

Differential operators in Spherical coordinate with the use of Mathematica

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The differential operator is one of the most important programs in Mathematica. The use of such techniques makes one so easy to solve the Schrodinger equation, and treat the commutation relations of angular momentum and linear momentum. Here we discuss the differential operators in the spherical coordinates with the use of Mathematica.

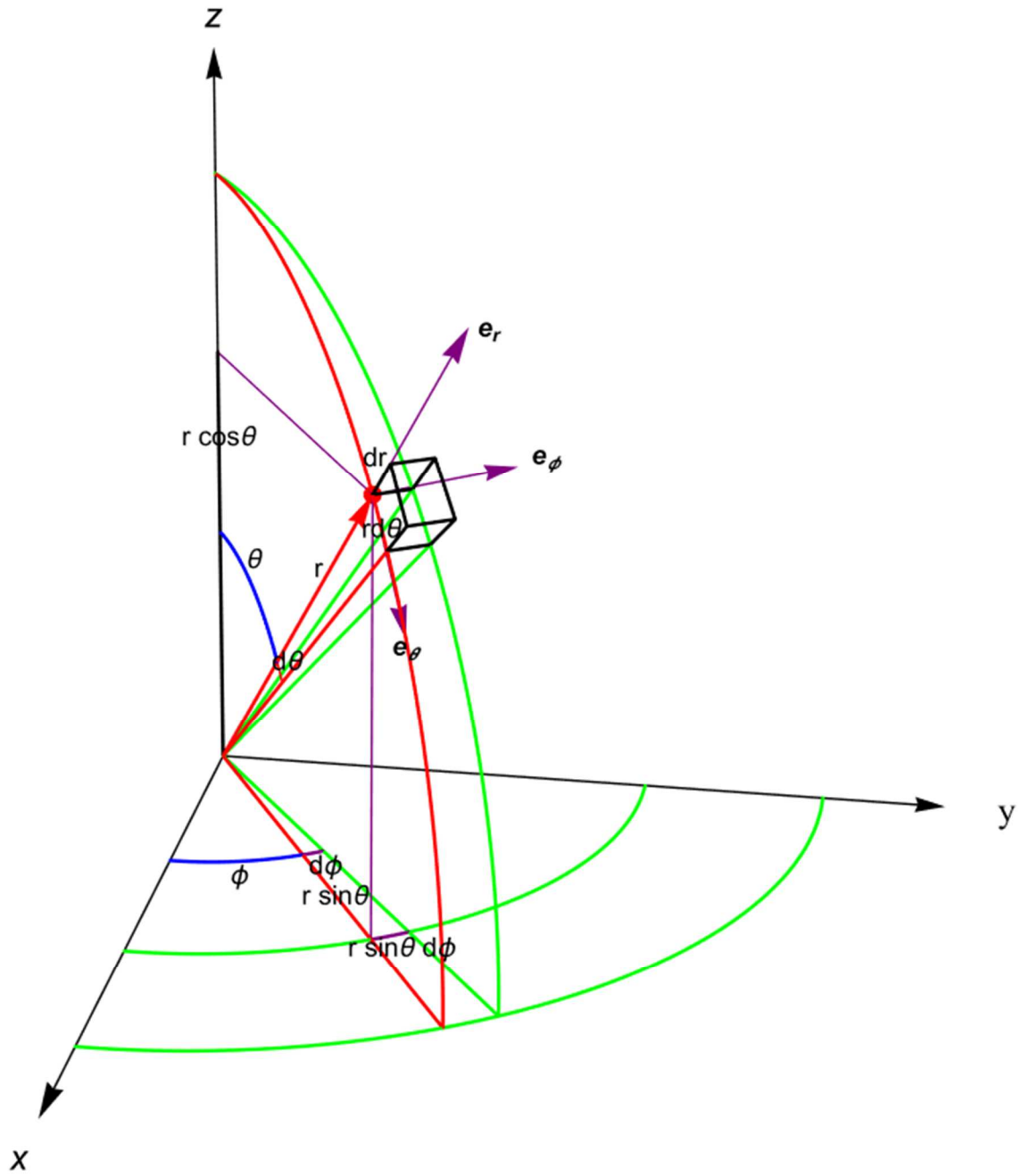


Fig. Spherical coordinates.

1. Vector analysis in spherical coordinates

$$\mathbf{r} = \mathbf{e}_x r \sin \theta \cos \phi + \mathbf{e}_y r \sin \theta \sin \phi + \mathbf{e}_z r \cos \theta$$

The spherical polar unit vectors in terms of cartesian unit vectors,

$$\mathbf{e}_r = \frac{\partial \mathbf{r}}{\partial r} = \mathbf{r} = \mathbf{e}_x \sin \theta \cos \phi + \mathbf{e}_y \sin \theta \sin \phi + \mathbf{e}_z \cos \theta ,$$

$$\mathbf{e}_\theta = \frac{1}{r} \frac{\partial \mathbf{r}}{\partial \theta} = \mathbf{e}_x \cos \theta \cos \phi + \mathbf{e}_y \cos \theta \sin \phi - \mathbf{e}_z \sin \theta ,$$

$$\mathbf{e}_\phi = \frac{1}{r \sin \theta} \frac{\partial \mathbf{r}}{\partial \phi} = -\mathbf{e}_x \sin \phi + \mathbf{e}_y \cos \phi ,$$

$$\begin{pmatrix} \mathbf{e}_r \\ \mathbf{e}_\theta \\ \mathbf{e}_\phi \end{pmatrix} = \begin{pmatrix} \sin \theta \cos \phi & \sin \theta \sin \phi & \cos \theta \\ \cos \theta \cos \phi & \cos \theta \sin \phi & -\sin \theta \\ -\sin \phi & \cos \phi & 0 \end{pmatrix} \begin{pmatrix} \mathbf{e}_x \\ \mathbf{e}_y \\ \mathbf{e}_z \end{pmatrix} .$$

