磁気トロイダル多極子

固体物理ミクロな多極氏による電子物性の表現論(その3)
式(17)，電気トロイダル多極子を磁気双極子とPauli行列の表式から求める

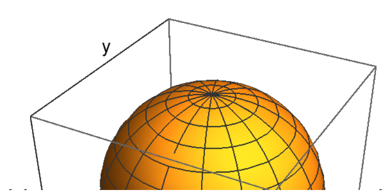
G’ ∝ M⊗σ

Global parameters

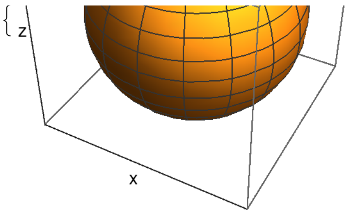
In[∘]:=
```
r = Sqrt[x^2 + y^2 + z^2];
rbm = {x, y, z};
tospherical = {x → r * Sin[θ] Cos[ϕ],
   y → r * Sin[θ] Sin[ϕ], z → r * Cos[θ], x^2 + y^2 + z^2 → r^2, Sqrt[x^2 + y^2 + z^2] → r};
tocartesian = {Sin[θ] → Sqrt[x^2 + y^2]/r, Cos[θ] → z/r,
   Sin[ϕ] → y/Sqrt[x^2 + y^2], Cos[ϕ] → x/Sqrt[x^2 + y^2]};
L[f_] := -I * {x, y, z} × Grad[f, {x, y, z}]
```

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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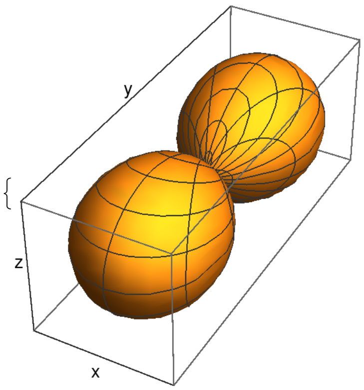

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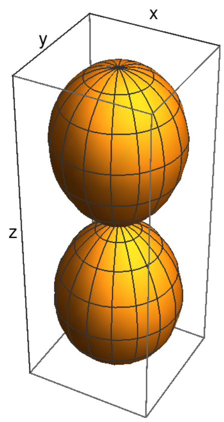

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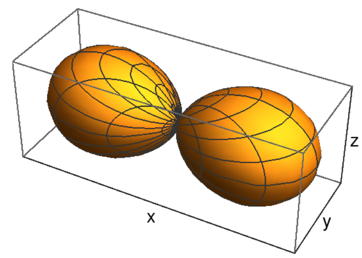

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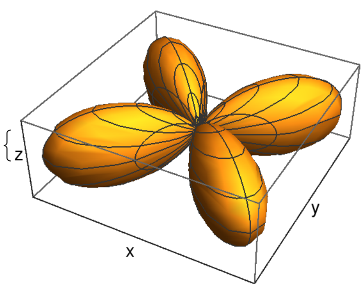

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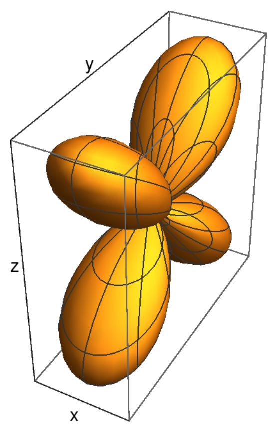

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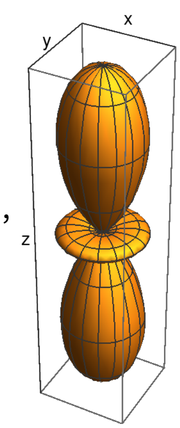

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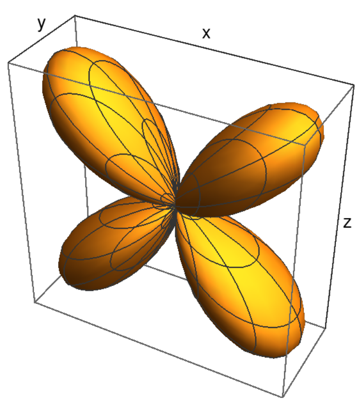

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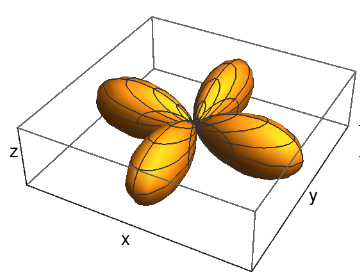

}}

Basis

In[∘]:=
```
A = Sqrt[3/(4 * π)];
phix = A * x/r;
phiy = A * y/r;
phiz = A * z/r;
phip = {phix, phiy, phiz}
```

Out[∘]=

$$\left\{\frac{\sqrt{\frac{3}{\pi}}\ x}{2\sqrt{x^2+y^2+z^2}}, \frac{\sqrt{\frac{3}{\pi}}\ y}{2\sqrt{x^2+y^2+z^2}}, \frac{\sqrt{\frac{3}{\pi}}\ z}{2\sqrt{x^2+y^2+z^2}}\right\}$$

Magnetic Multipole

In[∘]:=
```
Clear[M, magneticpole]
M[l_, m_, basis_, basis2_, θ_: θ, ϕ_: ϕ] :=
 Module[{μB = 1},
  magneticpole[b_] := -μB * Grad[Olm[l, m], {x, y, z}].(2 * L[b])/(l + 1);
  ket := Map[magneticpole, basis2];
  Mmat = ReplaceAll[KroneckerProduct[basis*, ket], tospherical] // FullSimplify;
  Mmat = Integrate[Mmat * Sin[θ], {θ, 0, π}, {ϕ, 0, 2 π}];
  Mmat
 ]
(Mx = -M[1, 1, phip, phip]) // MatrixForm
(Mz = -M[1, 0, phip, phip]) // MatrixForm
(My = -M[1, -1, phip, phip]) // MatrixForm
```

Out[∘]//MatrixForm=

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

Out[∘]//MatrixForm=

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

Out[∘]//MatrixForm=

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

In[•]:=
```
Mbm = {Mx, My, Mz};
σ = Table[PauliMatrix[k], {k, 3}];
σ[[2]]⊗Mx - σ[[1]]⊗My // MatrixForm
σ[[3]]⊗My - σ[[2]]⊗Mz // MatrixForm
σ[[1]]⊗Mz - σ[[3]]⊗Mx // MatrixForm
```

Out[•]//MatrixForm=

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

Out[•]//MatrixForm=

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

Out[•]//MatrixForm=

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