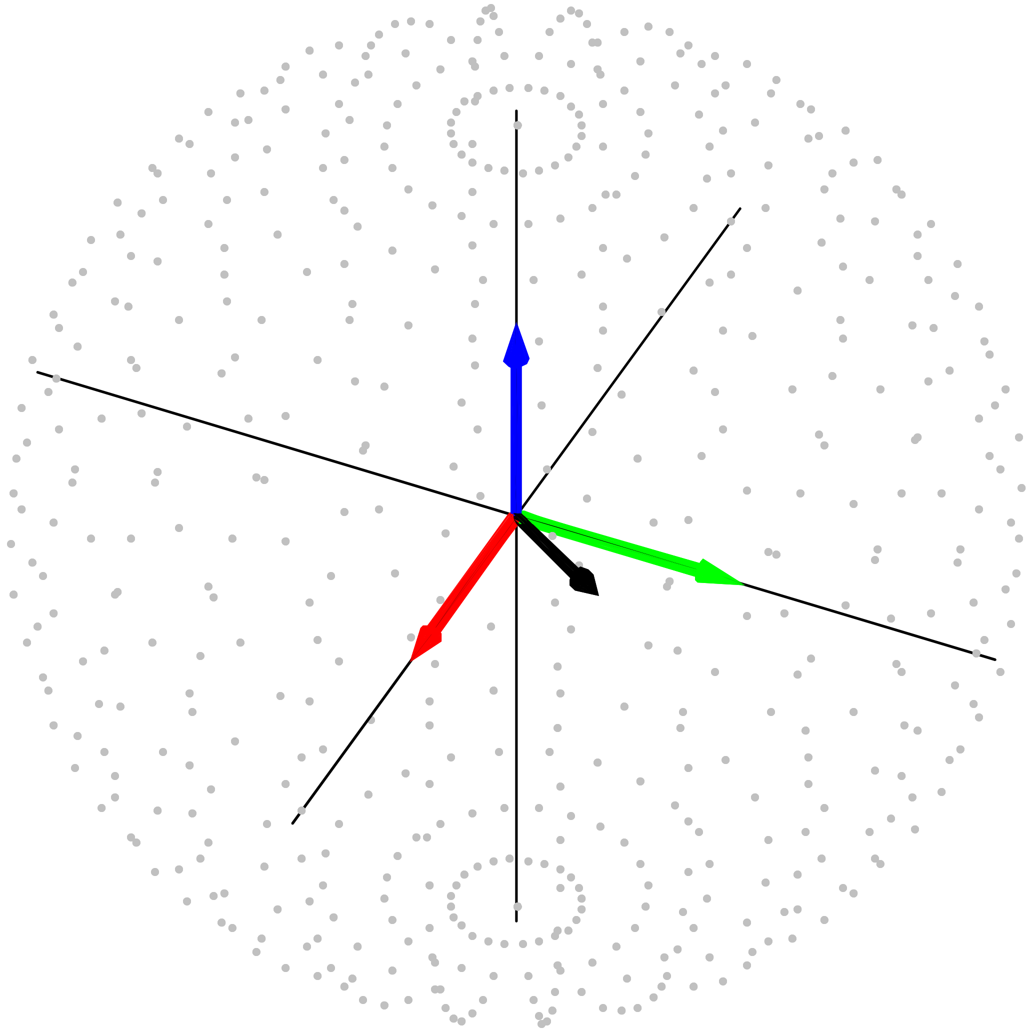
Plotting basis { v1, v2, v3 }

```
> 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]);
```



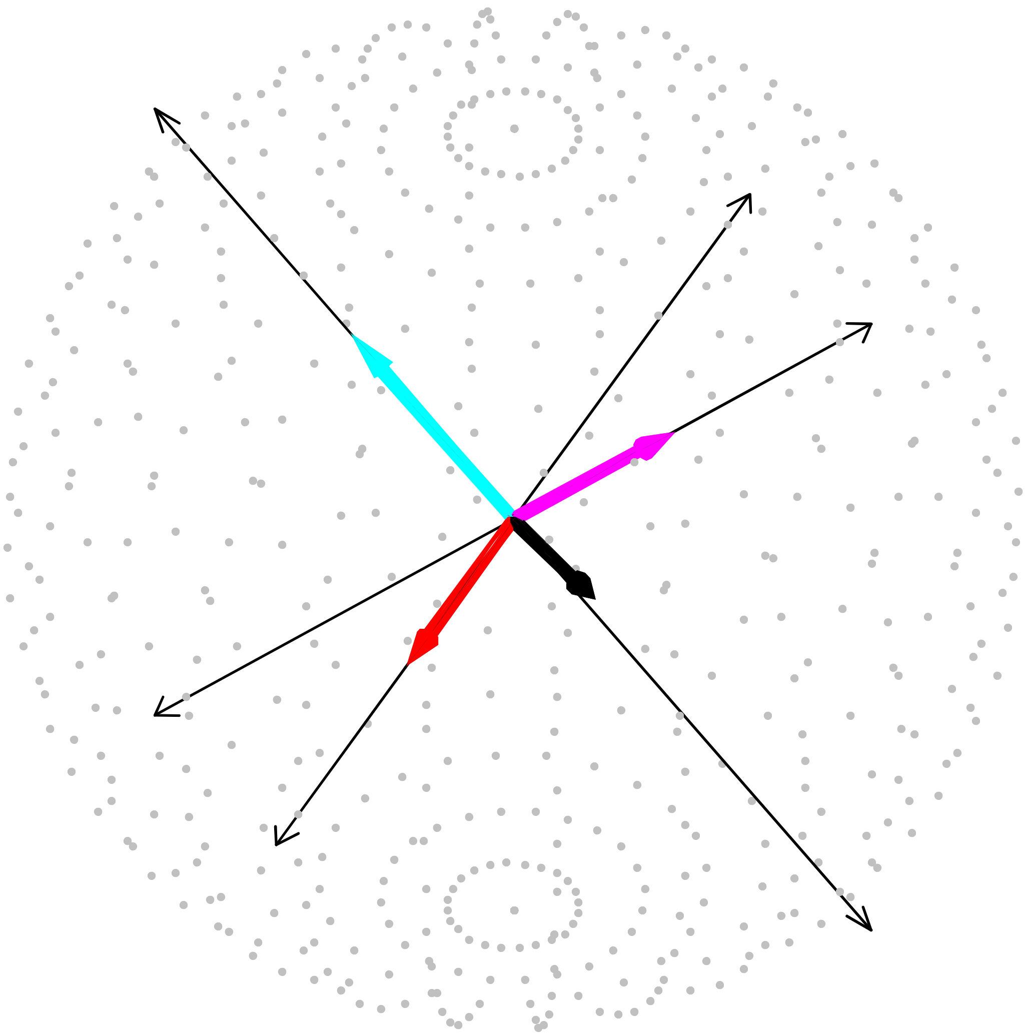
Plotting the state vector Y and the standard basis