The Cartesian unit vectors in terms of spherical polar unit vectors,

$$\begin{pmatrix} \mathbf{e}_x \\ \mathbf{e}_y \\ \mathbf{e}_z \end{pmatrix} = \begin{pmatrix} \sin \theta \cos \phi & \cos \theta \cos \phi & -\sin \phi \\ \sin \theta \sin \phi & \cos \theta \sin \phi & \cos \phi \\ \cos \theta & -\sin \theta & 0 \end{pmatrix} \begin{pmatrix} \mathbf{e}_r \\ \mathbf{e}_\theta \\ \mathbf{e}_\phi \end{pmatrix} ,$$

$$\mathbf{e}_x = \mathbf{e}_r \sin \theta \cos \phi + \mathbf{e}_\theta \cos \theta \cos \phi - \mathbf{e}_\phi \sin \phi ,$$

$$\mathbf{e}_y = \mathbf{e}_r \sin \theta \sin \phi + \mathbf{e}_\theta \cos \theta \sin \phi + \mathbf{e}_\phi \cos \phi ,$$

$$\mathbf{e}_z = \mathbf{e}_r \cos \theta - \mathbf{e}_\theta \sin \theta .$$

$$\mathbf{r} = \mathbf{e}_r r = x \mathbf{e}_x + y \mathbf{e}_y + z \mathbf{e}_z .$$

$$r = |\mathbf{r}| = \sqrt{x^2 + y^2 + z^2} .$$

$$d\mathbf{r} = \mathbf{e}_r dr + \mathbf{e}_\theta r d\theta + \mathbf{e}_\phi r \sin \theta d\phi .$$

The radial linear momentum

$$p_r = \frac{1}{2} \left(\frac{\mathbf{r}}{r} \cdot \mathbf{p} + \mathbf{p} \cdot \frac{\mathbf{r}}{r} \right) \quad p_r = \frac{\hbar}{ir} \frac{\partial}{\partial r} (r)$$

((**Mathematica**))

Here we use the following notations in the Mathematica program for the spherical coordinates.

$$u_x \rightarrow \mathbf{e}_x = \mathbf{e}_r \sin \theta \cos \phi + \mathbf{e}_\theta \cos \theta \cos \phi - \mathbf{e}_\phi \sin \phi$$

$$u_y \rightarrow \mathbf{e}_y = \mathbf{e}_r \sin \theta \sin \phi + \mathbf{e}_\theta \cos \theta \sin \phi + \mathbf{e}_\phi \cos \phi$$

$$u_z \rightarrow \mathbf{e}_z = \mathbf{e}_r \cos \theta - \mathbf{e}_\theta \sin \theta$$

$$u_r \rightarrow \mathbf{e}_r$$

$$x \rightarrow \mathbf{e}_x \cdot r \mathbf{e}_r$$

$$y \rightarrow \mathbf{e}_y \cdot r \mathbf{e}_r$$

$$z \rightarrow \mathbf{e}_z \cdot r \mathbf{e}_r$$

$$\text{Lap} \rightarrow \nabla^2$$

$$\text{Gra} \rightarrow \text{grad}, \nabla$$

$$\text{Diva} \rightarrow \text{div}$$

$$\text{Curla} \rightarrow \text{curl} \quad \text{or} \quad \text{rot}$$

$$L \rightarrow \mathbf{L} = \mathbf{r} \times \mathbf{p}$$

$$L_x \rightarrow \mathbf{e}_x \cdot \mathbf{L}$$

$$L_y \rightarrow \mathbf{e}_y \cdot \mathbf{L}$$

$$L_z \rightarrow \mathbf{e}_z \cdot \mathbf{L}$$

$$LP \rightarrow L_x + iL_y$$

$$LM \rightarrow L_x - iL_y$$

$$Leq \rightarrow \mathbf{L}^2 = L_x^2 + L_y^2 + L_z^2$$

$$p \rightarrow \mathbf{p} = \frac{\hbar}{i} \nabla$$

$$p_x \rightarrow \mathbf{e}_x \cdot \mathbf{p} = \frac{\hbar}{i} \mathbf{e}_x \cdot \nabla$$

$$p_y \rightarrow \mathbf{e}_y \cdot \mathbf{p} = \frac{\hbar}{i} \mathbf{e}_y \cdot \nabla .$$

$$p_z \rightarrow \mathbf{e}_z \cdot \mathbf{p} = \frac{\hbar}{i} \mathbf{e}_z \cdot \nabla .$$

$$Peq \rightarrow \mathbf{p}^2 = p_x^2 + p_y^2 + p_z^2 .$$

$$prq \rightarrow p_r \quad (\text{radial linear momentum}).$$

$$pq \rightarrow \frac{\hbar}{ir} \frac{\partial}{\partial r} r \quad (\text{radial linear momentum, simplified form}).$$

$$\mathbf{r} \rightarrow r \mathbf{e}_r$$

$$x \rightarrow \mathbf{e}_x \cdot r \mathbf{e}_r = r \sin \theta \cos \phi.$$

$$y \rightarrow \mathbf{e}_y \cdot r \mathbf{e}_r = r \sin \theta \sin \phi.$$

$$z \rightarrow r \mathbf{e}_r \cdot \mathbf{e}_z = r \cos \theta.$$

((Mathematica))

```

Clear["Global`"];
ux = {Sin[θ] Cos[φ], Cos[θ] Cos[φ], -Sin[φ]};
uy = {Sin[θ] Sin[φ], Cos[θ] Sin[φ], Cos[φ]};
uz = {Cos[θ], -Sin[θ], 0};
ur = {1, 0, 0};
x = r ur.ux;
y = r ur.uy;
z = r ur.uz;
Lap := Laplacian[#, {r, θ, φ}, "Spherical"] &;
Gra := Grad[#, {r, θ, φ}, "Spherical"] &;
Diva := Div[#, {r, θ, φ}, "Spherical"] &;
Curla := Curl[#, {r, θ, φ}, "Spherical"] &;
L := (-i ħ (Cross[(ur r), Gra[#]])) & // Simplify;
Lx := (ux.L[#] &) // Simplify;
Ly := (uy.L[#] &) // Simplify;
Lz := (uz.L[#] &) // Simplify;
LP := (Lx[#] + i Ly[#]) & // Simplify;
LM = (Lx[#] - i Ly[#]) & // Simplify;
Leq := (Nest[Lx, #, 2] + Nest[Ly, #, 2] + Nest[Lz, #, 2]) &;
p := (-i ħ Gra[#]) &;
px := (ux.p[#] &;
py := (uy.p[#] &;
pz := (uz.p[#] &;
Peq := (Nest[px, #, 2] + Nest[py, #, 2] + Nest[pz, #, 2]) &;
prq := ( (-i ħ / 2 ur . Gra[#] + (-i ħ / 2 Diva[# ur]) ) &;
pq := (ħ / (i r) D[r #, r] &;

