Global parameters

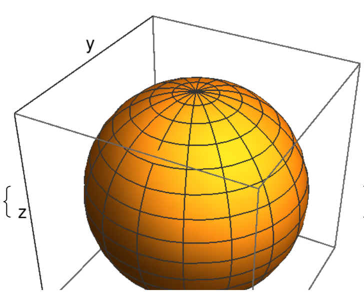
In[•]:=
```
r = Sqrt[x^2 + y^2 + z^2];
rbm = {x, y, z};
topolar = {x → r * Sin[θ] Cos[ϕ],
   y → r * Sin[θ] Sin[ϕ], z → r * Cos[θ], x^2 + y^2 + z^2 → r^2, Sqrt[x^2 + y^2 + z^2] → r};
tocartesian = {Sin[θ] → Sqrt[x^2 + y^2]/r, Cos[θ] → z/r,
   Sin[ϕ] → y/Sqrt[x^2 + y^2], Cos[ϕ] → x/Sqrt[x^2 + y^2]};
L[f_] := -I * {x, y, z} × Grad[f, {x, y, z}]
Lx[f_] := -I * (y * D[f, z] - z * D[f, y])
Ly[f_] := -I * (z * D[f, x] - x * D[f, z])
Lz[f_] := -I * (x * D[f, y] - y * D[f, x])

σ = Table[PauliMatrix[k], {k, 3}];
```

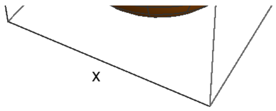
In[•]:=
```
Y[l_, m_, θ_: θ, ϕ_: ϕ] :=
 If[m == 0, SphericalHarmonicY[l, m, θ, ϕ],
   If[m < 0, I * 1/Sqrt[2]
     (SphericalHarmonicY[l, -m, θ, ϕ] + (-1)^(Abs[m]+1) * SphericalHarmonicY[l, m, θ, ϕ]),
    1/Sqrt[2] (SphericalHarmonicY[l, -m, θ, ϕ] +
      (-1)^Abs[m] * SphericalHarmonicY[l, m, θ, ϕ])]] // FullSimplify
Yxyz[l_, m_, θ_: θ, ϕ_: ϕ] := ReplaceAll[
   TrigExpand[Y[l, m, θ, ϕ]], tocartesian
  ] // Simplify
Olm[l_, m_, θ_: θ, ϕ_: ϕ] := Sqrt[(4 π)/(2 l + 1)] * r^l * Yxyz[l, m, θ, ϕ]
```

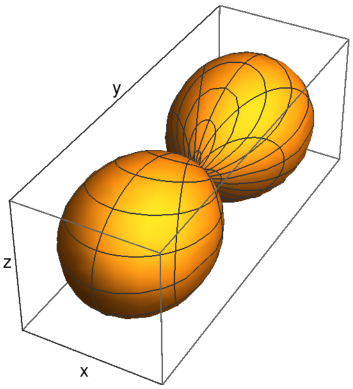
In[•]:=
```
Table[SphericalPlot3D[Evaluate[Y[l, m, θ, ϕ]^2],
   {θ, 0, Pi}, {ϕ, 0, 2 π}, AxesLabel → {"x", "y", "z"}, Ticks → None,
   DisplayFunction → Identity, PlotRange → All], {l, 0, 2}, {m, -l, l}] // Short
```