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



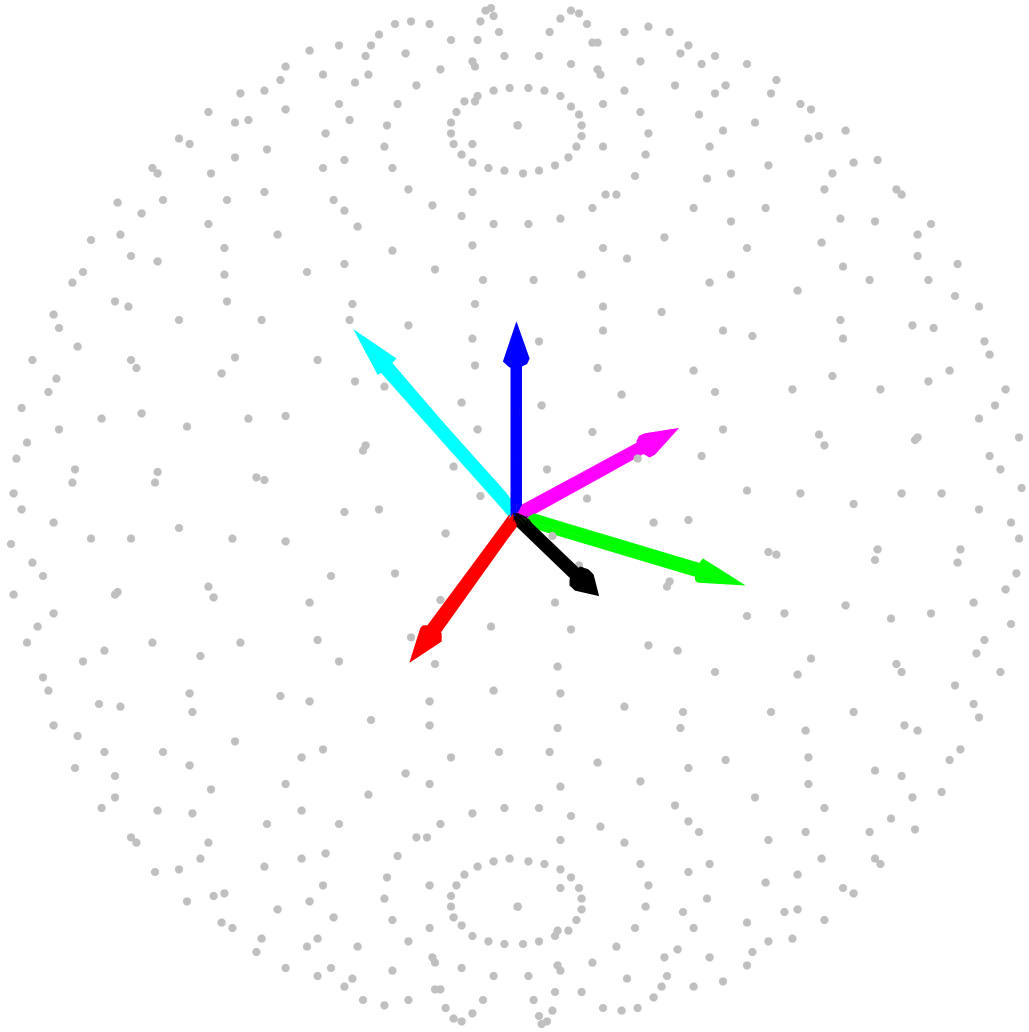
Plotting the state vector Y and basis { v1, v2, v3 }

> 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]);