```

2. Grad, Laplacian, Div, Curl

$$\nabla = \mathbf{e}_r \frac{\partial}{\partial r} + \mathbf{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \mathbf{e}_\phi \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi}$$

$$\begin{aligned} \nabla^2 &= \frac{1}{r^2} \left(2r \frac{\partial}{\partial r} + r^2 \frac{\partial^2}{\partial r^2} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \\ &\quad + \frac{1}{r^2} \left(\cot \theta \frac{\partial}{\partial \theta} + \frac{\partial^2}{\partial \theta^2} \right) \\ &= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \end{aligned}$$

$$\begin{aligned} \nabla \cdot \mathbf{V} &= \frac{1}{r} \left(2V_r + r \frac{\partial V_r}{\partial r} \right) + \frac{1}{r} \left(\cot \theta V_\theta + \frac{\partial V_\theta}{\partial \theta} \right) + \frac{1}{r \sin \theta} \frac{\partial V_\phi}{\partial \phi} \\ &= \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 V_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta V_\theta) + \frac{1}{r \sin \theta} \frac{\partial V_\phi}{\partial \phi} \end{aligned}$$

$$\nabla^2 \psi = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2}$$

$$\nabla \times \mathbf{V} = \frac{1}{r^2 \sin \theta} \begin{vmatrix} \mathbf{e}_r & r\mathbf{e}_\theta & r \sin \theta \mathbf{e}_\phi \\ \frac{\partial}{\partial r} & \frac{\partial}{\partial \theta} & \frac{\partial}{\partial \phi} \\ V_r & rV_\theta & r \sin \theta V_\phi \end{vmatrix}$$

((**Mathematica**))

eq1 = Gra[ψ[r, θ, φ]] // Simplify

$$\left\{ \psi^{(1,\theta,\theta)}[r, \theta, \phi], \frac{\psi^{(\theta,1,\theta)}[r, \theta, \phi]}{r}, \frac{\text{Csc}[\theta] \psi^{(\theta,\theta,1)}[r, \theta, \phi]}{r} \right\}$$

eq2 = Lap[ψ[r, θ, φ]] // Simplify

$$\frac{1}{r^2} \left(\text{Csc}[\theta]^2 \psi^{(\theta,\theta,2)}[r, \theta, \phi] + \text{Cot}[\theta] \psi^{(\theta,1,\theta)}[r, \theta, \phi] + \psi^{(\theta,2,\theta)}[r, \theta, \phi] + 2r \psi^{(1,\theta,\theta)}[r, \theta, \phi] + r^2 \psi^{(2,\theta,\theta)}[r, \theta, \phi] \right)$$

eq3 = Diva[{Vr[r, θ, φ], Vθ[r, θ, φ], Vφ[r, θ, φ]}] // Simplify

$$\frac{1}{r} \left(2Vr[r, \theta, \phi] + \text{Cot}[\theta] V\theta[r, \theta, \phi] + \text{Csc}[\theta] V\phi^{(\theta,\theta,1)}[r, \theta, \phi] + V\theta^{(\theta,1,\theta)}[r, \theta, \phi] + rVr^{(1,\theta,\theta)}[r, \theta, \phi] \right)$$

eq4 = Curla[{Vr[r, θ, φ], Vθ[r, θ, φ], Vφ[r, θ, φ]}] // Simplify

$$\left\{ \frac{1}{r} \left(\text{Cot}[\theta] V\phi[r, \theta, \phi] - \text{Csc}[\theta] V\theta^{(\theta,\theta,1)}[r, \theta, \phi] + V\phi^{(\theta,1,\theta)}[r, \theta, \phi] \right), -\frac{1}{r} \left(V\phi[r, \theta, \phi] - \text{Csc}[\theta] Vr^{(\theta,\theta,1)}[r, \theta, \phi] + rV\phi^{(1,\theta,\theta)}[r, \theta, \phi] \right), \frac{V\theta[r, \theta, \phi] - Vr^{(\theta,1,\theta)}[r, \theta, \phi] + rV\theta^{(1,\theta,\theta)}[r, \theta, \phi]}{r} \right\}$$

3. Angular momentum

In quantum mechanics, the angular momentum is defined as follows.

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} = \frac{\hbar}{i} \mathbf{r} \times \nabla = -i\hbar \left(\mathbf{e}_\phi \frac{\partial}{\partial \theta} - \mathbf{e}_\theta \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} \right)$$

$$L_x = \mathbf{e}_x \cdot \mathbf{L} = i\hbar(\sin\phi \frac{\partial}{\partial\theta} + \cot\theta \cos\phi \frac{\partial}{\partial\phi})$$

$$L_y = \mathbf{e}_y \cdot \mathbf{L} = i\hbar(-\cos\phi \frac{\partial}{\partial\theta} + \cot\theta \sin\phi \frac{\partial}{\partial\phi})$$

$$L_z = \mathbf{e}_z \cdot \mathbf{L} = -i\hbar \frac{\partial}{\partial\phi}$$

The Ladder operator:

$$L_+ = L_x + iL_y = \hbar e^{i\phi} (\frac{\partial}{\partial\theta} + i \cot\theta \frac{\partial}{\partial\phi})$$

$$L_- = L_x - iL_y = -\hbar e^{-i\phi} (\frac{\partial}{\partial\theta} - i \cot\theta \frac{\partial}{\partial\phi})$$

$$\begin{aligned} \mathbf{L}^2 &= L_x^2 + L_y^2 + L_z^2 \\ &= -\hbar^2 [\csc^2(\theta) \frac{\partial^2}{\partial\phi^2} + \cot\theta \frac{\partial}{\partial\theta} + \frac{\partial^2}{\partial\theta^2}] \\ &= -\hbar^2 [\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} (\sin\theta \frac{\partial}{\partial\theta}) + \frac{1}{\sin^2(\theta)} \frac{\partial^2}{\partial\phi^2}] \end{aligned}$$