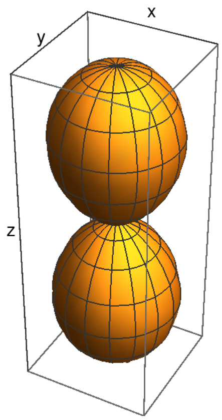
Out[•]//Short= {{

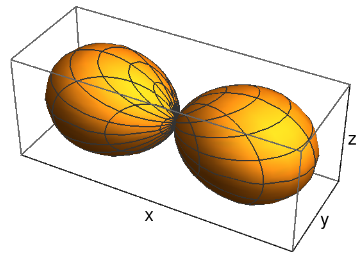


},

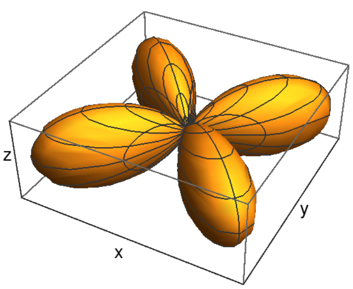


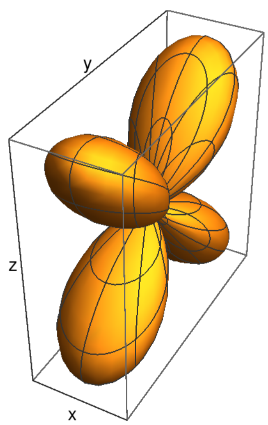
{ 

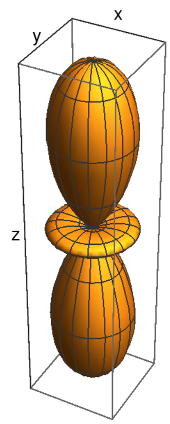
, 

, 

},

{ 

, 

, 

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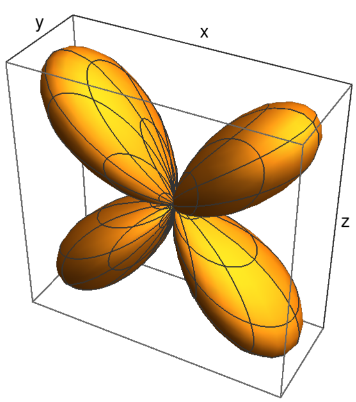
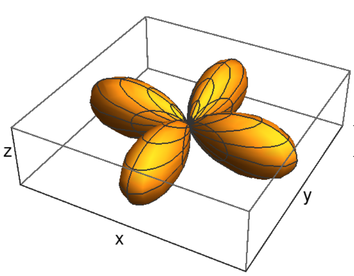


, 

}}

Basis

In[•]:=
$$A = \sqrt{\frac{3}{4\,\pi}};$$

$$phix = A * \frac{x}{r};$$

$$phiy = A * \frac{y}{r};$$

$$phiz = A * \frac{z}{r};$$

$$s_{up} = \{1, 0\};\ s_{down} = \{0, 1\};$$

$$\phi 32p = \frac{-I}{\sqrt{2}} * \left(phix * s_{up} + I * phiy * s_{up}\right);$$

$$\phi 12p = \frac{-I}{\sqrt{6}} * \left(phix * s_{down} + I * phiy * s_{down}\right) + I * \sqrt{\frac{2}{3}} * phiz * s_{up};$$

$$\phi 12m = \frac{I}{\sqrt{6}} * \left(phix * s_{up} - I * phiy * s_{up}\right) + I * \sqrt{\frac{2}{3}} * phiz * s_{down};$$

$$\phi 32m = \frac{I}{\sqrt{2}} * \left(phix * s_{down} - I * phiy * s_{down}\right);$$

$$\phi spinor = \{\phi 32p, \phi 12p, \phi 12m, \phi 32m\};$$

Electric Multipole

In[•]:=
```
Q[l_, m_, basis_, basis2_, θ_: θ, ϕ_: ϕ] :=
 Module[{e = 1},
  electricpole = -e * Olm[l, m];
  ket = Table[basis2[[i]]*.basis[[j]] * electricpole, {i, 1, 4}, {j, 1, 4}];
  Qmat = ReplaceAll[ket, topolar];
  Qmat = Integrate[Qmat * Sin[θ], {θ, 0, π}, {ϕ, 0, 2 π}];
  normalize = Sqrt[Tr[Qmat.Qmat]] / 2;
  normalize = If[
    NumberQ[normalize] && Equal[normalize, 0], 1, normalize
   ];
  Qmat / normalize
 ]
Q[0, 0, ϕspinor, ϕspinor] // MatrixForm
Q[2, -2, ϕspinor, ϕspinor] // MatrixForm
```

Out[•]//MatrixForm=

$$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

Out[•]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & \frac{i\,(x^2+y^2+z^2)}{\sqrt{(x^2+y^2+z^2)^2}} & 0 \\ 0 & 0 & 0 & \frac{i\,(x^2+y^2+z^2)}{\sqrt{(x^2+y^2+z^2)^2}} \\ -\frac{i\,(x^2+y^2+z^2)}{\sqrt{(x^2+y^2+z^2)^2}} & 0 & 0 & 0 \\ 0 & -\frac{i\,(x^2+y^2+z^2)}{\sqrt{(x^2+y^2+z^2)^2}} & 0 & 0 \end{pmatrix}$$

Magnetic Multipole

In[•]:=
```
M[l_, m_, basis_, basis2_, θ_: θ, ϕ_: ϕ] :=
 Module[{μB = 1},
  ml[b_] := (2 * {Lx[b], Ly[b], Lz[b]})/(l + 1) + σ.b;
  magneticpole[b_] := -μB * Grad[Olm[l, m], {x, y, z}].ml[b];
  ket = Map[magneticpole, basis];
  ket = Table[basis2[[i]]*.ket[[j]], {i, 1, 4}, {j, 1, 4}];
  Mmat = ReplaceAll[ket, topolar] // FullSimplify;
  Mmat = Integrate[Mmat * Sin[θ], {θ, 0, π}, {ϕ, 0, 2 π}];
  normalize = Sqrt[Tr[Mmat.Mmat]]/2;
  normalize = If[
    NumberQ[normalize] && Equal[normalize, 0], 1, normalize
   ];
  Mmat/normalize
 ]
M[1, -1, ϕspinor, ϕspinor] // MatrixForm
M[1, 1, ϕspinor,  ϕspinor] // MatrixForm
```

