

In[1]:= Needs ["SpinDynamica`"]

SpinDynamica version 3.0.1 loaded

 **ModifyBuiltIn:** The following built-in routines have been modified in SpinDynamica:
{Chop, Dot, Duration, Exp, Expand, ExpandAll, NumericQ, Plus, Power, Simplify, Times, WignerD}.
Evaluate ??symbol to generate the additional definitions for symbol.

In[2]:= ? AxesToEuler

AxesToEuler[system2,system1,opts] gives the Euler angles $\Omega_{21}=\{\alpha_{21},\beta_{21},\gamma_{21}\}$ by which each axis of system2 may be rotated around the system1 axes in order to be brought into coincide with the corresponding axis of system1:

$$e_{\mu 1}=R_{z1}(\alpha_{21})R_{y1}(\beta_{21})R_{z1}(\gamma_{21}).e_{\mu 2}, \text{ where } \mu \in \{x,y,z\}.$$

The same result is generated by rotating around the system2 axes:

$$e_{\mu 1}=R_{z2}(\alpha_{21})R_{y2}(\beta_{21})R_{z2}(\gamma_{21}).e_{\mu 2}, \text{ where } \mu \in \{x,y,z\}.$$

The same result is also generated by using "moving axes", where the axes follow the Euler rotations, but in this case the angles are applied in reverse order:

$$e_{\mu 1}=R_{z2}'(\gamma_{21})R_{y2}'(\beta_{21})R_{z2}'(\alpha_{21}).e_{\mu 2},$$

where the primed axes of system1 follow the rotation.

In a typical application, system2 is the principal axis system P of an anisotropic interaction, and system1 is a reference axis system such as a molecular frame M, or the laboratory frame L. The routine AxesToEuler[P,M] then generates the Euler angles Ω_{PM} which would be used in spherical tensor realisations of the spin Hamiltonian.

Each of system1 and system2 may have the form {Z} or {X,Z} or {X,Y,Z}. Here Z,X and Y are 3-vectors. If only Z is specified, the two remaining axes are constructed. If X and Z is specified, the z-axis of the constructed system is equal to Z and the x-axis is in the XZ plane. If all three axes are specified, they must be a right-handed orthogonal set. If system1 is missing, the system {ex,ey,ez} is assumed.

AxesToEuler also accepts axis definitions containing symbolic angles; in this case the symbolic result assumes that all angles are in the first quadrant (i.e. greater than 0 and less than $\pi/2$).

generate a randomly oriented Axis system (specifying the z-axis)

In[3]:= **vecz = RandomReal[{-1, 1}, {3}]**

Out[3]= {0.394581, -0.159527, -0.412323}

In[4]:= **axes = AxisSystem[vecz]**

Out[4]= {{0.74607, 0.240267, 0.621009},
{0., -0.932631, 0.360833}, {0.665868, -0.269206, -0.695807}}

derive the Euler angles relating the axis system to the original frame

In[5]:= **{ α , β , γ } = AxesToEuler[axes]**

Out[5]= {0.526364, 2.34034, -2.75739}

In[6]:= **{ α , β , γ } / °**

Out[6]= {30.1584, 134.092, -157.987}

rotate the axis system back to the original position

```
In[7]:= Chop@RotateEuler[axes, {α, β, γ}]
Out[7]= {{1., 0, 0}, {0, 1., 0}, {0, 0, 1.}}
```

generate a randomly oriented Axis system (specifying two axes)

```
In[8]:= vecx = RandomReal[{-1, 1}, {3}]
vecz = RandomReal[{-1, 1}, {3}]
Out[8]= {0.00705992, -0.289924, -0.926157}
Out[9]= {-0.641769, 0.0301905, -0.0273466}
In[10]:= axes = AxisSystem[vecx, vecz]
Out[10]= {{0.0265384, -0.299698, -0.953665},
          {-0.0575177, -0.952878, 0.29785}, {-0.997992, 0.0469481, -0.0425258}}
```

derive the Euler angles relating the axis system to the original frame

```
In[11]:= {α, β, γ} = AxesToEuler[axes]
Out[11]= {2.83887, 1.61333, 0.0470079}
In[12]:= {α, β, γ} / °
Out[12]= {162.655, 92.4373, 2.69336}
```

rotate the axis system back to the original position

```
In[13]:= Chop@RotateEuler[axes, {α, β, γ}]
Out[13]= {{1., 0, 0}, {0, 1., 0}, {0, 0, 1.}}
```