((**Mathematica**))


```

eq0 = L[ψ[r, θ, φ]] // Simplify
{0, i ħ Csc[θ] ψ(θ,θ,1)[r, θ, φ], -i ħ ψ(θ,1,θ)[r, θ, φ]}

eq1 = Lx[ψ[r, θ, φ]] // Simplify
i ħ (Cos[φ] Cot[θ] ψ(θ,θ,1)[r, θ, φ] +
      Sin[φ] ψ(θ,1,θ)[r, θ, φ])

eq2 = Ly[ψ[r, θ, φ]] // Simplify
i ħ (Cot[θ] Sin[φ] ψ(θ,θ,1)[r, θ, φ] -
      Cos[φ] ψ(θ,1,θ)[r, θ, φ])

eq3 = Lz[ψ[r, θ, φ]] // Simplify
-i ħ ψ(θ,θ,1)[r, θ, φ]

eq4 = LP[ψ[r, θ, φ]] // Simplify
ħ (Cos[φ] + i Sin[φ])
  (i Cot[θ] ψ(θ,θ,1)[r, θ, φ] + ψ(θ,1,θ)[r, θ, φ])

eq5 = LM[ψ[r, θ, φ]] // Simplify
ħ (i Cos[φ] + Sin[φ])
  (Cot[θ] ψ(θ,θ,1)[r, θ, φ] + i ψ(θ,1,θ)[r, θ, φ])

eq6 = Leq[ψ[r, θ, φ]] // Simplify
-ħ2 (Csc[θ]2 ψ(θ,θ,2)[r, θ, φ] +
      Cot[θ] ψ(θ,1,θ)[r, θ, φ] + ψ(θ,2,θ)[r, θ, φ])

```

4. Radial linear momentum

The radial linear momentum in the quantum mechanics is defined by

$$p_r = \frac{1}{2} \left(\frac{\mathbf{r}}{r} \cdot \mathbf{p} + \mathbf{p} \cdot \frac{\mathbf{r}}{r} \right) = \frac{\hbar}{2i} \left(\frac{\mathbf{r}}{r} \cdot \nabla + \nabla \cdot \frac{\mathbf{r}}{r} \right)$$

or

$$p_r = \frac{\hbar}{ir} \frac{\partial}{\partial r} r = \frac{\hbar}{i} \left(\frac{1}{r} + \frac{\partial}{\partial r} \right).$$

Commutation relation

$$[p_r, r] = \frac{\hbar}{i}.$$

((**Mathematica**))

Radial linear momentum

`prq[ψ[r, θ, φ]] // Simplify`

$$-\frac{i\hbar\left(\psi[r,\theta,\phi]+r\psi^{(1,\theta,\theta)}[r,\theta,\phi]\right)}{r}$$

Commutation relation: `prq r - r prq = -iħ`

`prq[r ψ[r, θ, φ]] - r prq[ψ[r, θ, φ]] // Simplify`

$$-i\hbar\psi[r,\theta,\phi]$$

5. Relation between p and L

We show that $\mathbf{p}^2$ can be expressed by

$$\mathbf{p}^2 = p_r^2 + \frac{1}{r^2} \mathbf{L}^2$$

where

$$\begin{aligned} \mathbf{p}^2 &= -\hbar^2 \nabla^2 \\ &= -\hbar^2 \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \end{aligned}$$

$$\mathbf{L}^2 = L_x^2 + L_y^2 + L_z^2 = -\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2(\theta)} \frac{\partial^2}{\partial \phi^2} \right]$$

$$p_r^2 = \frac{\hbar}{ir} \frac{\partial}{\partial r} \left(r \frac{\hbar}{ir} \frac{\partial}{\partial r} r \right) = -\frac{\hbar^2}{r} \frac{\partial^2}{\partial r^2} r = -\frac{\hbar^2}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right)$$

$$\begin{aligned} \mathbf{p}^2 &= p_r^2 + \frac{1}{r^2} \mathbf{L}^2 \\ &= -\hbar^2 \left[\frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2(\theta)} \frac{\partial^2}{\partial \phi^2} \right] \\ &= -\hbar^2 \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2(\theta)} \frac{\partial^2}{\partial \phi^2} \right] \end{aligned}$$

((**Mathematica**))

eq1 = Peq[ψ[r, θ, φ]] // Simplify

$$-\frac{1}{r^2} \hbar^2 \left(\text{Csc}[\theta]^2 \psi^{(\theta, \theta, 2)}[r, \theta, \phi] + \right. \\ \left. \text{Cot}[\theta] \psi^{(\theta, 1, \theta)}[r, \theta, \phi] + \psi^{(\theta, 2, \theta)}[r, \theta, \phi] + \right. \\ \left. 2 r \psi^{(1, \theta, \theta)}[r, \theta, \phi] + r^2 \psi^{(2, \theta, \theta)}[r, \theta, \phi] \right)$$

eq2 = Nest[prq, ψ[r, θ, φ], 2] // Simplify

$$-\frac{\hbar^2 \left(2 \psi^{(1, \theta, \theta)}[r, \theta, \phi] + r \psi^{(2, \theta, \theta)}[r, \theta, \phi] \right)}{r}$$

eq3 = $\frac{1}{r^2}$ Leq[ψ[r, θ, φ]] // FullSimplify

$$-\frac{1}{r^2} \hbar^2 \left(\text{Csc}[\theta]^2 \psi^{(\theta, \theta, 2)}[r, \theta, \phi] + \right. \\ \left. \text{Cot}[\theta] \psi^{(\theta, 1, \theta)}[r, \theta, \phi] + \psi^{(\theta, 2, \theta)}[r, \theta, \phi] \right)$$

eq23 = eq2 + eq3 // Simplify

$$-\frac{1}{r^2} \hbar^2 \left(\text{Csc}[\theta]^2 \psi^{(\theta, \theta, 2)}[r, \theta, \phi] + \right. \\ \left. \text{Cot}[\theta] \psi^{(\theta, 1, \theta)}[r, \theta, \phi] + \psi^{(\theta, 2, \theta)}[r, \theta, \phi] + \right. \\ \left. 2 r \psi^{(1, \theta, \theta)}[r, \theta, \phi] + r^2 \psi^{(2, \theta, \theta)}[r, \theta, \phi] \right)$$

eq1 - eq23 // Simplify

0

6. Commutation relation

$$[L_i, x_j] = i\hbar \sum_k \varepsilon_{ijk} x_k$$

$$[L_x, L_y] = i\hbar L_z, \quad [L_y, L_z] = i\hbar L_x, \quad [L_z, L_x] = i\hbar L_y$$

$$[\mathbf{L}^2, L_x] = 0, \quad [\mathbf{L}^2, L_y] = 0, \quad [\mathbf{L}^2, L_z] = 0$$

$$[L^2, L_{\pm}] = 0, \quad [L_+, L_-] = 2\hbar \hat{L}_z,$$

$$[L_z, L_+] = \hbar L_+ \quad [L_z, L_-] = -\hbar L_-$$

$$[L_+, L_-] = 2\hbar L_z$$

$$\mathbf{L}^2 = \frac{1}{2}(L_+ L_- + L_- L_+) + L_z^2$$

((**Levi-Civita symbol**))

ε_{ijk} is the Levi Civita symbol. $\varepsilon_{123} = \varepsilon_{231} = \varepsilon_{312} = 1$ (even permutation).
 $\varepsilon_{321} = \varepsilon_{132} = \varepsilon_{213} = -1$ (odd permutation). $\varepsilon_{ijk} = 0$ if $i = j$, or $j = k$, or $k = i$.