Out[•]//MatrixForm=

$$\begin{pmatrix} 0 & i\sqrt{\frac{3}{5}} & 0 & 0 \\ -i\sqrt{\frac{3}{5}} & 0 & \frac{2i}{\sqrt{5}} & 0 \\ 0 & -\frac{2i}{\sqrt{5}} & 0 & i\sqrt{\frac{3}{5}} \\ 0 & 0 & -i\sqrt{\frac{3}{5}} & 0 \end{pmatrix}$$

Out[•]//MatrixForm=

$$\begin{pmatrix} 0 & -\sqrt{\frac{3}{5}} & 0 & 0 \\ -\sqrt{\frac{3}{5}} & 0 & -\frac{2}{\sqrt{5}} & 0 \\ 0 & -\frac{2}{\sqrt{5}} & 0 & -\sqrt{\frac{3}{5}} \\ 0 & 0 & -\sqrt{\frac{3}{5}} & 0 \end{pmatrix}$$

Toroidal Multipole

トロイダルはl=2の項が活性となるが，Q(l=2)と完全に比例関係にある

In[•]:=
```
Clear[T, troidalpole, t]

T[l_, m_, basis_, basis2_, θ_: θ, ϕ_: ϕ] :=
 Module[{μB = 1},
  t[b_] := LeviCivitaTensor[3].({x, y, z}/(l + 1)).(2 * {Lx[b], Ly[b], Lz[b]}/(l + 2) + σ.b);
  troidalpole[b_] := -μB * Grad[Olm[l, m], {x, y, z}].t[b];
  ket = Map[troidalpole, basis];
  ket = Table[basis2[[i]]*.ket[[j]], {i, 1, 4}, {j, 1, 4}];
  Tmat = ReplaceAll[ket, topolar] // FullSimplify;
  Tmat = Integrate[Tmat * Sin[θ], {θ, 0, π}, {ϕ, 0, 2 π}];
  normalize = Sqrt[Tr[Tmat.Tmat]]/2;
  normalize = If[
    NumberQ[normalize] && Equal[normalize, 0], 1, normalize
   ];
  Tmat/normalize
 ]
T[2, -2, ϕspinor,  ϕspinor] // MatrixForm // FullSimplify
T[1, -1, ϕspinor, ϕspinor] // MatrixForm // FullSimplify
```

Out[•]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & \frac{x^2+y^2+z^2}{\sqrt{-(x^2+y^2+z^2)^2}} & 0 \\ 0 & 0 & 0 & \frac{x^2+y^2+z^2}{\sqrt{-(x^2+y^2+z^2)^2}} \\ \frac{\sqrt{-(x^2+y^2+z^2)^2}}{x^2+y^2+z^2} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{-(x^2+y^2+z^2)^2}}{x^2+y^2+z^2} & 0 & 0 \end{pmatrix}$$

Out[•]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Electric Toroidal Multipole

In[∘]:=
```
Clear[G]
Clear[electrictroidal]

G[l_, m_, basis_, basis2_, θ_: θ, ϕ_: ϕ] :=
 Module[{e = 1},
  mα[b_] := (2 * {Lx[b], Ly[b], Lz[b]})/(l + 1) + σ.b;
  tβ[b_] := LeviCivitaTensor[3].({x, y, z}/(l + 1)).((2 * {Lx[b], Ly[b], Lz[b]})/(l + 2) + σ.b);
  g[b_] := Sum[-e * mα[ -tβ[b][[i]] ][[j]] *
     D[Olm[l, m], rbm[[i]], rbm[[j]]], {i, 1, 3}, {j, 1, 3}];
  ket = Map[g, basis];
  bracket = Table[basis2[[i]]*.ket[[j]], {i, 1, 4}, {j, 1, 4}];
  Gmat = ReplaceAll[bracket, topolar] // FullSimplify;
  Gmat = Integrate[Gmat * Sin[θ], {θ, 0, π}, {ϕ, 0, 2 π}];
  normalize = Sqrt[Tr[Gmat.Gmat]]/2;
  normalize = If[
    NumberQ[normalize] && Equal[normalize, 0], 1, normalize
   ];
  Gmat/normalize
 ]
G[1, -1, ϕspinor, ϕspinor] // MatrixForm // FullSimplify
G[2, -2, ϕspinor, ϕspinor] // MatrixForm // FullSimplify
```

Out[∘]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Out[∘]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$