((**Mathematica**))

The commutation relations can be easily proved through Mathematica

$$L_x[y \psi[r, \theta, \phi]] - y L_x[\psi[r, \theta, \phi]] -$$

$$\frac{i \hbar}{2} z \psi[r, \theta, \phi] // \text{FullSimplify}$$

0

$$L_y[z \psi[r, \theta, \phi]] - z L_y[\psi[r, \theta, \phi]] -$$

$$\frac{i \hbar}{2} x \psi[r, \theta, \phi] // \text{FullSimplify}$$

0

$$L_z[x \psi[r, \theta, \phi]] - x L_z[\psi[r, \theta, \phi]] -$$

$$\frac{i \hbar}{2} y \psi[r, \theta, \phi] // \text{FullSimplify}$$

0

$$L_x[L_y[\psi[r, \theta, \phi]]] - L_y[L_x[\psi[r, \theta, \phi]]] -$$

$$\frac{i \hbar}{2} L_z[\psi[r, \theta, \phi]] // \text{FullSimplify}$$

0

$$L_y[L_z[\psi[r, \theta, \phi]]] - L_z[L_y[\psi[r, \theta, \phi]]] -$$

$$\frac{i \hbar}{2} L_x[\psi[r, \theta, \phi]] // \text{FullSimplify}$$

0

$$L_z[L_x[\psi[r, \theta, \phi]]] - L_x[L_z[\psi[r, \theta, \phi]]] -$$

$$\frac{i \hbar}{2} L_y[\psi[r, \theta, \phi]] // \text{FullSimplify}$$

0

Leq[Ly[ψ[r, θ, φ]]] - Ly[Leq[ψ[r, θ, φ]]] // FullSimplify

0

LP[LM[ψ[r, θ, φ]]] - LM[LP[ψ[r, θ, φ]]] - 2 ħ Lz[ψ[r, θ, φ]] // FullSimplify

0

Leq[Lz[ψ[r, θ, φ]]] - Lz[Leq[ψ[r, θ, φ]]] // FullSimplify

0

Leq[LP[ψ[r, θ, φ]]] - LP[Leq[ψ[r, θ, φ]]] // FullSimplify // FullSimplify

0

Leq[LM[ψ[r, θ, φ]]] - LM[Leq[ψ[r, θ, φ]]] // FullSimplify // FullSimplify

0

Lz[LP[ψ[r, θ, φ]]] - LP[Lz[ψ[r, θ, φ]]] - ħ LP[ψ[r, θ, φ]] // FullSimplify

0

Lz[LM[ψ[r, θ, φ]]] - LM[Lz[ψ[r, θ, φ]]] + ħ LM[ψ[r, θ, φ]] // FullSimplify

0

```

eq1 = (LP[LM[ψ[r, θ, φ]]] + LM[LP[ψ[r, θ, φ]]]) /
      2 // FullSimplify;
eq2 = Lx[Lx[ψ[r, θ, φ]]] + Ly[Ly[ψ[r, θ, φ]]] //
      FullSimplify;

(eq1 - eq2) // Simplify

0

```

7. Relations

$$[L^2, x_k] = (-i\hbar) \sum_{i,j} \varepsilon_{ijk} (L_i x_j + x_j L_i)$$

We show that

$$\begin{aligned}
[L^2, x] &= (-i\hbar)(L_y z + z L_y - L_z y - y L_z) \\
&= 2r\hbar^2 (\cos\phi \sin\theta + \sin\phi \csc\theta \frac{\partial}{\partial\phi} - \cos\phi \cos\theta \frac{\partial}{\partial\theta})
\end{aligned}$$

$$\begin{aligned}
[L^2, y] &= (-i\hbar)(L_z x + x L_z - L_x z - z L_x) \\
&= 2r\hbar^2 (\sin\phi \sin\theta - \cos\phi \csc\theta \frac{\partial}{\partial\phi} - \sin\phi \cos\theta \frac{\partial}{\partial\theta})
\end{aligned}$$

$$\begin{aligned}
[L^2, z] &= (-i\hbar)(L_x y + y L_x - L_y x - x L_y) \\
&= 2r\hbar^2 (\cos\theta + \sin\theta \frac{\partial}{\partial\theta})
\end{aligned}$$

through Mathematica.

((Mathematica))


```
eq1 = Leq[x  $\psi$ [r,  $\theta$ ,  $\phi$ ]] - x Leq[ $\psi$ [r,  $\theta$ ,  $\phi$ ]] //
FullSimplify
```

```
2 r  $\hbar^2$  (Cos[ $\phi$ ] Sin[ $\theta$ ]  $\psi$ [r,  $\theta$ ,  $\phi$ ] +
Csc[ $\theta$ ] Sin[ $\phi$ ]  $\psi^{(\theta, \theta, 1)}$ [r,  $\theta$ ,  $\phi$ ] -
Cos[ $\theta$ ] Cos[ $\phi$ ]  $\psi^{(\theta, 1, \theta)}$ [r,  $\theta$ ,  $\phi$ ])
```

```
eq11 =
```

```
(-i  $\hbar$ ) (Ly[z  $\psi$ [r,  $\theta$ ,  $\phi$ ]] + z Ly[ $\psi$ [r,  $\theta$ ,  $\phi$ ]] -
Lz[y  $\psi$ [r,  $\theta$ ,  $\phi$ ]] - y Lz[ $\psi$ [r,  $\theta$ ,  $\phi$ ]]) // Simplify
```

```
2 r  $\hbar^2$  (Cos[ $\phi$ ] Sin[ $\theta$ ]  $\psi$ [r,  $\theta$ ,  $\phi$ ] +
Csc[ $\theta$ ] Sin[ $\phi$ ]  $\psi^{(\theta, \theta, 1)}$ [r,  $\theta$ ,  $\phi$ ] -
Cos[ $\theta$ ] Cos[ $\phi$ ]  $\psi^{(\theta, 1, \theta)}$ [r,  $\theta$ ,  $\phi$ ])
```

```
eq1 - eq11 // Simplify
```

```
0
```

```
eq2 = Leq[y ψ[r, θ, φ]] - y Leq[ψ[r, θ, φ]] // Simplify
```

$$r \hbar^2 \left(2 \sin[\theta] \sin[\phi] \psi[r, \theta, \phi] - 2 \left(\cos[\phi] \csc[\theta] \psi^{(\theta, \theta, 1)}[r, \theta, \phi] + \cos[\theta] \sin[\phi] \psi^{(\theta, 1, \theta)}[r, \theta, \phi] \right) \right)$$

```
eq21 =
```

```
(-i ħ) (Lz[x ψ[r, θ, φ]] + x Lz[ψ[r, θ, φ]] -  
Lx[z ψ[r, θ, φ]] - z Lx[ψ[r, θ, φ]]) // Simplify
```

$$-2 r \hbar^2 \left(-\sin[\theta] \sin[\phi] \psi[r, \theta, \phi] + \cos[\phi] \csc[\theta] \psi^{(\theta, \theta, 1)}[r, \theta, \phi] + \cos[\theta] \sin[\phi] \psi^{(\theta, 1, \theta)}[r, \theta, \phi] \right)$$

```
eq2 - eq21 // Simplify
```

```
0
```

```
eq3 = Leq[z ψ[r, θ, φ]] - z Leq[ψ[r, θ, φ]] //  
FullSimplify
```

$$2 r \hbar^2 \left(\cos[\theta] \psi[r, \theta, \phi] + \sin[\theta] \psi^{(\theta, 1, \theta)}[r, \theta, \phi] \right)$$

```
eq31 =
```

```
(-i ħ) (Lx[y ψ[r, θ, φ]] + y Lx[ψ[r, θ, φ]] -  
Ly[x ψ[r, θ, φ]] - x Ly[ψ[r, θ, φ]]) // Simplify
```

$$2 r \hbar^2 \left(\cos[\theta] \psi[r, \theta, \phi] + \sin[\theta] \psi^{(\theta, 1, \theta)}[r, \theta, \phi] \right)$$

```
eq3 - eq31 // Simplify
```

```
0
```

We show that

$$[L^2, [L^2, x]] = 2\hbar^2 (xL^2 + L^2x)$$

((Proof))

((Mathematica))

```
eq1 =
  Leq[Leq[x ψ[r, θ, φ]]] - Leq[x Leq[ψ[r, θ, φ]]] -
    Leq[x Leq[ψ[r, θ, φ]]] + x Leq[Leq[ψ[r, θ, φ]]] //
  FullSimplify

2 r ħ^4 (2 Csc[θ] Sin[φ] ψ^(θ,θ,1)[r, θ, φ] - 2 Cos[φ]
  Sin[θ] (-ψ[r, θ, φ] + Csc[θ]^2 ψ^(θ,θ,2)[r, θ, φ] +
    2 Cot[θ] ψ^(θ,1,θ)[r, θ, φ] + ψ^(θ,2,θ)[r, θ, φ])

eq2 = 2 ħ^2 (x Leq[ψ[r, θ, φ]] + Leq[x ψ[r, θ, φ]]) //
  FullSimplify

2 r ħ^4 (2 Csc[θ] Sin[φ] ψ^(θ,θ,1)[r, θ, φ] - 2 Cos[φ]
  Sin[θ] (-ψ[r, θ, φ] + Csc[θ]^2 ψ^(θ,θ,2)[r, θ, φ] +
    2 Cot[θ] ψ^(θ,1,θ)[r, θ, φ] + ψ^(θ,2,θ)[r, θ, φ])

eq1 - eq2
0
```

9. Commutation relations for the radial momentum

$$[r, p_r] = i\hbar$$

$$[r, p_r^2] = i2\hbar p_r$$

$$[r, p_r^3] = i3\hbar p_r^2$$

$$[r, p_r^n] = in\hbar p_r^{n-1}$$

$$[p_r, r] = -i\hbar$$

$$[p_r, r^2] = -i2\hbar r.$$

$$[p_r, r^3] = -i3\hbar r^2.$$

$$[p_r, r^n] = -in\hbar r^{n-1}.$$

$$[p_r, \frac{1}{r}] = \frac{i\hbar}{r^2}.$$

$$[p_r, \frac{1}{r^2}] = \frac{2i\hbar}{r^3}.$$

$$[p_r^2, \frac{1}{r^2}] = \frac{-2\hbar^2}{r^4} (1 - 2r \frac{\partial}{\partial r}).$$

$$\begin{aligned} [p_r^2, \frac{1}{r}] &= -[\frac{1}{r}, p_r^2] \\ &= 2[p_r, \frac{1}{r}]p_r \\ &= \frac{2i\hbar}{r^2} p_r \\ &= \frac{2\hbar^2}{r^2} \frac{\partial}{\partial r} \end{aligned}$$

((**Mathematica**))

Commutation relations of quantum mechanical radial angular momentum and power of r

```
Clear["Global`*"]; Pr =  $\frac{1}{r} \frac{\hbar}{i} D[r \#, r] \&;$ 
```

```
Pr[Pr[ψ[r, θ, φ]]] // Simplify
```

$$-\frac{\hbar^2 \left(2 \psi^{(1, \theta, \theta)}[r, \theta, \phi] + r \psi^{(2, \theta, \theta)}[r, \theta, \phi] \right)}{r}$$

```
Pr[r ψ[r, θ, φ]] - r Pr[ψ[r, θ, φ]] // Simplify
```

$$-i \hbar \psi[r, \theta, \phi]$$

```
Pr[r^2 ψ[r, θ, φ]] - r^2 Pr[ψ[r, θ, φ]] // Simplify
```

$$-2 i r \hbar \psi[r, \theta, \phi]$$

```
Pr[r^n ψ[r, θ, φ]] - r^n Pr[ψ[r, θ, φ]] // Simplify
```

$$-i n r^{-1+n} \hbar \psi[r, \theta, \phi]$$

```
r Nest[Pr, ψ[r, θ, φ], 2] - Nest[Pr, r ψ[r, θ, φ], 2] -  
2 i ħ Pr[ψ[r, θ, φ]] // Simplify
```

$$0$$

```
r Nest[Pr, ψ[r, θ, φ], 3] - Nest[Pr, r ψ[r, θ, φ], 3] -  
3 i ħ Nest[Pr, ψ[r, θ, φ], 2] // Simplify
```

$$0$$

$$\text{Pr}\left[\frac{1}{r} \psi[r, \theta, \phi]\right] - \frac{1}{r} \text{Pr}[\psi[r, \theta, \phi]] // \text{Simplify}$$

$$\frac{i \hbar \psi[r, \theta, \phi]}{r^2}$$

$$\text{Pr}\left[\frac{1}{r^2} \psi[r, \theta, \phi]\right] - \frac{1}{r^2} \text{Pr}[\psi[r, \theta, \phi]] // \text{Simplify}$$

$$\frac{2 i \hbar \psi[r, \theta, \phi]}{r^3}$$

$$\text{Nest}\left[\text{Pr}, \frac{1}{r^2} \psi[r, \theta, \phi], 2\right] - \frac{1}{r^2} \text{Nest}[\text{Pr}, \psi[r, \theta, \phi], 2] //$$

Simplify

$$- \frac{2 \hbar^2 \left(\psi[r, \theta, \phi] - 2 r \psi^{(1, \theta, \theta)}[r, \theta, \phi] \right)}{r^4}$$

$$\text{Nest}\left[\text{Pr}, \frac{1}{r} \psi[r, \theta, \phi], 2\right] - \frac{1}{r} \text{Nest}[\text{Pr}, \psi[r, \theta, \phi], 2] //$$

Simplify

$$\frac{2 \hbar^2 \psi^{(1, \theta, \theta)}[r, \theta, \phi]}{r^2}$$

10. Example (Townsend)

We show that

$$\mathbf{L}^2 = \mathbf{r}^2 \mathbf{p}^2 - (\mathbf{r} \cdot \mathbf{p})^2 + i \hbar (\mathbf{r} \cdot \mathbf{p})$$

((Proof))

$$\mathbf{L}^2 = -\hbar^2 \left(\frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{\partial^2}{\partial \theta^2} \right)$$

$$\mathbf{r}^2 \mathbf{p}^2 = -\hbar^2 \left(\frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{\partial^2}{\partial \theta^2} + 2r \frac{\partial}{\partial r} + r^2 \frac{\partial^2}{\partial r^2} \right)$$

$$-(\mathbf{r} \cdot \mathbf{p})(\mathbf{r} \cdot \mathbf{p}) = r\hbar^2 \left(\frac{\partial}{\partial r} + r \frac{\partial^2}{\partial r^2} \right)$$

$$i\hbar(\mathbf{r} \cdot \mathbf{p}) = \hbar^2 r \frac{\partial}{\partial r}$$

Thus, we have

$$\begin{aligned} \mathbf{r}^2 \mathbf{p}^2 - (\mathbf{r} \cdot \mathbf{p})^2 + i\hbar(\mathbf{r} \cdot \mathbf{p}) &= -\hbar^2 \left(\frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{\partial^2}{\partial \theta^2} + 2r \frac{\partial}{\partial r} + r^2 \frac{\partial^2}{\partial r^2} \right) \\ &\quad + \hbar^2 \left(2r \frac{\partial}{\partial r} + r^2 \frac{\partial^2}{\partial r^2} \right) \\ &= -\hbar^2 \left(\frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{\partial^2}{\partial \theta^2} \right) \\ &= \mathbf{L}^2 \end{aligned}$$

((Mathematica))

```
eq0 = Leq[ψ[r, θ, φ]] // FullSimplify
```

$$-\hbar^2 \left(\text{Csc}[\theta]^2 \psi^{(\theta, \theta, 2)}[r, \theta, \phi] + \text{Cot}[\theta] \psi^{(\theta, 1, \theta)}[r, \theta, \phi] + \psi^{(\theta, 2, \theta)}[r, \theta, \phi] \right)$$

```
eq1 = r^2 Peq[ψ[r, θ, φ]] // Simplify
```

$$-\hbar^2 \left(\text{Csc}[\theta]^2 \psi^{(\theta, \theta, 2)}[r, \theta, \phi] + \text{Cot}[\theta] \psi^{(\theta, 1, \theta)}[r, \theta, \phi] + \psi^{(\theta, 2, \theta)}[r, \theta, \phi] + 2r \psi^{(1, \theta, \theta)}[r, \theta, \phi] + r^2 \psi^{(2, \theta, \theta)}[r, \theta, \phi] \right)$$

```
eq2 = -(r ur).p[(r ur).p[ψ[r, θ, φ]]] // Simplify
```

$$r \hbar^2 \left(\psi^{(1, \theta, \theta)}[r, \theta, \phi] + r \psi^{(2, \theta, \theta)}[r, \theta, \phi] \right)$$

```
eq3 = I hbar (r ur) . p[psi[r, theta, phi]] // Simplify
```

```
r hbar^2 psi^(1,0,0)[r, theta, phi]
```

```
eq123 = eq1 + eq2 + eq3 // Simplify
```

```
-hbar^2 (Csc[theta]^2 psi^(0,0,2)[r, theta, phi] +  
Cot[theta] psi^(0,1,0)[r, theta, phi] + psi^(0,2,0)[r, theta, phi])
```

```
eq0 - eq123 // Simplify
```

```
0
```

11. Runge-Lenz operator in spherical coordinates (Sakurai and Napolitano)

The detail of the Runge-Lenz method will be discussed elsewhere. Here we show that the commutation relations associated with the Runge-Lenz operator:

$$\mathbf{M} = \frac{1}{2\mu} (\mathbf{p} \times \mathbf{L} - \mathbf{L} \times \mathbf{p}) - \frac{Ze^2}{r} \mathbf{r}.$$

can be proved using the differential operators in the spherical coordinates (just one of the exercises). We note that

$$M_x = \frac{1}{2\mu} (p_y L_z - p_z L_y - L_y p_z + L_z p_y) - \frac{Ze^2}{r} x.$$

The Hamiltonian is defined by

$$H = \frac{\mathbf{p}^2}{2\mu} - \frac{Ze^2}{r}.$$

where μ is the reduced mass. We show that

(a)

$$[\mathbf{M}, H] = 0,$$

(b)

$$\mathbf{L} \cdot \mathbf{M} = 0 = \mathbf{M} \cdot \mathbf{L},$$

(c)

$$\mathbf{M}^2 = \frac{2}{\mu} H(\mathbf{L}^2 + \hbar^2) + Z^2 e^4$$

((Mathematica))

```
Clear["Global`"];
ux = {Sin[θ] Cos[φ], Cos[θ] Cos[φ], -Sin[φ]};
uy = {Sin[θ] Sin[φ], Cos[θ] Sin[φ], Cos[φ]};
uz = {Cos[θ], -Sin[θ], 0};
ur = {1, θ, 0};
x = r ur.ux;
y = r ur.uy;
z = r ur.uz;
Lap := Laplacian[#, {r, θ, φ}, "Spherical"] &;
Gra := Grad[#, {r, θ, φ}, "Spherical"] &;
Diva := Div[#, {r, θ, φ}, "Spherical"] &;
Curla := Curl[#, {r, θ, φ}, "Spherical"] &;
L := (-I ħ (Cross[(ur r), Gra[#]])) & // Simplify;
Lx := (ux.L[#] &) // Simplify;
Ly := (uy.L[#] &) // Simplify;
Lz := (uz.L[#] &) // Simplify;
LP := (Lx[#] + I Ly[#]) & // Simplify;
LM = (Lx[#] - I Ly[#]) & // Simplify;
Leq := (Nest[Lx, #, 2] + Nest[Ly, #, 2] + Nest[Lz, #, 2]) &;
```

```

p := (-i ħ Gra[#]) &;
px := (ux.p[#]) &;
py := (uy.p[#]) &;
pz := (uz.p[#]) &;
Peq := (Nest[px, #, 2] + Nest[py, #, 2] + Nest[pz, #, 2]) &;
prq :=  $\left( \frac{-i \hbar}{2} \text{ur} \cdot \text{Gra}[\#] + \frac{-i \hbar}{2} \text{Diva}[\# \text{ur}] \right) \&;$ 
pq :=  $\frac{\hbar}{i r} \text{D}[r \#, r] \&;$ 

```

$$M_x = \frac{1}{2\mu} (p_y L_z - p_z L_y - L_y p_z + L_z p_y) - \frac{Z e^2}{r} x$$

$$H = \frac{1}{2\mu} p^2 - \frac{Z e^2}{r}$$

```

Mx :=  $\left( \frac{1}{2\mu} (p_y[L_z[\#]] - p_z[L_y[\#]] \right.$ 
       $\left. - L_y[p_z[\#]] + L_z[p_y[\#]]) - \frac{Z e^2}{r} x \# \right) \& // \text{FullSimplify};$ 

```

$$M_y := \left(\frac{1}{2\mu} (p_z[L_x[\#]] - p_x[L_z[\#]] - L_z[p_x[\#]] + L_x[p_z[\#]]) - \frac{Ze^2}{r} y \# \right) \& // \text{FullSimplify};$$

$$M_z := \left(\frac{1}{2\mu} (p_x[L_y[\#]] - p_y[L_x[\#]] - L_x[p_y[\#]] + L_y[p_x[\#]]) - \frac{Ze^2}{r} z \# \right) \& // \text{FullSimplify};$$

$$H1 = \left(\frac{1}{2\mu} \text{Peq}[\#] - \frac{Ze^2}{r} \# \right) \&;$$

Proof of

$$[M_x, H]=0, [M_y, H]=0, [M_z, H]=0$$

```
Mx[H1[ψ[r, θ, φ]]] - H1[Mx[ψ[r, θ, φ]]] // FullSimplify
0
```

```
My[H1[ψ[r, θ, φ]]] - H1[My[ψ[r, θ, φ]]] // FullSimplify
0
```

```
Mz[H1[ψ[r, θ, φ]]] - H1[Mz[ψ[r, θ, φ]]] // FullSimplify
0
```

$$M^2 = M_x^2 + M_y^2 + M_z^2$$

$$M^2 = \frac{2}{\mu} (H L^2 + \hbar^2 H) + Z^2 e^4$$

```
eq1 = Mx[Mx[ψ[r, θ, φ]]] + My[My[ψ[r, θ, φ]]] +
      Mz[Mz[ψ[r, θ, φ]]] // FullSimplify;
```

```
s11 = ħ^2 H1[ψ[r, θ, φ]] // FullSimplify;
```

```
s12 = H1[Leq[ψ[r, θ, φ]]] // FullSimplify;
```

```
s13 = \frac{2}{\mu} (s11 + s12) + Z^2 e^4 ψ[r, θ, φ];
```

```
eq1 - s13 // FullSimplify
```

```
0
```

$$L_x M_x + L_y M_y + L_z M_z = 0$$

$L_x[M_x[\psi[r, \theta, \phi]]] + L_y[My[\psi[r, \theta, \phi]]] + L_z[Mz[\psi[r, \theta, \phi]]] //$
 FullSimplify

0

$$M_x L_x + M_y L_y + M_z L_z = 0$$

0

$M_x[L_x[\psi[r, \theta, \phi]]] + M_y[L_y[\psi[r, \theta, \phi]]] + M_z[L_z[\psi[r, \theta, \phi]]] //$
 FullSimplify

0

$$M_x L_y - L_y M_x - i \hbar M_z = 0$$

$M_x[L_y[\psi[r, \theta, \phi]]] - L_y[M_x[\psi[r, \theta, \phi]]] - i \hbar M_z[\psi[r, \theta, \phi]] //$
 Simplify

0

$$M_x M_y - M_y M_x + \frac{i 2 \hbar}{\mu} H L_z = 0$$

$M_x[M_y[\psi[r, \theta, \phi]]] - M_y[M_x[\psi[r, \theta, \phi]]] +$
 $i \frac{2 \hbar}{\mu} H [L_z[\psi[r, \theta, \phi]]] //$ Simplify

0

12. Conclusion

Using the above formula, one can derive the Schrödinger equation of hydrogen in the spherical coordinates. We will discuss this problem later.

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